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BOUNDARY-LAYER TRANSITION DETECTION IN CRYOGENIC WIND TUNNEL USING FLUORESCENT PAINTS.

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Applications of Temperature and Pressure Sensitive Paints

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Summary

Luminescent molecular probes imbedded in a polymer binder form a temperature or pressure paint. On excitation by light of the proper wavelength, the luminescence, which is quenched either thermally or by oxygen, is detected by a camera or photodetector. From the detected luminescent intensity, temperature and pressure can be determined. The basic photophysics, calibration, accuracy and time response of a luminescent paints is described followed by applications in low speed, transonic, supersonic and cryogenic wind tunnels and in rotating machinery.

Introduction

The use of luminescent molecular probes for measuring surface temperature and pressure on wind tunnel models and flight vehicles offers the promise of enhanced spatial resolution and lower costs compared to traditional techniques. These new sensors are called temperature-sensitive paint (TSP) and pressure-sensitive paint (PSP). Traditionally, arrays of thermocouples and pressure taps have been used to obtain surface temperature and pressure distributions. These techniques can be very labor-intensive and model/flight vehicle preparation costs are high when detailed maps of temperature and pressure are desired. Further, the spatial resolution is limited by the number of instrumentation locations chosen. By comparison, the TSP and PSP techniques provide a way to obtain simple, inexpensive, full-field measurements of temperature and pressure with much higher spatial resolution. Both TSP and PSP incorporate luminescent molecules in a paint which can be applied to any aerodynamic model surface. Figure 1 shows a schematic of a paint layer incorporating a luminescent molecule.

The paint layer is composed of luminescent molecules and a polymer binder material. The resulting 'paint' can be applied to a surface using a brush or sprayer. As the paint dries, the solvent evaporates and leaves behind a polymer matrix with luminescent molecules embedded in it. Light of the proper wavelength to excite the luminescent molecules in the paint is directed at the model and luminescent light of a longer wavelength is emitted by the molecules. Figure 2 shows the spectra for a typical luminescent ruthenium molecule. Using the proper filters, the excitation light and luminescent emission light can be separated and the intensity of the luminescent light can be determined using a photodetector. Through the photo-physical processes known as thermal- and oxygen-quenching, the luminescent intensity of the paint emission is related to temperature or pressure. Hence, from the detected luminescent intensity, temperature and pressure can be determined.

The polymer binder is an important ingredient of a luminescent paint used to adhere the paint to the surface of interest. In some cases, the polymer matrix is a passive anchor. In other cases, however, the polymer may affect significantly the photophysical behavior of the paint through a complicated interaction between the luminescent molecules and the macro-molecules of the polymer. A good polymer binder should be robust enough to sustain skin friction and other forces on the surface of an aerodynamic model. Also, it must be easy to apply and repair to the surface in a smooth, thin film. For TSPs, many commercially available resins and epoxies can be chosen serve as polymer binders if they are not oxygen permeable and do not degrade the activity of the luminophore molecules. In contrast, a good polymer binder for a PSP must have high oxygen permeability besides being robust and easy to apply.

Two recent papers (Liu et al. 1997 and Gouterman 1997) provide excellent reviews of the foundations and history of TSP and PSP and contain extensive reference lists.

Measurement Systems

The measurement systems are the same for both TSPs and PSPs. The essential elements of the systems include illumination sources, optical filters, photodetectors and data acquisition/processing units. This section provides a brief description of two measurement systems: the CCD camera system and the laser scanning system. Intensity based measurements are considered first and then lifetime and multi-luminophore systems.

CCD Camera System

The CCD camera system for luminescent paints is the most commonly used in aerodynamic testing. A schematic of this system is shown in Figure 3. The luminescent paint (TSP or PSP) is coated on the surface of the model. The paint is excited to luminesce by the illumination source, such as a lamp or a laser. The luminescent intensity image is filtered optically to eliminate the illuminating light and then captured by a CCD camera and transferred to a computer with a frame grabber board for image processing. Both wind-on image (at temperature and pressure to be determined) and wind-off image (at a known constant temperature and pressure) are obtained. The ratio between the wind-on and wind-off images is taken after the dark current level image is subtracted from both images, yielding a relative luminescent intensity image. Using the calibration relations, the surface temperature and pressure distributions can be computed from the relative luminescent intensity image.

Selection of the appropriate illumination sources depends on the absorption spectrum of the paint and the optical access of the facility. The source must provide a large number of photons in the wavelength band of absorption. A variety of illumination sources are available. Lasers with fiber-optic delivery systems have been used in wind tunnel tests (Morris et al. 1993b, Crites 1993, Bukov et al.. 1992, Engler et al. 1995). Other light sources reported in literature include a xenon arc light with a blue filter (McLachlan et al. 1993a), incandescent tungsten/halogen lamps (Dowgwillo et al. 1994) and fluorescent UV lamps (Liu et al. 1995a, 1995b). Morris et al. (1993a) and Crites (1993) discussed the characteristics of some illumination sources. For imaging the surface, scientific grade cooled CCD digital cameras can provide high intensity resolution (12 and 16 bits) and high spatial resolution (up to 2048 × 2048 pixels). Since the scientific grade CCD camera exhibits good linearity and high signal-to-noise ratio (SNR), it is particularly suitable to quantitative luminescent intensity measurements.

A necessary step in data processing is taking the ratio between the wind-on luminescence image and the wind-off reference image at a known reference temperature and pressure. The image ratio process can eliminate the effects of spatial non-uniformity in illumination light, coating thickness, and luminophore concentration. However, since aerodynamic forces may cause model motion and deformation in high-speed wind tunnel tests, the wind-on image may not align with the wind-off image. The ratio between the non-aligned images leads to considerable errors in calculating temperature and pressure using the calibration relations. Also, some distinct flow characteristics, such as shocks, transition and separation locations, could be smeared. In order to correct this non-alignment, an image registration method was suggested by Bell and McLachlan (1996) and Donovan et al. (1993).

Laser Scanning System

A laser scanning system for TSPs and PSPs is shown in Figure 4. A low power laser is focused to a small point and scanned over the surface of the model using computer controlled mirrors The laser illumination excites the paint on the model and luminescence is detected by a low noise photodetector (e.g. a PMT). The photodetector signal is digitized with a high resolution A/D converter and processed to obtain temperature and pressure. The mirror is synchronized to the data acquisition so that the position of the laser spot on the model is accurately known.

Compared with the CCD camera system, it takes longer to obtain full-surface temperature and pressure distributions using the laser scanning system. However, this system has some advantages. (Hamner et al. 1994)

(i) Luminescence is detected by a low noise photodetector. Before the analog output from the PMT is digitized, filtering and other SNR enhancement techniques are available to improve the measurement resolution. The signal is then digitized with a high resolution (12 to 24 bit) A/D converter. Additional noise reduction can be accomplished by using a lock-in amplifier if the laser intensity is modulated.
(ii) The laser scanning system can be used for measurement in a facility where optical access is very limited and the CCD camera system is difficult to use.
(iii) The system provides uniform illumination over the surface by scanning a single light spot.
(iv) The system can be easily adapted for measurement of luminescent lifetime or phase shift if a pulsed laser or modulated laser is used.

Lifetime-based detection systems

A promising method for making temperature and pressure measurements is to determin the luminescent lifetime of the paint rather than the luminescent intensity. Compared with the intensity-based method, the greatest advantage of this method is that the lifetime-temperature or -pressure relation is not dependent on illumination intensity. Therefore, the calibration relation is intrinsic for a particular paint and the image ratio process is not required. Also, the lifetime measurement is insensitive to luminophore concentration, paint thickness, photodegradation, tubid paint surface and dirty optical surfaces. The temperature and pressure can be directly obtained from the measured lifetime. The lifetime measurement technique in photochemistry is well-developed (Szmacinski and Lakowicz 1995, Papkovsky 1995). The basic configuration of this system is similar to either the CCD camera or the laser scanning system, except a pulsed excitation light is used. After each pulse, the luminescence decay is detected and acquired by a computer. Then, temperature or pressure is obtained by using the calibration relation. Using a lifetime detection system, Davies et al. (1995) measured the pressure distributions on a cylinder in subsonic flow and on a wedge at Mach 2. Comparison with data obtained by conventional pressure taps was favorable.

A frequency-domain method detects the phase angle between the luminescence emission and harmonically modulated excitation light. If the modulation frequency is fixed, the phase angle is a function of the lifetime and hence is dependent on temperature and pressure. The phase angle can be measured using a lock-in amplifier. Campbell et al. (1994) gave a calibration between phase angle and temperature for Ru(bpy)-Shellac paint at 100 kHz modulation frequency. A simple phase detection system using blue LED excitation was used to measure surface temperature on an electrically heated steel foil on which a round air jet impinged (Campbell et al. 1994). Torgerson et al. (1996) measured the pressure distribution in a low-speed impinging jet using a laser scanning system with an optical modulator.

Multi-Luminophore System

Use of the normal CCD camera or laser scanning system requires a ratio between the wind-on and wind-off luminescent images. This image ratio method inevitably causes inaccuracy in determining temperature and pressure because the image registration is never perfect. A two-color luminophore paint would eliminate the need for a wind-off reference image. Two-color luminescent TSP is made by combining a temperature-sensitive luminophore with a temperature-insensitive reference luminophore. Similarly, two-color luminescent PSP consists of a pressure-sensitive luminophore with a pressure-insensitive reference luminophore. The probe luminophore and reference luminophore can be excited by the same illumination. However, there is ideally no overlap between the emission spectra of the probe luminophore and reference luminophore such that two color luminescent images can be completely separated by optical filters. The ratio between these two color images can eliminate effects of spatial non-uniformity in illumination, paint thickness and luminophore concentration. Besides the aforementioned combinations, a temperature sensitive luminophore which is not quenched by oxygen can be combined with an oxygen sensitive luminophore. This dual luminophore temperature/pressure paint can be used for temperature correction in PSP measurement. Furthermore, a multi-color PSP can be developed to correct simultaneously the effects of both temperature variation and non-uniformities in lighting, paint thickness and concentration.

Some preliminary experiments indeed indicate that a two-color PSP can correct variations in illumination (Oglesby et al. 1995, Harris and Gouterman 1995). Three pressure sensitive paints with internal temperature sensitive luminophore have also been tested by Oglesby et al. (1996). Their results show that the dual luminophore paint enables point-by-point correction of temperature effects of PSP measurement. Only recently, a two-color PSP was used to measure pressure distribution in a low speed impinging jet (Torgerson et al. 1996).

Temperature Sensitive Paints

This section will describe the photophysics, calibration, accuracy, time response of temperature sensitive paint.

Photophysics

For a TSP, it is assumed that the paint layer is not oxygen-permeable so that $[O_2] = 0$. Hence, the quantum yield is simply given by

$$\Phi = \frac{I}{I_a} = \frac{k_L}{k_L + k_D} = k_L \tau_0 \qquad (1)$$

The deactivation term k_D may be decomposed into a temperature-independent part k_0 and a temperature-dependent part k_1 that is related to thermally activated intersystem crossing (i.e. $k_D = k_0 + k_1$). The rate k_1 can be assumed to have an Arrhenius form (Bennett and McCartin 1966, Schanze et al. (1997)

$$k_1 = C \exp(-E/RT) \qquad (2)$$

where C is a constant, E is the Arrhenius activation energy, R is the universal gas constant and T is the thermodynamic temperature (in Kelvin).

The relation (1) can be approximately written in the simple Arrhenius form

$$\ln \frac{I(T)}{I(T_{ref})} = \frac{E}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right) \qquad (3)$$

Theoretically speaking, the Arrhenius plot of $\ln[I(T)/I(T_{ref})]$ versus $1/T$ gives a straight line of slope E/R. Tests indicate that the simple Arrhenius relation does fit experimental data over a certain temperature range. However, for some paints, the data may not fully obey the simple Arrhenius relation over a wider range of temperature. As an alternative, the relation between the luminescence intensity and temperature can be expressed in a functional form

$$\frac{I(T)}{I(T_{ref})} = F(T/T_{ref}) \qquad (4)$$

The empirical expression $F(T/T_{ref})$ could be a polynomial, exponential or other functions to fit the experimental data over a certain temperature range. Both (3) and (4) are operational forms of the calibration relation for a TSP used for data reduction in practical applications.

TSP Calibration

In order to quantitatively measure temperature with the TSP coatings, a calibration relating luminescent intensity or lifetime to temperature is needed. A calibration rig consists of a temperature controlled sample and appropriate illumination source and luminescent detector.

Typical temperature dependencies of luminescent intensity are shown in Figure 5 for some TSPs. Several TSPs have high temperature sensitivity in cryogenic temperature range. Others can be used in a temperature range from -20 to 105 ^{0}C. Figure 6 gives a lifetime calibration of two TSPs.

Accuracy

The accuracy of the temperature measurement has been shown to depend primarily on calibration accuracy, but is in the range of 1 degree. (see Liu et al. 1995b for a detailed analysis)

Time Response

There are two characteristic time scales that are related to the time response of the paint. One is the luminescent lifetime which represents an intrinsic physical limit for the achievable temporal resolution of the paint. Luminescent paint usually has a lifetime ranging from 10^{-10} seconds to milliseconds. Another is the time scale of the thermal diffusion in the TSP layer. In a forced convection-dominated case, the thermal diffusion time can be expressed by $\tau = \rho c \ell / h$, where. ρ is the density, c is the specific

heat, ℓ is the paint thickness and h is the convection heat transfer coefficient. In general, the diffusion time is much larger than the lifetimes of most luminescent paints. Therefore, the time response of the luminescent paint is mainly limited by the diffusion processes for both TSP and PSP measurements.
Figure 7 shows a the temperature response of the TSP paint subjected to the pulsed laser heating.(Liu et al.,1995c). The surface temperature increases rapidly after the pulsed laser beam is turned on and then gradually decays due to natural convection. By fitting the experimental data with the asymptotic solutions, it is found that $\tau_1 = 0.25$ ms(heating) and $\tau_2 = 25$ ms (cooling).

TSP Applications

Transition Detection
TSP has also been utilized as an approach to flow transition detection (Campbell 1994, McLachlan et al. 1993b). Since convective heat transfer is much higher in turbulent flow than in laminar flow, TSP can visualize the surface temperature difference between turbulent and laminar regions. In low speed wind tunnel tests, the model is typically heated or cooled to enhance temperature variation across the transition line. Using EuTTA-dope paint, Campbell et al. (1992, 1993) visualized transition patterns on a symmetric NACA 65_4-021 airfoil in a low-speed wind tunnel. (Figure 8). Recently, a cryogenic TSP systems have been developed at Purdue, the University of Florida NASA Langley and National Aerospace Laboratory (NAL), Japan. Several TSP formulations have been successfully used to detect transition on airfoils in a 0.1m transonic cryogenic wind tunnel at the NAL in Japan (Figure 9 from Asai et al. 1997a) and a 0.3m cryogenic wind tunnel at NASA-Langley (Figure 10 from Popernack et al.).
Quantitative Heat Transfer
Global surface heat transfer mapping on a waverider model in Mach 10 flow has been obtained using EuTTA-dope paint (Liu et al. 1995b).
A thin Mylar insulating layer covered the windward side of the model, and EuTTA-dope paint was applied on the insulating layer. The temporal evolution of surface temperature distributions was obtained and then heat flux was calculated using a simple heat transfer model. Figure 11 shows a representative map of heat flux on the windward side of the waverider. The bright and dark regions correspond to high and low heat transfer, respectively. The low heat transfer region near the leading edge corresponds to laminar flow. Transition from laminar to turbulent flow can be easily identified by an abrupt change from low to high heat transfer. Figure 12 shows a typical heat transfer history. The TSP measurement is in good agreement with data obtained by thermocouples.

Pressure Sensitive Paints

This section will describe the photophysics, calibration, accuracy, time response of pressure sensitive paint.

Photophysics
PSP operation is based on the principle that certain fluorescent molecules are quenched by the presence of oxygen. In the molecules of interest, oxygen interacts with the excited molecules and the excess energy is transferred to the oxygen in a collisional process, with no photons being emitted. This process, known as oxygen quenching, is the basis for the pressure sensitive paint method.
According to Henry's law, oxygen concentration is proportional to the partial pressure of oxygen, which is proportional to static pressure. The result is that if there is a locally high pressure area, the fluorescent molecules will be quenched by oxygen.
The quenching process is governed by the Stern Volmer equation which can be written as a ratio of intensities in order to remove the effects of concentration, thickness and illumination variations.

$$\frac{I_{ref}}{I} = A(T) + B(T)\left(\frac{P}{P_{ref}}\right) \qquad (5)$$

I_{ref} = fluorescence intensity at reference condition

P_{ref} = pressure at reference condition

A(T),B(T) = Stern Volmer constants

The result is that an increasing pressure causes the intensity of the paint to decrease. In using equation 5, an intensity map must be acquired at a reference condition, typically a flow off or slow rotation where the pressure is a known constant across the surface.
In this version of the Stern Volmer equation, the coefficients A and B are functions of temperature.

$$A(T) = a_1\left[1 + \frac{E_{nr}}{RT_{ref}}\left(\frac{T - T_{ref}}{T_{ref}}\right)\right],$$

$$B(T) = b_1\left[1 + \frac{E_p}{RT_{ref}}\left(\frac{T - T_{ref}}{T_{ref}}\right)\right]$$

E_{nr} = non-radiative activation energy
E_p = polymer activation energy

R = interaction distance

a_1, b_1 = constants

The temperature dependence of A is due to the thermal quenching as in TSP. The temperature dependence of B is due to the temperature dependence of diffusivity of the polymer binder.(Torgerson 1997 , Schanze et al.)
Calibration
Figure 13 shows Stern Volmer curves for various paints at room temperature. A calibration of Ru(ph_2-phen) in GE RTV 118 at several temperatures is given in Figure 14 and for PtTFPP in polystrene in Figure 15.
Accuracy
To estimate the uncertainty of the PSP measurement with a scientific-grade CCD camera system, Morris et al. (1993a) conducted a series of calibration experiments focused on a proprietary PSP paint sample in a pressure vessel which controlled both the temperature and pressure. After

averaging a 32 sequential images to improve the SNR, they found that the minimum pressure resolution near atmospheric pressure (13 to 16 psia) is about ± 0.05 psid for their system. Note that the above uncertainty estimates do not contain the contributions from some major error sources such as the temperature effects and model displacement. The uncertainty of PSP measurements depends strongly on a systematic error source associated with the temperature dependence of the paint. An analysis by Sajben (1993) indicates that the temperature uncertainty dominates the PSP measurement errors. Another major error source is model motion between the wind on and wind off images. To date, it has been necessary to perform an in-situ calibration of the PSP using standard pressure taps on the model in order to obtain reasonable accuracy.

Time Response

Based on the transient solution of the diffusion equation, the oxygen diffusion time for a thin PSP coating is on the order of $\tau = \ell^2 / D_m$, where ℓ is the coating thickness and D_m is the mass diffusivity of oxygen in the paint layer. Baron et al. (1993) studied the time response to oxygen concentration changes of several PSPs using a pressure jump apparatus. The PSPs that they investigated are PtOEP in GP-197 and MAX-100 polymer binders and H_2TFPP in Silica-W, Silica-B and TLC binders. They found that the response times for GP-197 and MAX-100 binder are 2.45 s and 0.4 s, respectively. The Silica-W and Silica-B show response times of 11 ms and 1.5 ms, respectively. The response time of the TLC is about 25 μs. Recently, using a similar set-up, Carroll et al. (1996) measured the step response of three PSPs: a proprietary PSP from McDonnell Douglas, PtOEP on a white primer layer, and PtOEP in GP-197. For the McDonnell Douglas paint with thickness ranging from 13 to 35 μm, the response time varies from 0.042 s to 0.42 s. The response time of PtOEP on a white primer layer is 45 ms. For PtOEP in GP-197, the response times are 1.4 s, 1.6 s and 2.6 s for the paint thickness of 22 μm, 26 μm and 32 μm, respectively. Bukov et al. (1992) reported that a proprietary fast-responding PSP coating developed by TsAGI has a time constant of 5 ms. Clearly, the diverse time constants of various PSPs result from the effects of the different polymer diffusivity, coating thickness and structure of the paint.

PSP Applications

Most of PSP measurements on aerodynamic models have been conducted in transonic and supersonic wind tunnels. Recently, the PSP technique has been used for pressure measurements in low-speed flows and rotating machinery.

Tests in Wind Tunnels

PSPs have been applied to pressure measurements in wind tunnel tests over a wide range of Mach numbers in order to examine the feasibility of this method. Kavandi et al. (1990) and McLachlan et al. (1993a) tested a two-dimensional airfoil (NACA-0012) over a Mach number range of 0.3 to 0.66. McLachlan et al. (1995a, 1995b) also tested a large generic transport wing/body configuration in transonic Mach number from 0.7 to 0.9. The PSP data not only provide good quantitative chordwise pressure results, but also show complicated two-dimensional pressure maps that would be difficult to deduce from the usual discrete tap data. Some experiments conducted in the McDonnell Douglas Research Laboratories (Morris et al. 1993b) include pressure measurements on a generic wing/body model (Mach number = 2 and angle of attack = 8 degree), a model of a high performance fighter (Mach number = 1.2), and a two-dimensional converging/diverging nozzle. Sellers and Brill (1994) conducted a demonstration test of a PSP in the Arnold Engineering Development Center transonic wind tunnel for an aircraft model. Using fast-responding PSP coatings developed at TsAGI, Troyanovsky et al. (1993) carried out a semi-quantitative pressure visualization for a shock/body interaction in a Mach 8 shock tube with 0.1 s duration, and Borovoy et al. (1995) determined the pressure distributions on a cylinder at Mach 6 in a shock wind tunnel with about 40 ms duration. In general, the PSP technique works well in high Mach number subsonic flows and supersonic flows since static pressure change is typically large. Morris (1995) and Shimbo et al. (1997) measured the pressure on delta wings at low Mach numbers ranging from 0.05 to 0.2. These results indicate the low pressure regions induced by leading edge vortices.

Figure 16 shows a typical surface pressure map in the interaction of a cylinder mounted normal to a flat floor with a supersonic turbulent boundary layer at a freestream Mach number of 2.5. In this test carried out in the Purdue University supersonic wind tunnel, the incoming boundary layer thickness is 4 mm, the cylinder height is 15 mm, and the cylinder diameter is 4.8 mm. The PSP, Ru(ph_2-phen) in GE RTV 118, was applied to the floor surface for pressure measurement. The pressure map clearly indicates a pressure rise induced by a bow shock ahead the cylinder and a low pressure region in the turbulent wake behind the cylinder.

Transonic Airfoil - Lifetime Method

The laser scanning method for pressure and temperature sensitive paints was demonstrated in the Boeing Company model transonic wind tunnel. (Torgerson 1997) The arifoil was 10% thick with a sharp leading edge and a small amount of camber. It had 19 pressure taps along the upper surface to compare with the pressures found from the paints. The laser used was a small air-cooled argon-ion laser. The beam was modulated using an electro-optic modulator, enabling the signal to be processed by a two phase lock-in amplifier. Both intensity and phase were recorded during the scan over the airfoil, so that a comparison between intensity and lifetime methods could be made. Results in Figure 17 show both methods compare favorably with the pressure tap data. The phase measurements have the advantage that wind off data is not required.

Cryogenic Pressure Paint

Recently, Asai et al. 1997b demonstrated the feasibility of using luminescent coatings for surface pressure measurements in a cryogenic wind tunnel. Calibrations of a new anodized layer (Figures 18 and 19) show extremely high oxygen sensitivity. By injecting a small of oxygen (250 ppm) into the NAL transonic cryogenic tunnel excellent comparison between pressure taps and PSP was obtained for flow over a 14% circular-arc bump model. (Figure 20)

Rotating Machinery

The PSP/TSP technique provides a promising tool for measuring surface pressure distributions on a high-speed rotating blade at a high spatial resolution. Instrumentation is particularly difficult in the rotating environment and the pressure taps weaken the structure of the rotating blade. Recently, a test was performed to measure the chordwise pressure distributions on the rotor blades of a high speed axial flow compressor shown in Figure 21 (Liu et al 1996b). TSP (Ru(bpy)-Shellac) and PSP (Ru(ph_2-phen) in GE RTV 118) were applied to alternating blades. The TSP provided the temperature distributions on the blades for temperature correction of the PSP results. A scanning laser system was used for excitation and detection of luminescence. Both the TSP and PSP were excited with an Argon laser and luminescence was detected with a Hamamatsu PMT. The pressure map of Figure 22 shows a strong suction surface shock wave. Comparisons to CFD over a range of rotational speeds (Figure 23) show good correlation but require care in interpretation since the error in the PSP is ~.1 psia because an in-situ calibration was not possible.

The same system was on used on an Allied Signal F109 gas turbine engine (Figure 24) giving the suction surface pressure map at 14000 rpm shown in Figure 25.

Conclusion

The fundamentals and applications of the TSP and PSP techniques have been discussed in this paper. The TSP technique has been used not only to visualize surface flow features such as boundary layer transition, shocks and separation, but also to obtain quantitative surface temperature and heat transfer maps with good accuracy. Applications of the PSP technique are focused on surface pressure measurements on airfoils, generic wing-body models aircraft models and turbomachinery over a wide range of Mach numbers. The field mapping capability of the TSP and PSP techniques is able to provide information about complicated flow characteristics that cannot be easily acquired using more conventional methods. Much effort has being made to improve essential elements of the measurement system including paint formulation, illumination, imaging, and data acquisition/processing hardware and software. Many groups are working to extend and refine TSP and PSP measurements so they will become a routine procedure in aerodynamics testing.

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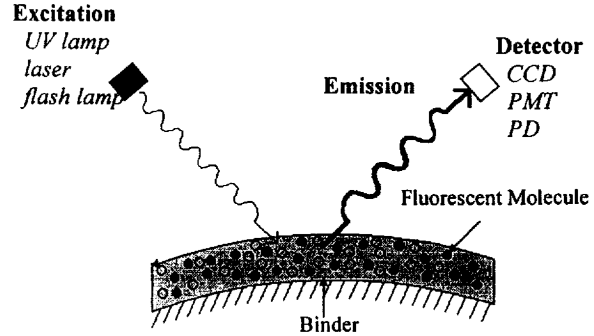

Figure 1: Schematic of TSP/PSP Layer

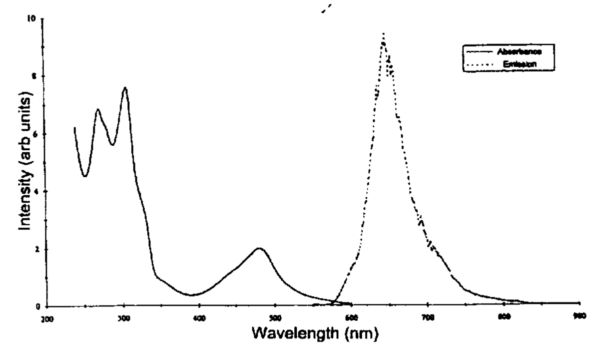

Figure 2: Excitation and Emission spectra of a Ruthenium based molecule

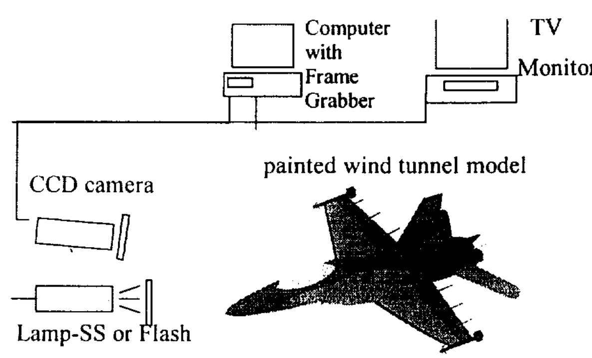

Figure 3: Schematic of CCD camera system

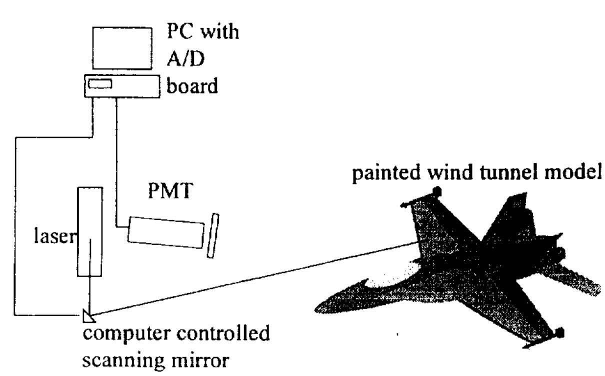

Figure 4: Schematic of laser scanning system

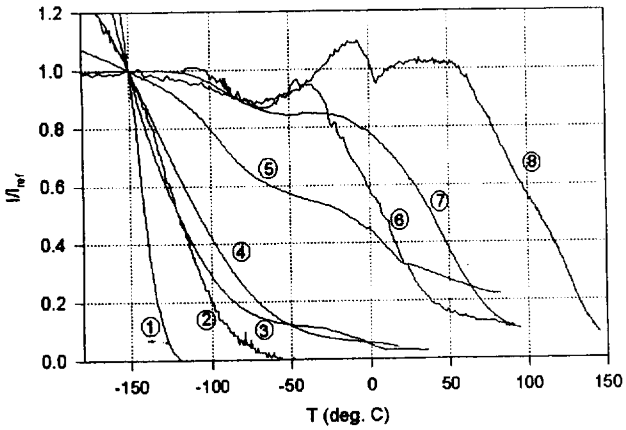

Figure 5.Temperature dependence of luminescence intensity for several TSP formulations: (1) Ru(trpy) in Ethanol/ Methanol, (2) Ru(trpy)(phtrpy) in GP-197, (3) Ru(VH127) in GP-197, (4) Ru(trpy) in Du Pont Chroma Clear, (5) Ru(trpy)/Zeolite in GP-197, (6) EuTTA in dope, (7) Ru(bpy) in Du Pont Chroma Clear, (8) Perylenedicarboximide in Sucrose Octaacetate. (T_{ref} = -150 °C).

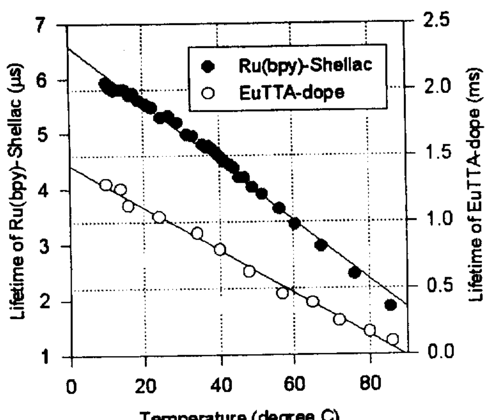

Figure 6 Lifetime-temperature relations for Ru(bpy)-Shellac and EuTTA-dope paints.

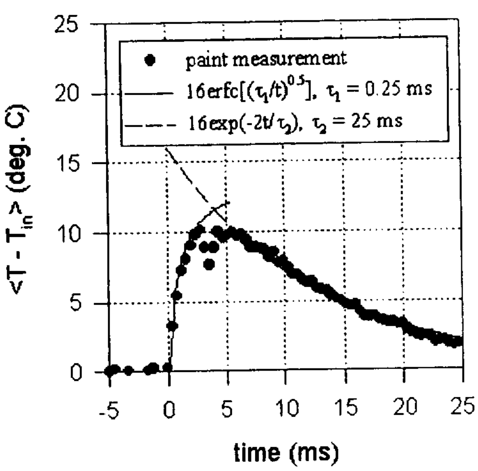

Figure 7 Temperature response of Ru(bpy)-Shellac paint to pulsed laser heating on steel foil.

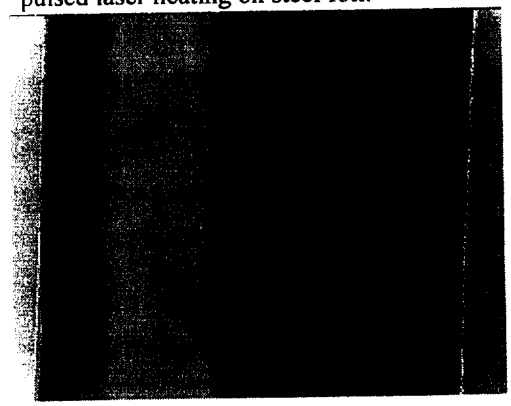

Figure 8. Transition at low speed on a NACA 65-021 Airfoil

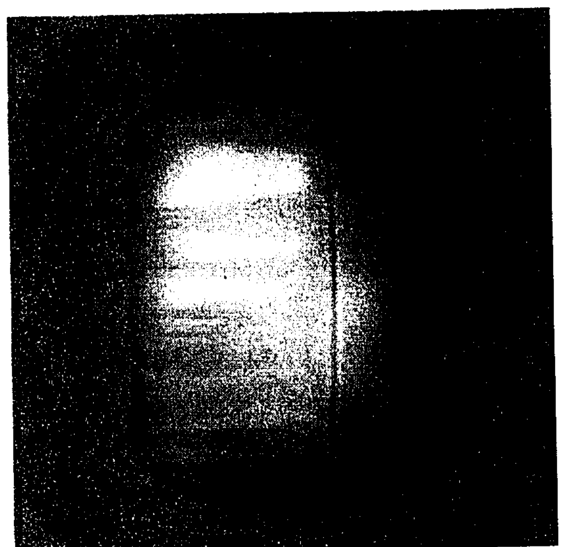

Figure 9. Transition on a NACA 64A021 at M=.82 and T=120 K in NAL cryogenic wind tunnel.

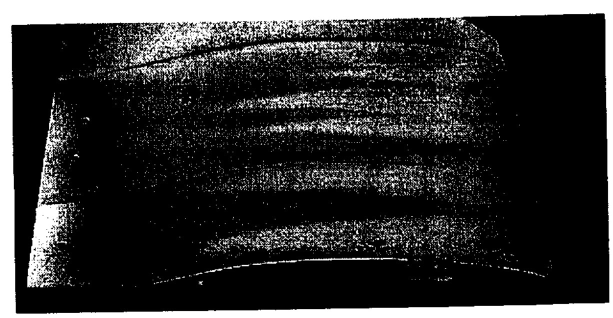

Figure 10. Transition on a HSNLF in the NASA .3 meter cryogenic wind tunnel.

Figure 11. Transition on a Waverider model at M=10.

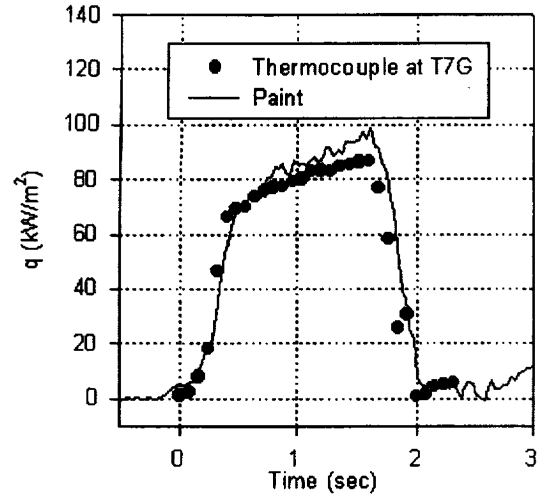

Figure 12 Heat transfer history on a Mach 10 waverider model at location T7G.

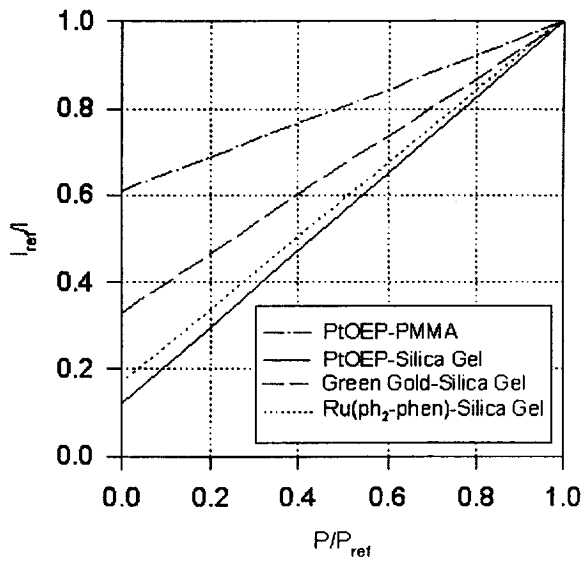

Figure 13 Stern-Volmer plots for several PSPs at ambient temperature (22 °C), where P_{ref} is the ambient pressure and I_{ref} is the luminescence intensity at ambient conditions.

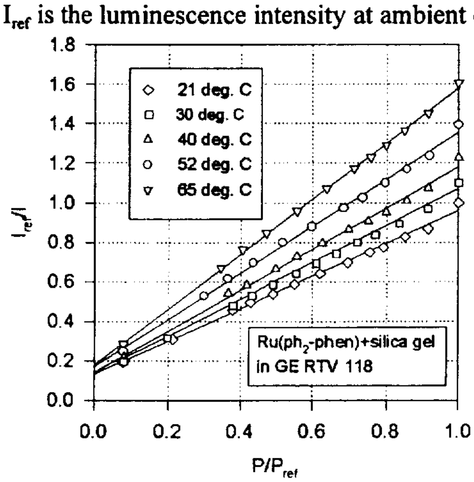

Figure 14. Calibration of Ruthenium based PSP.

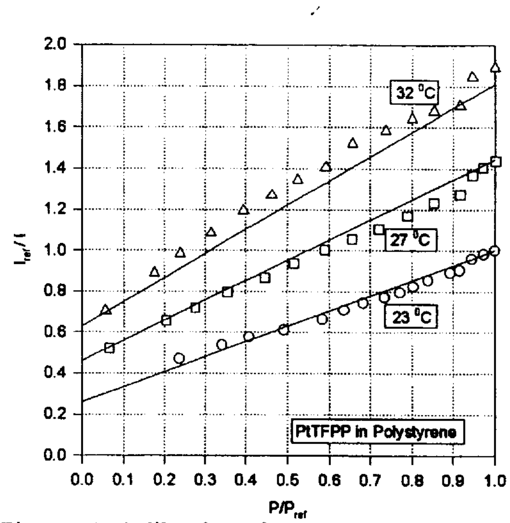

Figure 15. Calibration of PtTFPP pressure paint.

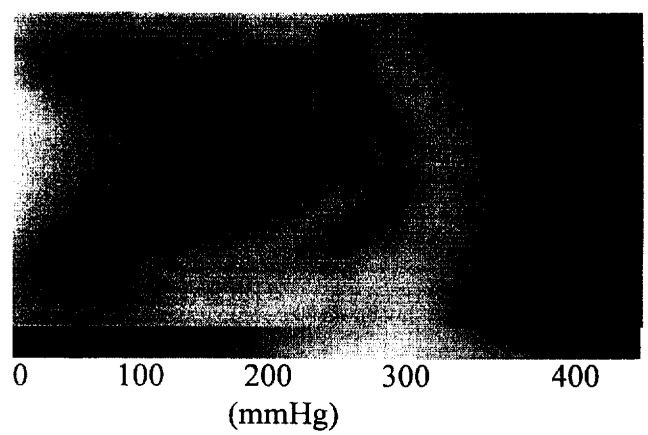

Figure 16. Pressure map for cylinder/boundary layer interaction at M=2.5.

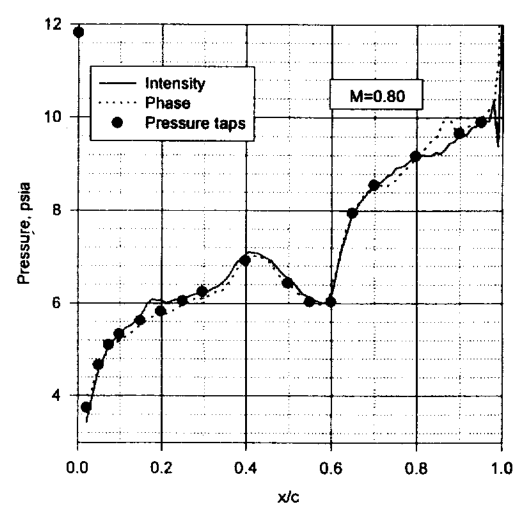

Figure 17. Pressure distribution on a transonic airfoil using both intensity and lifetime based methods.

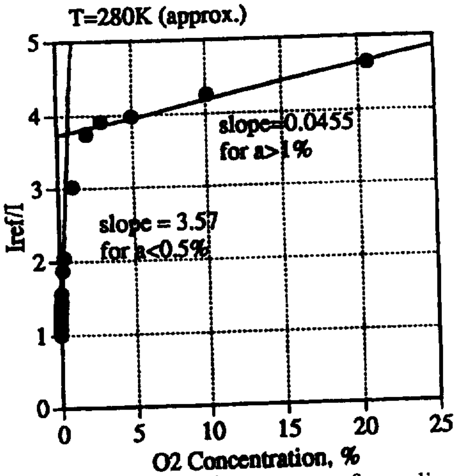

Figure 18. Calibration curve of anodized luminescent coating.

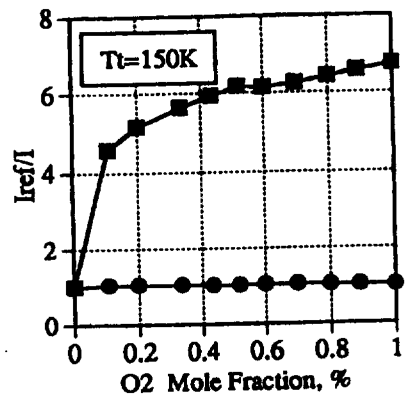

Figure 19. Calibration curve at cryogenic temperature.

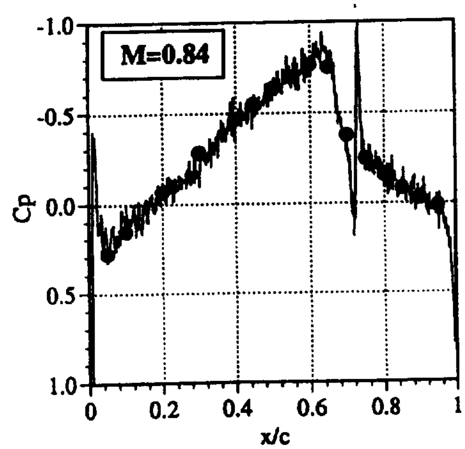

Figure 20. Comparison of luminescent paint and pressure tap data at T= 100K.

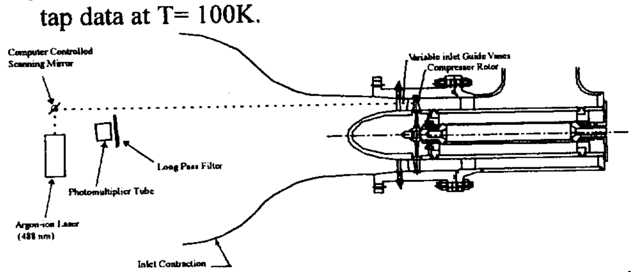

Figure 21. Transonic compressor rig with laser scanning system

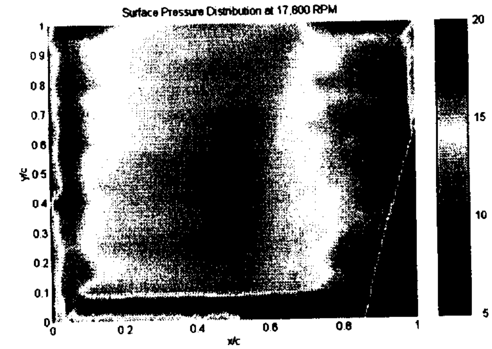

Figure22. Compressor blade suction surface pressure map at 17,800 rpm (scale in psia).

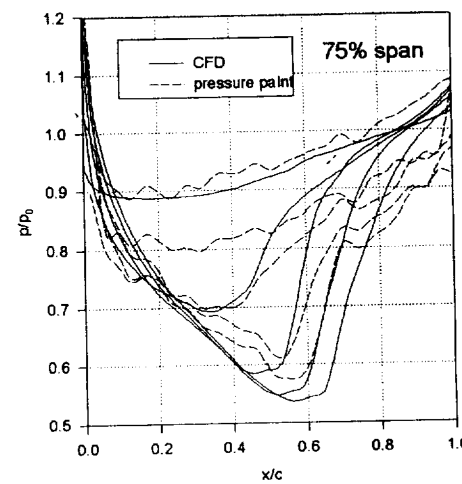

Figure 23. Comparison of PSP data and CFD results.

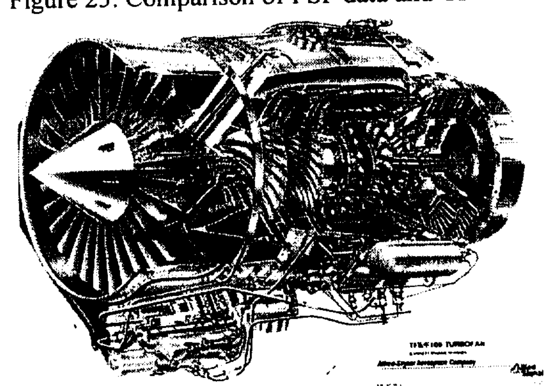

Figure 24. Allied F109 turbofan engine.

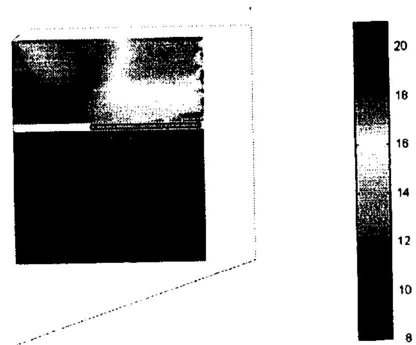

Figure 25. Fan blade pressure distribution at 14,000rpm (scale in psia).

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KEYWORDS

Pressure-Sensitive Paint, Anodized Aluminum, Cryogenic Wind Tunnel

ABSTRACT

Anodized aluminum pressure-sensitive paint has been used to measure the surface pressure distributions of wind tunnel models in a cryogenic wind tunnel. A thin, uniform anodized aluminum layer was directly coated onto the wind tunnel models by an electrochemical process. The resulting coating has an extremely high oxygen sensitivity for very low mole fractions of oxygen in the working gas (~150ppm). Numerous types of anodized aluminum PSPs were calibrated to optimize the sensitivity and the uniformity and to prevent the aging of anodized aluminum PSP. The luminophore deposition affected the sensitivity, and the phosphoric acid modification improved the uniformity and reduced the aging. To demonstrate this technology, a flat model and a 14% thick circular arc bump model were tested in the 0.1m Transonic Cryogenic Wind Tunnel at NAL. Surface pressure distributions on the models were clearly captured.

INTRODUCTION

Pressure-sensitive paint (PSP) measures the surface pressure distributions of wind tunnel models.

This technology is based on a photophysical phenomena known as oxygen quenching. Currently, PSP is applied to aircraft development wind tunnel testing. Using PSP, surface pressure distributions over the entire surface of a wind tunnel model can be obtained using a standard imaging camera and imaging processing techniques. However, one can say that the potential of the paint technology has not been fully exploited. One of the challenging areas to apply PSP is the use in a cryogenic wind tunnel. The idea of the cryogenic wind tunnel was developed at NASA Langley[1] to operate at high Reynolds number flows by lowering the working gas temperature by the continuous injection of liquid nitrogen. Hence, the working gas is practically pure nitrogen. In addition, a normal PSP cannot be used at cryogenic temperatures, since the oxygen quenching hardly occurs because of the low oxygen permeation in a normal PSP binder.

Asai[2] developed a new type of PSP which uses anodized aluminum as a binder. This PSP is extremely sensitive to oxygen since the luminophore is directly attached on the porous wall opened to the working gas. This new type of PSP is called anodized aluminum pressure sensitive paint (AA-PSP).

In our previous papers[3,4], the surface pressure measurements in a cryogenic wind tunnel using AA-PSP were discussed. Successful results were obtained for some AA-PSPs, showing the correspondence between pressure distributions from AA-PSP and from pressure taps. However, AA-PSP has not been fully developed. Uniformity was not reliably obtained, and the luminescent intensity and the sensitivity were changed by the day (aging).

In this paper, four factors of AA-PSPs, which are the anodization process, materials, phosphoric acid modification, and aging, are considered. Experimental results from a flat model and a 14% thick circular arc bump model tests in the 0.1m Transonic Cryogenic Wind Tunnel at National Aerospace Laboratory (NAL) are also presented.

BACKGROUND

Theory

The relationship between the luminescent intensity and the surface pressure of the wind tunnel model can be described by the Stern-Volmer equation. The original Stern-Volmer equation is,

$$\frac{I_0}{I} = 1 + K_q[O_2] \qquad (1)$$

where, I_0 is the luminescent intensity without the oxygen quencher, I is the luminescent intensity, and K_q is the Stern-Volmer quenching constant. $[O_2]$ is the oxygen concentration, which is proportional to the partial pressure of oxygen, $p_{[O2]}$. In addition, $p_{[O2]}$ and the static pressure of the working gas, p, can be related by the mole fraction of oxygen, $\bar{\phi}_{o2}$, which is a constant in the atmosphere (21%) but varies in a cryogenic wind tunnel. Equation (1) is rewritten as

$$\frac{I_0}{I} = 1 + K\bar{\phi}_{o2}\,p_{[O2]} \qquad (2)$$

where K is the quenching constant with respect to $p_{[O2]}$. The luminescent intensities can be related to the static gas pressures from equation (2).

One way to set the reference is to use an image with no-wind condition (wind-off condition). However, it is impossible to obtain a wind-off condition in a cryogenic wind tunnel since the test gas is cooled by the continuous injection of liquid nitrogen. An alternate way to set the reference is to use a low-speed condition. Taking a ratio between a low-speed condition and a wind-on condition, one can obtain the Stern-Volmer equation,

$$\frac{I_{ref}}{I} = A + B\frac{p_{[O2]}}{p_{[O2]ref}} \tag{3}$$

where $A = \dfrac{1}{1 + K\overline{\phi_{O2}}p_{[O2]ref}}$ and $B = \dfrac{K\overline{\phi_{O2}}p_{[O2]ref}}{1 + K\overline{\phi_{O2}}p_{[O2]ref}}$.

The coefficients A and B can be obtained by subjecting the PSP coating to a series of known partial pressures of oxygen.

Anodized Aluminum PSP (AA-PSP)

Anodized aluminum PSP (AA-PSP) uses anodized aluminum as a binder, and the luminophore is directly deposited on the anodized aluminum surface. The anodized aluminum is created from aluminum by an electrochemical process known as anodization. Hence, an aluminum model surface becomes the anodized aluminum surface by anodization. Spraying is not required to coat PSP onto the wind tunnel model for AA-PSP. By the anodization technique, an uniform AA-PSP coating can be obtained.

Anodized aluminum has micropores, 20 to 100nm in diameter, distributed on the surface. Since the anodized layer grows inward to the model surface, the thickness increase of the model surface is less than the anodized layer thickness.

Sensitivity

Stern-Volmer plots of AA-PSP show non-linearity, which can be fit with Freundlich isotherm,

$$\frac{I_{ref}}{I} = A + B\left(\frac{p_{[O2]}}{p_{[O2]ref}}\right)^{\gamma} \tag{4}$$

Since the Stern-Volmer plot is non-linear, we used the slope at $p_{[O2]}/p_{[O2]ref}=1$ to represent the pressure sensitivity, σ, such as,

$$\sigma = \left.\frac{\Delta(I_{ref}/I)}{\Delta(p_{[O2]}/p_{[O2]ref})}\right|_{p_{[O2]}/p_{[O2]ref}=1} \tag{5}$$

Uniformity

In our previous experiments, some AA-PSPs had spatial variations in Stern-Volmer constants. This means that the same calibration constants cannot be used to convert pressures from the luminescent intensity image at different spatial points. Uniformity of the calibration constants at different points on the AA-PSP model was necessary to obtain the pressure distributions.

Aging

The luminescent intensity and the sensitivity were lowered by aging, which occurs to AA-PSP within one day. One day after the experiment, for example, thè luminescent intensity was changed by 10% for one of the AA-PSPs in previous experiments.

DESCRIPTION OF EXPERIMENTS

AA-PSP Conditions

The following four factors were considered for their effect on the sensitivity, uniformity, and aging.

1. Anodization Process (Pretreatment)

The anodized aluminum layer is prepared from an aluminum surface pretreatment and anodization[5]. Although the pretreatment is important to prepare the anodized aluminum layer, its influence on the pressure sensitivity has not been evaluated. The pretreatment requires mechanical polishing or electrochemical polishing which dissolves the aluminum surface to remove the microscopic bumps. Mechanical polishing, electropolishing, and non-polishing were considered.

2. Material (Alloy)

Pure aluminum is usually used for anodizing aluminum, however, pure aluminum is soft and expensive to use as a wind tunnel model. The cost of aluminum alloy is much less than that of pure aluminum. For aluminum alloys, some impurities are mixed to increase the strength. However, the impurities cause pits, which are locally dissolved holes, on the anodized aluminum surface. Pure aluminum, 2024 aluminum alloy, and 5052 aluminum alloy were used for preparing AA-PSP models.

3. Luminophore Deposition

Two types of luminophore depositions, electrochemical deposition and the dipping deposition, were considered. Electrochemical deposition was used in the previous experiments. For this deposition, the AA-PSP model surface was negatively charged to attract the anionized luminophore. We developed another way to deposit luminophore called the dipping deposition. For this deposition, AA-PSP models were just dipped into a luminophore-dichloromethane solution. In both depositions, bathophen ruthenium was used as a luminophore.

4. Anodized Layer Modification

The anodized aluminum layer consists of three types of layers (Figure 1)[6]. We assumed that aging occurs on the anodized aluminum surface. Hence, the outer cell layer was dissolved by phosphoric acid (H_3PO_4) to compare two different anodized aluminum surfaces. Figure 2 (a) and (b) show SEM (Scanning Electron Microscope) pictures of unmodified and H_3PO_4 modified anodized aluminum surfaces. These surfaces were prepared from non-polished, pure aluminum. The micropores became wide and the outer cell layer was removed for H_3PO_4 modified surface (Figure 2 (b)).

Table 1 shows a list of AA-PSP conditions employed in present experiments.

Cryogenic Wind Tunnel Facility

To demonstrate the capability of AA-PSP to measure the surface pressures of wind tunnel models, experiments were conducted in the 0.1m Transonic Cryogenic Wind Tunnel (0.1m TCWT) at NAL[7]. This facility is a closed-circuit, fan-driven wind tunnel operated with cryogenic nitrogen as the working gas. The maximum stagnation pressure is 200kPa with the stagnation temperature ranging from 90K to 200K. The test section is 0.1m square and is equipped with slotted top and bottom walls of 4% porosity and solid side walls.

Figure 3 shows a schematic diagram of the experimental setup. The cryogenic wind tunnel is operated by controlling both the liquid nitrogen injection and the gaseous nitrogen exhaust. Oxygen gas was injected through a strut located just downstream of the test section. A small amount of the exhaust gas was sampled and fed into a Zirconia (ZrO_2) oxygen sensor to monitor the mole fractions of oxygen in the flow. The Zirconia sensor was calibrated prior to each run using a standard gas with known oxygen concentration.

Optical Equipment and Model

Figure 4 represents a schematic of the optical setup. The wind tunnel model was installed on one side of the wall of the wind tunnel test section. The optical access is gained through a 70mm diameter observation window on the opposite side of the wall. AA-PSP was excited by a Xenon light with a band pass filter (475±50nm). A dichroic mirror was used to separate the luminescence from the excitation light. The luminescence from the AA-PSP was detected by a digital camera with a cooled CCD. This camera has a 12-bit intensity resolution and 1000 x 1018 spatial resolution. An infrared rejection filter (900nm) and a red long pass filter (620nm) were placed over the camera lens.

In the present experiment, two types of models, a flat model and a 14% circular arc bump model, were used. A Flat model has six removable strips, which are 5mm wide and 50mm chord, mounted on one side of the wall of the test section (Figure 5 (a)). An arc bump model is a 14% thick circular arc bump with 50mm chord with 16 static pressure taps on the centerline. Four removable 8mm wide strips are mounted in spanwise locations (Figure 5 (b)). AA-PSP was applied onto the removable strips for both models. Tap pressures were measured by an electric pressure scanner located outside the tunnel.

Test Conditions

1 Flat Model Tests

Flat model tests were conducted prior to the arc bump model tests. The objective of this test was to optimize the sensitivity of AA-PSP, so that the pressure distributions on the wind tunnel model were not necessary. The anodization process, materials, and the luminophore deposition were considered. AA-PSP1 through AA-PSP6 is listed in Table 1. The partial pressures of oxygen on the flat model were changed by controlling the mole fractions of oxygen in the working gas ranging from 4ppm to 500ppm. The Mach number was kept at 0.40 and the stagnation temperature and the stagnation pressure were set as 100K and 190kPa, respectively.

2 Arc Bump Model Tests

14% circular arc bump models were employed to obtain the pressure distributions. A low-speed condition was taken as a reference and the Mach number of the flow was changed from 0.40 to 0.84. The mole fractions of oxygen was fixed at 150ppm, and the stagnation temperature and the stagnation pressure were kept at 100K and 190kPa, respectively.

The phosphoric acid modification was considered for uniformity and aging.

RESULTS AND DISCUSSION

Flat Model Tests

Sensitivity

Figure 6 shows the Stern-Volmer plots of AA-PSP1 through AA-PSP6. Each AA-PSPs has combinations of polishings, materials, and luminophore depositions. The main factor affecting the sensitivity was the luminophore deposition. The difference in materials and the difference in polishings did not change the sensitivity as much as the luminophore deposition. Taking 14Pa of the partial pressure of oxygen as a reference, the sensitivity was determined from equation (5). Higher sensitivity was obtained by the AA-PSP with the dipping deposition. The sensitivity was 0.40 to 0.53 for the AA-PSP with the dipping deposition and 0.13 with the electrochemical deposition.

Arc Bump Model Tests

From flat model results, non-polished, pure aluminum was used for preparing AA-PSP models. The AA-PSPs with the electrochemical deposition (AA-PSP7) and with the dipping deposition (AA-PSP8) were applied on arc bump model surfaces. To consider the uniformity and the aging, AA-PSP with the phosphoric acid modification and dipping deposition (AA-PSP9) was also applied.

Uniformity

Figure 7 (a) through (c) shows Stern-Volmer plots near pressure tap locations forAA-PSP7, AA-PSP8, and AA-PSP9. The partial pressure of oxygen at 14Pa was used as a reference. The partial pressures of oxygen on the model were changed by controlling the mole fractions of oxygen at Mach 0.40. It is clear that uniformity was not obtained for AA-PSP8. On the other hand, AA-PSP7 and AA-PSP9 were uniform. However, low sensitivity was obtained for AA-PSP7 because of the electrochemical deposition. Uniformity was obtained for the high sensitivity AA-PSP by using the phosphoric acid modification.

Pressure Distribution

We used *in situ* calibration to convert the luminescent intensity image to pressures. The calibration curves were obtained from pressure tap measurements and the luminescent intensity image at corresponding tap locations on AA-PSP. A low-speed image (Mach 0.40) was taken as a reference.

Figure 8 (a) shows *in situ* calibration curves of AA-PSP7 and AA-PSP8 models at M=0.82. Linear lines could fit to all *in situ* calibration curves, which indicates that temperature effects were negligible. Since the model surface is fairly isothermal in a cryogenic flow, we can use a single calibration curve for the entire surface of the model. Using these calibration curves, pressure coefficient, Cp, distributions were obtained from luminescent intensity images. Cp distributions of AA-PSP7 model had larger noise than that of AA-PSP8 model because of lower sensitivity (Figure 8(b)). Cp distributions of AA-PSP8 model did not correspond to the pressure tap measurements because of the poor uniformity (Figure 8 (c)). Both the uniformity and high sensitivity are necessary to obtain high signal to noise pressure distributions.

The Mach number was changed from 0.75 to 0.84 for AA-PSP9 model. Using the *in situ* calibration curves shown in Figure 9 (a), Cp distributions of AA-PSP9 model were obtained at different Mach numbers (Figure 9 (b) through (e)). At M=0.82 and 0.84, the shock wave strength and locations were clearly identified. The main source of error comes from errors in the calibration. Other error sources, such as camera shot noise, are much smaller. The error bars were estimated from the calibration error, and shown at 20%, 50%, and 85% of the chord (Figure 9 (b) through (e)).

Aging

Figure 10 (a) and (b) show Cp distributions of (a) AA-PSP9 and (b) AA-PSP7 models after six days from the previous arc bump model test. It is clear that AA-PSP7, which was not modified by phosphoric acid, was totally aged. Aging was reduced by the phosphoric acid modification. This suggests that the outer cell layer causes aging, since it was reduced by removing the outer layer.

CONCLUSIONS

1) Different types of AA-PSP were evaluated. The difference in the pretreatment and the difference in aluminum materials did not affect the sensitivity. Aluminum alloys can be used to increase the strength and to reduce the cost of the model.
2) The luminophore deposition changed the sensitivity. The dipped deposition method gave higher sensitivity than the electrochemical deposition method.
3) Uniformity was improved and the aging was reduced by the phosphoric acid modification. This suggests that aging occurs at the outer cell layer of the anodized aluminum surface.
4) With the uniformity and high sensitivity, AA-PSP can be used as a pressure sensor in cryogenic wind tunnel tests. Using the intensity image taken at a low speed condition as a reference, surface pressure distributions over the arc bump model were obtained. The AA-PSP data agreed with pressure tap data. The pressure jump due to a shock wave was clearly identified at transonic Mach numbers.

ACKNOWLEDGEMENTS

This work has been done as an international collaboration between Purdue University, USA, and National Aerospace Laboratory (NAL), Japan. The authors wish to thank Science and Technology Agency (STA), Japan, and the NASA Langley Research Center, USA, for their support of this work. The authors would like to thank Prof. H. Masuda at Tokyo Metropolitan University for his advice on how to prepare anodized aluminum layers, and H. Kanda at NÀL for his supports in optical setups.

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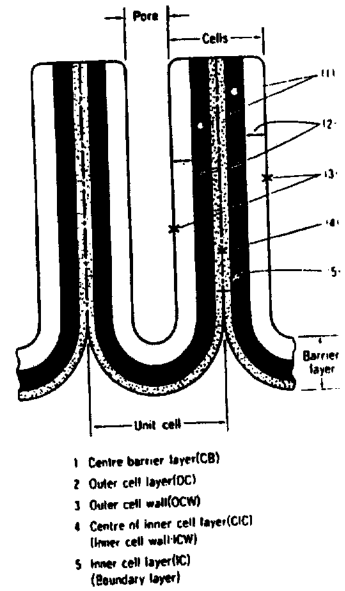


Figure 1 Composition of micropore (obtained from Wada, K.[6]).

(a) (b)

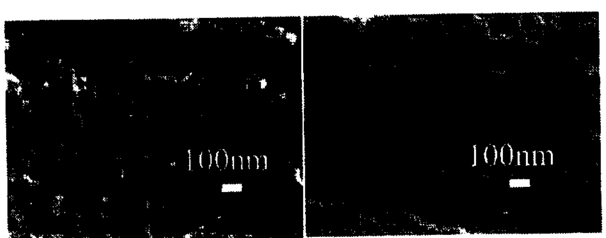


Figure 2 SEM pictures of (a) unmodified and of (b) phosphoric acid modified anodized aluminum surfaces.

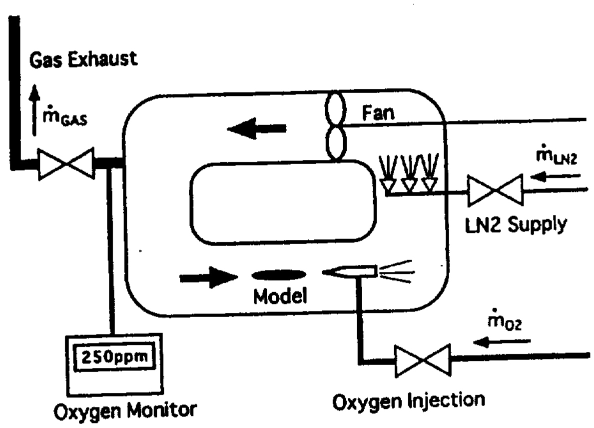


Figure 3 Schematic diagram of experimental setup in NAL 0.1m Transonic Cryogenic Wind Tunnel.

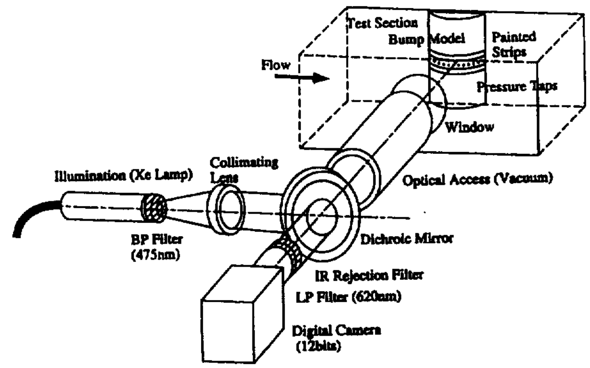


Figure 4 Schematic of optical setup in NAL 0.1m Transonic Cryogenic Wind Tunnel.

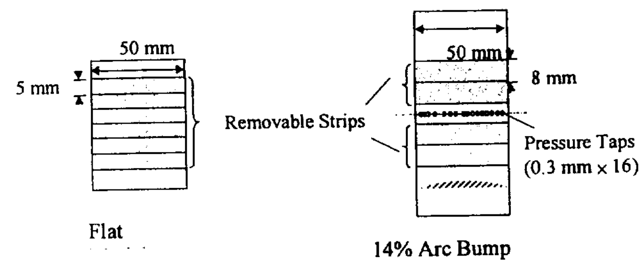


Figure 5 Schematic of (a) a flat model and (b) a 14% thick arc bump model.

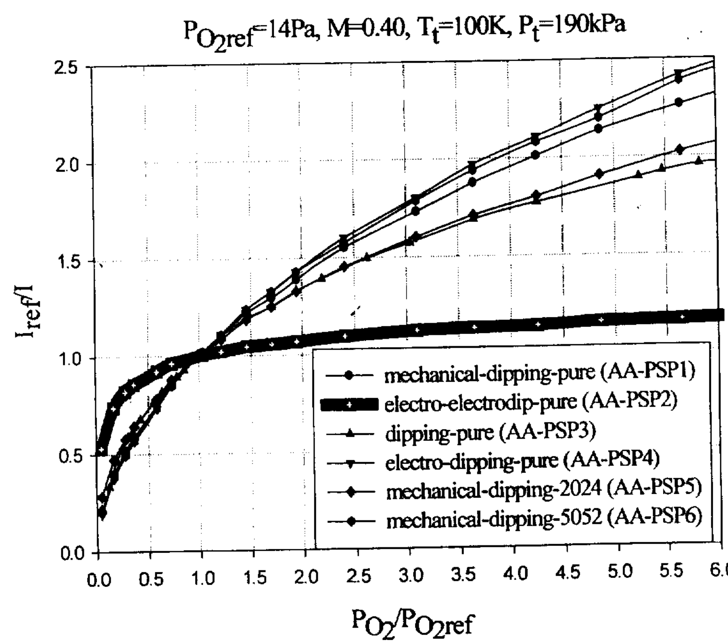


Figure 6 Stern-Volmer curves of different AA-PSPs (flat model tests).

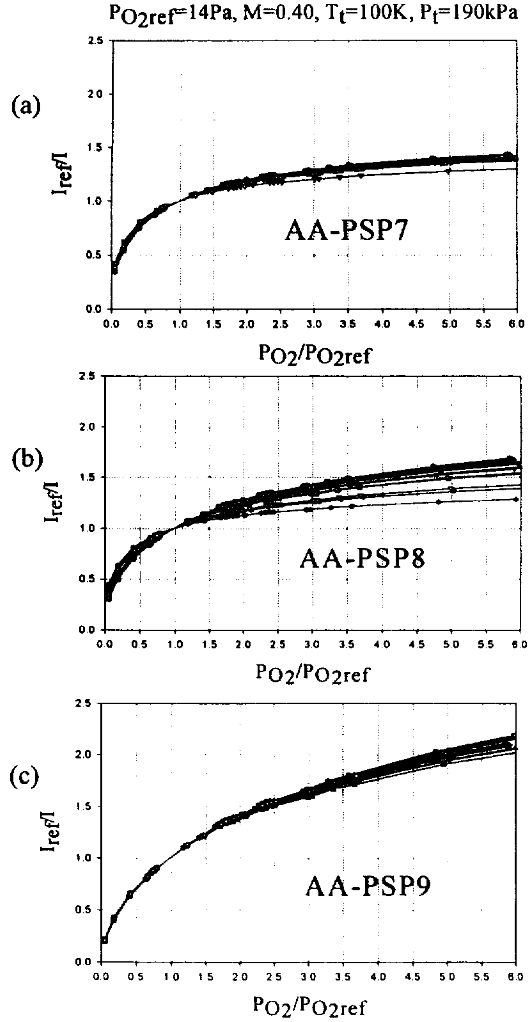
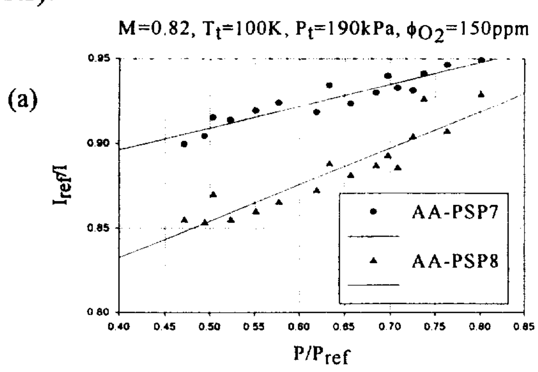


Figure 7 Stern-Volmer curves of different AA-PSPs near pressure tap locations (arc bump model tests).



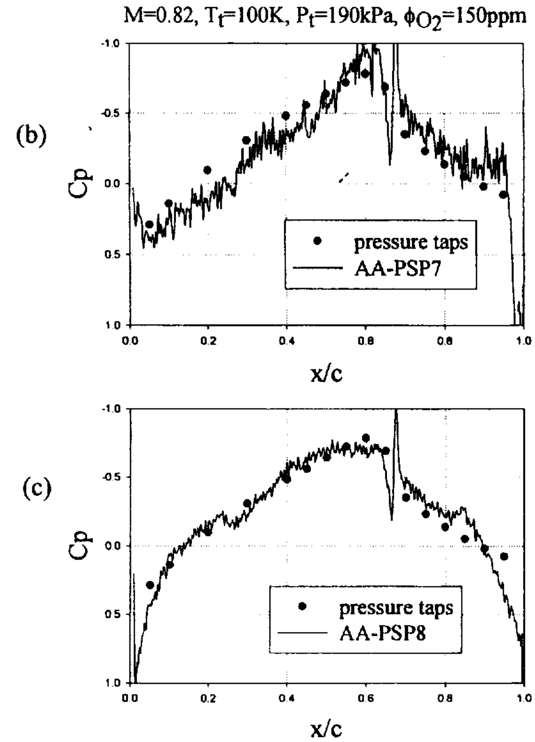
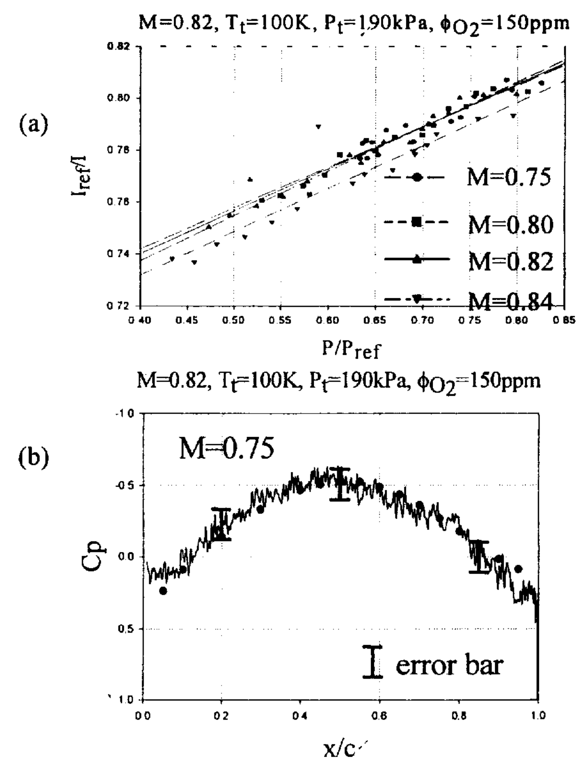


Figure 8 *in situ* calibration curves and Cp distributions for AA-PSP7 and AA-PSP8 at M=0.82.



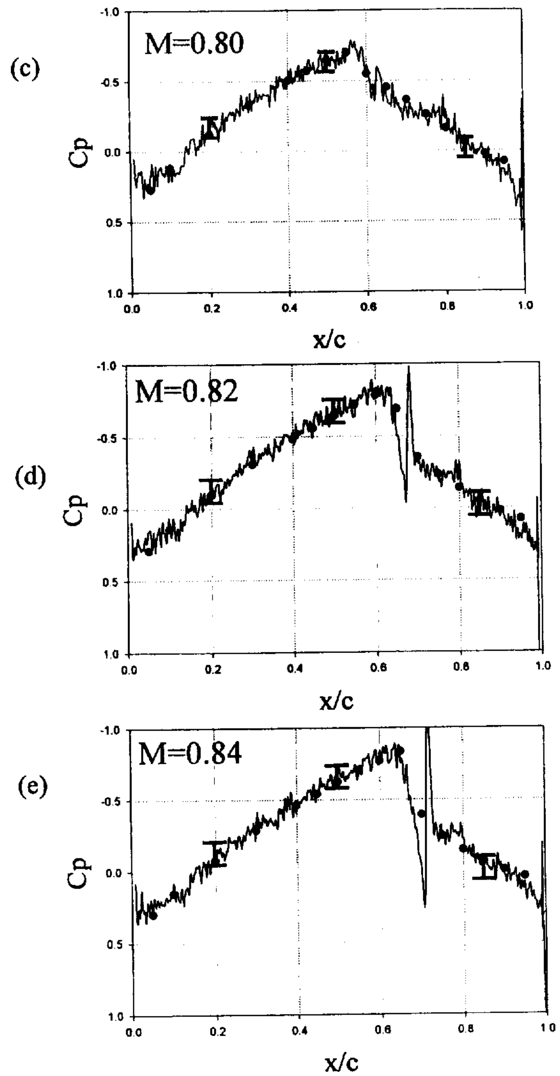


Figure 9 *in situ* calibration curves and Cp distributions of AA-PSP9 at different Mach numbers.

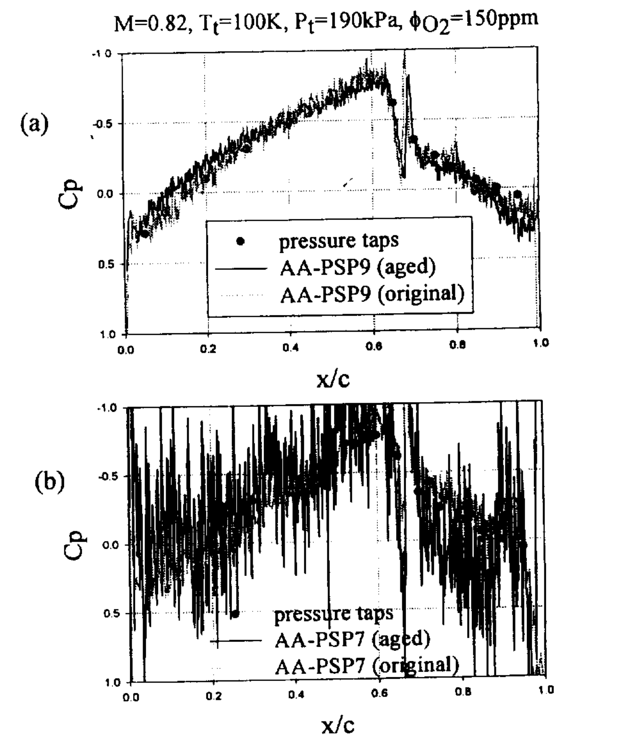


Figure 10 Aging of (a) AA-PSP9 and (b) AA-PSP7 (after 6 days in the wind tunnel).

Table 1 Anodized Aluminum PSP conditions

AA-PSP	Test	Pretreatment	Material	Deposition	Modification
1	Flat Model	mechanical	pure aluminum	dipping	no
2	Flat Model	electrochemical	pure aluminum	electrochemical	no
3	Flat Model	none	pure aluminum	dipping	no
4	Flat Model	electrochemical	pure aluminum	dipping	no
5	Flat Model	mechanical	2024 alloy	dipping	no
6	Flat Model	mechanical	5052 alloy	dipping	no
7	Arc Bump Model	none	pure aluminum	electrochemical	no
8	Arc Bump Model	none	pure aluminum	dipping	no
9	Arc Bump Model	none	pure aluminum	dipping	yes

POROUS POLYMER/CERAMIC COMPOSITES FOR LUMINESCENCE-BASED TEMPERATURE AND PRESSURE MEASUREMENT

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ABSTRACT

Porous Polymer/ceramic films were processed via tape casting. Upon doping with luminescent molecules such as platinum(II) octaethylporphine and [Ru(4,7-diphenyl-1,10-phenanthroline)$_3$]Cl_2, the films were used as pressure sensors, yielding a Stern-Volmer constant of A ranging from 0.02 to 0.61. These films also exhibited very fast response times (~1 ms). Tape cast films doped with Rhodamine B were used as temperature sensors under cryogenic conditions. The temperature sensitivity of the doped films increased with increasing Rhodamine B concentration.

INTRODUCTION

Recently, luminescence-based sensors for temperature and pressure measurement have received a great deal of attention for aerodynamics applications [1-3]. These sensors, based on the phenomena of oxygen and thermal luminescence quenching, potentially provide inexpensive, non-intrusive, high resolution pressure and temperature mapping of aerodynamic model surfaces.

Pressure sensors typically consist of a luminescent molecule (luminophore) housed in a polymer binder [4]. When exposed to radiation of the proper wavelength, the luminophore will be excited to a singlet state. It may return to its ground state by emitting a photon of a longer wavelength. Certain luminophores can transfer excited state energy to a quencher molecule, such as O_2, that has diffused into the sensor from the environment, causing a radiationless transition to the ground state. This phenomenon is known as oxygen quenching. The rate at which these two relaxation processes compete is dependent on the partial pressure of oxygen, with a higher oxygen pressure quenching the molecules more effectively. By filtering the excitation radiation from the emission radiation, photodetection of oxygen quenching makes pressure measurement possible. Oxygen quenching generally follows a Stern-Volmer relationship:

$$\frac{I_{ref}}{I} = A + B\left(\frac{P}{P_{ref}}\right)^{\gamma} \qquad (1)$$

where A, B, and γ are constants. I_{ref} and P_{ref} are a reference intensity and pressure, respectively. These reference values correct for non-uniformities in excitation illumination, luminophore deposition, and photodetector sensitivity.

While polymers are mechanically robust, their effectiveness as a housing medium for luminophores is limited by material properties such as O_2 permeability (permeability representing the product of the diffusivity and the solubility). A low O_2 solubility will decrease the sensitivity $\left(\frac{d\left(\frac{I_{ref}}{I}\right)}{d\left(\frac{P}{P_{ref}}\right)}\right)$ of the sensor, while a low O_2 diffusivity will lengthen the response time of the sensor to changes in O_2 pressure [1]. Several polymers have a high O_2 solubility:

However, most also display a low O_2 diffusivity, thus limiting the overall effectiveness of the sensor.

If a luminophore could be adsorbed or bonded to a porous surface, it would produce a sensor that would have a very fast response time to changes in oxygen pressure. Porous polymer membranes are commercially available, but are costly to apply for large-scale wind tunnel tests. Ceramic films provide a low cost alternative; however, due to challenges in processing ceramic films to conform to surfaces for aerodynamic testing, as well as their inherent brittle behavior, ceramics have yet to find widespread use as luminophore housings for luminescent pressure sensors.

Tape casting is a widely used process for preparing ceramic substrates for electronic packaging [6]. Prior to firing, tape cast films are composed of ceramic powder held together with a polymeric binder. Tape cast films are good candidates to house luminophores for luminescent pressure sensors. The films are porous, which may shorten response time, yet they are mechanically robust due the polymer, facilitating handling, and providing a film that will withstand the stresses of aerodynamic testing.

Tape casting may also be used to process luminescent temperature sensors by using luminophores that are sensitive to their thermal environment. The luminophore is again excited by absorption of a photon. The excited molecule deactivates through the emission of a photon. A rise in temperature of the luminescent molecule will increase the probability that the molecule will return to the ground state by a vibrational (radiationless) process. This is known as thermal quenching, and may be expressed in functional form as:

$$\frac{I(T)}{I(T_{ref})} = F(T/T_{ref}) \qquad (2)$$

where $F(T/T_{ref})$ is an empirical expression that may be a polynomial, or another function best fitting the experimental data.

While there are several effective temperature sensors near room temperature, few luminophores have exhibited temperature sensitivity at cryogenic temperatures (120-200 K) [1,5]. The sensors currently used exhibit sensitivity over only a small temperature range, making tests in cryogenic wind tunnels more difficult [5].

EXPERIMENTAL PROCEDURE

Ceramic/polymer composite films were processed from an aqueous suspension of ceramic powder via tape casting. The suspension was prepared by dispersing Al_2O_3 (Reynolds Aluminum Co., specific surface area=8.5 m^2/g) in water (83 wt% Al_2O_3) using a polyelectrolyte surfactant (D-3021, Rohm & Haas). The suspension was ball-milled for one hour to eliminate agglomerates, and subsequently mixed with 7.5 wt% (relative to the suspension) of a poly(acrylic) binder emulsion (B-1035, Rohm & Haas). The suspension was cast onto a silicone-coated Mylar™ sheet (Richard E. Mistler, Inc.) using a doctor blade to form films ranging in thickness from 0.1-0.2 mm.

Two different luminophores were used in this study, platinum(II) octaethylporphine (PtOEP) (Porphyrin Products) dissolved in toluene, and [Ru(4,7-diphenyl-1,10-phenanthroline)$_3$]Cl_2 (Ru(dpp)Cl_2) (GFS Chem.) dissolved in methanol. Tape cast coupon samples were dipped into the luminophore solutions, and subsequently dried in air. The individual components of the tape cast composites were also prepared for calibration. The polymeric binder was cast onto Mylar™ via a doctor blade technique and allowed to dry. Coupons were again cut and dipped into the two luminophore solutions. The Al_2O_3 powder was pressed in a die at 5000 psi, and the resulting porous powder compact was dipped into the luminophore solutions and dried in air.

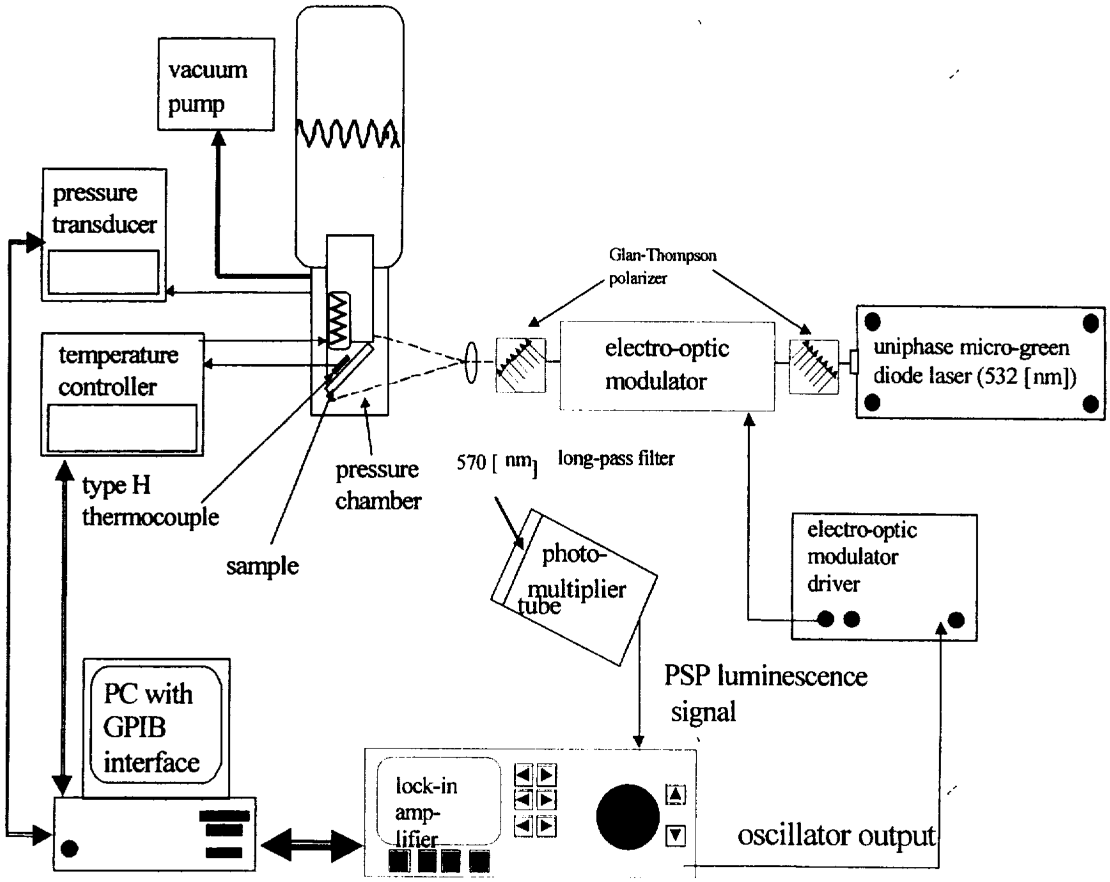

Figure 1. Apparatus used for pressure calibrations.

For the temperature sensors, tape cast coupons were dipped into solutions of Rhodamine B (RhB) (Aldrich) dissolved in methanol, and subsequently dried in air. To vary the amount of RhB in a given sample, coupons were prepared using RhB solution concentrations ranging from $2.09*10^{-4}$ to 0.02 molar.

The experimental apparatus used to calibrate the pressure sensors is shown in Figure 1. The sample is enclosed in a test chamber with optical access, and the chamber pressure is controlled by a vacuum pump and monitored by an absolute pressure gauge. Dry air (21% O_2) of varying absolute pressure is fed into the chamber, and the partial pressure of oxygen in the calibration chamber is determined by combining the pressure measurement from the absolute pressure gauge and the test gas composition.

Measurements of the pressure sensor's luminescent intensity were made using phase sensitive detection. The sample was illuminated with 532 nm radiation from a 50 mW Uniphase Micro-Green diode laser. The laser radiation was passed through an electro-optic modulator which was driven by a sinusoidal reference from a lock-in amplifier resulting in a modulated illumination signal for the sample. The luminescent signal from the sample was collected through a 570 nm long pass filter onto a photo-multiplier tube. The photo-multiplier tube signal was demodulated by the lock-in amplifier using a 1-second integration time. The bandwidth narrowing characteristics of the phase sensitive detection scheme resulted in improved signal to noise ratio, and improved accuracy in the sensor calibrations. The entire calibration process was controlled by a LabView™-based data acquisition program on a personal computer.

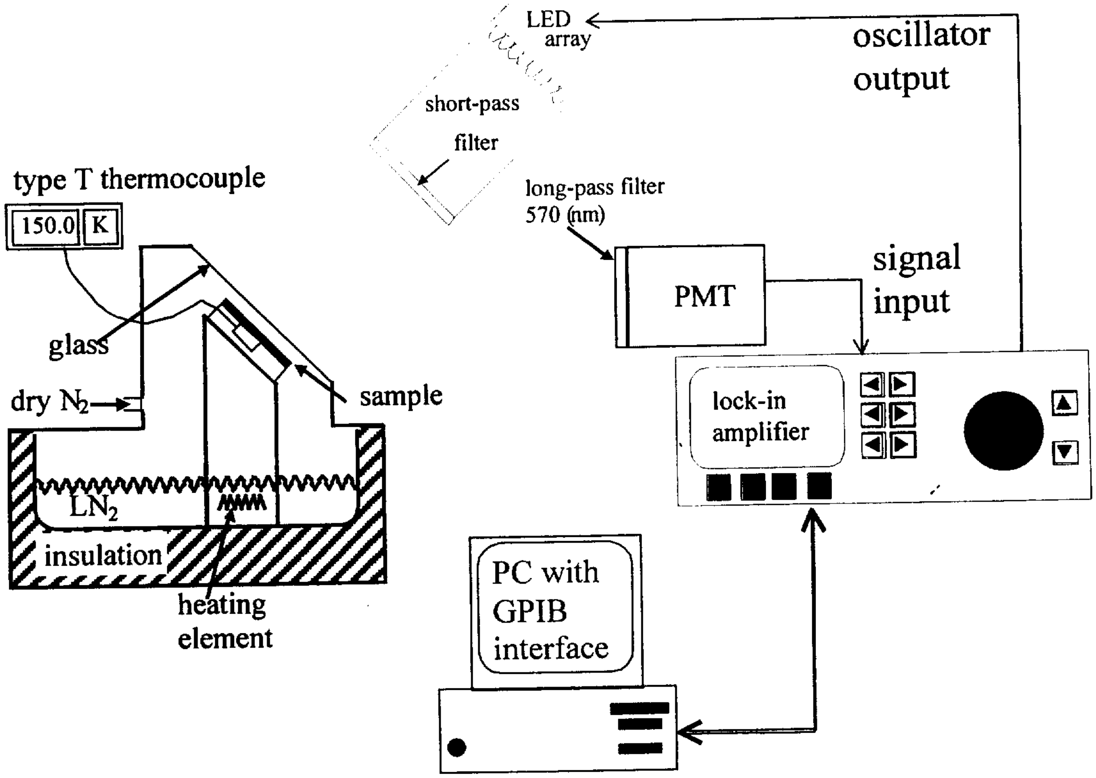

Figure 2. Apparatus used for temperature sensor calibrations.

The experimental apparatus used to calibrate the temperature sensors in the cryogenic range is shown in Figure 2. The temperature sensor was placed on a copper rod rising from a liquid nitrogen bath. A type T thermocouple was placed between the sensor and the copper rod. Good thermal contact between the sensor, thermocouple, and copper rod was ensured by the use of thermal grease. The sensor and bath were enclosed in a small chamber allowing optical access through a single window. Dry nitrogen was bled through the enclosure to prevent water from condensing on the paint sample. Accurate measurements of the luminescent intensity of the sensor were accomplished using phase sensitive detection. The sensor was excited with sinusoidally modulated illumination from a green LED array. The luminescent signal from the sensor was collected through a 570 nm long pass filter onto a photo-multiplier tube. The photo-multiplier tube signal was again demodulated by the lock-in amplifier with a 1-second integration time.

RESULTS AND DISCUSSION

The tape cast films exhibited excellent mechanical properties. They were flexible and scratch resistant. They have successfully withstood the stresses that are seen in sonic jet impingement experiments, wind tunnel tests, and flight tests for *in-situ* pressure measurements.

Stern-Volmer plots for tape cast films doped with either the PtOEP or Ru(dpp)Cl_2 are shown in Figure 3. Films doped with PtOEP exhibited greater pressure sensitivity (larger slope) compared to films doped with Ru(dpp)Cl_2. When the luminophores were housed in the binder alone, they exhibited the same behavior as the tape cast film. However, the pressure sensitivity of luminophores housed in Al_2O_3 powder compacts differed significantly from the tape cast

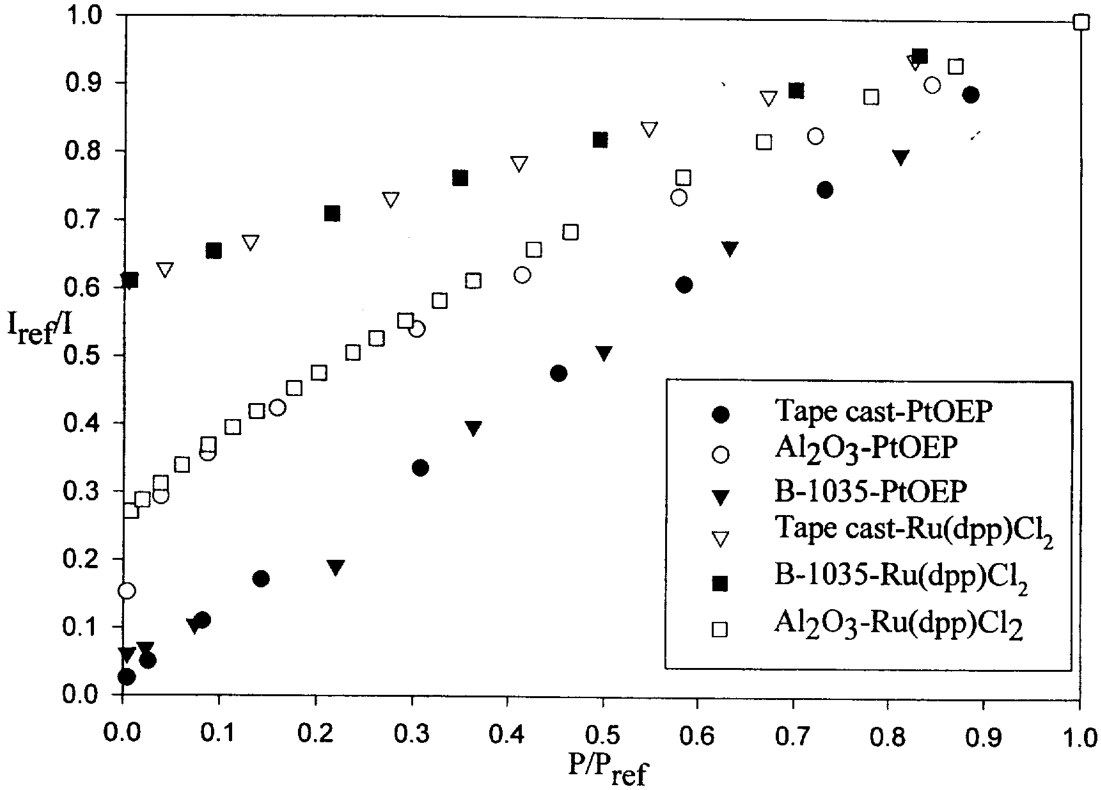

Figure 3. Stern-Volmer data for tape cast components and films doped with different luminophores.

films. When housed in Al_2O_3 powder compacts, PtOEP and Ru(dpp)Cl_2 exhibited similar pressure sensitivity. Compared to the powder compact with the same luminophore, the PtOEP tape cast film exhibited a greater pressure sensitivity, while the Ru(dpp)Cl_2 tape cast film had a lower pressure sensitivity. This implies that the polymer plays a dominant role in determining the pressure sensitivity characteristics of the tape cast films. Preliminary measurements indicated that the tape cast films exhibited response times on the order of 1 ms. Microtomed cross sections of the tape cast films showed that there is a continuous interconnecting network of pore channels throughout the film. This may account for the observed rapid response times, because the porosity provides a fast diffusion path for oxygen.

Tape cast temperature sensors of varying RhB concentration were calibrated over a broad range of cryogenic temperatures (Fig. 4). At low RhB concentrations, the films were nearly insensitive to temperature variations, while at higher concentrations, the films showed good temperature sensitivity. However, the luminescent intensity of the sensor decreased both with increasing temperature due to more available vibrational modes for radiationless deactivation, and with increasing RhB concentration due to self-quenching effects. A larger luminescent intensity facilitates data acquisition by increasing photodetection efficiency. Therefore, the effective range of a temperature sensor depends on both the temperature sensitivity and the luminescent intensity. The film with intermediate RhB concentration exhibited an effective operating range of 130-260 K while the higher concentration had a range of 130-210 K. While the temperature sensitivity of the intermediate concentration was less than that of the highest concentration sensor, it still exhibited sufficient thermal quenching for data acquisition purposes.

CRYOGENIC TEMPERATURE- AND PRESSURE-SENSITIVE FLUORESCENT PAINTS

A Thesis
Submitted to the Faculty
of
Purdue University
by

Richard German Erausquin Jr.

In Partial Fulfillment of the
Requirements for the Degree
of
Master of Science in Aeronautics and Astronautics

December 1998

To my wonderful wife, Heather.
Her willingness to assume the greater burdens of family
and work have enabled the achievement of this goal.
Words alone cannot convey my appreciation for the
patience and love she has shown over the years.

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ABSTRACT

Erausquin, Richard G. Jr. M.S.A.A., Purdue University, December 1998. Cryogenic Temperature- and Pressure- Sensitive Fluorescent Paints. Major Professor: John P. Sullivan.

The use of pressure- and temperature-sensitive fluorescent paints to make aerodynamic measurements has been well documented. The present work describes the extension of that research into the realm of cryogenic wind tunnel testing. Cryogenic wind tunnels are capable of simulating in-flight transonic Reynolds Numbers by lowering the operating temperature of the working gas to near liquid nitrogen temperatures. While this process enables testing in a dynamically similar flow, there are inherent difficulties in obtaining measurements. The use of pressure- and temperature-sensitive paints in cryogenic wind tunnels offers better economics and simplicity in measurement. The objective of this research is the development of pressure- and temperature-sensitive paints that function under the conditions experienced in a cryogenic wind tunnel. The problems associated with the extension of paint technology into the cryogenic realm are discussed and methods for preparing different coatings examined. These coating preparation methods include increasing pressure-paint layer porosity using previously untried methods of surface depositing luminescent molecules that alleviate poor diffusivity at cryogenic conditions. Issues associated with molecular properties and the ability to change those properties in an effort to design temperature-sensitive paints that respond with better sensitivity over specific temperature ranges are investigated. Apparatus for conducting cryogenic calibrations of pressure- and temperature-sensitive paints are described and calibrations conducted. Results of these calibrations show temperature response can be slightly affected by molecular design of luminescent molecules and that paint layers can be created that show sensitivity to oxygen concentration in the low temperature and low oxygen conditions found in cryogenic wind tunnels.

CHAPTER 1: INTRODUCTION

In recent years, temperature-sensitive paints (TSP's) and pressure-sensitive paints (PSP's) have attracted much attention in the aerospace community. These paints are commonly composed of a luminescent compound and a binder. A luminescent compound is one that adsorbs radiative energy (light) of a particular wavelength and emits light of a slightly longer wavelength. Through the photophysical phenomena of thermal and oxygen quenching of luminescence, emission intensity of the paint can be related to temperature and pressure. Hence from the detected luminescence intensity, temperature or pressure on the painted surface can be determined. In general, emission intensity increases with decreasing temperature and decreasing oxygen concentration.

Currently, TSP's and PSP's are being applied to aircraft development and wind tunnel testing. Much success in obtaining temperature and pressure maps on wind tunnel model surfaces has been documented. These paints can be used to generate high-resolution temperature and pressure maps, detect boundary layer transition, and examine shock/boundary layer interactions.

Temperature measurements on wind tunnel models can sometimes incorporate a large number of thermocouples or similar measurement devices. These are complex systems that are expensive to instrument and do not yield continuous temperature distributions. On the other hand, temperature-sensitive paint measurements are fairly simple, inexpensive, and can yield full surface temperature maps.

Pressure-sensitive paints similarly offer several advantages over traditional methods of measuring pressure distributions on wind tunnel models. Pressure taps are complex and expensive (~$200 per tap) to install on wind tunnel models, cannot give continuous pressure distributions, and aerodynamics and structural dynamics of the model can be seriously altered by the modifications required for pressure tap installation. Using PSP's alleviates all of these concerns. The continuous distributions obtained from PSP's allow for better comparisons with computational results and data rates are much higher than conventional techniques which increases efficiency of wind tunnel usage.

One recent, and very challenging, extension of the paint technology has been its application in cryogenic wind tunnel testing. Cryogenic wind tunnel technology was developed at NASA Langley as a means of simulating high Reynolds number flows. By cooling the wind tunnel test gas to near liquid nitrogen (LN_2) temperature, significant increases in Reynolds number can be obtained. Full-scale flight Reynolds numbers have been obtained with sub-scale models in cryogenic wind tunnel facilities such as the National Transonic Facility (NTF), European Transonic Wind Tunnel Facility (ETW), and the 0.1-m Transonic Cryogenic Wind Tunnel at The National Aerospace Laboratory (NAL) in Japan. Typically, these wind tunnels operate at temperatures in the range of 90 to 180 K. Naturally, these types of facilities are expensive to operate and the conditions limit tunnel access. Cryogenic TSP's and PSP's require limited access and less tunnel operating time, thus reducing the cost. Like room temperature paints, they are also easier to implement than current techniques.

There are many challenges in the development of cryogenic TSP's and PSP's. The environment is very harsh, thus adversely affecting the coating. The extremely low temperatures have been observed to severely decrease diffusion of oxygen into the commonly used polymer binders for PSP's. Brittleness of the binder also becomes a major concern at these temperatures because any cracking or flaking of the binder would destroy the coating. In addition, most work with TSP's has concentrated on temperatures near room temperature. Compounds that are temperature sensitive under cryogenic conditions are difficult to obtain. Another concern with cryogenic PSP's is the need for molecular oxygen in the working gas to serve as a quencher. The problem that arises is that since the working gas in a cryogenic wind tunnel is pure nitrogen, oxygen needs to be added to the flow. Injecting large amounts of oxygen is, however, not permissible from the standpoints of safety and cost. Thus, only small concentrations of oxygen are allowed to exist in the working gas, yielding a necessity for highly sensitive PSP coatings.

Once a coating has been found to respond to temperature or pressure it must be calibrated to obtain a relation between emission intensity and temperature or pressure. Under room temperature conditions, this is a fairly straightforward process. Calibrations under cryogenic conditions, however, require the use of specialized test stands designed specifically for that purpose. The design of such test stands, calibration methods, and calibration results for cryogenic TSP's and PSP's are presented herein.

Another interesting aspect of the luminescent molecules is that recent photophysical theory has suggested that temperature response can be affected by the molecular structure itself. Through modification of currently utilized luminescent molecules, the region of temperature over which the luminophore shows a response can be changed. It has also been postulated that the sensitivity can also be affected. Attempts have been made to create temperature sensitive molecules that exhibit a response over a specific region of temperature with a high sensitivity.

CHAPTER 2: LITERATURE REVIEW

Thermal and oxygen quenching of luminescence has been observed since as early as 1931[1], however it has not been until the past two decades that luminescent molecules have seen widespread use as temperature and oxygen sensors. Two driving forces in the development of these sensors have been the areas of biosensing and aerodynamics.

In the realm of biosensing, much effort has been made in the area of luminescent oxygen sensors. Papkovsky[2] created a prototype fiber-optic intensity-based oxygen sensor using a derivative of PtOEP. Shriver-Lake, et. al.[3] adapted a biosensor to utilize dyes excited above 600 nm and coupled easily to proteins to enable easy detection of blood toxins. A low cost instrument based on light-emitting diodes and photodiodes was created by Trettnak, et. al.[4] Another interesting quality of Trettnak's device was that the flow-through cell was thermally stabilized to alleviate temperature effects on the luminescent molecules. In the ultimate application, Poole et. al[5] demonstrated the measurement of microvascular plasma P_{O2} in vivo in a rat's costal diaphragm. While many of these sensors use intensity-based methods, biomedical researchers have also investigated fluorescence lifetime or phase based methods of making oxygen measurements. Szmacinski and Lackowicz[6] describe their method for externally modulating excitation light sources to enable measurements based on lifetime methods. Lifetime and phase methods in biosensing have also been investigated by Holst et. al.[7] and Keeffe et. al.[8] Another interesting aspect of Keffe's work was that the luminescent molecule was immobilized in a Sol-gel matrix, a previously untried binder in aerodynamics circles. Another interesting investigation of binder effects from the biosensing community is the work of He et. al.[9] In this work, He examines the effects of entrapping a Ruthenium based complex in a silicone polymer binder.

Much of the early success of luminescent paints in aerodynamics came from temperature-sensitive paints. Campbell. et. al.[10] calibrated many aromatic hydrocarbon and transition metal based TSP's. The calibrated paints were then used to perform steady state and unsteady heat transfer measurements on subsonic, supersonic, and hypersonic models. Heat transfer in a shock-turbulent boundary layer interaction, heat transfer on a wall shear flow, and heat transfer of an excited circular impinging jet were measured using temperature-sensitive paints by Liu[11]. More recently, work by Shen and Schanze[12] has focused on the actual synthesis of new temperature-sensitive paints that can be designed to respond over certain regions of temperature by choice of ligand structure.

Pressure-sensitive paints have been used in numerous aerodynamic measurements. Kavandi, et. al.[13] conducted measurements on a 2-D NACA 0012 airfoil. McDonnell Douglas conducted tests on a generic wing/body model at Mach 2, a Mach 1.2 high performance fighter, and a converging-diverging nozzle[14]. McDonnell Douglas[15] and Torgerson[16] (of Purdue University) have also made efforts at PSP measurements in low speed flows. In a very challenging extension of the technique, pressure measurements on the fan blades of rotating machinery have been made using PSP's by Burns[17] and Torgerson[16]. An excellent review of both TSP's and PSP's is given by Liu, et. al.[24]

To date, very little work has been done in implementing TSP's and PSP's under cryogenic conditions. Campbell[10] calibrated many different compounds and discovered a number of excellent TSP's that function in the cryogenic range. Cryogenic TSP's were used by Asai, et. al. to detect boundary-layer transition in a cryogenic wind tunnel over a temperature range of 90 to 150 K in both subsonic and transonic flows[18]. In cooperation with this research, Asai et. al. produced and tested a new coating technique for obtaining PSP measurements in a cryogenic wind tunnel[19]. Using this new coating, accurate resolution of the pressure distribution on a circular arc bump model was accomplished. Oglesby et. al. have also conducted cryogenic PSP experiments with this new type of coating and have noted marked divergence from traditional linear Stern-Volmer response[20]. It should be noted that non-linear Stern-Volmer responses have been noted for various paints containing $[Ru(ph_2\text{-}phen)_3]$[21] and Platinum Porphyrin complexes[22]. These PSP's exhibit a downward curve in the Stern-Volmer response at lower oxygen concentrations, thus exhibiting higher sensitivity at these low partial pressures. As previously noted, this is desirable in the low oxygen environment of a cryogenic wind tunnel.

CHAPTER 3: THEORY

The photophysical processes behind the behavior of TSP's and PSP's have been thoroughly presented in literature, but will be covered for completeness. On the macro scale, a luminescent molecule is embedded in a polymer binder and placed on the surface to be measured. Absorbing a photon of light of a particular wavelength excites the luminescent molecules. In the process of returning to the ground state, the luminescent molecules emit photons of Stokes shifted light. The general term for the emitted light is luminescence. This process is depicted below in Figure 3.1, and a typical absorption and emission spectra is shown in Figure 3.2.

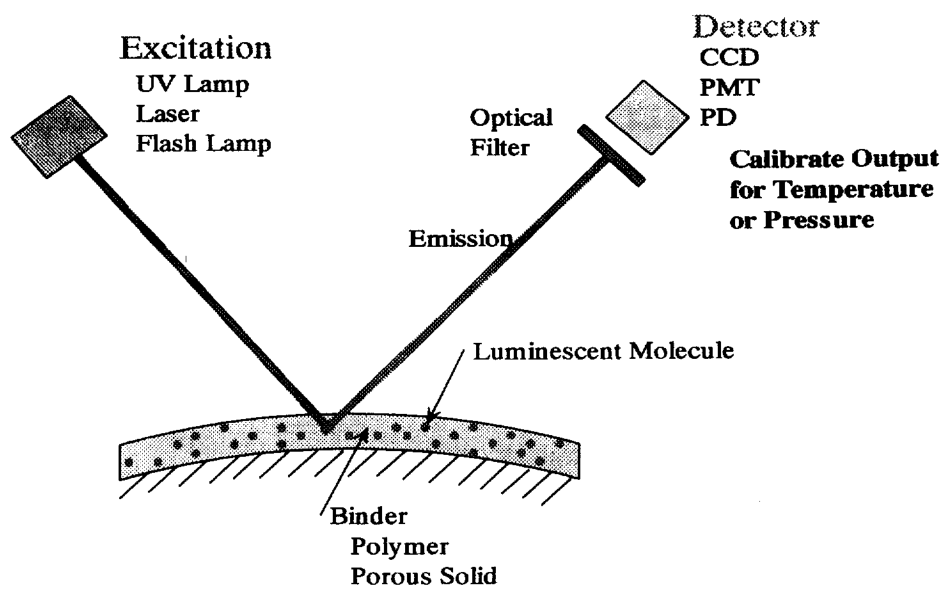

Figure 3.1: Luminescent Paint Layer

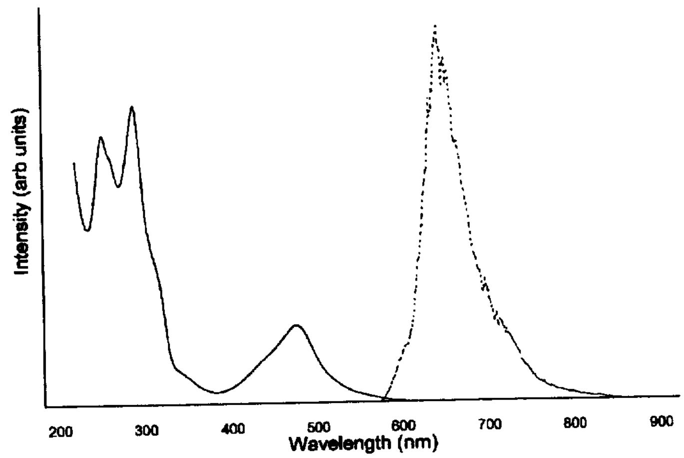

Figure 3.2: Absorption and Emission Spectrum for [Ru(ph$_2$-phen)$_3$]

3.1 Electrochemical Theory

On a molecular scale, once the photon is adsorbed, an electron jumps from the singlet ground state S_o to the excited state S_i (i>1). Within picoseconds, the excited state relaxes to the lowest excited singlet state S_1 through radiationless internal conversion. There is a small possibility that an intersystem crossing from S_1 to the T_1 triplet state may occur at this point, otherwise the electron remains in the S_1 state for a short period of time. Once the electron is in either the lowest excited singlet or triplet state, the remaining excess energy must be dissipated in order for the electron to transition back to the ground state S_o. It is at this point, where a distinction is drawn as to what process happens next: fluorescence, phosphorescence, or radiationless deactivation (quenching). All of these processes are illustrated below in Figure 3.3.

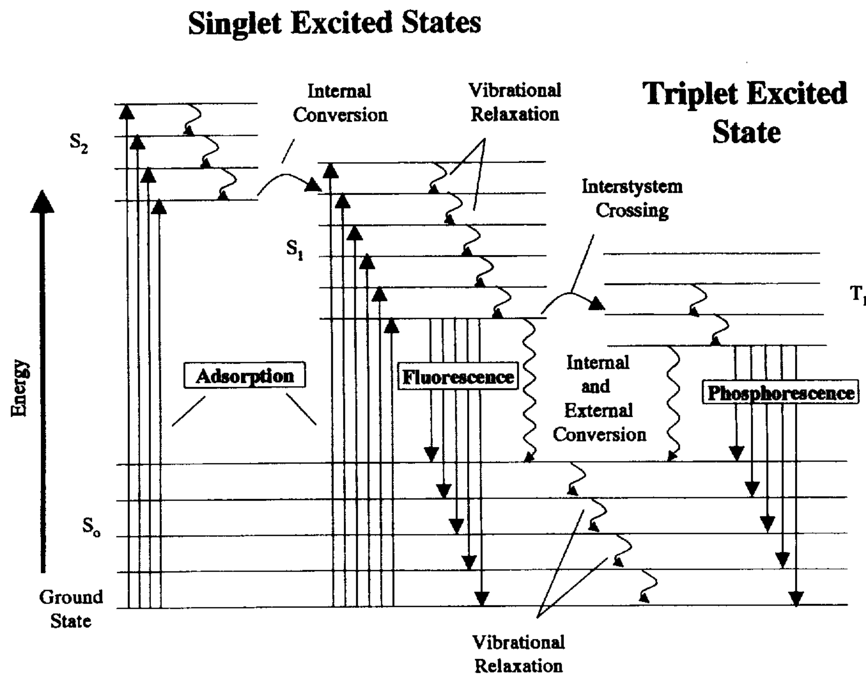

Figure 3.3: Energy Level Diagram

Electrons remaining in the S_1 excited state can do so for only a short period of time. In order to relax to the singlet ground state, the excess energy must be dissipated. This is accomplished through the emission of a photon of light of a longer wavelength than the excitation light. The emission of a photon during a transition from S_1 to S_0 is called fluorescence. The other method of transitioning from S_1 to S_0 is through internal or external conversion, commonly known as quenching. When a molecule is quenched, the S_1 to S_0 transition occurs without the emission of a photon of light.

If an intersystem crossing from the first singlet excited state to the first triplet excited state occurs prior to relaxation to the ground state, a slightly different process takes place. As with transitions from the first singlet excited state, energy is dissipated through the emission of a photon of light of a longer wavelength than the excitation light, or through a radiationless deactivation process. The light emitted in the T_1 to S_0 transition is called phosphorescence. The difference between fluorescence and phosphorescence comes from the fact that transitions into the triplet excited state involve a spin flip of the electron. Phosphorescence occurs much less than fluorescence because the transition from the excited triplet state to the ground singlet state is spin forbidden according to the Pauli Principle and thus exhibits a longer lifetime than a singlet excitation. It should be noted that second- and third-row transition metals exhibit a spin-orbit coupling where effects of the heavy metal atom can lead to a loss of distinction between singlet and triplet states.[23] In TSP's and PSP's the radiationless deactivation processes are of interest. Radiationless deactivation, or quenching, can occur through thermal or oxygen quenching of the molecule.

3.1.1 Molecular Structure

The luminophores used in this research are based on second and third row transition metals. A metal atom is bonded to a ligand molecule. The ligand is a molecule based on benzene structures. The structure of the bond between the metal and ligand is a major factor in determining temperature sensitivity. As an example of one of these atoms, a 2-D figure of the [Ru(trpy)] molecule is shown below. In three dimensions another trpy ligand molecule is bonded to the Ru opposite and perpendicularly out of plane with the trpy ligand shown below.

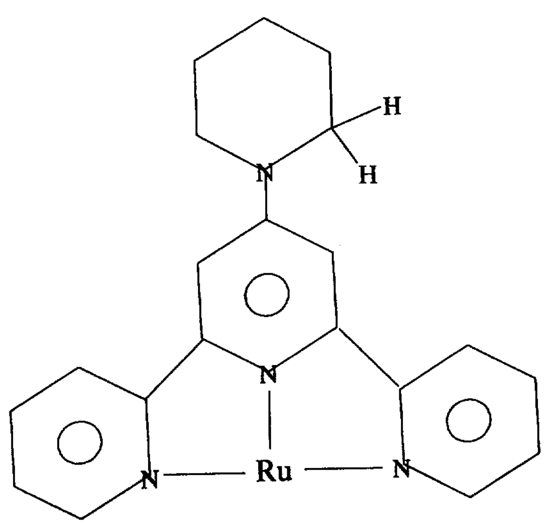

Figure 3.4: Structure of the [Ru(trpy)] molecule

An anion is added to neutralize the charge of the luminescent molecule. Anion quenching has been noted in some molecules, however it does not exhibit a large effect. The size of the anion used determines the solubility of the luminescent molecule and thus effects the kind of solvent used or whether or not the molecule dissolves directly into certain polymer binders.

3.1.2 Thermal Quenching

Thermal quenching of luminescence is based on the metal-to-ligand bond as mentioned in Section 3.1.1. At higher temperatures, the metal-to-ligand bond begins to elongate and shrink in a spring-like fashion. As temperature increases, more energy is lost to this vibration. Statistically, a system containing molecules experiencing energy loss due to this vibration can be modeled using Boltzman statistics. Figure 3.5 below shows the model used to describe a molecule's entry into the theoretical quenching state.

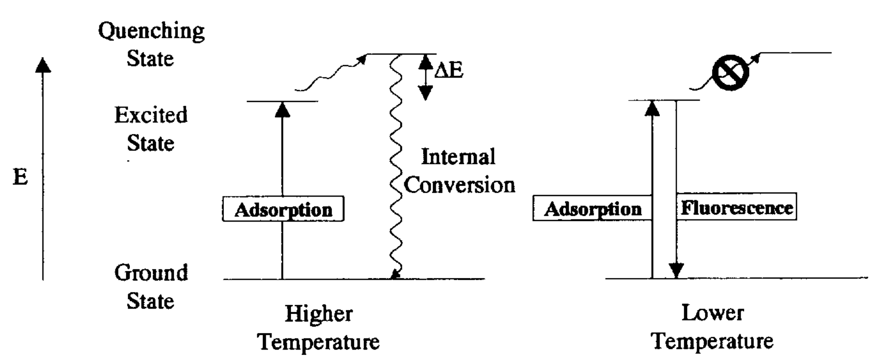

Figure 3.5: Quenching State Model

At higher temperatures, enough excess energy exists to allow some of the molecules to transition into the quenching state. Once in the quenching state, the molecule goes through a non-radiative internal conversion to return to the ground state. At lower temperatures, not enough excess energy exists to enter the quenching state thus the molecule must transition to the ground state by emitting excess energy in the form of a photon of light (fluorescence). It is the Boltzman statistics that describe the rate constant k_D, used in Section 3.2.

From this discussion, it should be apparent that the properties of the metal-to-ligand bond have a large effect on rate parameters. These effects are controlled by the type of bond and bond angle. Stronger bonds allow for less rigidity, thus adversely effecting vibrations between the metal and ligand. Bond angle effects the distribution of molecular orbitals, thus effecting the energy gap, E, between the excited state and quenching state.

3.1.3 Oxygen Quenching

Oxygen quenching of luminescence is an entirely separate process from thermal quenching. The unexcited valence electrons in an O_2 molecule naturally exist in the degenerate triplet state. When two electrons inhabit a degenerate triplet state in a molecule they have the same spin. When an O_2 molecule in the triplet state comes in close proximity to an excited luminescent molecule in the triplet state (see 3.1), the electrons of opposite spin undergo a simultaneous transfer between the O_2 molecule and the luminophore. This process returns the luminophore to the ground state, thus quenching the fluorescence, and returns the oxygen molecule to the singlet state.

It should be noted that singlet O_2 is very reactive and may cause a destructive reaction with nearby luminescent molecules. This is the cause of photodegradation in pressure-sensitive paints (see 7.1.1 for a complete discussion). Metal porphyrin complexes like PtOEP are very susceptible to reactions with singlet O_2, transition metals are not as likely to react.

3.2 Quantitative Theory

The entire photophysical process is best quantified through the quantum yield (quantum efficiency) of luminescence Φ.

$$\Phi = \frac{\text{rate of luminescence emission}}{\text{rate of excitation}} = \frac{I}{I_a} \tag{3.1}$$

where I is the luminescence intensity and I_a is the adsorption intensity. In the steady-state condition, the quantum yield in the presence of the quencher, $[O_2]$, is given by the following model:

$$\Phi = \frac{I}{I_a} = \frac{k_L}{k_L + k_D + k_Q[O_2]} = k_L \tau \tag{3.2}$$

where k_L is the rate constant for luminescence emission, k_D is the rate constant for deactivation and is temperature dependent, k_Q is the rate constant for quenching, $[O_2]$ is the local concentration of oxygen, and τ is the lifetime of the excited molecule, given by:

$$\tau = 1/(k_L + k_D + k_Q[O_2]) \tag{3.3}$$

Thus the process of thermal quenching affects quantum yield through k_D, and oxygen quenching affects quantum yield through the dependence on $[O_2]$ and k_Q. Dividing (3.2) by the maximum luminescence intensity I_o at $[O_2]=0$ yields the Stern-Volmer equation:

$$\frac{I_o}{I} = 1 + k_Q \tau_o [O_2] = 1 + K_Q [O_2] \tag{3.4}$$

where τ_o is simply the rate constant at $[O_2]=0$ and K_Q is the product of k_Q and τ_o. Since $[O_2]$ is proportional to the oxygen partial pressure, $p_{[O2]}$, equation (3.4) can be written:

$$\frac{I_o}{I} = 1 + K\, p_{[O_2]} \tag{3.5}$$

where K is the quenching constant with respect to $p_{[O2]}$. For a constant mole fraction of oxygen in the gas, the partial pressure of oxygen can be related to the local static pressure by:

$$p = \overline{\Phi}_{o_2}\, p_{[O_2]} \tag{3.6}$$

where p is the local static pressure and $\overline{\Phi}_{o_2}$ is the mole fraction of oxygen in the working gas. The mole fraction is 0.21 for air and can be varied in a cryogenic wind tunnel. Using equations (3.5) and (3.6) an expression for the sensitivity of the luminescent coating to static pressure can be obtained:

$$\frac{\Delta\left(I_0/I\right)}{\Delta p} = K\overline{\Phi}_{[O_2]} \tag{3.7}$$

From equation (3.7) it can be noted that the sensitivity of a paint with quenching constant K will decrease with decreasing mole fraction. Thus in a cryogenic wind tunnel where the mole fraction of oxygen is low in the nitrogen-based cryogenic working gas, a paint with large quenching constant, K, is needed.

By using the ratio of I_o/I, spatial nonuniformities in the coating thickness, uneven luminophore concentration, and non-uniform excitation light are ratioed out of the result. It is however, very difficult to obtain a zero oxygen condition, even in a cryogenic wind tunnel where residual oxygen in the liquid nitrogen can have a large effect on the emitted intensity from these very sensitive PSP's. This problem can be alleviated by taking equation (3.4) at intensity I and ratioing it with an intensity measured at a known reference condition, I_{ref}. Factoring out adsorption intensity I_a yields the functional form of the Stern-Volmer equation shown below:

$$\frac{I_{ref}}{I} = A(T) + B(T)\frac{p_{[o_2]}}{p_{[O_2]ref}} = a(T) + b(T)\frac{p}{p_{ref}} \tag{3.8}$$
$$A(T) + B(T) = a(T) + b(T) = 1$$

where A and B are experimentally determined coefficients, I is the measured intensity, I_{ref} is a reference intensity, $p_{[O2]}$ is the oxygen partial pressure, and $p_{[O2]ref}$ is a reference partial pressure. Due to the temperature dependence of the oxygen permeability of the binder and k_D (τ_o), the coefficients A and B are temperature dependent thus requiring surface temperature to be known. The constants A and B can be determined through the following relation and experimental determination of the constants a_1 and b_1 in the following[16]:

$$A = a_1\left[1 + \frac{E_{nr}}{RT_{ref}}\left(\frac{T - T_{ref}}{T_{ref}}\right)\right]$$
$$B = b_1\left[1 + \frac{E_p}{RT_{ref}}\left(\frac{T - T_{ref}}{T_{ref}}\right)\right] \tag{3.9}$$

where E_{nr} is the non-radiative activation energy, E_p is the polymer activation energy, R is the interaction distance, T is the surface temperature in K, T_{ref} is the reference temperature in K, and a_1 and b_1 are experimentally determined constants. These constants can be obtained through a calibration where oxygen partial pressures are varied (or static pressure of a constant oxygen mole fraction gas is varied) at known constant temperature. Equation (3.8) can be more generally expressed as a power series expansion on the partial pressure ratio to account for some non-linear effects, however the second order polynomial expression has been shown to be sufficiently accurate to this point.

For TSP's, the assumption of a non oxygen-permeable paint allows $[O_2]$ to be set to zero in equation (3.2) yielding:

$$\Phi = \frac{I}{I_a} = \frac{k_L}{k_L + k_D} = k_L \tau_0 \tag{3.10}$$

As noted previously, the rate constant k_D is temperature dependent. It can be decomposed into a temperature-independent part and temperature-dependent part, $k_D = k_0 + k_1$. The thermal deactivation rate k_1 can be assumed as the Arrhenius form[24]:

$$k_1 = C \exp\left(-E/_{RT}\right) \tag{3.11}$$

where C is a pre-exponential constant, E is the Arrhenius activation energy, R is the universal gas constant, and T is the thermodynamic temperature in Kelvin. Substituting equation (3.11) into (3.10) and then subtracting the inverse of equation (3.10) at absolute zero from the inverse of equation (3.10) at temperature T yields the following:

$$\frac{I_a}{I(T)} - \frac{I_a}{I(0)} = A\, k_L^{-1} \exp\left(-E/_{RT}\right) \tag{3.12}$$

The adsorption intensity I_a can be excluded from the above expression by dividing (3.12) by the reference intensity I_{ref} at a known constant temperature T_{ref} yielding:

$$\ln \frac{I(T)\left[I(0) - I_{ref}(T_{ref})\right]}{I_{ref}(T_{ref})\left[I(0) - I(T)\right]} = \frac{E}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right) \tag{3.13}$$

Since I(0) is much larger than I(T) and $I_{ref}(T_{ref})$ it follows that:

$$\frac{\left[I(0) - I_{ref}(T_{ref})\right]}{\left[I(0) - I(T)\right]} \approx 1.0 \tag{3.14}$$

and

$$\ln \frac{I(T)}{I_{ref}(T_{ref})} = \frac{E}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right) \tag{3.15}$$

Thus theorectially speaking, a plot of the log of the intensity ratio versus ($1/T - 1/T_{ref}$) yields a straight line of slope E/R. Since the ratioing process corrects for non-uniformities, the slope of the Arrhenius plot can be used to compare the sensitivity of respective temperature paints.

While the linear relation holds for many luminescent compounds in solution, some compounds in rigid matrices show non-linearities over certain temperature ranges. Alternatively, the temperature dependence can be expressed in a functional form:

$$\frac{I(T)}{I_{ref}(T)} = F(T/T_{ref}) \tag{3.16}$$

The functional form could be a polynomial, exponential, or other function that fits the experimental data over a certain temperature range.

CHAPTER 4: PAINT COMPOSITION, PREPARATION, AND MEASUREMENT TECHNIQUES

4.1 Paint Composition and Preparation Techniques

A TSP or PSP is generally composed of two components, a luminescent molecule and binder. Some new methods of attaching luminescent molecules to surfaces have also been investigated in order to make more sensitive cryogenic PSP's.

4.1.1 Luminescent Molecules

The luminescent molecules calibrated in this research were based on second- and third-row transition metals. These metals readily undergo the addition or subtraction of electrons to produce different oxidation states, which makes them attractive as photoredox reagents[23]. Their likelihood to donate electrons to electron-accepting substituents is desired because this has been shown to increase quantum yield and excited state lifetime[36]. Another positive attribute of the transition metals is that they are naturally structured to carry out photochemical reactions using visible light[23].

For temperature-sensitive paint research, emphasis was placed on the $[Ru(trpy)_2]$ family of luminescent molecules. This family exhibits very intense emissions at low temperatures and are nearly fully quenched at room temperature[25]. Thus, they are an excellent choice for temperature sensors under cryogenic conditions. The structure of $[Ru(trpy)_2]$ molecules offers several advantages significant to this research. Various $[Ru(trpy)_2]$ molecules can be easily synthesized with different ligands[36]. As noted in Section 3.1.1, the dynamics of the metal-to-ligand bond and the electron donating or accepting characteristics of the ligand[36] have a significant effect on the temperature sensitivity of the luminescent molecule. This includes the rate constant and region of temperature over which the molecule responds. A main effort in this research was to calibrate $[Ru(trpy)_2]$ type molecules with various ligands to determine if the response could be "tuned". This would enable the synthesis of molecules specifically designed to respond with high sensitivity in a specific region of temperature.

For cryogenic pressure-sensitive paint research, the emphasis was placed more on the binder than on the luminescent molecule. The reasoning being that the permeability of the binder has a significant effect on the response of the paint (see discussion in section 4.1.3). Thus, three luminescent molecules known to exhibit good sensitivity at lower oxygen concentrations were chosen for this research. The first, $[Ru(ph_2\text{-}phen)_3]$ has been used for many different measurements at room temperature and has a good record of accomplishment. The other two luminescent molecules chosen were Platinum porphyrins, Pt(meso-tetra flourophenyl) Porphyrin (PtTFPP) and Pt(octa-ethyl) Porphyrin (PtOEP). Both have been observed to exhibit non-linear Stern-Volmer behavior in a rigid matrix, but this non-linear behavior exhibits greater sensitivity at lower oxygen partial pressures. As noted previously, good quenching behavior at low oxygen partial pressures is needed for cryogenic wind tunnel measurements.

With the exception of the porphyrin complexes, a standard nomenclature has been used throughout this document to describe the luminescent molecules. The nomenclature is of the following form:

[atom(ligands)](anion)

4.1.2 Temperature-sensitive Paint Preparation

The preparation of temperature-sensitive paint layers is generally a simple process. Two essential ingredients are required, the luminescent molecule and the binder used to hold the luminescent molecules to the surface. While some luminescent molecules will dissolve directly into certain polymers, in general it is necessary to first dissolve the luminescent molecules into a solvent, then mix with a binder which is also soluble in the solvent used. After the paint is mixed it can be applied to the surface on which a temperature measurement is desired. The solvent typically fully evaporates before the polymer is completely dry, leaving a layer where the luminescent molecules are suspended within the polymer matrix.

Generally, polymer binders are used to attach the luminescent molecules to the surface. Polymer binders are typically chosen because of their ability to form thin layers and their solubility in common organic solvents. Different binders have been shown to have contrasting effects on adsorption and emission spectra, luminescent intensity (lifetime) and temperature dependence[35]. Binder choice is often the result of experience plus trial and error. Another concern in choosing a binder for TSP measurements is oxygen permeability. Since both oxygen and temperature quench luminescent molecules, it is desirable to de-couple the effects. This is easily accomplished in TSP's by choosing a binder that has low oxygen permeability.

The mixture may be applied to the surface using a variety of methods. The two most common application methods are spray and dipping. Spraying the paint onto the surface using an airbrush produces a thin, fairly uniform coating. This is desirable so that non-uniformity in the layer does not adversely effect the measurements. Dipping the surface into the paint solution and slowly withdrawing it produces thin films. Uniformity depends on the rate at which the surface is withdrawn from the paint mixture and on surface adhesion properties. In general, this method produces coatings uniform to the eye and acceptable for conducting measurements.

As this research is focused on TSP's operating in the cryogenic temperature range, it is necessary to examine what effects cold temperatures have on paint layers. The main concern is that the layer will become too brittle and crack at the extremely cold temperatures. Whether or not the layer will crack is dependent on the amount of contraction the material suffers with lowering temperature and the thickness of the layer. Experience has shown that thicker layers tend to crack more than thinner layers under the same cryogenic conditions. The overall likelihood of a layer to crack is difficult to quantify, thus trial and error generally identifies which particular binders are best to use and how thick the coating should be.

4.1.3 Pressure-sensitive Paint Preparation

In general, the PSP molecule is absorbed into a polymer binder, which is highly oxygen permeable, and applied to the surface being measured. This is completed in a similar manner to that used to mix and apply TSP's. Factors such as test environment and response time influence the choice of molecule and binder. As with TSP's, the binder can affect a luminescent molecules absorption and emission spectra, luminescent intensity (lifetime) and temperature dependence.

Generally, binders with higher diffusivity produce more sensitive PSP's with faster response times. Baron et al[26]. suggest fast responding coatings based on silica coatings applied to aluminum plates or a commercial porous silica thin-layer chromatography (TLC) plates. These types of coatings have been used to measure pressure distributions in impinging jets[27] and rotating propeller blades[28]. Torgerson et. al.[29] have used less porous binders such as GE 118 RTV and model airplane dope to make measurements on a low speed impinging jet. GE RTV 118 mixed with silica particles was used as a binder for [Ru(ph$_2$-phen)$_3$] in high-speed axial compressor fan blade pressure distribution measurements[30]. While the most sensitive response is obtained with silica coatings, these are often difficult to apply to wind tunnel models. RTV based binders can be more easily sprayed onto the model, but tend to be less permeable to oxygen.

Oxygen permeability of the layer becomes an even larger issue at the low temperatures being investigated for this work. Permeability of gaseous oxygen into the paint layer is obtained from the following relation:

$$P = P_o e^{-E/kT} \tag{4.1}$$

where P is the coefficient of permeability, E is the thermal activation energy, k is Boltzman's constant, and T is temperature in Kelvin. It can be seen from equation (4.1) above that permeability will decrease exponentially with decreasing temperature.

Because permeability becomes so low at cryogenic temperatures, methods of increasing permeability needed to be found. Some of the low temperature effects on permeability of the RTV and GP-197 based paints have been alleviated by adding large amounts of silica to the paint mixture. While this increases the porosity of the binder, it also has an adverse effect on the ductility of the paint layer. In addition, several new methods of depositing the luminescent molecules onto the surface using little or no polymer were examined. Those methods are outlined in the following sections.

4.1.3.1 Anodized Aluminum

To alleviate some of the poor effects of low temperature on binders, a new method of depositing the luminescent molecule onto the model was developed by Asai et. al[31]. In this method, an electrochemical anodizing process is used to produce a thin layer of porous alumina containing a luminophore. Aluminum and lead strips are placed in a bath of 20% (by concentration) sulfuric acid and 10 Volts (~0.6 A) placed across the two strips with the positive lead attached to the aluminum and the negative lead to the Pb. The voltage is applied to the two strips for approximately 10 to 30 minutes. Next the luminescent molecule is dissolved in a bath of Ethanol and the two strips are placed in the Ethanol bath with the aluminum surface to be coated facing the lead strip. A voltage of 20 Volts (~0.01A) is then placed across the two strips with the negative lead attached to the aluminum and the positive lead attached to the Pb. The voltage is applied for 5 to 10 minutes depending on the desired coating thickness. The resulting coating is very uniform, tough, and has an extremely high sensitivity to oxygen at cryogenic temperatures.

4.1.3.2 Hydrothermal Coating

A coating method in which a thin coating of polymer and titania can be created through hydrothermal crystallization[32] was tried. This offers the possibility of creating a coating with high quantum yield. Since only a small weight percent of polymer is required, this coating also offers the possibility of minimizing the cryogenic effects on the polymer. To create the mixture, the polymer (Kraton D1102 shell / polystyrene-polybutaediene co-polymer) is dissolved in toluene. Next, a titanium precursor (titanium diisopropoxide bis(ethyl acetoacetate)) is added. The ratio of TiO_2 to polymer in the final coating is controlled at this step. The mixture is applied to a surface which is subsequently dipped into a solution of water and a luminophore ([Ru(ph$_2$-phen)$_3$] in this case) where a hydrolyzing process takes place, forming the coating containing TiO_2, polymer, and luminescent molecule. The ratio of TiO_2 to polymer can vary significantly, however 80/20 and 99/1 were tested in this research.

4.1.3.3 Sol-gel

The Sol-gel process is used to produce high quality glasses and ceramics[33]. In optical sensors, silica or titania is commonly used in the production of the Sol-gel layer. These glasses are produced through a process of hydrolysis and condensation polymerization of the metal alkoxide solution containing the silica or titania. Following this, a temperature program is undertaken to control the densification process. Through selection of process parameters, a microporous glass can be produced. This structure can be used as a support matrix for the luminophores, which are added to the precursor solution. This structure grows around the luminescent molecules and encapsulates them in a nanometer-scale cage-like structure small enough to hold the luminescent molecule, yet large enough to allow the quenching reagent (oxygen) to pass through.

4.1.3.4 Tape Casting

Tape casting is a commonly used method of producing extremely thin layers of ceramic powders[34]. Again, some polymer is needed but considerably less polymer is in the coating than in traditional paints. To create a tape cast coating, a backing is passed through a bath containing a solution of aqueous ceramic slurry with polymer emulsion as shown below in Figure 4.1.

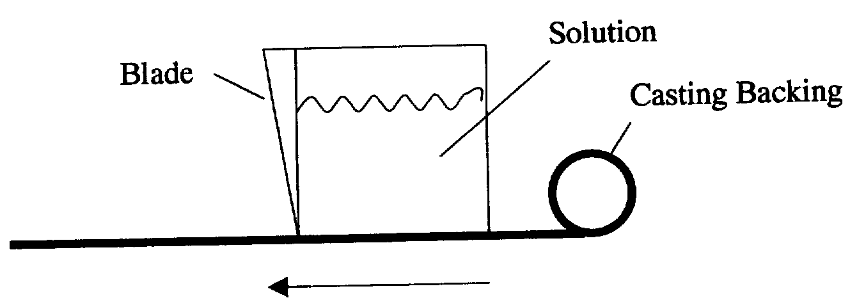

Figure 4.1: Tape Casting Method

The blade controls the thickness of the layer as the backing passes out of the solution. The solution then dries onto the backing. Final coatings can be approximately 0.5 mm thick. Once the coating is dry, it can be dipped into a solution containing a dissolved luminophore, which is soaked into the coating.

4.1.3.5 Porous Filters

Certain filters may retain their porosity under cryogenic temperatures. Soaking luminescent molecules into the filters creates a PSP that retains its porosity under cryogenic conditions. The choice of filters is primarily a trial and error process. Two such paints were tested in this work.

4.2 Measurement Techniques

Two possible measurements can be used to relate to temperature or pressure in a TSP or PSP coating. Both are acquired in similar manners. The first is based on the intensity of the emitted light from the paint. The second involves AC measurement of the lifetime or phase of the emitted light.

4.2.1 Intensity Based

Measurement of fluorescent intensity is currently the most common method of gathering experimental data from temperature- and pressure-sensitive paints. Blue or UV lamps are used to excite the paint and fluorescent emissions are collected with a CCD camera or photodetector and PC based frame digitizer board. For paint calibration, integrated measurements using a photodetector are used to relate intensity on a small painted surface to temperature or pressure.

For full surface mapping a CCD camera is used to take an image of the entire surface. The digitized image is then processed to get pixel intensities and flow-off and flow-on images are divided to remove non-uniformities in paint thickness and lighting. This ratio is then converted to temperature or pressure readings based on calibration data, yielding a temperature or pressure map of the entire surface. Resolutions of 8 bits and 640X480 pixels are available in standard CCD cameras, however resolutions of 16 bits are available in more expensive cooled, scientific CCD arrays. The biggest disadvantage to this method is that model movement can cause displacement between the flow-off and flow-on images. This problem is commonly alleviated by the use of image mapping and spatial transformations.

Improved resolution and noise characteristics can be achieved through the use of a laser scanning system. Instead of taking an image of the entire surface, a focused laser spot is scanned over the surface, exciting the paint. A low noise photo-multiplier tube or photo-diode is used to measure the emission intensity at each spot in the scan. After amplifying and filtering, the signal is digitized with a high resolution A/D converter. Through the use of computer controlled scanning mirrors or a rotary stage, the scan area and resolution can be user-specified. An added advantage is that the laser provides fairly uniform excitation intensity, while variations can be easily monitored.

4.2.2 Lifetime Based

By modulating the intensity of the excitation light, fluorescence decay curves can be recorded. Typically several curves are recorded and averaged using a digital oscilloscope or A/D board. An exponential curve can then be fitted to the data and the lifetime calculated. The advantage to using lifetime measurements is that the measurements are independent of luminophore concentration and lighting effects. There is however, a disadvantage when using a laser scanning system in conjunction with this method. The disadvantage is that a large amount of computing time is required to fit a curve to each data point on the surface.

A related method that requires less computing time is measurement of phase. Similar to lifetime measurements, the excitation intensity is modulated but the phase shift between the excitation and fluorescence signals is measured instead of decay. This measurement can be easily completed using a lock-in amplifier and has the added advantage of rejection of AC noise at frequencies other than the frequency of the modulation. Torgerson[29] notes that for systems with small pressure changes (i.e. low speed aerodynamic tests), signal-to-noise ratio can be significantly increased through the use of the scanning system with a lock-in amplifier. By modulating the laser beam, producing an AC fluorescent signal, and making use of the lock-in amplifier, electrical bandwidth can be decreased to well below 1 Hz, increasing the signal-to-noise ratio. The other method used to increase signal-to-noise ratio is to increase the excitation intensity, however care must be taken not to photodegrade the paint. Many popular luminescent compounds, such as the porphyrin family, are highly susceptible to photodegradation.

CHAPTER 5: TEMPERATURE CALIBRATIONS

In order to make effective surface temperature measurements using temperature-sensitive paint, a calibration relating the surface temperature to paint emission intensity must be performed. The apparatus used to perform these calibrations is shown in Figure 5.1. Each sample consisted of a temperature-sensitive paint applied to an aluminum block (1" x 1" x 0.25"). A 0.125" diameter hole was drilled in the block, parallel to and near the painted surface, for the temperature probe. These samples were then placed on the sample stand and illuminated with light of the correct wavelength to excite the fluorescence.

5.1 Calibration Apparatus

The calibration rig consists of five basic components: an excitation source, a sample stand, an intensity measurement system, a thermometer to measure sample temperature, and a personal computer (PC) to collect the data. Details concerning the specific components are given in the following sections and a diagram of the entire system is shown in Figure 5.1.

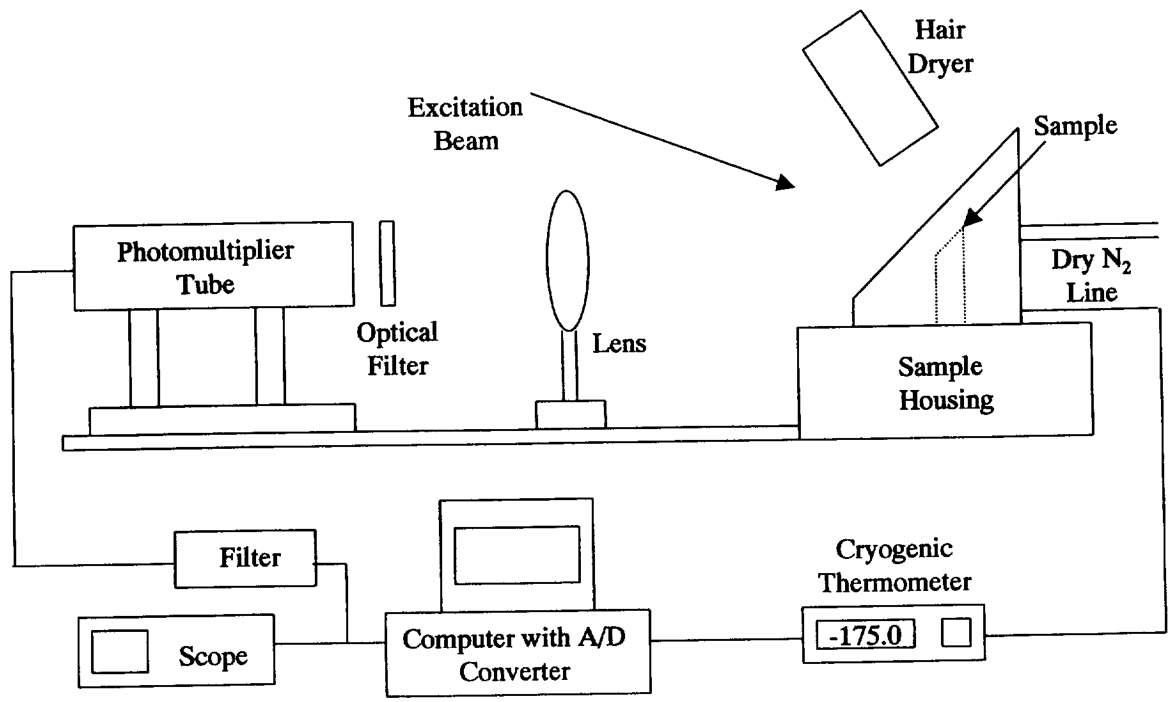

Figure 5.1: Temperature Calibration System

5.1.1 Excitation Source

Paints were excited using either an Argon ion (Ar+) laser or Ultraviolet (UV) light. The UV lamp was a 100-watt mercury arc lamp equipped with a filter. The lamp had a peak emission at 365 nm and little radiation at other wavelengths. In the case of Ar+ laser excitation, either an air-cooled or a water-cooled Argon ion (Ar+) laser was used. The air-cooled laser is a low power (5 mW), multiline (515, 488, and 457 nm) Ar+ laser. The water-cooled Ar+ laser has 5 watts peak power and emissions at various peaks with 488 nm (blue-green) and 514 nm (green) being the strongest.

5.1.2 Sample Stand

Since the area of interest in these experiments was the response of temperature-sensitive paints under cryogenic temperatures, a sample stand capable of attaining temperatures between –180 °C and room temperature was required. A stand capable of operating in this temperature range was used in previous investigations by Campbell[35] and was used again for these experiments. The design of the stand is shown below in Figure 5.2.

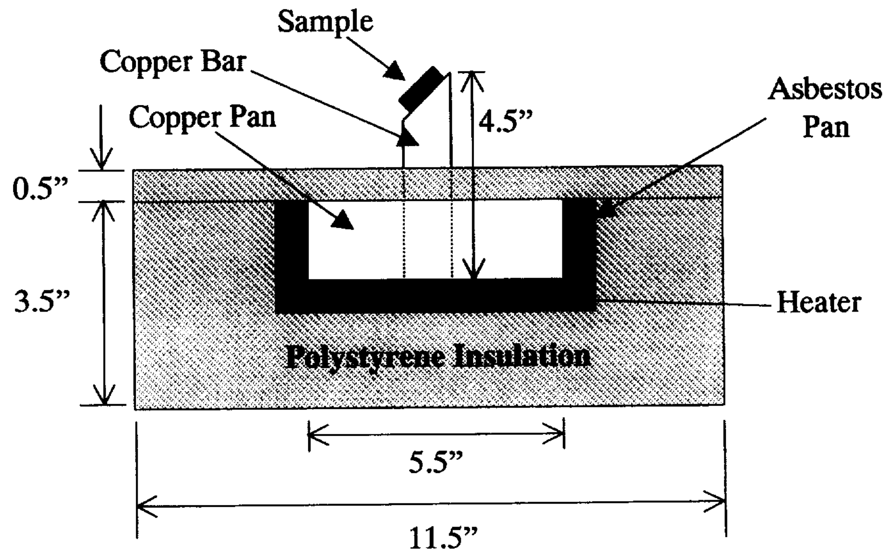

Figure 5.2: Cross Section of Sample Stand

The test stand consists of a 5.5" x 5.5" x 1.5" copper pan with a solid copper bar welded perpendicular to the pan's bottom. The copper bar has a diameter of 1" and is approximately 4.5" tall. It is cut at a 45° angle at its top and a small ledge is bolted to the bar allowing the sample block to rest on the sloped surface.

Underneath the pan rests a 3" diameter heating pad attached to the copper with heat sink compound. The copper fixtures rest inside another pan (6.5" x 6.5" x 2.25") consisting of asbestos blocks with fiberglass insulation placed between the copper and asbestos. The assembly of copper and asbestos rests inside a square hole recessed into a large block of polystyrene insulation. Another block of polystyrene with a small hole for the copper bar is placed over the copper pan. This block also contains a hole for pouring liquid nitrogen into the copper pan. The gaps between the polystyrene sheets are sealed with duct tape along the edges.

To isolate the sample from room air to allow cooling to near liquid nitrogen temperature, a housing of aluminum with a glass window sits atop the polystyrene box surrounding the copper bar and sample. The housing is sealed to the top of the box with duct tape. A line from a nitrogen bottle was attached to the back of the housing in order to purge the box of air prior to each calibration, eliminating the possibility of icing or condensation occurring on the sample surface. In addition, the glass window was heated with hot air from a hair dryer to prevent fogging at the low temperatures.

5.1.3 Emission Intensity Measurement

The intensity of the paint's fluorescent emissions was measured using a Photomultiplier tube (PMT) from EMI corporation. The light emitted from the sample was collected by a large lens and the image focused onto the PMT through a long-pass glass/interference optical filter. The filter cut-off frequency was determined by the wavelength of the particular paint's emission. Filters utilized in this research had cut-off frequencies of 550, 580, or 600 nm. The output of the PMT was passed through a Wavetech model 452 low pass digital filter with cut-off set to 30 Hz. This setting reduced any higher frequency fluctuations such as 60 Hz line noise. The output was connected to a PC equipped with a 12-bit analog-to-digital (A/D) board (DAS-1600).

5.1.4 Sample Temperature Measurement

Sample temperature was monitored using an Omega CY7-SD7 cryogenic silicon diode sensor and Omega CYD-208 cryogenic thermometer. The sensor was soldered onto a 0.125" copper wire which fit into the hole on the sample drilled near the painted surface. The sensor was connected to the thermometer with 32 gage copper wires, purchased from Omega (CYW4-32-25). The PC read the temperature from the thermometer through a serial port connection.

5.1.5 Data Collection

Calibration data was collected using a PC via a Quick Basic Program. The program reads voltage from the PMT via an A/D board and reads sample temperature through the serial port.

5.1.6 Calibration Procedure

First, a trickle flow of nitrogen gas through the calibration rig is initiated. This purges ambient air from the rig to avoid condensation or icing on the sample. Next, the sample is cooled to approximately –175 °C by filling the copper pan with liquid nitrogen through the liquid nitrogen pouring hole in the top of the calibration rig. Once the sample is at its coldest temperature, the emitted fluorescence will be at the highest and the PMT supply voltage can be set to yield the highest resolution. After ensuring the PMT is within the linear detection range, the PMT is covered and the Quick Basic program is used to obtain a reading of the DC offset of the PMT. After this, the PMT is uncovered and the program takes data points (temperature, PMT output voltage) at regular intervals as the sample warms from liquid nitrogen temperature to room temperature. As sample warming slows, a current is applied to the heating pad to increase the rate of warming until the calibration ends.

5.2 Calibration Results

A total of 26 paints were made and calibrated during this research. Plots of the calibration results are included in Appendix A. Two plots are presented for each paint: relative intensity versus temperature and an Arrhenius plot. Since experimental data is usually presented as an intensity ratio, presenting calibration data as an intensity ratio versus temperature gives direct insight when deciding what paint to use in an experiment based on the calibration data. Campbell[35] found that comparisons of paint sensitivity could be made by comparing the slopes of intensity ratio versus temperature for various paints. For each paint a useful range of sensitivity is identified. The useful range is determined by identifying the temperature region where the paint exhibits sharp intensity changes with temperature (i.e. the largest slope). A linear regression was performed over the useful range of each paint and a regression line is marked on each intensity ratio plot in Appendix A.

5.2.1 General Results

Fluorescent compounds based on Copper, Platinum, Rhodium, Ruthenium, and Osmium were tested. Emphasis was placed on the $[Ru(trpy)_2]$ family of compounds because they have been shown to be temperature dependent in the region of interest by Campbell[35] and Maestri et. al.[36] and derivatives with larger Stokes shifts into the red could be formulated[36]. A discussion of the different Ruthenium compounds is given in section 5.2.2. Early in this research the binder of choice was determined to be DuPont Chromaclear® due to its low oxygen diffusivity and good surface adhesion at cryogenic temperatures.

For the purpose of comparison, the average slope of each paint's intensity ratio versus temperature over it's useful range was calculated by linear regression. Plots of the calibration data can be found in Appendix A. The useful range and intensity ratio slope of each paint are tabulated below in Table 5.1.

Table 5.1: Intensity Ratio Slope Data for Calibrated TSP's

Paint	Fig.	Useful Range (°C)	Intensity Ratio Slope $(\Delta(I/I_{ref})/\Delta T)$	Comments
$[Cu(ph_2\text{-}phen)_2](PF_6)_2$ in GP-197	A.1	-150 to -80	-0.0073	Calibration Failed
PtPFPP in CC	A.2	45 to 100	-0.0107	Easily photodegraded
PtPFPP in Polyurethane	A.3	0 to 75	-0.0062	Easily photodegraded
$[Rh(bzq)_2Cl]_2$ in CC	A.4	-175 to -130	-0.0191	
$[Rh(bzq)_2(phen)](PF_6)$ in CC	A.5	-100 to -50	-0.0107	
$[Ru(bipy)_3](DS)_2$ in CC	A.6	0 to 75	-0.0096	
$[Ru(bipy)_3](TFPB)_2$ in CC	A.7	0 to 75	-0.0095	
$[Ru(ph_2\text{-}phen)_3](DS)_2$ in CC	A.8	20 to 90	-0.0077	
[Ru(trpy)] in CC	A.9	-175 to -85	-0.0112	
$[Ru(trpy)(4'\text{-}C_6F_5\text{-}trpy)](NO_3)_2$ in CC	A.10	-175 to -50	-0.0081	
$[Ru(trpy)(4'\text{-}Cl\text{-}trpy)](Cl_2)$ in CC	A.11	-175 to -50	-0.0106	
$[Ru(trpy)(4'\text{-}NC\text{-}trpy)](NO_3)_2$ in CC	A.12	-150 to -50	-0.0078	
$[Ru(phtrpy)(Cltrpy)](NO_3)_2$ in CC	A.13	-175 to -50	-0.0093	
$[Ru(trpy)(4'\text{-}TfO\text{-}trpy)](NO_3)_2$ in CC	A.14	-175 to -50	-0.0101	
$[Ru(trpy)(MeStrpy)](NO_3)_2$ in CC	A.15	-175 to -75	-0.0105	
$[Ru(trpy_2)(NO_2Phtrpy)](PF_6)$ in CC	A.16	-175 to -75	-0.0087	Not very stable
$[Ru(trpy)(phtrpy)](PF_6)_2$ in GP-197	A.17	-175 to -50	-0.0114	
$[Ru(trpy)(phtrpy)](PF_6)_2$ in CC	A.18	-150 to -100	-0.0142	
$[Ru(trpy)(ppd\text{-}trpy)](TFPB)_2$ in CC	A.19	-175 to -50	-0.0097	
$[Ru(trpy)(phyphen)](TFPB)_2$ in CC	A.20	-175 to -50	-0.0090	
$[Ru(trpy)(SO_2Me\text{-}trpy)](PF_6)_2$ in CC	A.21	-175 to -75	-0.0104	
$[Ru(trpy)_2](DS)_2$ in CC	A.22	-150 to -75	-0.0122	Calibration Failed
$[Ru(trpy_2)](TFPB)_2$ in CC	A.23	-170 to -75	-0.0114	
$[Ru(ppd\text{-}trpy)_2](TFPB)_2$ in CC	A.24	-175 to -75	-0.0149	
$[Os(trpy)_2](PF_6)_2$ in CC	A.25	0 to 75	-0.0041	
$[Ru(trpy)(Vh127)](PF_6)_2$ in GP-197	A.26	-175 to -75	-0.0154	

In general, the Ruthenium and Rhodium compounds exhibited the best response in the temperature range of interest. Compounds based on these two elements exhibited sensitivity from –175 °C to –75 or –50 °C. While $[Cu(ph_2\text{-}phen)_2](PF_6)_2$ exhibited sensitivity at –150 °C, it had a small useful range and comparatively poor intensity ratio slope. Osmium compounds with both terpyridine and bipyridene ligands were tested but only $[Os(trpy)_2](PF_6)_2$ was calibratable. It was desirable to test Osmium based compounds since they can be excited by red laser light and emit in the infa-red range of the spectrum. While a paint that could be excited by a relatively cheap red laser was desired, the useful range was above 0°C and the intensity ratio slope was very poor. The Platinum Porphyrin compounds also did not exhibit temperature sensitivity in the desired temperature range. $[Rh(bzq)_2Cl]_2$ exhibited a large intensity ratio slope over a fairly small useful range (-175°C to –130°C) while $[Rh(bzq)_2(phen)](PF_6)$ had a similar but shifted useful range (-100 °C to -50 °C) which was outside our desired temperature range. Overall, the Ru(trpy) based compounds showed the best intensity ratio slope over good useful ranges.

5.2.2 $[Ru(trpy)_2]$ based compounds

The objective in investigating various $[Ru(trpy)_2]$ based compounds was to obtain a compound which exhibited a response similar to the response of $[Ru(trpy)(VH\text{-}127)](PF_6)_2$, which was received from Thummel at the University of Houston. While the VH-127 compound exhibits a very good temperature response in cryogenic conditions, it is very hard to synthesize while the other Ru(trpy) compounds calibrated here were relatively easy to synthesize. By using various ligands as electron donating or electron accepting groups, the "activation" temperature of the luminescent response to temperature could be moved and hopefully designed. All compounds were synthesized by C. Cunningham of the Purdue University chemistry department and were mixed into paints and calibrated using the calibration apparatus described in section 5.1. Figure 5.3 below shows a comparison of several of the synthesized compounds.

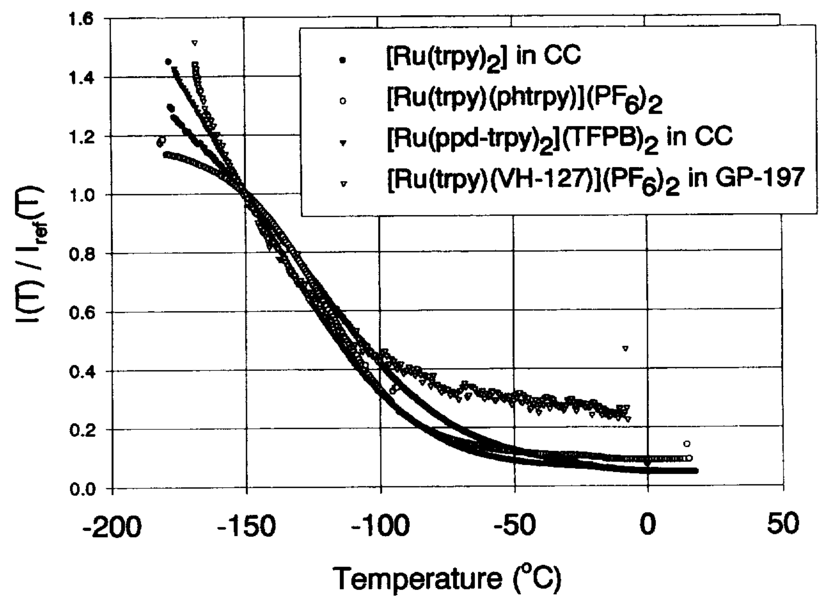

Figure 5.3: Comparison of Ru(trpy) based paints

As can be seen from the above plot and the slopes in Table 5.1, the response of the paints to temperature is very similar for these compounds. As expected, [Ru(trpy)$_2$] has the shallowest slope, while changing the ligand structure produced steeper slopes. While the increases in slope were not as significant as hoped, most interesting is that the response and intensity ratio slope of [Ru(ppd-trpy)$_2$](PF$_6$)$_2$ were very similar to that of [Ru(trpy)(VH-127)](PF$_6$)$_2$ which met our goal as [Ru(ppd-trpy)$_2$](PF$_6$)$_2$ is simpler to synthesize. The major difference between these two compounds was that the [Ru(trpy)(VH-127)](PF$_6$)$_2$ exhibited a linear Arrhenius response while the [Ru(ppd-trpy)$_2$](PF$_6$)$_2$ did not. This however does not affect the researcher's ability to calibrate and fit a function to the paint's response. Other Ruthenium based compounds produced good responses in the temperature region of interest with useful sensitivity, but slopes were shallower than that of [Ru(ppd-trpy)$_2$](PF$_6$)$_2$.

5.2.3 Effects of Polymer Binders

In chemistry circles, the luminescence of transition metal complexes is typically studied in solution. The effect of a solid matrix on fluorescent compounds is a very complex question and is beyond the current scope. In the interest of completeness, some of the effects are illustrated with the current data.

As previously noted, the mobility of the metal-to-ligand bonds affects the vibrational energy of the bonds. Suspension in a rigid matrix restricts this mobility. Through this restriction the vibrational energy associated with vibrational (temperature) quenching is limited, reducing the sensitivity of the compound to changes in temperature. Interactions between different polymer binders and luminescent molecules have different effects on the mobility of the metal-to-ligand bonds, producing different results. This is illustrated by Figure 5.4 and Figure 5.5 below.

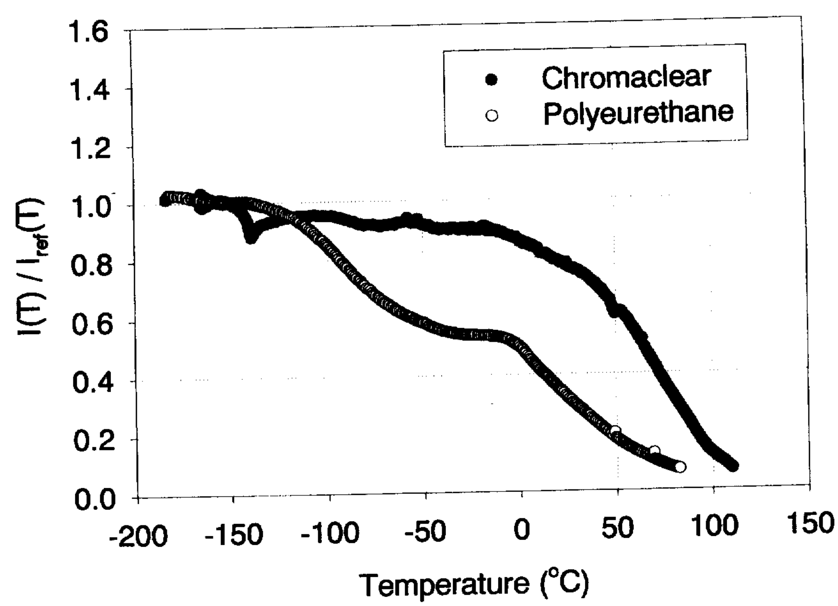

Figure 5.4: Effects of Polymer binder on PtPFPP

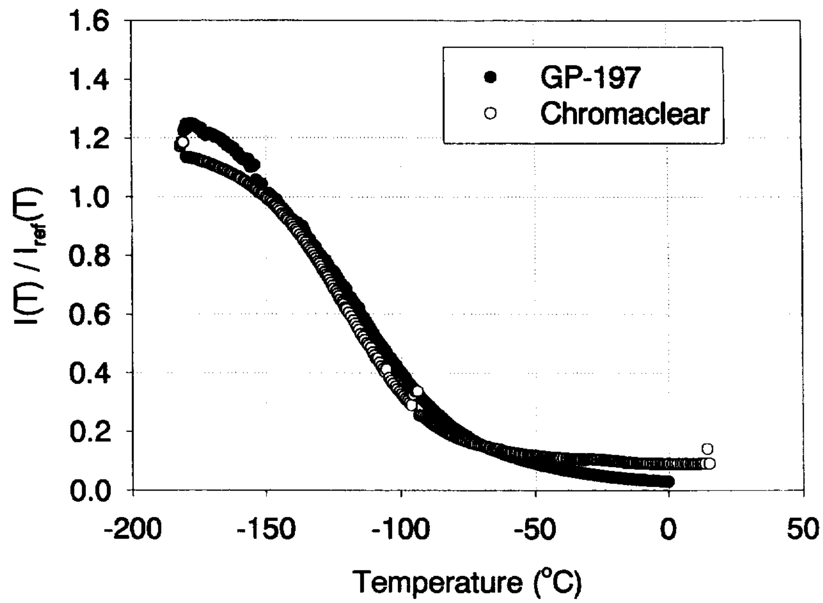

Figure 5.5: Effects of Polymer Binder on [Ru(trpy)(phtrpy)]$(PF_6)_2$

While the calibration results for PtPFPP in Chromaclear® and Polyurethane were significantly different, there was only a slight difference seen between [Ru(trpy)(phtrpy)]$(PF_6)_2$ in Chromaclear® and in GP-197. Thus, it should be noted that if one compound does not respond well in one binder, it may respond better in another (or vice versa). In this research it was decided to use one suitable binder and test different luminescent molecules in that binder.

Another interesting note is that the Arrhenius plots (see appendix A) are not linear for most of these paints. As noted in Chapter 3, theory states that the response of the paint should be linear when plotted in the Arrhenius form. With the exception of $[Rh(bzq)_2](Cl_2)$ and [Ru(trpy)(VH-127)]$(PF_6)_2$, it can be seen from Figures A.1-A.26 that many of the Arrhenius plots are non-linear over certain temperature ranges, notably the cryogenic. While this does not hinder the ability of the researcher to calibrate and fit a curve to the intensity data, is does indicate that other processes are affecting the response of the paint. One possible explanation of this could be effects of the binder. Increased rigidity of the polymer matrix at cryogenic temperatures could affect the molecular vibrations that produce the temperature response.

5.3 Application – Boundary Layer Transition Detection in Cryogenic Wind Tunnel

Two cryogenic temperature-sensitive paints found during Campbell's research[35] were applied to a NACA 64-A012 laminar airfoil placed in the 0.1-m Transonic Cryogenic Wind Tunnel at NAL, Japan. Testing was conducted by Asai, et. al.[18] and is presented here to illustrate one application of cryogenic temperature-sensitive paints.

5.3.1 Wind Tunnel and Experimental Setup

The 0.1-m Transonic Cryogenic Wind Tunnel is a closed-circuit, fan-driven wind tunnel operated with cryogenic nitrogen as the working gas. The tunnel has a maximum stagnation pressure of 200 Pa and stagnation temperatures can range from 90 K to 200 K. The test section is a 0.1 m square. A simple schematic showing the operation of the 0.1-m Transonic Cryogenic Wind Tunnel is shown below in Figure 5.6 and the optical system is shown in Figure 5.7.

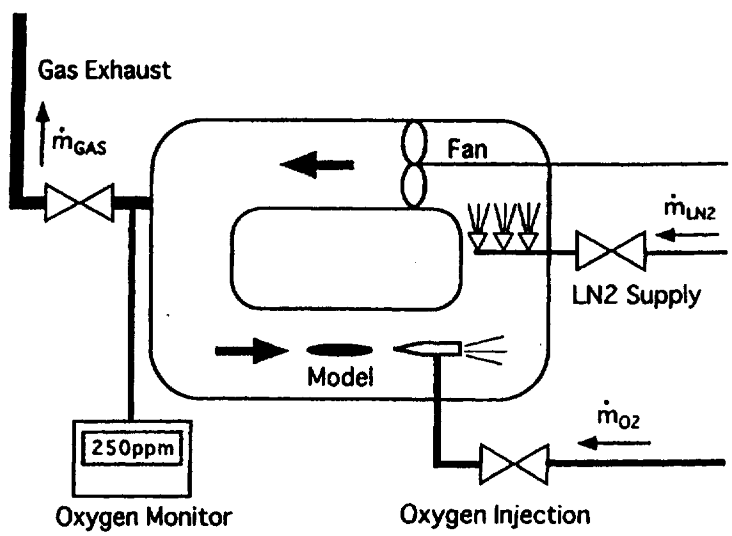

Figure 5.6: NAL 0.1-m Transonic Cryogenic Wind Tunnel Operation

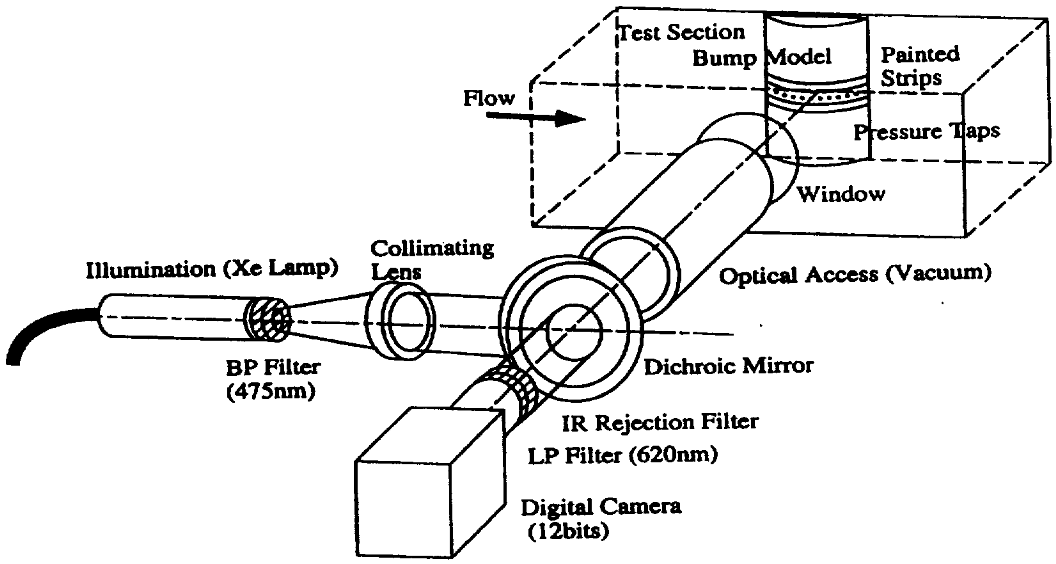

Figure 5.7: Optical System

A 300 W Xenon lamp with a light guide, band pass filter (470 +/- 50 nm), and a collating lens made up the excitation source. A dichroic mirror was used to separate paint emission from excitation light and a digital camera was used to measure the emission intensity of the paint.

5.3.2 Experiment and Results

[Ru(trpy)$_2$] in GP-197 and [Ru(trpy)(VH-127)] in GP-197 where applied to the airfoil. The Xenon lamp was used to excite the paint and images of the surfaces were recorded by the CCD camera. Two methods of enhancing the surface temperature signatures between the laminar and turbulent regions were used. The two methods were actively cooling or heating either the tunnel flow or model substrate. A sample image of the data obtained in this experiment is shown below.

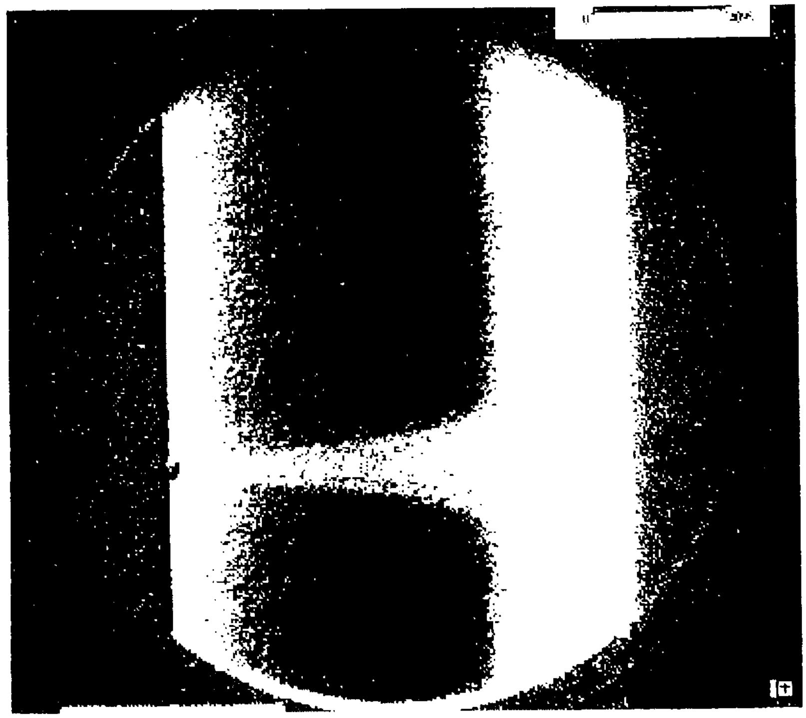

Figure 5.8: Transition on NACA 64-A012

The boundary layer transition is easily visualized in the above figure. The dark areas are laminar flow regions (low heat transfer) and the light areas are turbulent flow regions (high heat transfer). The boundary layer trip approximately 40 % up the chord is also clearly visible.

CHAPTER 6: PRESSURE CALIBRATIONS

Since measurements using Pressure-sensitive Paints (PSP's) under cryogenic temperatures had never been attempted prior to the inception of this work, simple initial experiments were conducted to determine if PSP's responded under cryogenic temperatures. Once it was determined that PSP's did respond cryogenically, a calibration relating the surface pressure to paint emission intensity needed to be performed in order to be able to make effective surface pressure measurements using pressure-sensitive paint. The apparatus used to perform these calibrations is shown in Figure 6.1, and it should be noted that the overall system is very similar to that used for temperature-sensitive paint calibrations. The main difference is that a more unique sample stand was necessary. As in the cryogenic temperature-sensitive paint calibrations, each sample consisted of a pressure-sensitive paint applied to an aluminum block (1" x 1" x 0.25"). These samples were placed in a modified cryostat and illuminated with light of the correct wavelength to excite the fluorescence.

6.1 Initial Feasibility Experiments

Initially it was not known if the pressure-sensitive paints would respond under cryogenic conditions. Thus, a simple experiment was conducted on various paints to see if they would respond. The sample stand used for temperature-sensitive paint calibrations (see Figure 5.2) was modified by adding a copper tube coiled around inside the liquid nitrogen pan. One end of the copper tube opened onto the sample and the other end was connected to a supply of dry oxygen gas. The sample was cooled as described in section 5.1.6 and then oxygen was allowed to flow through the copper tube, which cooled the gas, and then onto the surface of the sample. Visual inspection was made to determine if any observable change in emission intensity occurred. This was done repeatedly as the sample warmed up and the temperature at which a response was observed was recorded. The results of these initial experiments are shown below in Table 6.1.

Table 6.1: Results of Initial Cryogenic PSP Experiments

Compound	yes/ no	Notes
[Ru(ph_2-phen)$_3$] in Dope	no	
[Ru(ph_2-phen)$_3$] in GE 118	no	Responded above 200 K
[Ru(ph_2-phen)$_3$] in GE 118 + silica gel (dipped)	yes	Responded above 150 K
[Ru(ph_2-phen)$_3$] in GE 118 + silica gel (Toluene as solvent)	yes	Responded above 150 K
[Ru(ph_2-phen)$_3$] in GE 118 + silica gel particles (less than in prev sample) on Mylar	yes	Responded above 150 K.
[Ru(ph_2-phen)$_3$] in GE 118 + silica gel particles on Mylar	yes	Above 125 K
[Ru(ph_2-phen)$_3$] in GP-197	no	Responded above 235 K
[Ru(ph_2-phen)$_3$] in GP-197 + lots of silica	yes	Showed response at 90 K
PtTFPP in GP-197	no	Responded above 180 K
PtOEP in GP-197	no	Responded above 250 K
PtOEP in GP-197 + lots of silica gel	yes	Responded above 90 K. Very sensitive.
PtOEP in GP-197 + lots of silica gel (dipped)	yes	Responded above 90 K. Very sensitive.
[Ru(ph_2-phen)$_3$] on Porex Porous Polyethylene	no	
PtOEP on Porous Polyethylene	yes	Responded above 125 K.
[Ru(bipy)$_3$](DS)$_2$ on TLC	yes	Responded above 110 K.
[Ru(ph_2-phen)$_3$] on TLC	yes	Responded above 90 K. Very sensitive
PtOEP on Polystyrene	yes	Responded above 125 K. Not a very good response.
PtOEP in GP-197 soaked into ceramic #1	yes	Responded above 125 K.
PtOEP in GP-197 soaked into ceramic #10	no	Responded above 180 K.
PtOEP in GP-197 soaked into ceramic #2	yes	Responded above 125 K.
PtOEP in GP-197 soaked into ceramic #3	yes	Responded above 130 K
PtOEP in GP-197 soaked into ceramic #4	yes	Responded above 140 K.
PtOEP in GP-197 soaked into ceramic #5	yes	Responded above 150 K.
PtOEP in GP-197 soaked into ceramic #6	yes	Responded above 175 K.
PtOEP in GP-197 soaked into ceramic #7	yes	Responded above 140 K.
PtOEP in GP-197 soaked into ceramic #8	yes	Responded above 160 K.
PtOEP in GP-197 soaked into ceramic #9	yes	Responded above 125 K.
PtOEP in GP-197 soaked into filter paper	yes	Responded above 150 K.

Several significant observations can be made from the above results. Notably that paints using polymer binders from common room temperature PSP's showed no response at the desired conditions (below 150 K). The addition of silica gel to certain binders (GE RTV and GP-197) improved observed response by lowering the temperature at which a response was first observed. Finally, no ceramic binders worked in the region of interest.

6.2 Calibration Apparatus

The cryogenic pressure-sensitive paint calibration rig consists of eight basic components: an excitation source, a modified cryostat, an emission intensity measurement system, a temperature measurement and control system, an absolute pressure measurement and control system, the test gas, a vacuum pump, and a personal computer (PC) to collect the data. Details concerning the specific components are given in the following sections and a diagram of the entire system is shown in Figure 6.1.

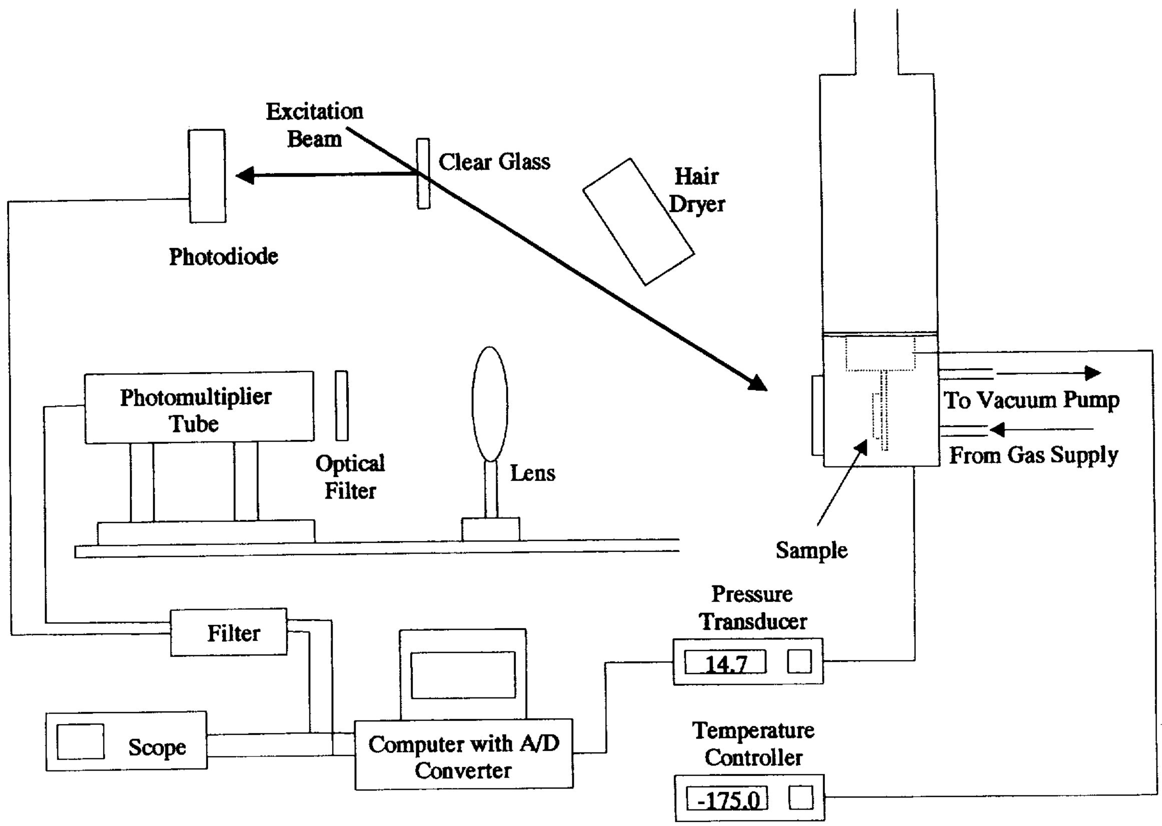

Figure 6.1: Pressure Calibration System

6.2.1 Excitation Source

Paints were excited using either an Argon (Ar+) laser or frequency doubled yag laser. In the case of Ar+ laser excitation, either an air-cooled or water-cooled Argon ion (Ar+) laser was used. The air-cooled laser is a low power (5 mW), multiline (515, 488, and 457 nm) Ar+ laser. The water-cooled Ar+ laser has 5 watts peak power and emissions at various peaks with 488 nm (blue-green) and 514 nm (green) being the strongest. The frequency doubled yag has 50 mW peak power with emission at 532 nm.

Excitation source intensity was measured using a Nu systems model 2001 photodiode and recorded on the PC through an A/D board. The excitation light was reflected off a piece of clear glass and focused onto the photodiode. This measurement was used to correct calibration data for fluctuations in the intensity of the excitation source.

6.2.2 Modified Cryostat

In addition to operating at cryogenic temperatures, the test stand for the cryogenic pressure-sensitive paints had to be a sealed vessel so that partial pressure of oxygen could be controlled. A modified Keltran PF cryostat was used for this purpose. The modified cryostat is shown below in Figure 6.2.

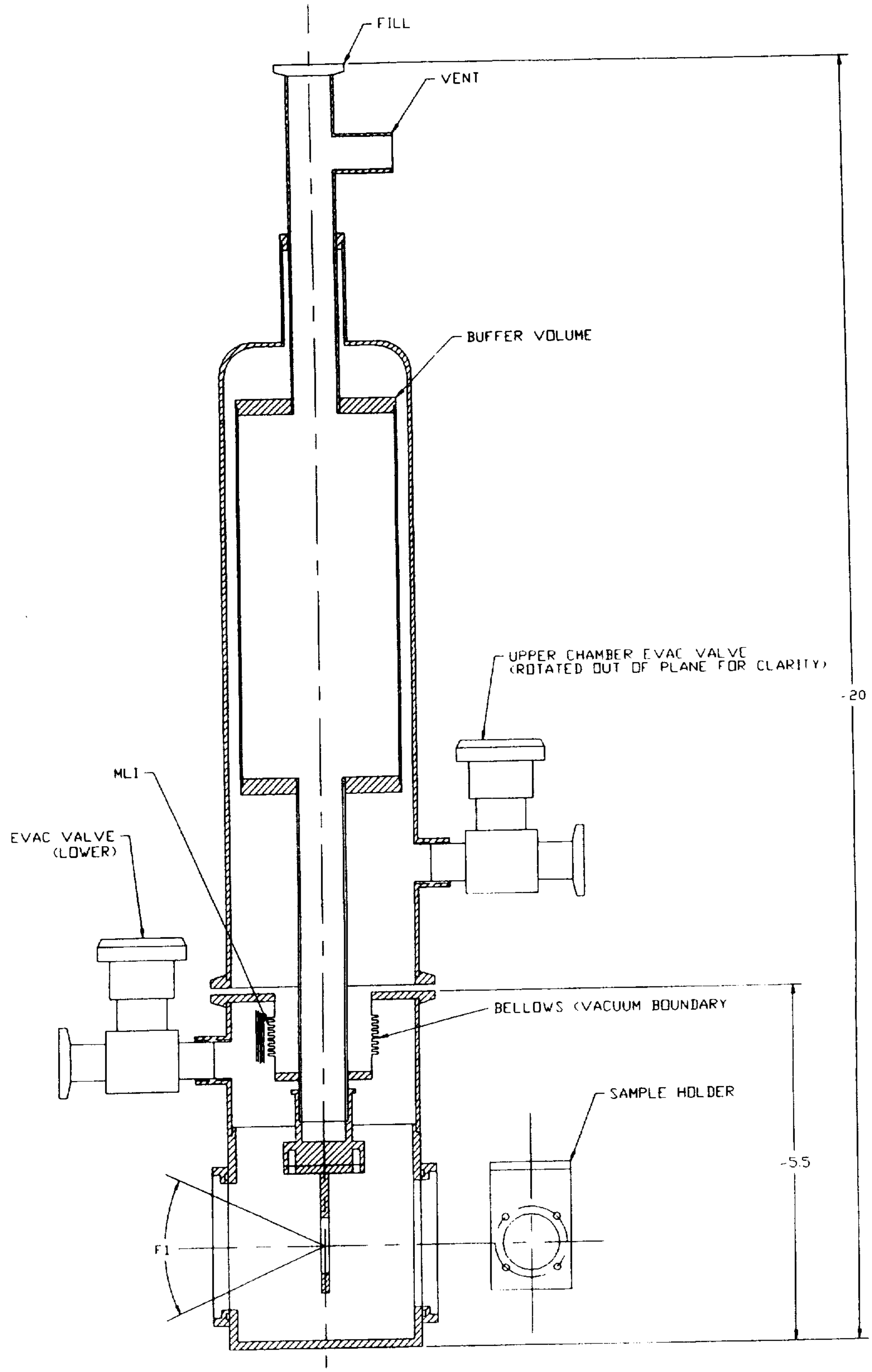

Figure 6.2: Modified Keltran PF Cryostat

Liquid nitrogen is used to cool the device to cryogenic temperatures and is contained in the buffer volume. In most standard cryostats, experiments are conducted solely under vacuum, thus the vacuum insulation jacket surrounding the buffer volume is simply extended around the sample holder so that one evacuation valve is needed to evacuate the entire unit. For our purpose however, it is necessary to fill the space surrounding the test sample with a gas mixture containing oxygen. Because the surface of the buffer volume is always near liquid nitrogen temperature (~77 K), any oxygen in a gas surrounding the buffer volume would condense on the surface of the buffer since the condensation temperature of oxygen (~90 K at 14.7 PSI) is above that of nitrogen. In addition, the presence of a gas in the system significantly increases the heat transfer to the outside, reducing test time available at cryogenic conditions. Thus, it was necessary to modify the basic design of the cryostat to better suit our requirements. The solution was to introduce a bellows between the buffer volume area of the cryostat and the test chamber area containing the sample (see Figure 6.2), thus separating the liquid nitrogen storage portion from the actual test chamber where gas would be introduced into the unit. Two valves were added to the lower portion to allow for filling and evacuation of test gasses.

There is one window on the lower portion allowing optical access to the sample, which is mounted on the copper sample holder. The sample holder is attached to the base of the lower tube leading from the buffer volume, allowing liquid nitrogen to come in direct contact with the sample holder. Aluminum sample blocks with the PSP paint on one surface are attached to the sample holder with an aluminum bracket and four screws. The interior of the test chamber has been finished with black paint to reduce reflected excitation light from inside the test chamber.

Sample temperature is controlled through two devices, the variable temperature displacer and Nichrome wire heater. The variable temperature displacer is a stopper of specific diameter inserted into the tube leading from the liquid nitrogen buffer volume to the top of the sample holder. It's purpose is to restrict the flow of nitrogen onto the top of the sample holder, thus slowing the cooling process, reducing heat transfer, and slowing evaporation of liquid nitrogen coming into contact with the hotter sample holder. As liquid nitrogen trickles past the variable temperature displacer, the sample mount and sample (which is thermally attached to the holder) cool down. A Nichrome wire heater is wrapped around the upper portion of the sample holder to introduce heat into the system and raise the temperature of the sample and holder. There is also an RTD temperature sensor in the top of the sample holder. The heater and RTD are attached to a temperature controller, which applies current to the heater when the temperature from the RTD becomes lower than the desired set point. In order to conserve liquid nitrogen, it is desirable to have the smallest possible flow rate past the displacer while still cooling at a sufficient rate to maintain the desired cryogenic temperature. Several displacers are used, each sized for use over a specific range of cryogenic temperatures (i.e. one for use above 100 K, one for use above 150 K, etc.). With use of the proper displacer and proper filling procedures (see Section 6.2.9), desired temperatures can be maintained for several hours. Actual test time is much less since gas is repeatedly introduced into the test chamber, significantly increasing heat transfer out of the unit thus increasing the rate of liquid nitrogen depletion. Under continuous calibrations, the unit can remain at temperature for approximately ½ hour when using the proper displacer and procedures.

6.2.3 Emission Intensity Measurement

The emission intensity of the paints was measured using a Photomultiplier tube (PMT) from EMI corporation. The light emitted from the sample was collected by a large lens and the image focused onto the PMT through a long-pass glass/interference optical filter. The filter cut-off frequency was determined by wavelength of the particular paint's emission. PMT output was passed through a 30 Hz cutoff low pass digital filter to eliminate any higher frequency fluctuations such as 60 Hz line noise. The output of the digital filter was connected to a PC equipped with a 12-bit analog-to-digital (A/D) converter board (DAS-1800).

6.2.4 Sample Temperature Measurement and Control

Sample temperature was controlled using an Omega CN-76000 temperature controller. The controller used an RTD located above the sample holder to measure the temperature of the sample mount assembly. It was assumed that the aluminum sample block was in thermal equilibrium with the copper sample mount assembly and thus the RTD temperature was equal to the sample surface temperature. To control temperature, the CN-76000 provided a reference signal to the Nichrome wire heater power supply, which activated a relay that closed the circuit to send current through the heater. Use of the controller in conjunction with a properly sized liquid nitrogen displacer enabled sample temperature to be controlled to within +/- 2 ^{o}C.

6.2.5 Pressure Measurement and Control

Absolute pressure in the test chamber was measured with an Omega PX-142 absolute pressure transducer in conjunction with an Omega DP-41 indicator. The transducer was capable of measuring 0-15 PSI absolute pressure with a 1 % F.S. error. The DP-41 indicator was connected to the data collection PC through a RS-485 serial port connection.

Test chamber pressure is controlled using the valve panel depicted below in Figure 6.3. Vacuum can be pulled on the cryostat vacuum jacket by opening ball valve 1. Once vacuum exists in the vacuum jacket, it can be sealed by the valve on the cryostat itself and by closing ball valve 1. Vacuum can be pulled in the cryostat test chamber by opening ball valves 2, 3, and 4 and the needle valve. The test gas enters the chamber through the lower line and valve system. With ball valve 4 open and slightly opening then closing the needle valve, small changes in test chamber pressure can be produced. See section 6.2.9 for a complete description of the operation of the valves to produce the desired environments in the test chamber.

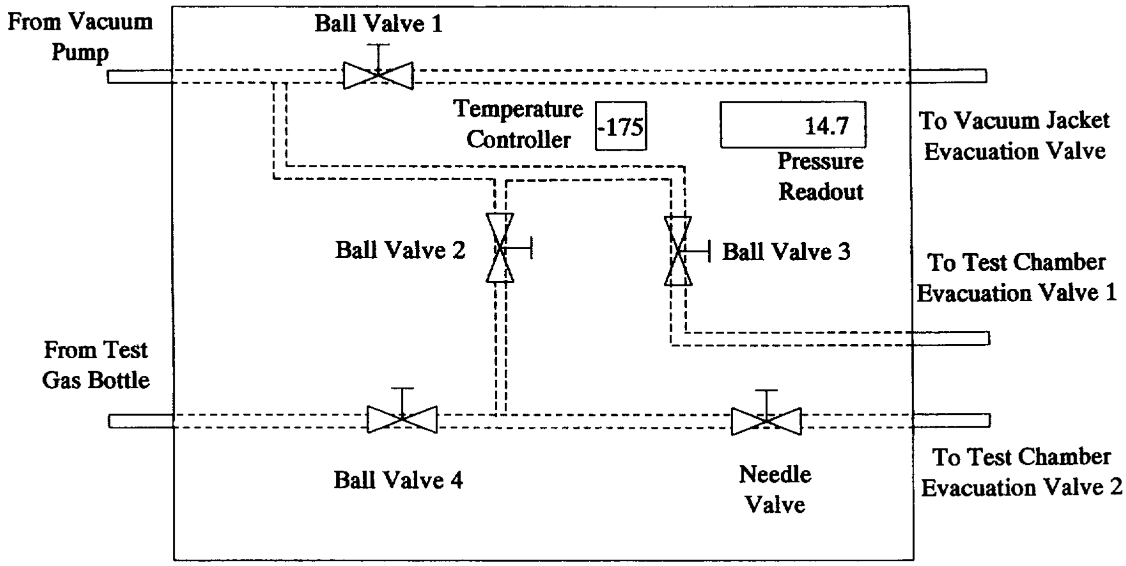

Figure 6.3: Valve Control Panel

6.2.6 Data Collection

Calibration data was collected using a PC via LabView® software. The computer reads voltage from the PMT and voltage from the photodiode via DAS-1800 A/D board and reads pressure from the DP-41 indicator via the serial port. Each data point is taken manually with the LabView® program. All data points for the test are corrected for laser intensity fluctuations and displayed graphically by the program in intensity ratio form.

6.2.7 Test Gasses

In order to calibrate cryogenic PSP's under the low oxygen partial pressures that are encountered in cryogenic wind tunnel testing, specialized test gasses were needed in order to achieve accurate resolution in the region of interest. These specialized gasses were dry mixtures of oxygen and nitrogen. The gasses available were 100 PPM, 250 PPM, 500 PPM, 0.1 %, 0.5 %, 1.0 %, and 2.0 % oxygen with the balance nitrogen, and dry air (21 % oxygen). Each gas was used to calibrate each sample between vacuum and 14.7 PSI. This allowed for proper resolution of the low partial pressures seen in cryogenic wind tunnel tests where oxygen concentrations are between 100 and 1000 PPM.

6.2.8 Vacuum Pump

An Edwards E2M0.7 rotary vacuum pump was used to evacuate the test chamber of the cryostat. The pumping capacity of the pump is 1.1 m^3/hr and the lowest observed pressures in the test chamber were less than 0.1 PSI.

6.2.9 Calibration Procedure

First, the test section is purged and evacuated several times with dry nitrogen using the procedure described below, to remove any ambient moisture or oxygen. Following the final purge, the test section is evacuated and the cryostat lower chamber evacuation valves closed (see Figure 6.2). The temperature controller is set to a value lower than 88 K so that the heater does not turn on during the cool down process. Next, liquid nitrogen is poured into the fill hole through a funnel until liquid is seen to be steadily streaming from the vent. At this point filling is stopped until the cryostat reaches its lowest temperature of approximately 88 K (about five minutes). Then more liquid is poured in to replace that evaporated during the final stage of the cool down. Once the buffer volume is full, the variable temperature displacer is inserted through the fill hole and adjusted so that it rests approximately 0.25 inches above the top of the sample holder (see Figure 6.2). This will slow the flow of liquid nitrogen to the top of the sample holder, allowing for slower rates of cooling while under constant temperature control.

With the sample at its lowest temperature and the cryostat readied for the test, the hair dryer is activated to alleviate condensation on the window, which may arise when the test gas is in the chamber. The temperature controller is set to the desired temperature and heating begins until the set point is reached and temperature control initiated. Then, the desired test gas is connected to the valve panel. Once above oxygen condensation temperature (~90 K), ball valves 2 and 3 and the needle valve (see Figure 6.3) are now opened to attain vacuum in the lines leading to the cryostat, allowing the cryostat lower evacuation valves to be opened. Next, the needle valve is set to a slightly open position and ball valves 2 and 3 are closed and ball valve 4 opened to allow test gas to flow into the test chamber until a pressure of ~14.7 PSI is attained. Ball valve 4 is then closed. Next ball valves 2 and 3 are opened again to pump out the gas in the chamber. This purge process is completed 4-5 successive times, leaving the chamber at vacuum. This ensures the composition of the residual gas inside the test chamber is indeed the intended composition. It should be noted that the test gasses should be used in order from lowest oxygen concentration to highest so as to have the paint at it's brightest intensity at the start of the calibration. The PMT supply voltage is then set to yield the highest resolution and a dark current data point is taken.

With the desired temperature attained and the test section at vacuum (with any residual gas being of the proper composition), the calibration can begin. With all panel valves in the closed position, ball valve 4 is opened so that test gas pressurizes the system up to the needle valve. An initial data point is taken, followed by the slight opening then closing of the needle valve to increase the pressure in the test section. A new data point is then taken and the process continued until the desired ending pressure is achieved (typically ~14.7 PSI).

Following this, the test chamber is evacuated as described above and the next desired test gas is connected to the valve panel. The chamber is purged 4-5 successive times as described above and the next calibration can be completed. The overall process can be continued until all test gases have been calibrated or the liquid nitrogen in the buffer volume is exhausted, whichever comes first. If the liquid nitrogen needs to be re-filled prior to having tested all gases, the test chamber should be brought to vacuum, closed off at the cryostat lower evacuation valves and the temperature controller disengaged. Following this, the liquid nitrogen can be refilled as described above without having to change any settings of additional electronic equipment such as the PMT. It should also be noted that care should be taken not to expose sensitive equipment, such as the PMT, to excess light while refilling the liquid nitrogen. Another important consideration is to make every effort to conserve the liquid nitrogen in the buffer volume. Time at cryogenic temperatures can be extended by always topping off the LN_2 level after the cryostat has reached it's coldest temperature and also keeping the test chamber at vacuum as much as possible so as to reduce heat transfer to the outside.

6.3 Calibration Results

A total of 22 paints were fashioned and calibrated during this research. Some paints were chosen as a result of the initial feasibility tests, others were synthesized using new methods in an effort to get the luminescent molecules deposited on the surface using little or no polymer. Because the binder was observed to have a large impact on PSP performance, results are organized by binder. In some cases, several different luminescent molecules were tested using the same type of binder. Although some results show non-linear behavior, data is plotted in the generally accepted Stern-Volmer form. The presentation in the following sections focuses primarily on the region of interest in cryogenic wind tunnel testing. More specifically, the region of interest includes temperatures of 150 K and 100 K and oxygen partial pressures between 0 and 100 Pa. Calibration data for oxygen partial pressures up to those found in the standard atmosphere can be found in Appendix B.

6.3.1 Anodized Aluminum

[Ru(ph_2-phen)$_3$] was deposited on the surface of pure aluminum and 2024 aluminum alloy using the anodizing process described in Section 4.1.3.1. Coatings were prepared by Hirotaka Sakaue of the Purdue University Aerospace Sciences Lab. Both coatings exhibited non-linear behavior and comparison of the room temperature response of the two paints shows that the coating on pure aluminum appears to exhibit better sensitivity, as shown below in Figure 6.4.

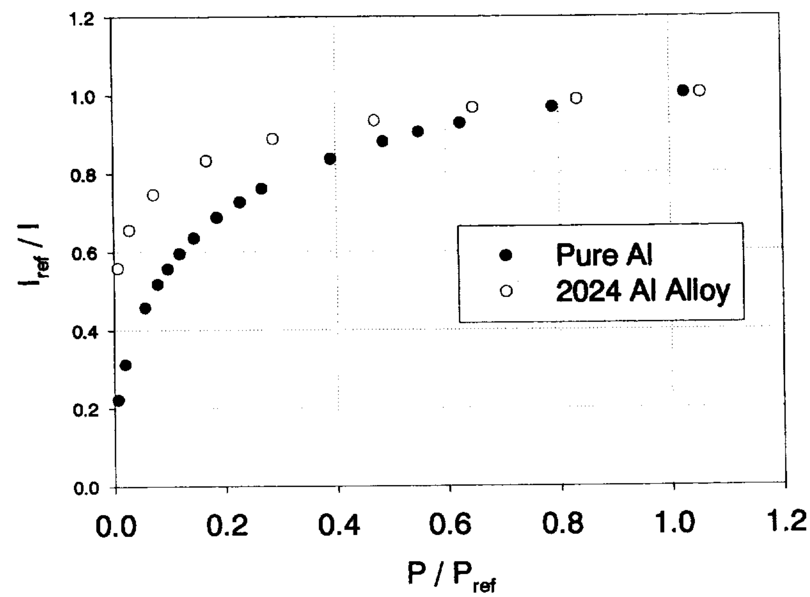

Figure 6.4: Stern-Volmer Response of Anodized Aluminum Paints

The data above was taken at room temperature using atmospheric pressure in PSI as the reference condition.

Under cryogenic conditions, examination of the overall response (shown in Appendix B) shows that the coating on the 2024 Alloy appears to respond better than pure aluminum at 150 K and the responses are the same at 100 K. This is contrary to comparisons made at standard conditions. Comparisons of the two responses in the region of interest for cryogenic wind tunnel testing are shown below in Figure 6.5 and Figure 6.6.

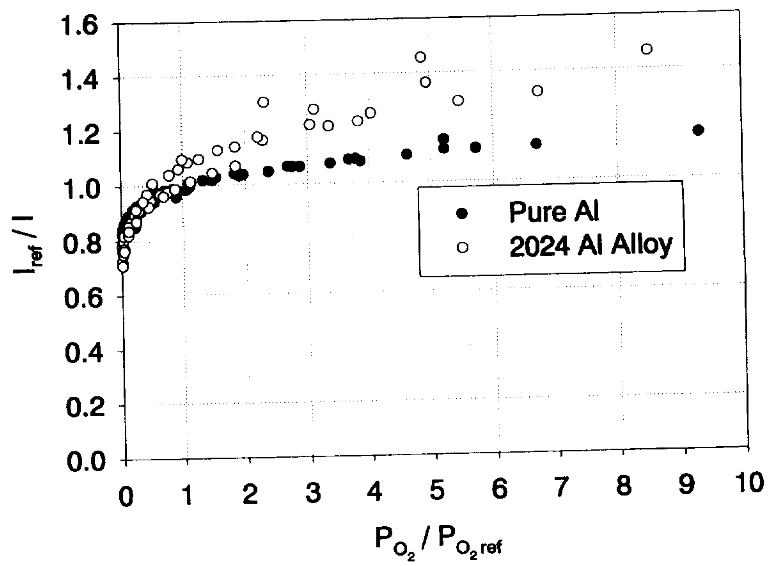

Figure 6.5: Comparison of Anodized Coatings at 150 K

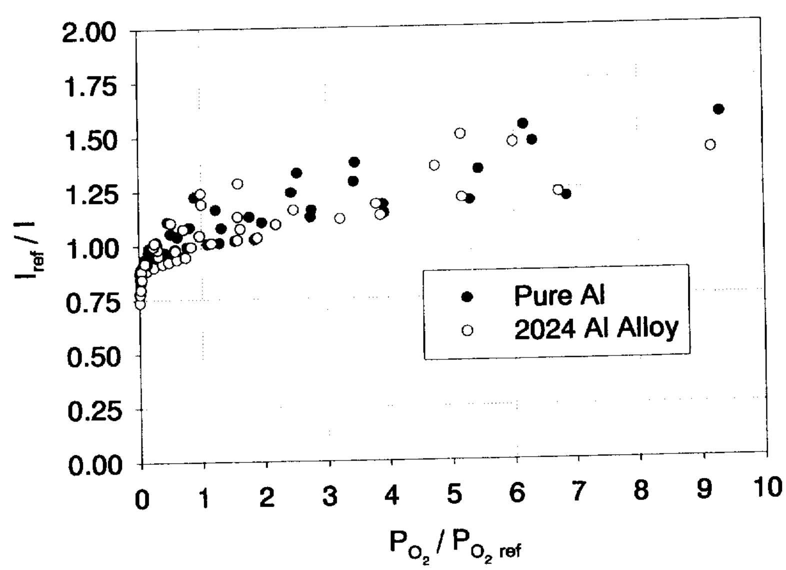

Figure 6.6: Comparison of Anodized Coatings at 100 K

In both figures, reference conditions are taken at an oxygen partial pressure of 14.0 Pa. At 150 K, the coating on the 2024 alloy shows approximately two times the sensitivity as the coating on the pure aluminum. At 100 K, there is no discernable difference between the two coatings, as the data is too noisy to give any insight into the response at this temperature.

6.3.2 GE RTV/Silica Gel

Luminescent coatings using GE RTV have been used in the past by several researchers[16,17]. The preliminary experiments described in Section 6.1 showed that paints with GE 110 RTV as the binder responded to oxygen at cryogenic temperatures when silica gel particles were added to the mixture. It was postulated that the addition of the silica gel increases the diffusivity of the coating. Using [Ru(ph$_2$-phen)$_3$] or PtTFPP as the sensor, paints with increasing concentrations of silica gel particles were tested. The specific binders tested were:

- 5 mg [Ru(ph$_2$-phen)$_3$]/5 mL RTV/0.5 g silica gel
- 5 mg [Ru(ph$_2$-phen)$_3$]/5 mL RTV/1.0 g silica gel
- 5 mg [Ru(ph$_2$-phen)$_3$]/5 mL RTV/2.5 g silica gel
- 10 mg PtTFPP/5 mL RTV/2.0 g silica gel

None of the coatings responded in the range of interest for cryogenic wind tunnel testing.

While none of the luminescent coatings responded at cryogenic conditions, the coatings did respond at temperatures above –60 °C. Although not cryogenic, this temperature range is of interest for conducting in-flight pressure measurements. A comparison of the response for the [Ru(ph$_2$-phen)$_3$]/5 ml RTV/X g Silica Gel coatings is shown below in Figure 6.7.

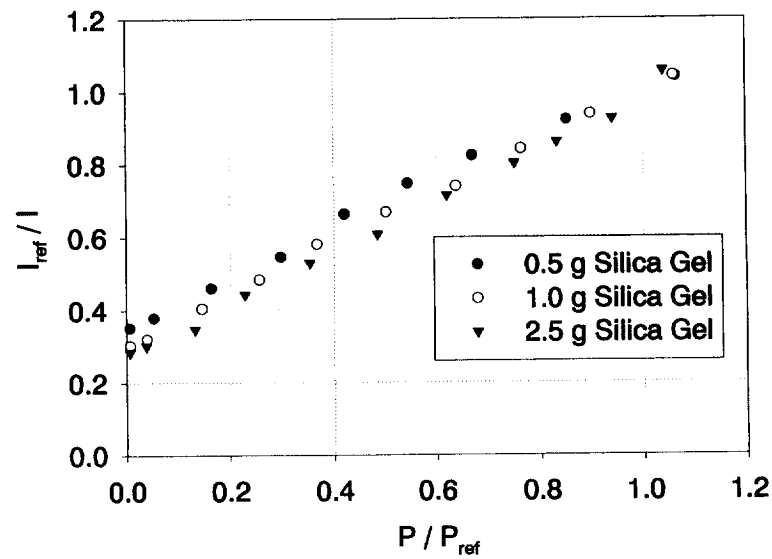

Figure 6.7: Comparison of [Ru(ph$_2$-phen)$_3$]/5 mL RTV/X g Silica Gel Paints

The above figure is in Stern-Volmer form with reference conditions taken at standard atmospheric pressure. The calibrations were done using air as the test gas at a temperature of –30 °C. The figure indicates that the addition of silica gel particles to the binder causes a small increase in the slope of the response. It should also be noted that the addition of silica gel causes the coating to become more powdery and harder to keep attached to the surface. Matrix calibrations for each paint at –30, -20, -15, and 25 °C are given in Appendix B. Another concern with this paint was hysteresis. The paints did not appear to return to their starting intensity once the test chamber was evacuated following calibration. Further investigation revealed that the paints apparently had a slow desorption rate of oxygen and that the [Ru(ph$_2$-phen)$_3$] based paints would indeed return to the starting intensity after 2-3 minutes under vacuum. Adsorption of oxygen seemed to be a much faster process with responses registering within 10 seconds of the introduction of additional gas. A coating of PtTFPP/5 mL RTV/2.0 g silica gel was also tested, but exhibited a much slower desorption rate (~ 15 min) and was deemed unusable.

6.3.3 GP-197/Silica Gel

While preliminary experiments showed that coatings using GP-197 as a binder were not very sensitive under cryogenic conditions, the addition of silica gel to the mixture appeared to dramatically increase the sensitivity. The following GP-197/silica gel coatings were prepared and tested under cryogenic conditions:

- 5 mg [Ru(ph_2-phen)$_3$] / 10 mL GP-197/1.0 g silica gel
- 5 mg [Ru(ph_2-phen)$_3$] / 10 mL GP-197/2.0 g silica gel
- 5 mg PtTFPP / 10 mL GP-197/2.0 g silica gel
- 6 mg PtOEP / 10 mL GP-197 / 2.0 g silica gel

Comparison plots in the region of interest are shown below in Figure 6.8 and Figure 6.9. Intensity data are normalized to 1.0 at an oxygen partial pressure of 14.0 Pa.

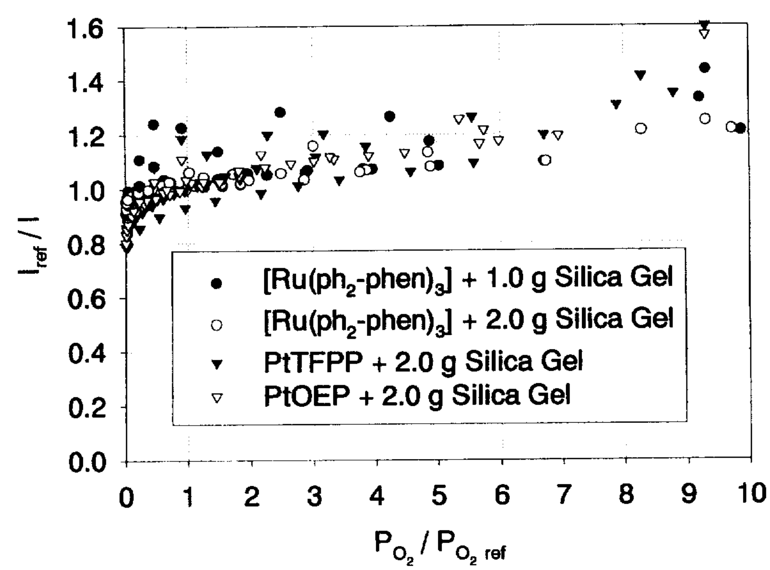

Figure 6.8: Comparison of GP-197/Silica Gel Coatings at 150 K

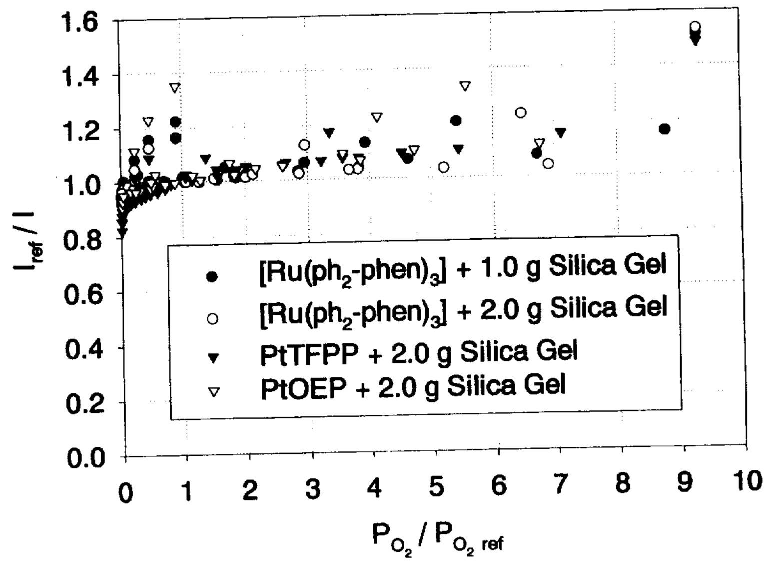

Figure 6.9: Comparison of GP-197/Silica Gel Coatings at 100 K

At both temperatures, no discernable differences can be observed. Resolution is generally too poor for these coatings to be useful. Information from the full range of pressure tested (see Appendix B) shows that these paints could be useful over a much larger range of partial pressures, but cannot provide the proper resolution over the small range needed in cryogenic wind tunnel testing.

6.3.4 Hydrothermal Coating

Two luminescent paints were prepared by Aaron Scroggin of the Purdue University Materials Engineering Department using the hydrothermal coating method described in Section 4.1.3.2. Both used [Ru(ph$_2$-phen)$_3$] as the luminescent pressure sensing molecule. One coating used 99% TiO_2 and 1% polymer, the other 80% TiO_2 and 20% polymer. Figure 6.10 below is a Stern-Volmer comparison of the two coatings at room temperature. Data is normalized to 1.0 at 14.7 PSI.

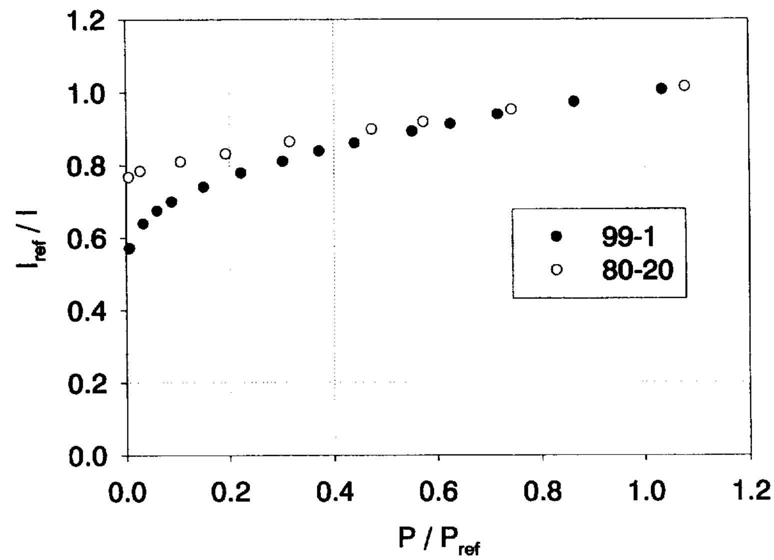

Figure 6.10: Comparison of Hydrothermal Coatings at Room Temperature

It can be seen from Figure 6.10 that slope of the response increases with decreasing amounts of polymer. Unfortunately, when tested at 150 K the coating containing 20% polymer did not respond and the coating with 1% polymer only showed a 5% drop in intensity between vacuum and atmospheric pressure air. Thus, neither coating could be considered further for use as a cryogenic PSP.

6.3.5 Polystyrene

Attempts were made to create paints using polystyrene as the binder. Coatings using [Ru(ph_2-phen)$_3$] in polystyrene and PtTFPP in polystyrene were created. The coating containing [Ru(ph_2-phen)$_3$] did not respond to oxygen at all. The PtTFPP/polystyrene coating showed the following response to air at room temperature (data is normalized to 1.0 at 14.7 PSI).

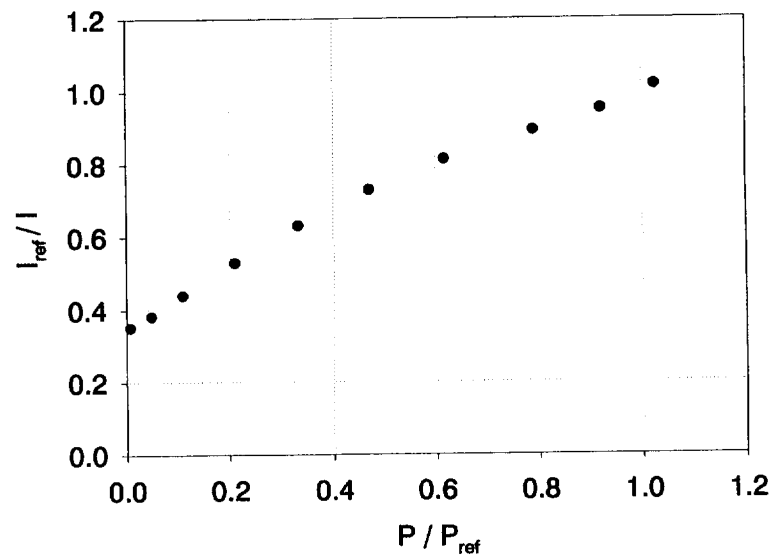

Figure 6.11: Stern-Volmer Response for PtTFPP/polystyrene in Air at 25 °C

The response follows the Stern-Volmer theory well and shows good sensitivity between vacuum and 15 PSI air. The coating, however, did not show any response to oxygen below a temperature of –25 °C and showed no temperature response below a temperature of –50 °C. Thus, this paint was of no use as a cryogenic PSP or TSP.

6.3.6 Sol Gel

Samples of [Ru(ph$_2$-phen)$_3$] in a Sol Gel binder were obtained from Jeff Jordan of Innovative Scientific Solutions, Incorporated (ISSI). Room temperature calibrations in air yielded the following Stern-Volmer response normalized to 1.0 at 14.7 PSI.

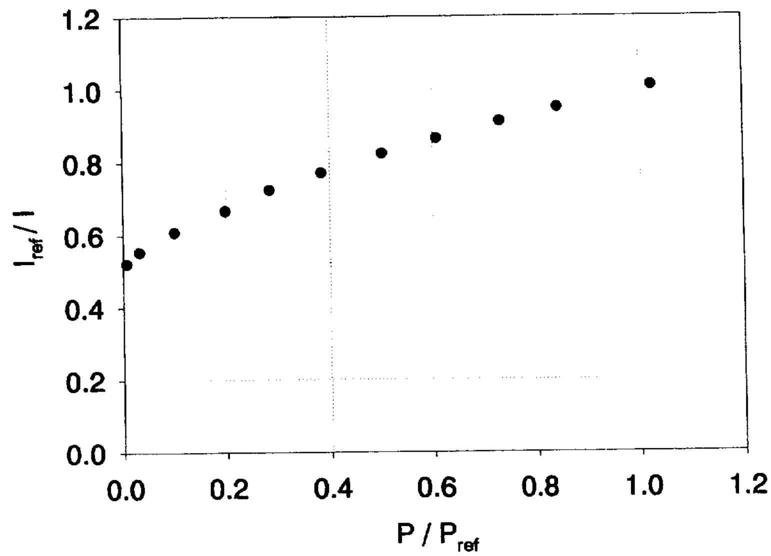

Figure 6.12: Stern-Volmer Response of [Ru(ph$_2$-phen)$_3$] in Sol Gel (25 °C, air)

This result agreed with similar tests on the sample conducted at ISSI. The sample however, did not respond to oxygen at temperatures below –70 °C.

6.3.7 Tape Casting

The Tape Casting method described in Section 4.1.3.4 was used to create PSP's using [Ru(ph$_2$-phen)$_3$] or PtTFPP as the luminescent molecule. These coatings were prepared by A. Scroggin of the Purdue University Materials Engineering Department. Room temperature calibrations in air yielded the following responses.

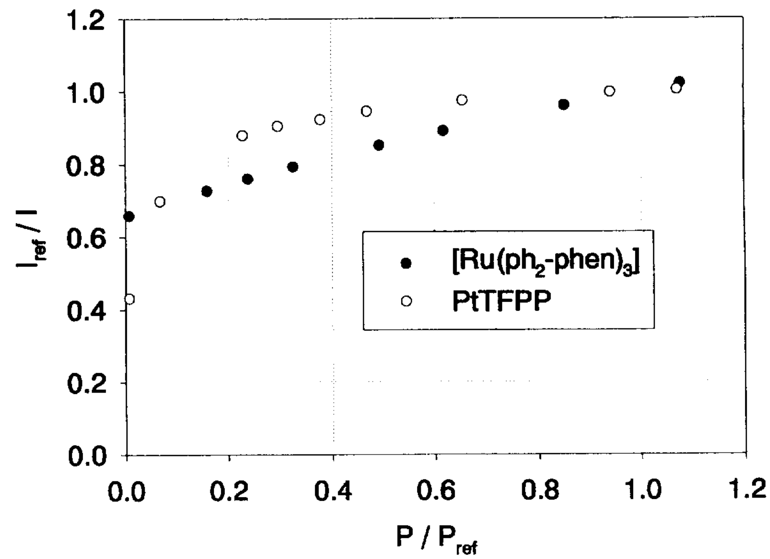

Figure 6.13: Stern-Volmer Responses of Tape Cast PSP's (25 °C, air)

While the [Ru(ph_2-phen)$_3$]/Tape Cast paint shows a linear response, the PtTFPP/Tape Cast paint is highly non-linear below P/P_{ref}=0.2. [Ru(ph_2-phen)$_3$]/Tape Cast shows no response to oxygen below –30 °C. PtTFPP/Tape Cast showed a 20% intensity drop between vacuum and 15 PSI air at 150 K and a 30% intensity drop at 200 K. While this response could be observed and calibrated, the paint is of little use in cryogenic wind tunnel testing as proper resolution of the low oxygen partial pressures cannot be obtained.

6.3.8 Thin-Layer Chromatography Plate

Based on results of the initial feasibility experiments, [Ru(ph_2-phen)$_3$], PtTFPP, and PtOEP where each soaked into standard grade Thin-Layer Chromatography (TLC) plates and calibrated under cryogenic conditions. Room temperature calibrations in air yielded the following results for these three paints.

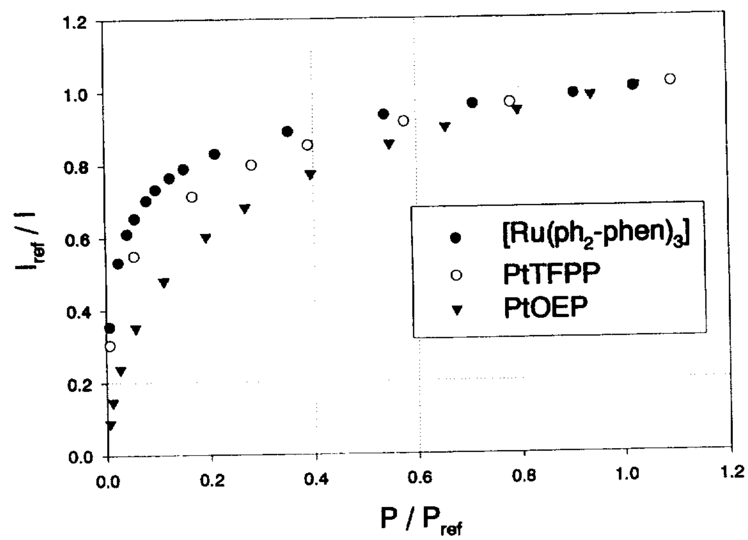

Figure 6.14: Stern-Volmer Response for TLC Based Paints (25 °C, air)

As can be seen above, all three paints show non-linear Stern-Volmer responses. PtOEP shows the steepest slope at low concentrations and [Ru(ph$_2$-phen)$_3$] shows the shallowest. All three paints responded well under cryogenic conditions and Figure 6.15 and Figure 6.16 below show comparisons of the three paints at 150 and 100 K respectively in the region of interest for cryogenic wind tunnel testing.

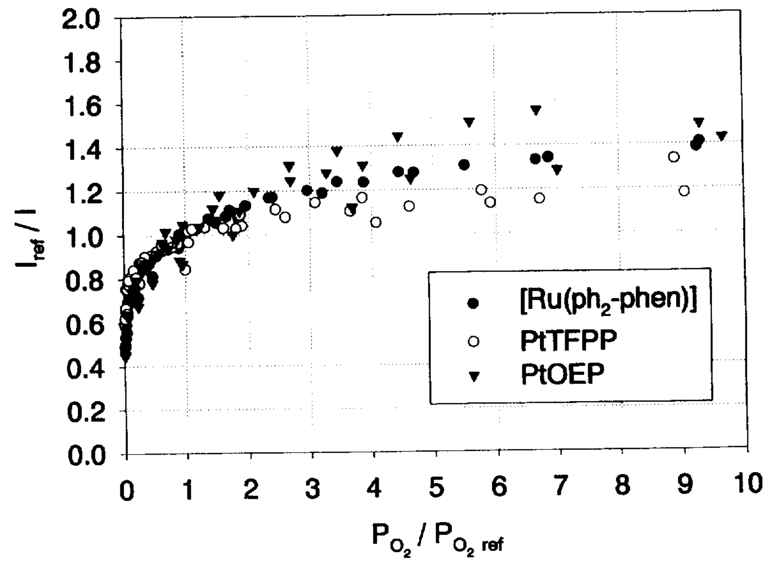

Figure 6.15: Comparison of TLC Based Paints at 150 K

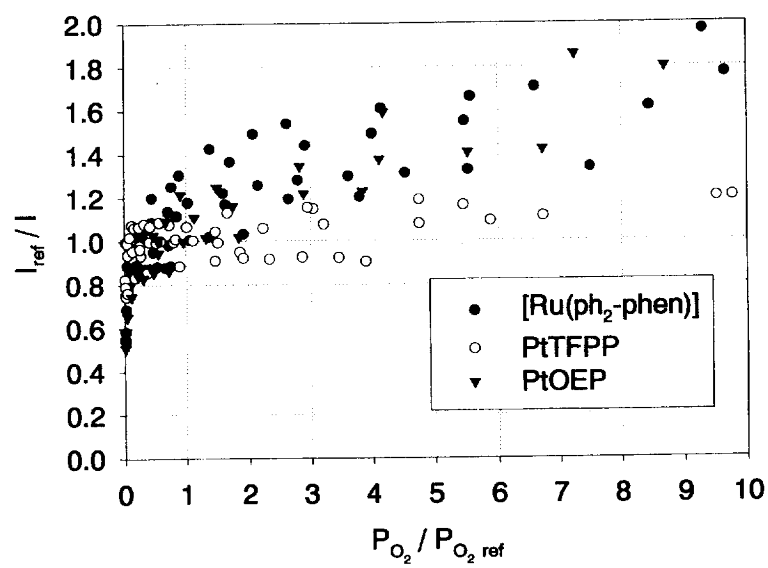

Figure 6.16: Comparison of TLC Based Paints at 100 K

At 150 K, PtOEP/TLC exhibits the largest intensity change over the region of interest. Followed by [Ru(ph_2-phen)$_3$] and PtTFPP. At 100 K, no discernable trends can be observed.

6.3.9 Filter Paper

Based on results of the initial feasibility experiments, [Ru(ph_2-phen)$_3$], PtTFPP, and PtOEP where each soaked into Whatman filter paper #1 (cat # 1001 042) and calibrated under cryogenic conditions. Room temperature calibrations in air yielded the following results for these three paints.

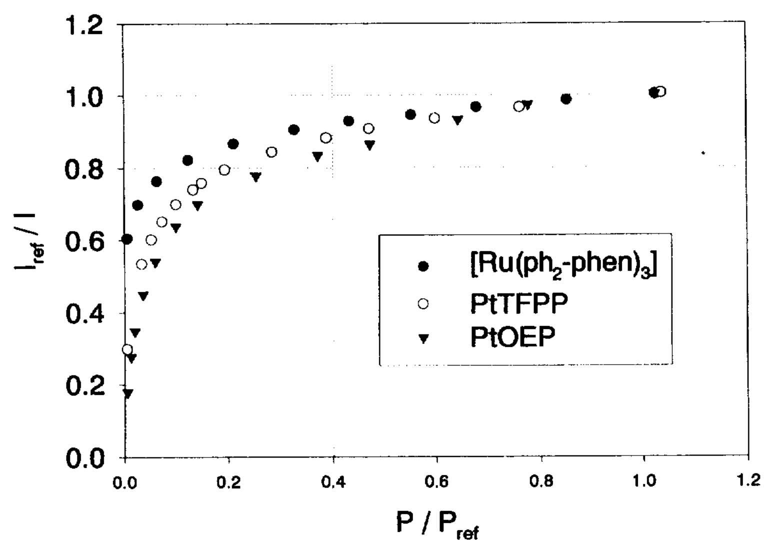

Figure 6.17: Stern-Volmer Responses for Filter Paper Based Paints (25 °C, air)

As with the TLC based paints, the filter paper based paints all show non-linear Stern-Volmer responses under room temperature conditions. PtOEP shows the steepest response at low pressures and [Ru(ph_2-phen)$_3$] shows the shallowest. All three paints responded well under cryogenic conditions. Figure 6.18 and Figure 6.19 below show comparisons of the responses at 150 and 100 K respectively.

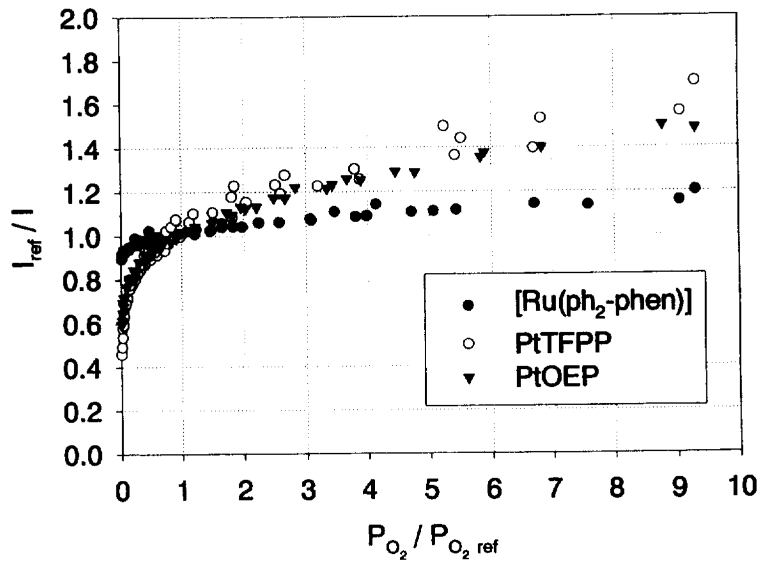

Figure 6.18: Response of Filter Paper Based Paints at 150 K

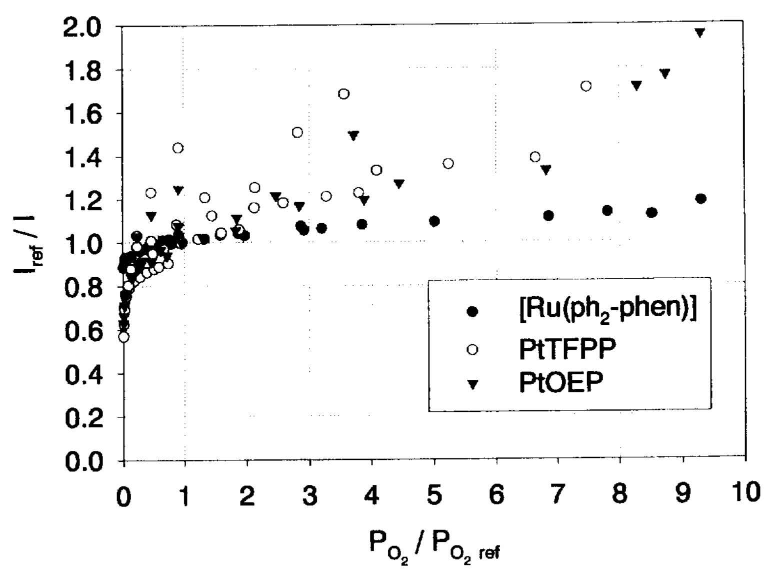

Figure 6.19: Response of Filter Paper Based Paints at 100 K

At 150 K, the PtOEP and PtTFPP paints responded with the steepest slopes and the [Ru(ph$_2$-phen)$_3$] was considerably shallower. No information could be derived from the response at 100 K.

6.3.10 Porous Polyethylene

Attempts were made to create paints using Porex X-7744 porous polyethylene filters. These particular filters had 7 μm pores. [Ru(ph$_2$-phen)$_3$] did not respond to oxygen when soaked into this material, but PtTFPP did respond at temperatures above –75 °C. This made it a good possibility for use as a flight test paint, as static temperatures at cruising altitudes are above this temperature. Figure 6.20 below shows a matrix calibration for PtTFPP in Porex for the temperature regime found at a cruising altitude of approximately 20-30,000 ft.

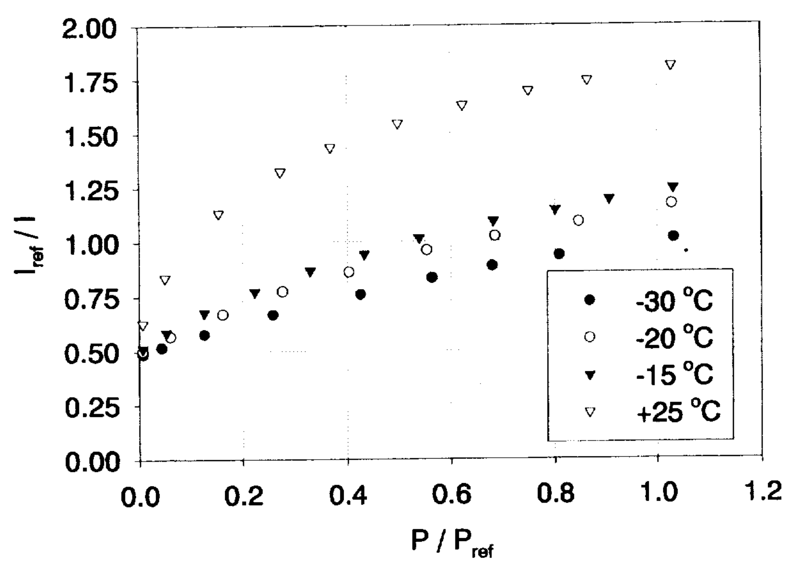

Figure 6.20: Matrix Calibration for PtTFPP in Porex Porous Polyethylene

6.3.11 Non-Collapse of Data at 100 K

Of the paints in the preceding sections which responded to oxygen under cryogenic conditions, none proved calibratable at 100 K while several were successfully calibrated at 150 K. A more detailed plot of the calibrations for [Ru(ph$_2$-phen)$_3$] on TLC at 150 K and 100 K are shown below in Figure 6.21 and Figure 6.22.

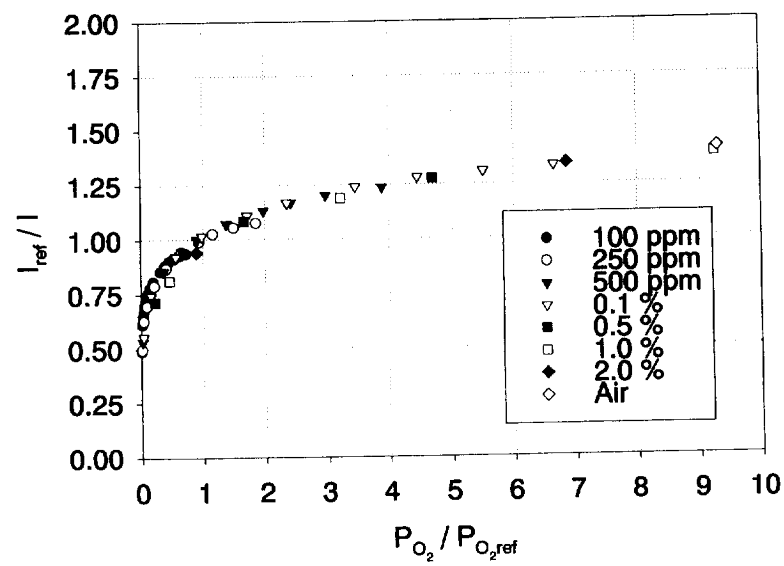

Figure 6.21: [Ru(ph$_2$-phen)$_3$] on TLC – 150 K

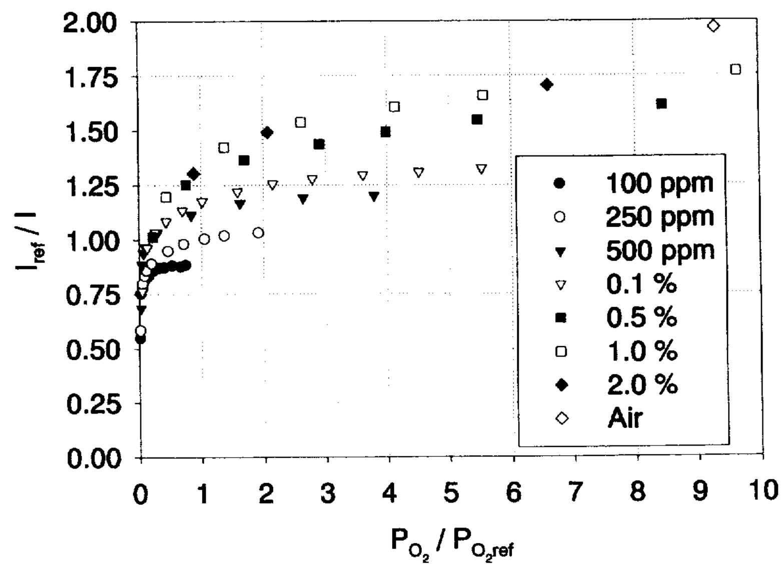

Figure 6.22: [Ru(ph$_2$-phen)$_3$] on TLC – 100 K

As described in section 5.1.6, different test gasses are used to resolve the small regions of partial pressure that are of interest in cryogenic wind tunnel testing. As discussed in section 3.2, theoretically, the data from different test gasses should collapse onto the same curve when plotted in Stern-Volmer form. The above figures show the data from each test gas. The data at 150 K collapses but the data does not collapse at 100 K. This phenomena was observed in all paints that responded to oxygen in this temperature range. The trend seen in the above data was observed even though individual test gas calibrations yielded repeatable results when normalized to the same reference conditions, as shown below in Figure 6.23. The data is from an anodized sample at 100 K in a 78 % nitrogen, 2 % oxygen gas mixture and is normalized to 1.0 at 14.7 psi static pressure.

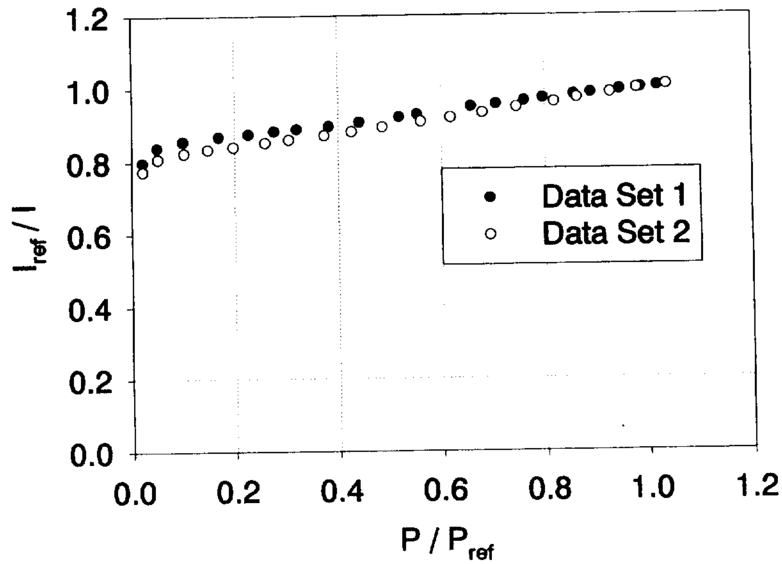

Figure 6.23: Repeated Calibration of Anodized Aluminum, 100 K, 2 % O_2

As an illustration to show this phenomena is not limited by luminophore and binder, Figure 6.24 and Figure 6.25 below show calibration results for PtTFPP on Filter Paper. Additional results are given in Appendix B.

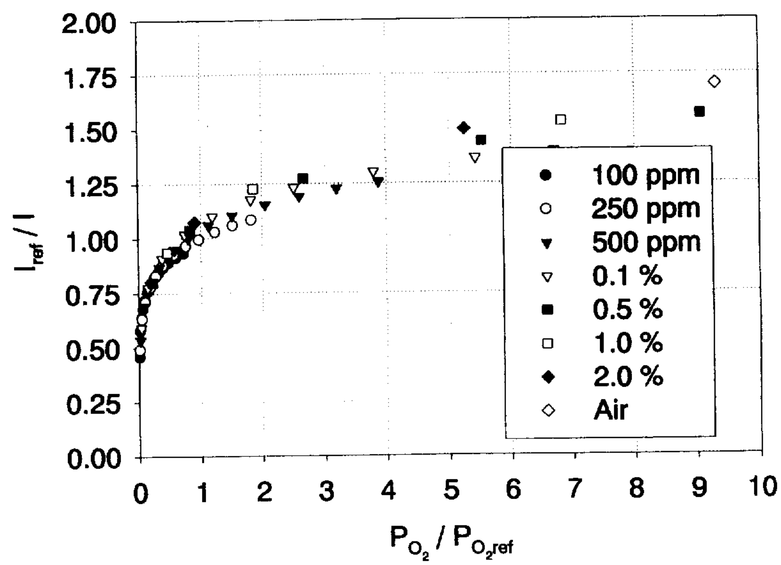

Figure 6.24: PtTFPP on Filter Paper – 150 K

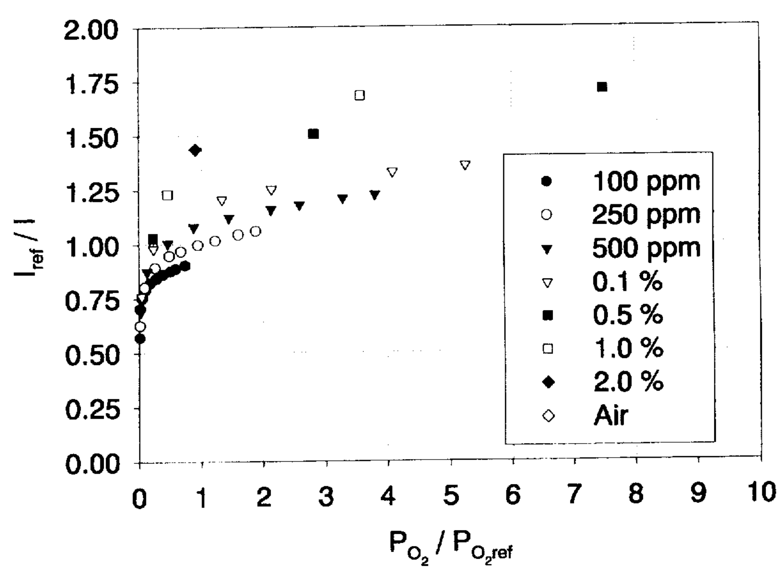

Figure 6.25: PtTFPP on Filter Paper – 100 K

This phenomena has also been observed by researchers at NASA Langley Research Center[20]. There is currently no explanation for this phenomena, however theories include nitrogen adsorption and occupation of quenching sites, condensation phenomena, or anomalies in the porous surface.

6.4 Application – PSP Data in NAL 0.1-m Transonic Cryogenic Wind Tunnel

Several of the cryogenic PSP's discovered during this research were tested in the 0.1-m Transonic Cryogenic Wind Tunnel at the National Aerospace Laboratory (NAL) in Japan[19]. A description of the wind tunnel and operating conditions was given in section 5.3.1. The paints were applied to strips on a circular arc bump model in the wind tunnel. The model had an array of pressure taps along the mid-chord. Oxygen injection provided the quencher for the PSP's. Quencher concentration was monitored using a ZrO_2 oxygen sensor. Figure 6.26 below shows an *a priori* calibration of [Ru(ph$_2$-phen)$_3$] in Anodized Aluminum at the 16 pressure tap locations.

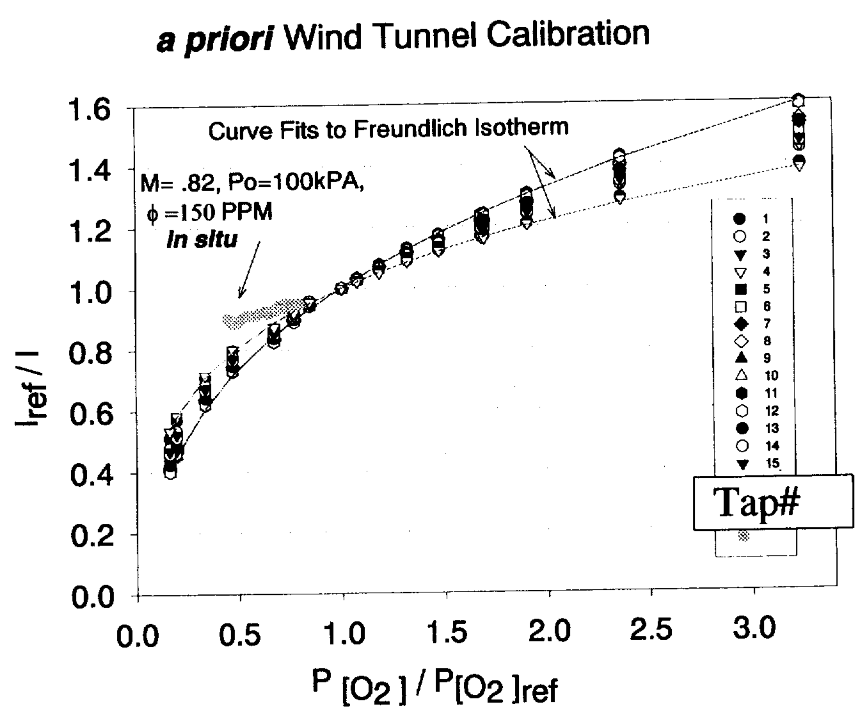

Figure 6.26: *a priori* calibration of [Ru(ph$_2$-phen)$_3$] in Anodized Aluminum

A C_p distribution over the bump is shown below in Figure 6.27.

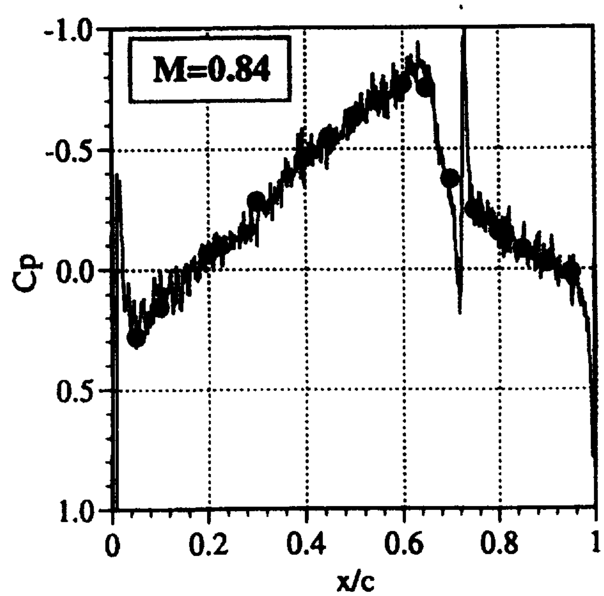

Figure 6.27: C_p Distribution Obtained from [Ru(ph$_2$-phen)$_3$] on Anodized Al

The spike at approximately 0.7 x/c is the shadowgraph of the shock wave on the surface of the model. The dots represent pressure data from taps at the corresponding location. From the figure it is seen that the paint data and pressure tap data agree well.

CHAPTER 7: SOURCES OF ERROR

The accuracy of TSP and PSP measurements depend generally on photochemical properties of the paint and the measurement system used. The error sources can be classified in 2 groups:

1) Errors resulting from Photochemical and Photophysical properties of the paint
   a) Photodegradation
   b) Hysteresis
2) Measurement System Errors
   a) Unstable illumination source
   b) Photodetector Noise/Dark Current Effects
   c) Non-linearity of photodetector response
   d) Wavelength overlap between illumination source and optical filters
   e) Leakage of atmospheric air into the test stand

Photodetector noise and illumination intensity fluctuations are random in nature, the remaining sources or error are systematic and must be procedurally addressed. A complete error analysis is difficult to obtain due to the many different components utilized in a TSP or PSP measurement system, however various sources of error can be individually addressed and minimized through proper procedures.

7.1 Errors Resulting From Photochemical and Photophysical Properties

7.1.1 Photodegradation

Photodegradation of a luminescent paint occurs when the emission light intensity of the paint decreases with exposure time to illumination light. It is dependent upon illumination intensity, exposure time, and the properties of the luminescent molecule itself. Photodegradation is caused by destructive reactions between singlet state O_2

molecules produced during the quenching process and the luminescent molecules. The Porphyrin family is very sensitive to singlet O_2, but molecules based on transition metals are not as sensitive.

Previous work[11] has shown that the calibration data for paints exhibiting various degrees of photodegradation roughly collapse onto the same curve through normalization. While this is true, photodegrading a paint is still undesirable since the emission intensity may fall below useful levels for detection. Since photodegradation results from exposure to singlet O_2, it can be significantly diminished in TSP's when using a binder with low oxygen permeability, which is already desirable. In addition, using minimal amounts of excitation light and limiting exposure time can diminish the effects of photodegradation.

7.1.2 Hysteresis

Hysteresis, or repeatability, occurs when calibration data does not match for consecutive calibrations. The causes of hysteresis vary depending on the type of coating being tested.

7.1.2.1 Temperature Hysteresis

Hysteresis in TSP's is mainly a function of the glass transition temperature, T_g[37]. When temperature of the polymer binder exceeds the glass transition temperature, the matrix undergoes a non-reversible transition from a relatively brittle glassy state to a soft and rubbery state. This transition effects the temperature dependence of the luminescent paint[11]. Either maintaining a temperature below the glass transition of the binder or pre-heating the binder to a temperature above T_g prior to calibration can eliminate the effects of temperature hysteresis. Depending on calibration conditions, either method of eliminating temperature hysteresis was used in this research.

7.1.2.2 Pressure Hysteresis

Hysteresis in PSP's can be caused by several factors. Glass transition causes hysteresis much the same as in TSP's and was avoided in the same manner as outlined in the above section. In addition, moisture can soak into the coatings containing silica and cause hysteresis. The water molecules occupy quenching sites on the surface that could otherwise be inhabited by a quencher. This decreases the paint's intensity and changes the calibration. Typically paints containing silica must be stored in dry conditions (in a desicator for example) and used within 72 hours before significant effects of moisture adsorption are observed. Similar aging effects have been observed with the anodized coatings, but this has not been directly correlated with moisture.

As a check for hysteresis which may have occurred during the calibration, room temperature calibrations in air were performed prior to and after exposure of each paint to cryogenic conditions. No significant changes in response were observed in any of the paints. Figure 7.1 below is an example of one of these checks. The calibration is for PtOEP on TLC plate at room temperature. Data is normalized to an intensity ration of 1.0 at 14.7 psi static pressure. As can be seen from the data below, only small variations in the response were observed.

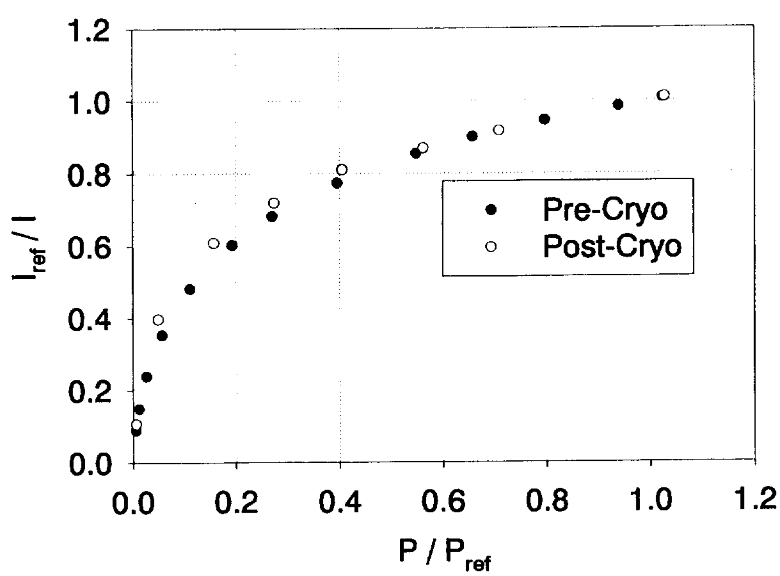

Figure 7.1: Hysteresis Check for PtOEP/TLC

As an additional check for hysteresis at low oxygen concentrations, the test chamber was purged repeatedly with nitrogen and brought to vacuum prior to and after each PSP calibration. Intensities were noted and if any significant differences (> 3 %) were detected, calibrations were repeated until repeatability was observed. Additionally, pre- and post-cryogenic exposure calibrations were conducted and results compared to observe if any hysteresis effects occurred. It was noted that some paints, such as those using GE RTV + silica gel binders, exhibited very low rates of desorption of oxygen while at cryogenic conditions. While these paints returned to the initial intensity after a significant time period (>15 min), the effect could be mistaken for hysteresis.

7.2 Measurement System Errors

7.2.1 Unstable Illumination Source

Fluctuations in the illumination source can cause associated fluctuations in emitted luminescence from the paint. In most cases in this research, the laser illumination sources had intensity fluctuations of less than 1.0 %, which was stable enough to not affect measurements. Since PSP's often exhibit less sensitivity to oxygen compared to TSP's sensitivity to temperature changes, laser emission was monitored and recorded for PSP calibrations. Fluctuations in laser intensity were corrected for by dividing each paint intensity reading by the associated laser emission intensity for that reading. For TSP calibrations, laser power was simply monitored for significant variations (> 1.0 %) where possible.

7.2.2 Photodetector Noise/Dark Current Effects

In addition to signal noise, there are two major sources of noise in photomultiplier tubes, shot noise and Johnson noise. Shot noise (dark noise) originates from the individual photons which eventually impact the PMT anode and is associated with the thermionic component of dark current[38]. The rms noise current from shot noise is given by:

$$I_{rms} = \mu(2ei_d B)^{1/2} \tag{7.1}$$

where μ is the photomultiplier gain, e is the charge on the electron, i_d is the dark emission current from the photocathode, and B is the bandwidth of the observation.

Johnson noise is thermal noise associated with the load resistance of the PMT and is given by the following:

$$I_{rms} = (4kTB / R)^{1/2} \tag{7.2}$$

where k is Boltzman's constant, T is the temperature in Kelvin, R is the load resistance, and B is the bandwidth of the observation.

From equation (7.2) it can be seen that the Johnson noise is dependent on the square root of the load resistance, assuming temperature is fairly constant. It has been shown that a load resistance of 50 ohms or greater will reduce the Johnson noise to a point where the shot noise (dark noise) far exceeds the Johnson noise[38].

Signal noise can be modeled with the following equation:

$$I_{rms} = \mu(2ei_s B)^{1/2} \tag{7.3}$$

where μ is the photomultiplier gain, e is the charge of an individual electron, i_s is the signal current, and B is the bandwidth of the measurement.

Noting that there is no correlation between shot noise and noise in the signal current, the noises may be added by summing their squares, yielding a total rms noise current of:

$$I_{rms} = \mu[2e(i_d + i_s)B]^{1/2} \tag{7.4}$$

In all cases, the PMT was operated at detection levels above that of the dark current, thus signal noise was the main contribution to overall noise. Regardless, digital low-pass filtering of the signal and averaging of A/D readings reduced both signal noise and shot noise in the system.

While dark current noise has minimal effects on the value of rms voltage readings, it can effect calculations of slope when using ratios to plot calibration data. Thus, dark current readings were taken at the start of each calibration and the rms voltage subtracted from each reading prior to ratioing. Dark current rms voltage values were typically on the order of 1,000 times less than the signal voltage levels.

7.2.3 Non-linearity of Photodetector Response

Care must be taken when using a PMT to operate the device within it's linear response range and also to not saturate the device. Linearity of the response is a function of incident light and supply voltage. As long as there is sufficient incident light and the supply voltage is set to an acceptable level, the response will be linear. This was checked prior to each calibration by reducing incident light by one half and observing if the voltage from the PMT dropped by approximately half. This test also will show if the device is saturated, as the signal would drop less than half. In addition, incident light can be slightly increased to see if signal increases, indicating the device is not saturated.

7.2.4 Wavelength Overlap Between Illumination Source and Optical Filters

All optical filters allow "bleed through" of wavelengths beyond the cut-off frequency of the filter. This could cause the PMT to detect some intensity associated with excitation light, which has passed through the optical filter. Care must be taken to use paints with sufficient Stokes shift to effectively filter out the excitation source intensity. Each excitation source and filter combination was tested by illuminating a piece of bare aluminum and checking the photodetector signal compared to a dark reading. In all cases, the effect of overlap was found to be negligible.

7.2.5 Leakage of Atmospheric Air Into the Test Stand

Since paints are sensitive to both oxygen and temperature, leakage of additional oxygen into the test stand can affect calibration results. The effects of leakage where not considered significant in temperature calibrations as the binders were relatively impermeable to oxygen and a trickle flow of nitrogen was maintained through the test stand.

Leakage, however, becomes a significant source of error for pressure calibrations especially since some of the paints being tested were highly sensitive under cryogenic conditions. Thus leakage of atmospheric air ($[O_2]$=21%) into the test chamber where much lower oxygen concentrations are present, can produce substantial changes in paint intensity. For example, the most sensitive PSP in this work showed a 60% change in intensity ratio over a 0.018 PSI change in oxygen partial pressure. Simple calculations using Dalton's Law shows that only 0.014 PSI leakage of atmospheric air into the test chamber could produce a 10% change in emission intensity. This amount of pressure increase is well within the measurement error of most pressure transducers and is thus considered undetectable without the purchase of expensive equipment. In lieu of purchasing better equipment, a simple test was conducted to observe any leakage effects. The most sensitive paint (PtOEP/filter paper) was placed in the test rig under vacuum at 150 K. The system was sealed by closing the proper valves on the control panel, just as it would be in a normal calibration. Paint intensity was monitored for a period of 10 minutes. The results are shown below in Figure 7.2.

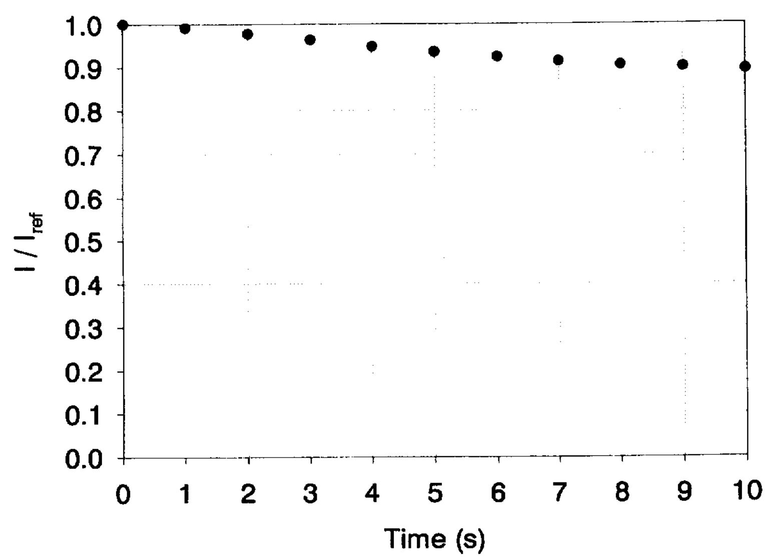

Figure 7.2: Intensity change in PtOEP/Filter Paper due to leakage

As can be seen from the figure, paint intensity changed by 10% over the 10 minute period, thus some leakage was assumed to exist. Using the calibration results for that paint, the leak rate is found to be 0.0014 PSI/min. Since data is taken with several test gasses and the test chamber purged between each test, the time scale of interest is the time it takes to conduct measurements with each test gas. It takes approximately 5 minutes to take data with each test gas, thus we are interested in the measurement error due to leakage over this period of time. Assuming leak rate remains constant throughout the 5 minute period, the error at the end of the 5 minutes is 5%. As outlined in section 5.1.6, measurements with each test gas start at vacuum and end near atmospheric pressure. Since the leak rate will decrease as the pressure differential between the test chamber and atmosphere decreases, the actual error is less.

CHAPTER 8: CONCLUSIONS AND RECOMMENDATIONS

While the use of temperature- and pressure-sensitive paints to make surface temperature and pressure measurements on aerodynamic models is well documented at near standard atmospheric conditions, little work has been done to extend this application to cryogenic wind tunnel testing. The objective of this research is to prove that extension possible through the design and calibration of temperature- and pressure-sensitive paints that respond under cryogenic conditions. Results indicate that extension of the technology into cryogenic wind tunnel testing is plausible and calibrations conducted under these conditions have been presented.

Many cryogenic temperature-sensitive paints were calibrated and found to respond in the region of interest for cryogenic testing (-175 to –50 °C). The $[Ru(trpy)_2]$ family of luminescent molecules was found to yield high intensity paints with excellent sensitivity in the region of interest. Through changes in the ligand structure of the basic $[Ru(trpy)_2]$ molecule, variations in slope and response range were obtained. The $[Ru(ppd\text{-}trpy)_2](PF_6)_2$ molecule was found to exhibit a 33% increase in response slope over the basic $[Ru(trpy)_2]$ molecule and responded over approximately the same temperature range. The response of this molecule was very similar to the response of $[Ru(trpy)(VH\text{-}127)](PF_6)_2$ (commonly considered the best response in this temperature region), but the $[Ru(ppd\text{-}trpy)_2](PF_6)_2$ molecule is much simpler and cheaper to synthesize. While the effects of the polymer binder were not a focus, they were outlined and illustrated.

While many pressure-sensitive paint formulations were tested under cryogenic conditions, only a few responded with reasonable sensitivity and resolution under the limited oxygen concentrations found in a cryogenic wind tunnel. These paints produced good data at 150 K, but no good responses were observed at 100 K. The paints that did respond well included the anodized paint layers and paints using TLC plate or filter paper as the binder. The anodized and TLC paints showed a 20-40% intensity change over the region of interest while the filter paper paints showed the same magnitude of change with the exception of PtTFPP/filter paper and PtOEP/filter paper which exhibited a 60%

intensity change. Although efforts were made to minimize the amount of polymer, none of the paints containing any type of polymer in the binder exhibited sensitivity under cryogenic conditions. However, porous polyethylene, tape cast, and RTV/silica gel paints were found to be good candidates for PSP's that operate in the temperature regions encountered during in-flight PSP measurements and should be considered for use in flight tests.

It is recommended that further investigation of porous surfaces be undertaken in an effort to understand the phenomena observed in PSP response at 100 K and also to expand binder choices beyond the limited options found in this research. Experiments to determine the nature of the 100 K response should also be conducted in an effort to explain and understand the origin of this behavior.

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APPENDIX A: TEMPERATURE CALIBRATION DATA

This appendix is a compilation of the temperature-sensitive paint calibration data produced during the course of this research. This appendix contains two tables and 26 figures. Table A.1 contains information concerning the formulation of the paint mixtures that were calibrated for this research. It should be noted that the amount of solvent used to dissolve the luminescent compound prior to mixing with the polymer binder is not critical. Only enough solvent to fully dissolve the compound is required. The solvent then evaporates into the atmosphere as the paint dries after application. Also, some compounds dissolved directly into the binder and no solvent was required. The choice of a base coat was dictated by two factors, adhesiveness of the binder to the metal and optical requirements. White base coats were used in order to allow more emitted light to be reflected back to the collection optics. Trial and error determined if a particular binder would better adhere to certain base coats. Table A.2 shows the excitation light and filters used in each calibration. Choice of excitation wavelength and filtration was dependent on the excitation and emission spectrum of each luminescent molecule and also on required excitation intensity. Figures A.1-A.26 show the results of each calibration. The top plot is intensity ratio versus temperature and the bottom plot is the Arrhenius form of the results. In all cases, the reference conditions were taken at –150 °C. A line representing the results of a linear regression over the useful range of sensitivity for each paint is shown on each intensity ratio plot.

Table A.1: TSP Paint Mixtures

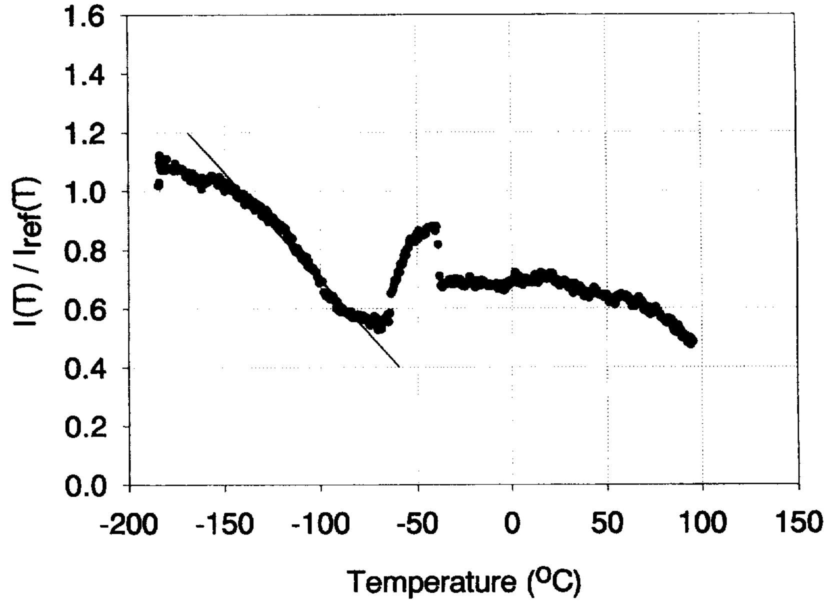
Paint (<compound> In <binder>)	Amount of Fluorophore (mg)	Amount of Binder (mL)	Solvent	Basecoat
$[Cu(ph_2\text{-}phen)_2](PF_6)_2$ in GP-197				None
PtPFPP in CC	100	25	Acetone	Chroma Base
PtPFPP in Polyurethane	100	20	Acetone	Chroma Base
$[Rh(bzq)_2Cl]_2$ in CC	50	25	Acetonitrile	Chroma Base
$[Rh(bzq)_2(phen)](PF_6)$ in CC	50	25	Acetonitrile	Chroma Base
$[Ru(bipy)_3](DS)_2$ in CC			Ethyl Alcohol	White Car Paint
$[Ru(bipy)_3](TFPB)_2$ in CC			None	Chroma Base
$[Ru(ph_2\text{-}phen)_3](DS)_2$ in CC			Ethyl Alcohol	Chroma Base
[Ru(trpy)] in CC	20	15	Acetone	Chroma Base
$[Ru(trpy)(4'\text{-}C_6F_5\text{-}trpy)](NO_3)_2$ in CC	6	20	Acetonitrile	Chroma Base
$[Ru(trpy)(4'\text{-}Cl\text{-}trpy)](Cl_2)$ in CC	8	22	Acetonitrile	Chroma Base
$[Ru(trpy)(4'\text{-}NC\text{-}trpy)](NO_3)_2$ in CC	13	22	Acetonitrile	Chroma Base
$[Ru(phtrpy)(Cltrpy)](NO_3)_2$ in CC	6	40	Acetonitrile	Chroma Base
$[Ru(trpy)(4'\text{-}TfO\text{-}trpy)](NO_3)_2$ in CC	12	20	Acetonitrile	Chroma Base
$[Ru(trpy)(MeStrpy)](NO_3)_2$ in CC	17	20	Acetonitrile	Chroma Base
$[Ru(trpy_2)(NO_2(Phtrpy)](PF_6)$ in CC			Acetone	Chroma Base
$[Ru(trpy)(phtrpy)](PF_6)_2$ in GP-197			None	White Car Paint
$[Ru(trpy)(phtrpy)](PF_6)_2$ in CC			Acetone	Chroma Base
$[Ru(trpy)(ppd\text{-}trpy)](TFPB)_2$ in CC	11	15	Acetone	Chroma Base
$[Ru(trpy)(phyphen)](TFPB)_2$ in CC	10	11	Acetone	Chroma Base

Table A.1: TSP Paint Mixtures (cont.)

$[Ru(trpy)(SO_2Me\text{-}trpy)](PF_6)_2$ in CC	10	15	Acetone	Chroma Base
$[Ru(trpy)_2](DS)_2$ in CC			Ethyl Alcohol	Chroma Base
$[Ru(trpy_2)](TFPB)_2$ in CC			Ethyl Alcohol	Chroma Base
$[Ru(ppd\text{-}trpy)_2](TFPB)_2$ in CC	8	10	Acetone	Chroma Base
$[Os(trpy)_2](PF_6)_2$ in CC	28	15	Acetone	Chroma Base
$[Ru(trpy)(Vh127)](PF_6)_2$ in GP-197	5	13	Acetone	White Krylon

Table A.2: TSP Calibration Settings

Paint (<compound> In <binder>)	Excitation		Optical Filter	
	Wavelength (nm)	Power (W)	Type	Cut-off (nm)
[Cu(ph$_2$-phen)$_2$](PF$_6$)$_2$ in GP-197	488		LP	550
PtPFPP in CC	488	0.005	LP	600
PtPFPP in Polyurethane	488	0.005	LP	600
[Rh(bzq)$_2$Cl]$_2$ in CC	UV lamp		LP	450
[Rh(bzq)$_2$(phen)](PF$_6$) in CC	UV lamp		LP	450
[Ru(bipy)$_3$](DS)$_2$ in CC	476	0.05	LP	550
[Ru(bipy)$_3$](TFPB)$_2$ in CC	488	0.13	LP	550
[Ru(ph$_2$-phen)$_3$](DS)$_2$ in CC	488	0.18	LP	550
[Ru(trpy)] in CC	488	0.12	LP	550
[Ru(trpy)(4'-C$_6$F$_5$-trpy)](NO$_3$)$_2$ in CC	488	0.005	LP	550
[Ru(trpy)(4'-Cl-trpy)](Cl$_2$) in CC	488	0.005	LP	550
[Ru(trpy)(4'-NC-trpy)](NO$_3$)$_2$ in CC	488	0.005	LP	550
[Ru(phtrpy)(Cltrpy)](NO$_3$)$_2$ in CC	488	0.005	LP	550
[Ru(trpy)(4'-TfO-trpy)](NO$_3$)$_2$ in CC	488	0.005	LP	550
[Ru(trpy)(MeStrpy)](NO$_3$)$_2$ in CC	488	0.005	LP	550
[Ru(trpy$_2$)(NO$_2$(Phtrpy)](PF$_6$) in CC	488		LP	550
[Ru(trpy)(phtrpy)](PF$_6$)$_2$ in GP-197	488		LP	550
[Ru(trpy)(phtrpy)](PF$_6$)$_2$ in CC	488		LP	550
[Ru(trpy)(ppd-trpy)](TFPB)$_2$ in CC	488	0.005	LP	550
[Ru(trpy)(phyphen)](TFPB)$_2$ in CC	488	0.005	LP	550
[Ru(trpy)(SO$_2$Me-trpy)](PF$_6$)$_2$ in CC	488	0.005	LP	550
[Ru(trpy)$_2$](DS)$_2$ in CC	488	0.005	LP	550
[Ru(trpy$_2$)](TFPB)$_2$ in CC	488	0.005	LP	550
[Ru(ppd-trpy)$_2$](TFPB)$_2$ in CC	488	0.005	LP	550
[Os(trpy)$_2$](PF$_6$)$_2$ in CC	632	0.01	LP	700
[Ru(trpy)(Vh127)](PF$_6$)$_2$ in GP-197	488	0.005	LP	550



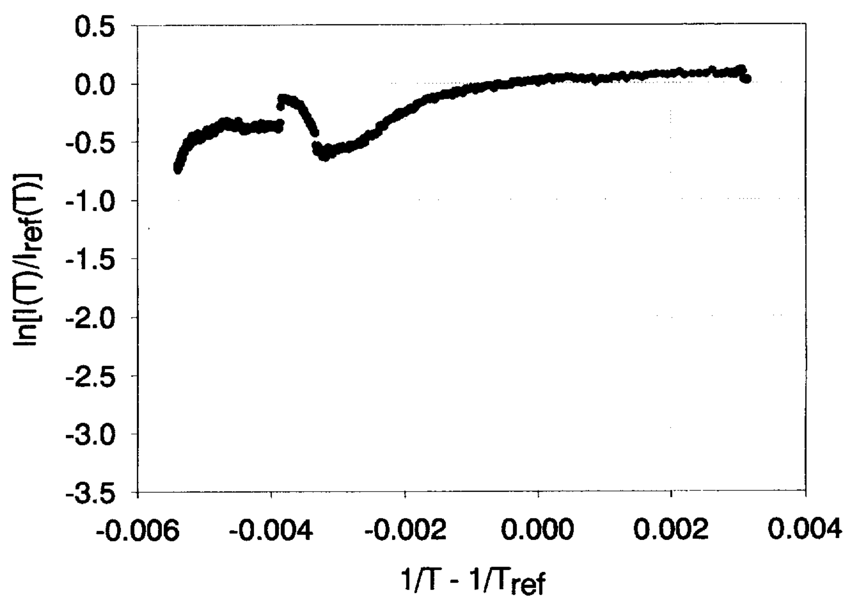
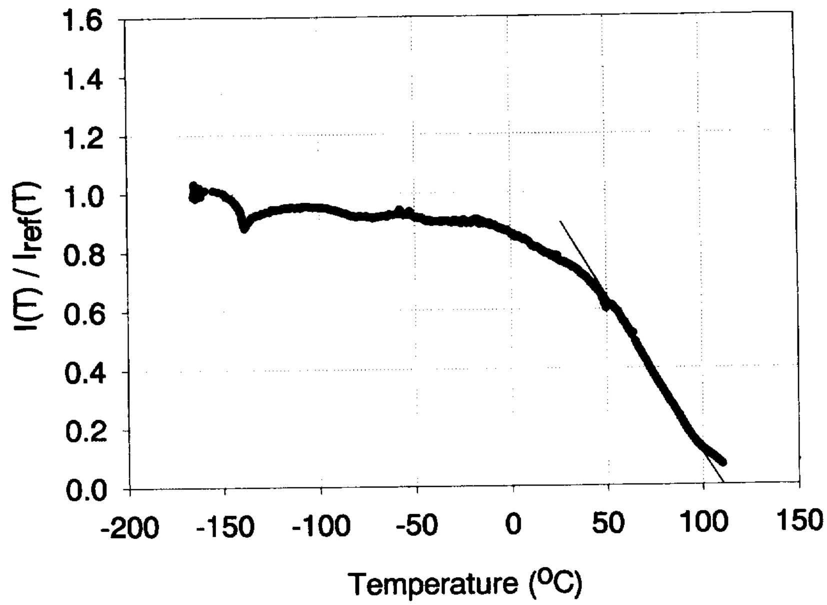


Figure A.1: $[Cu(ph_2\text{-}phen)_2](PF_6)_2$ in GP-197



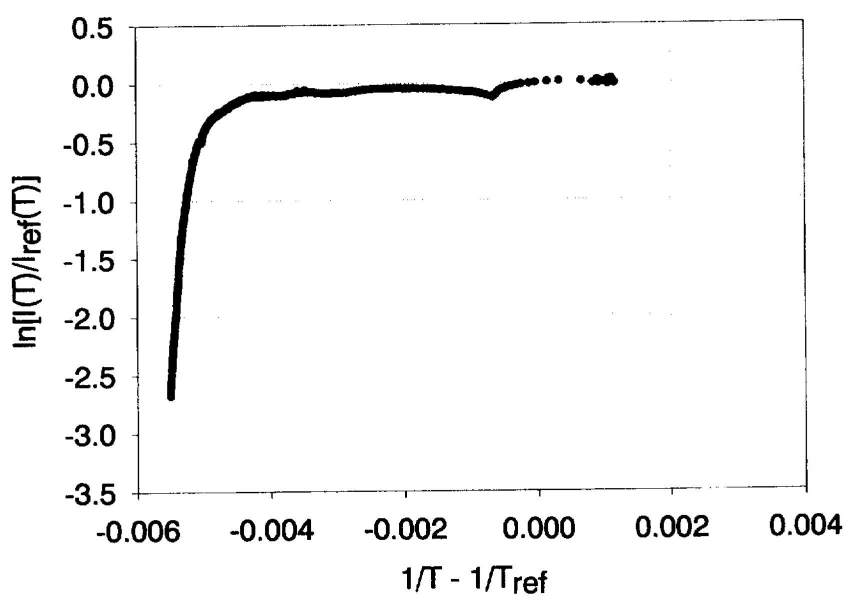
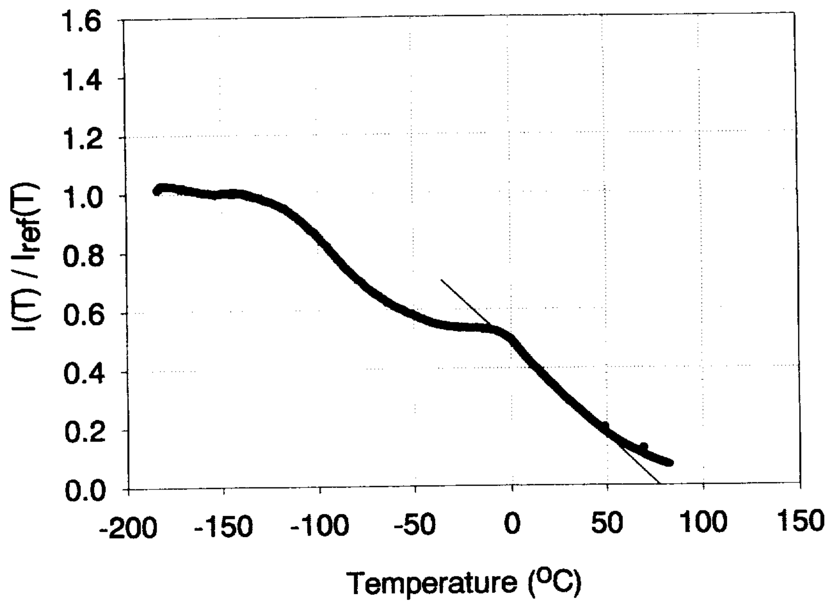


Figure A.2: PtPFPP in CC



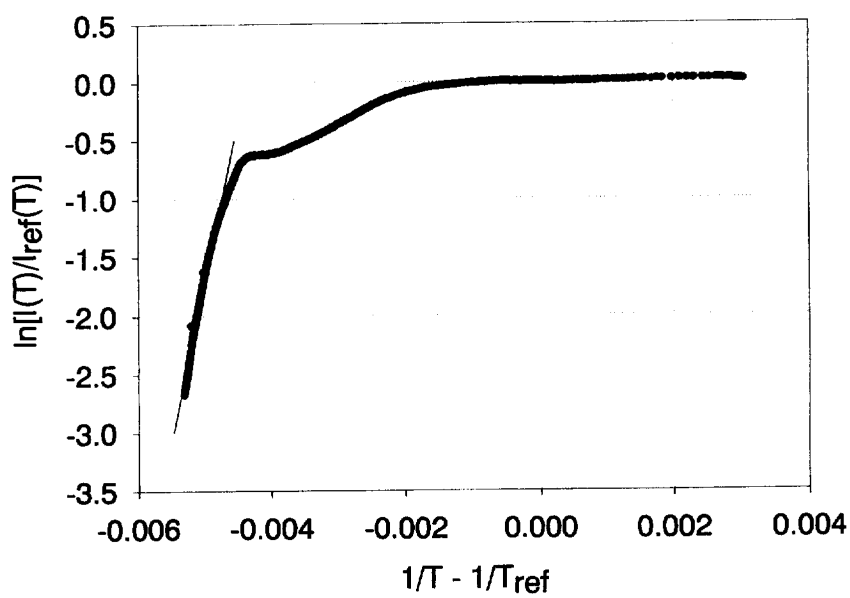
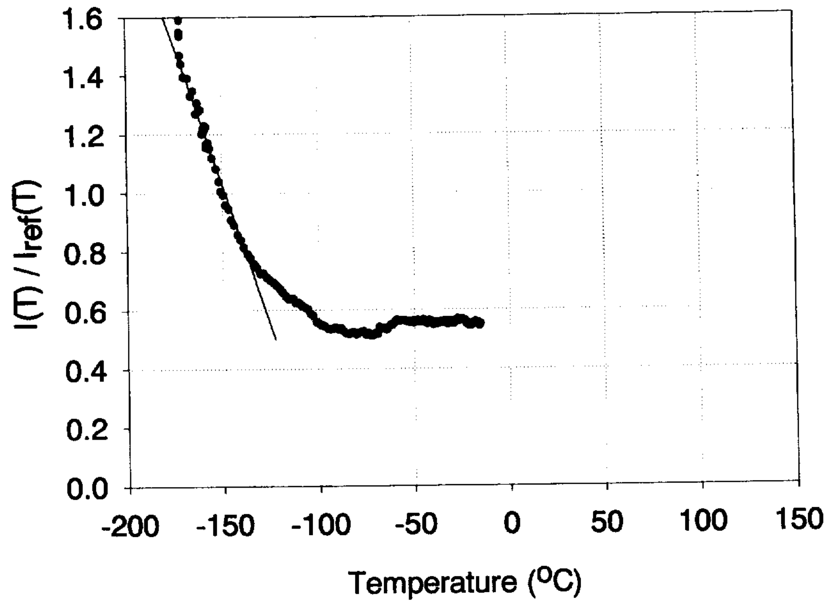


Figure A.3: PtPFPP in Polyurethane



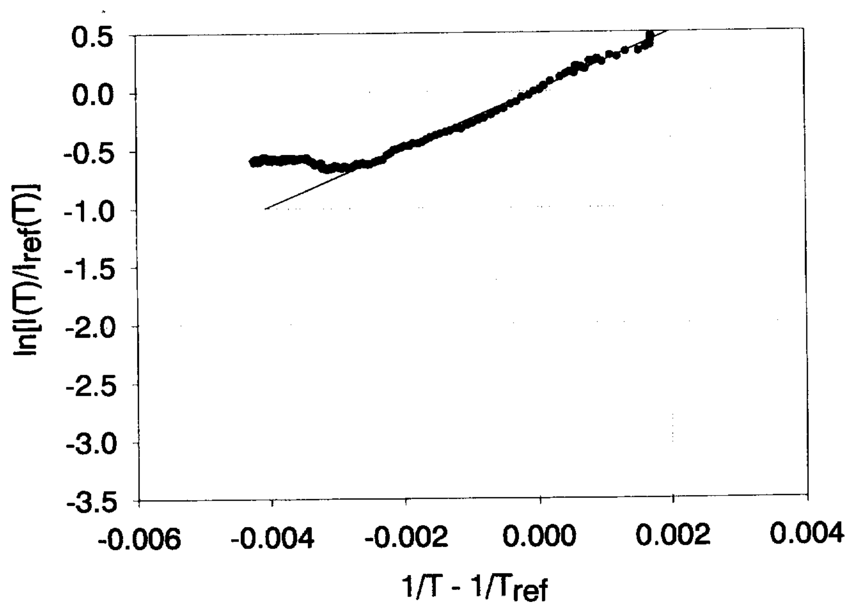


Figure A.4: $[Rh(bzq)_2Cl]_2$ in CC

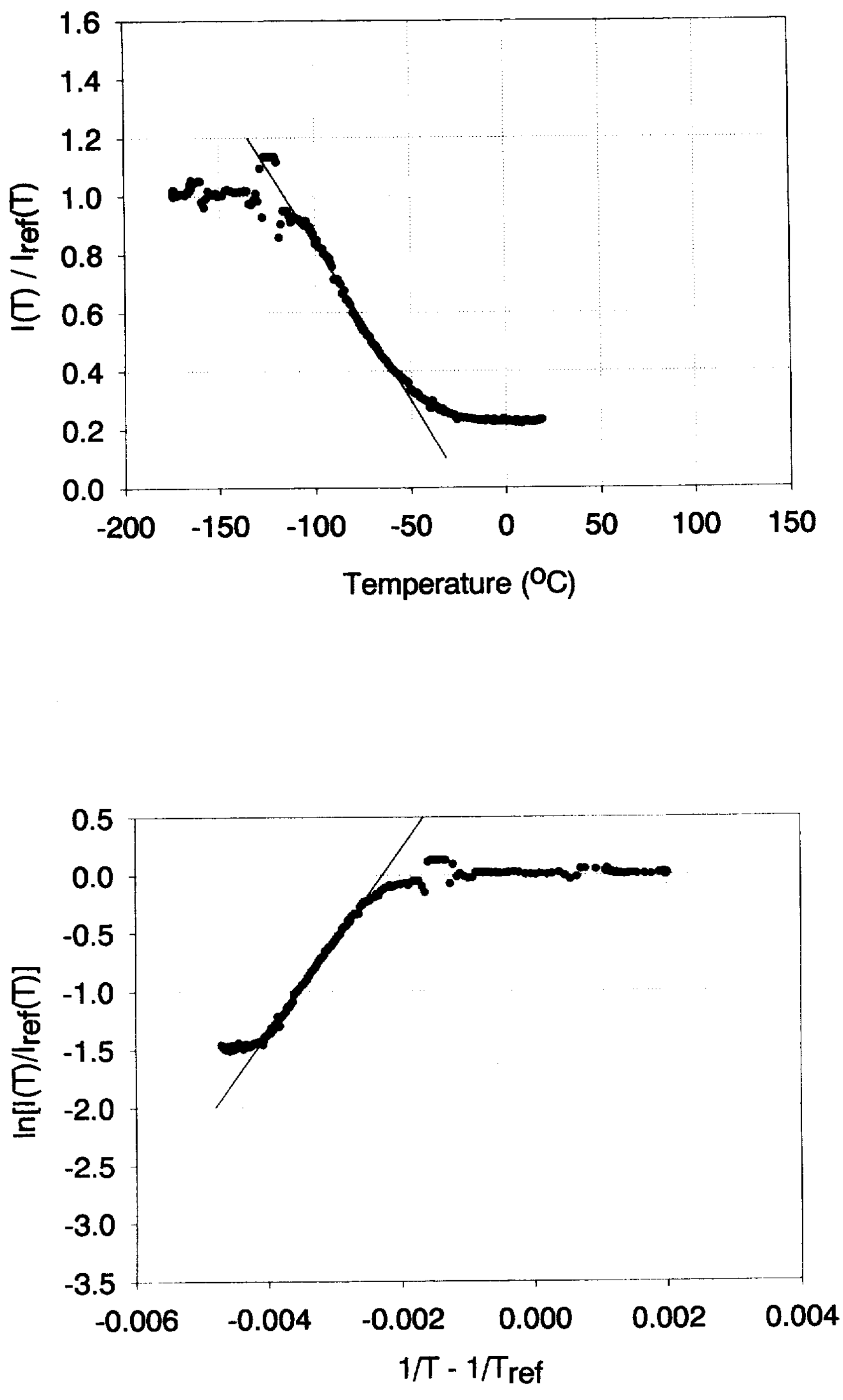
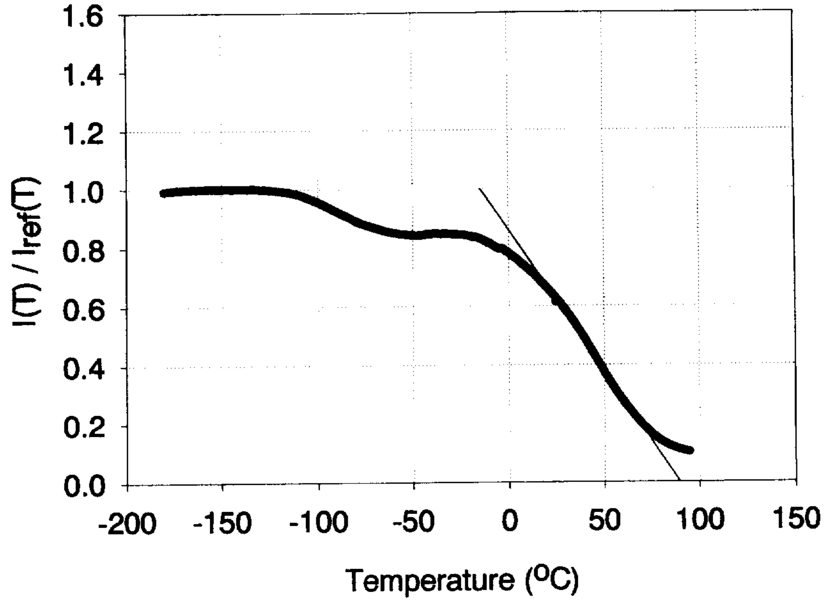


Figure A.5: $[Rh(bzq)_2(phen)](PF_6)$ in CC



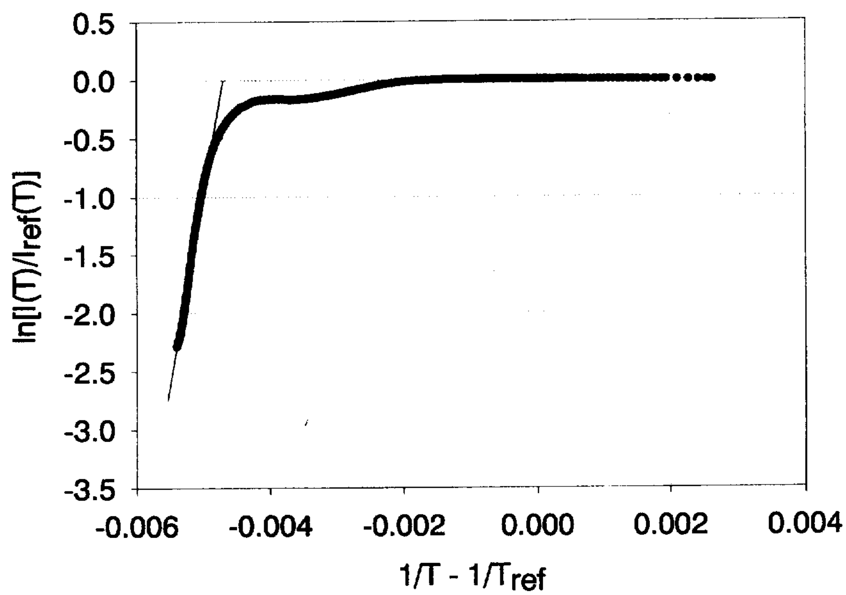


Figure A.6: $[Ru(bipy)_3](DS)_2$ in CC

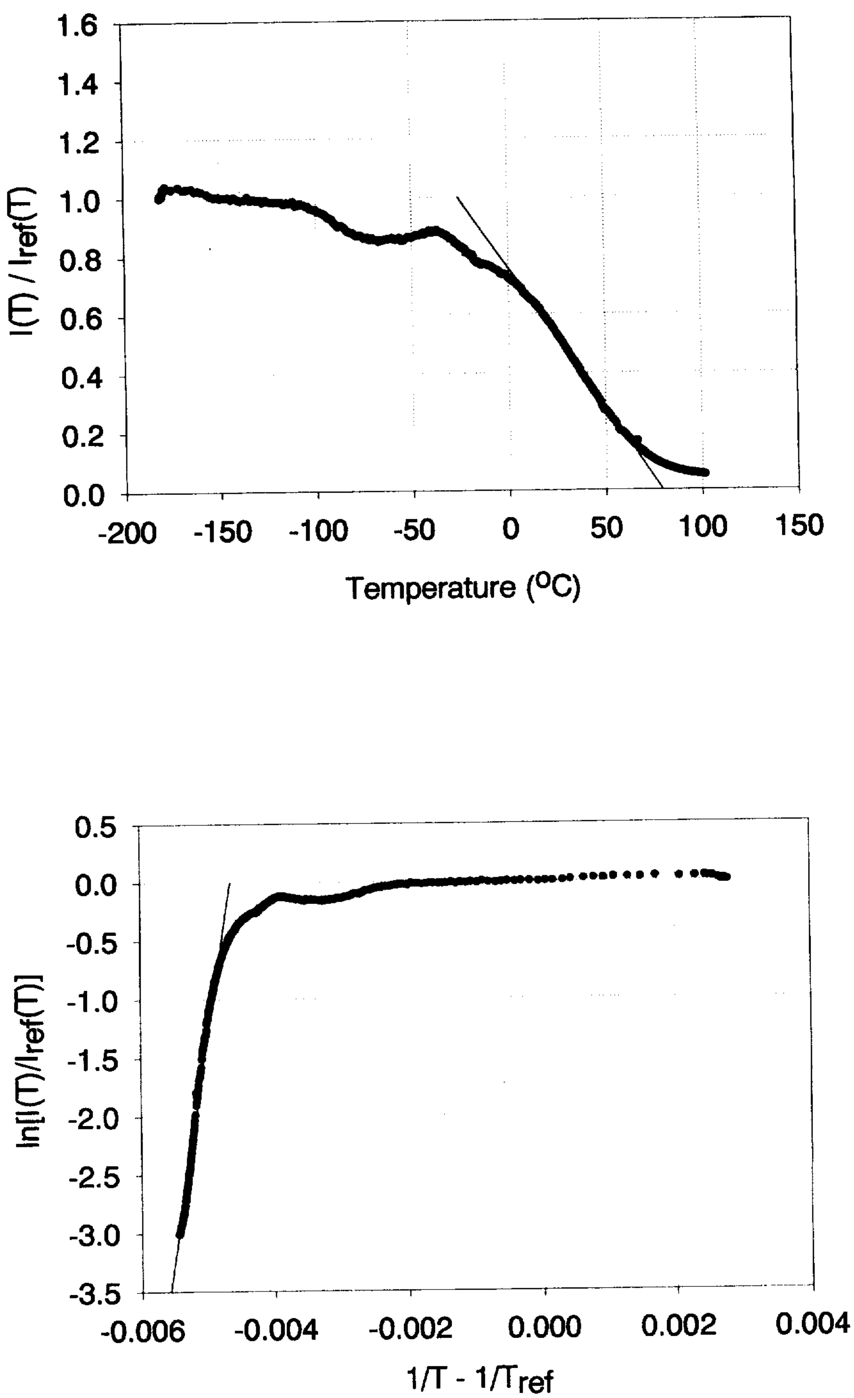
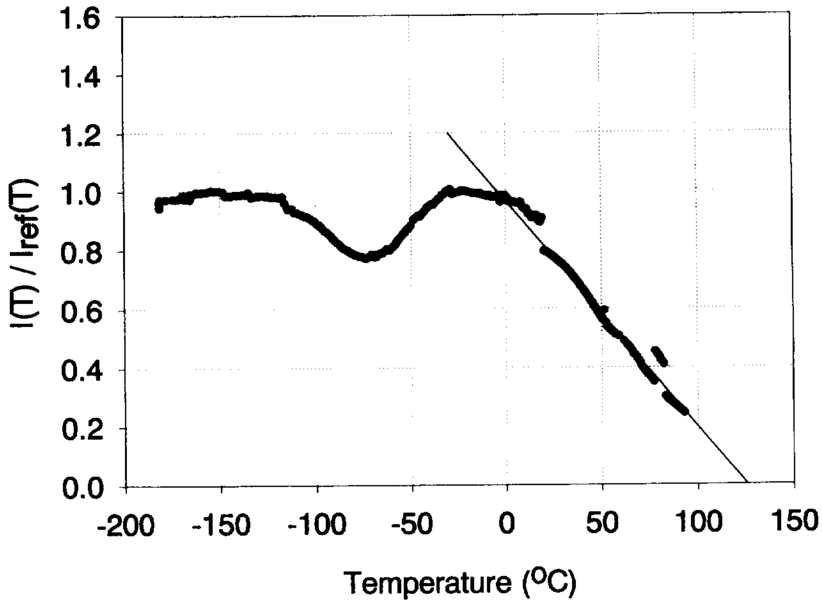


Figure A.7: $[Ru(bipy)_3](TFPB)_2$ in CC



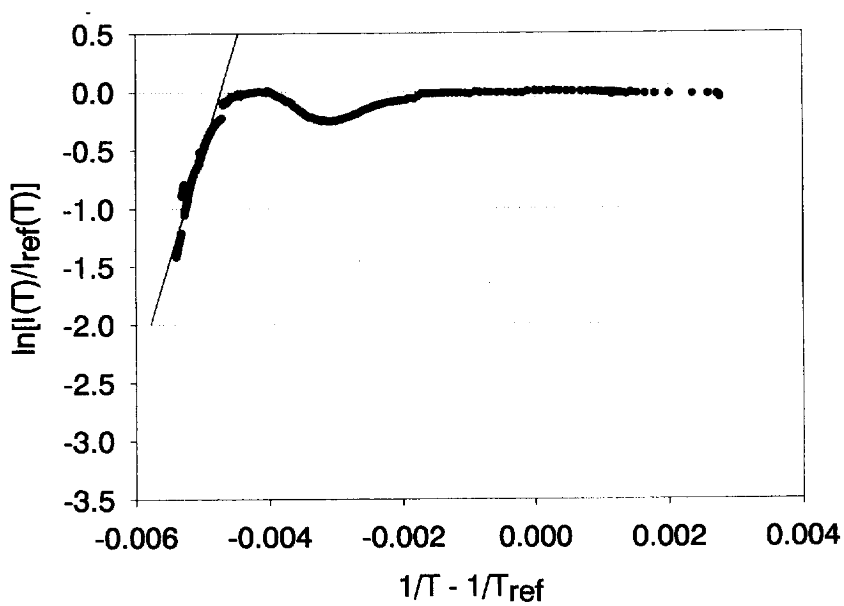
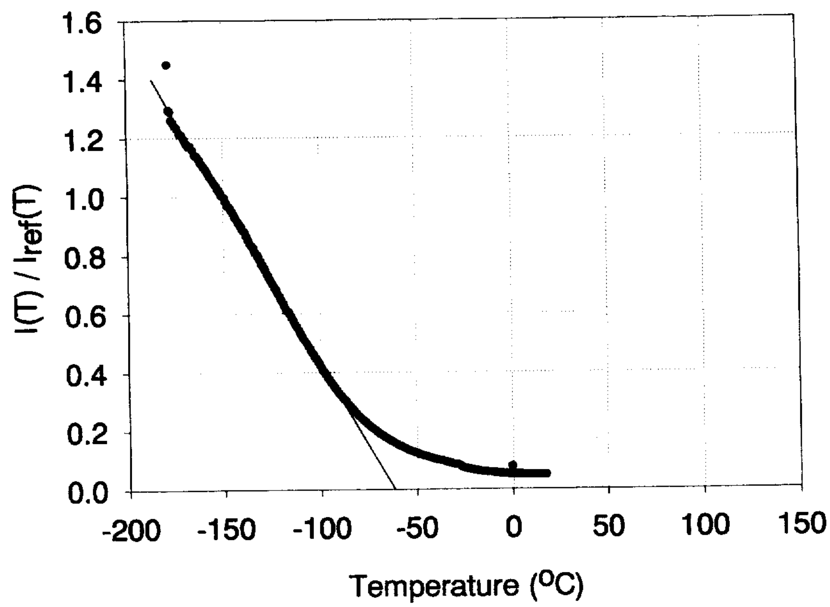


Figure A.8: $[Ru(ph_2\text{-}phen)_3](DS)_2$ in CC



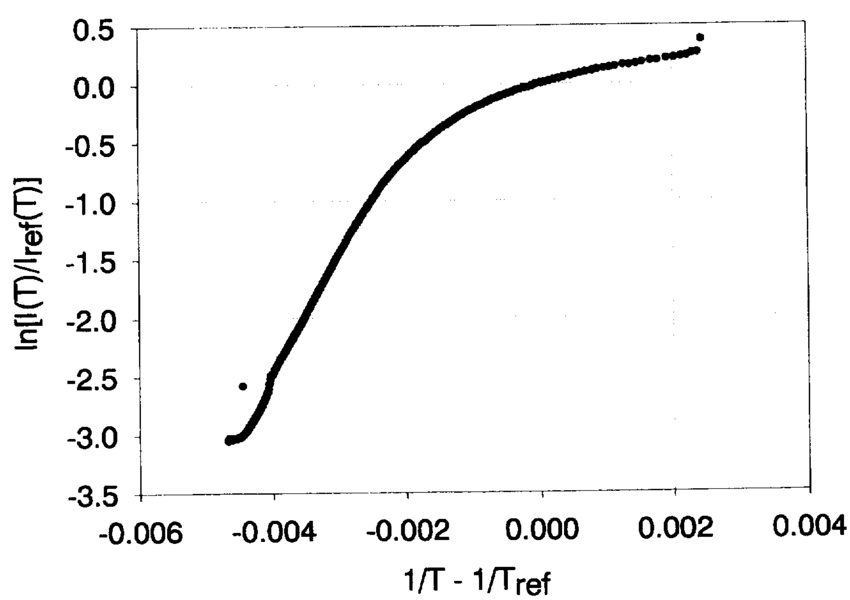


Figure A.9: [Ru(trpy)] in CC

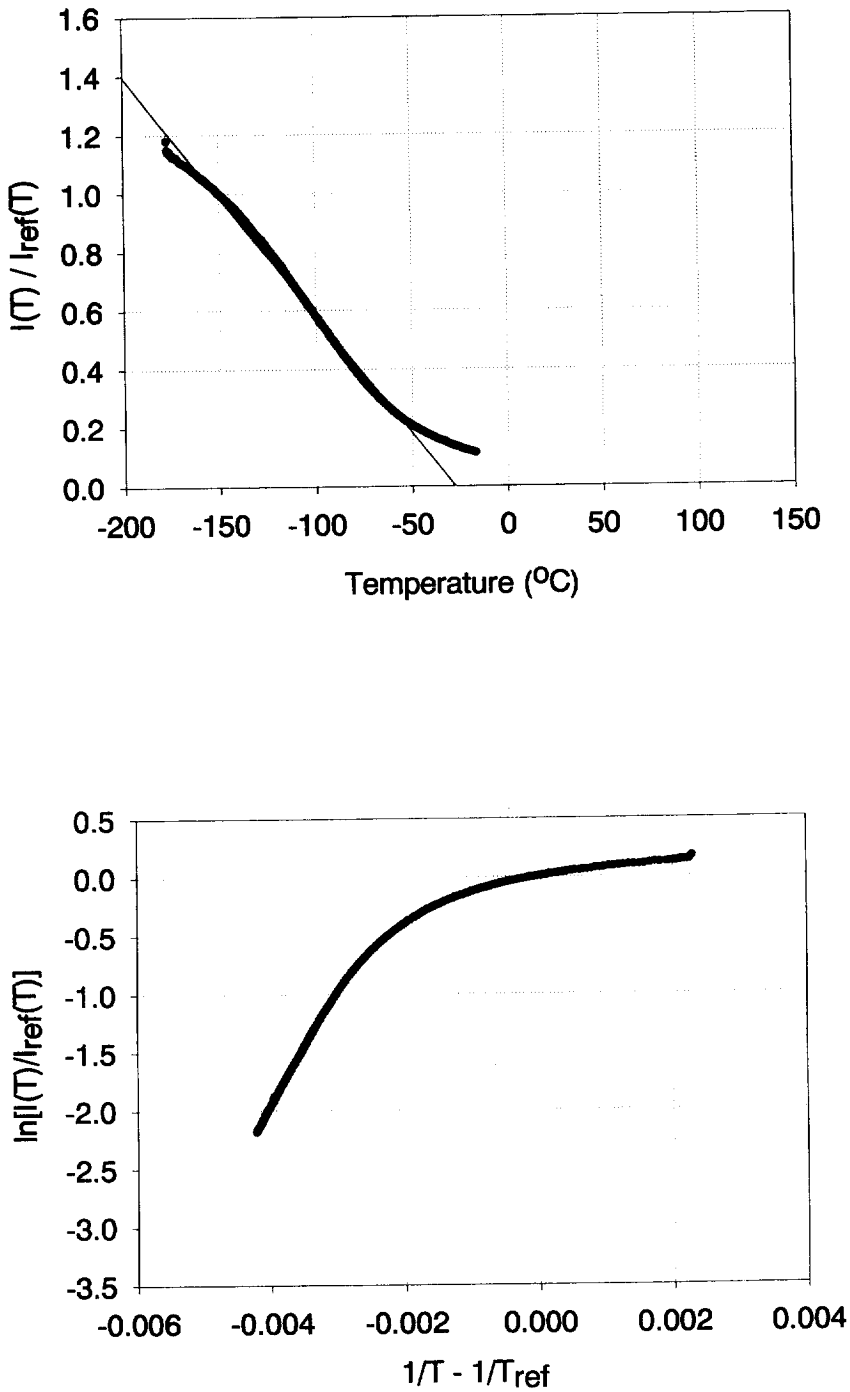
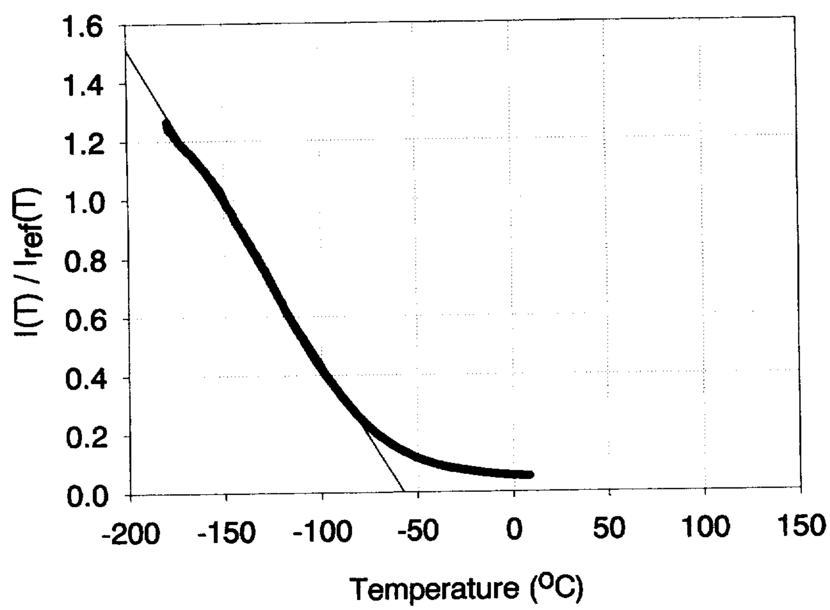


Figure A.10: $[Ru(trpy)(4'\text{-}C_6F_5\text{-}trpy)](NO_3)_2$ in CC



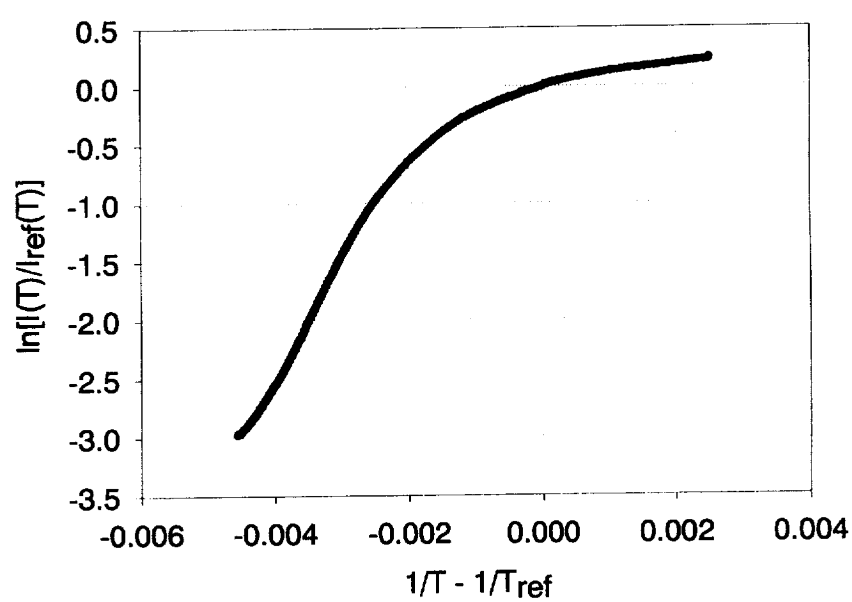
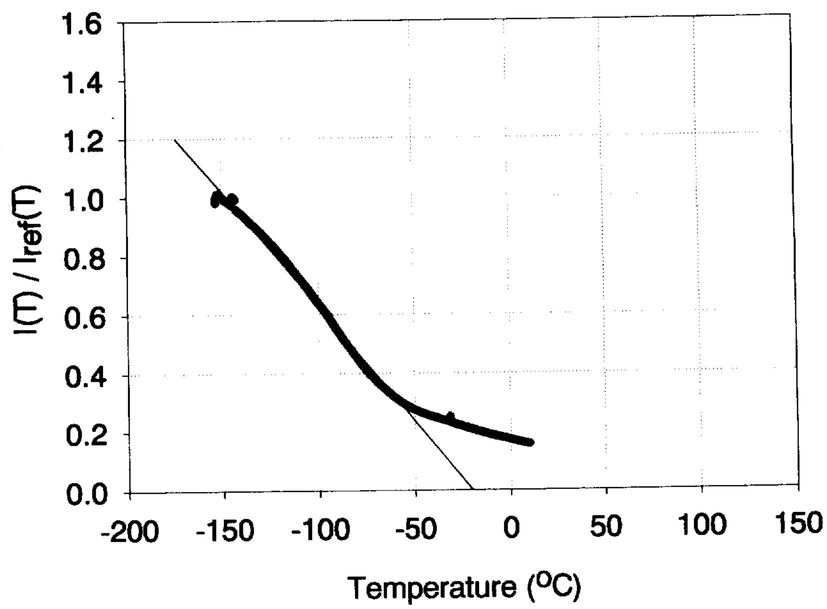


Figure A.11: [Ru(trpy)(4'-Cl-trpy)](Cl_2) in CC



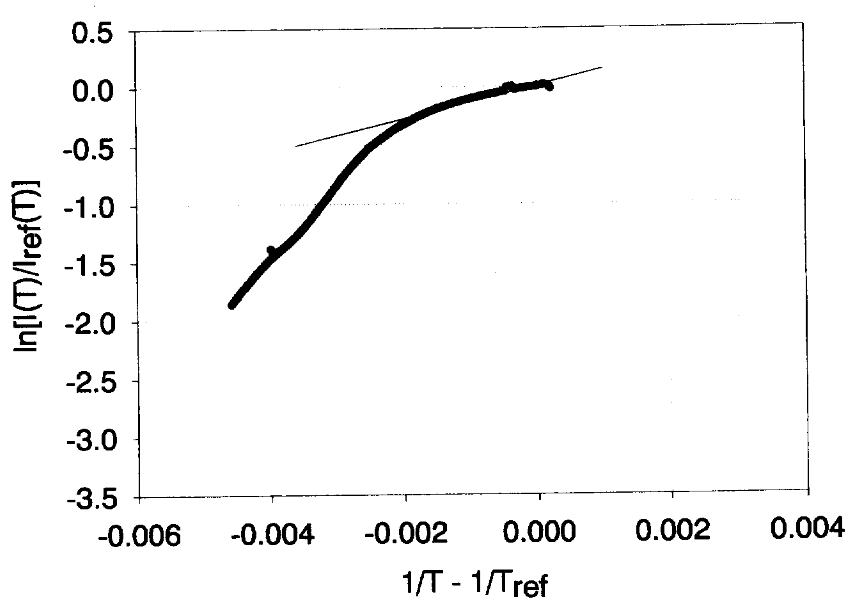
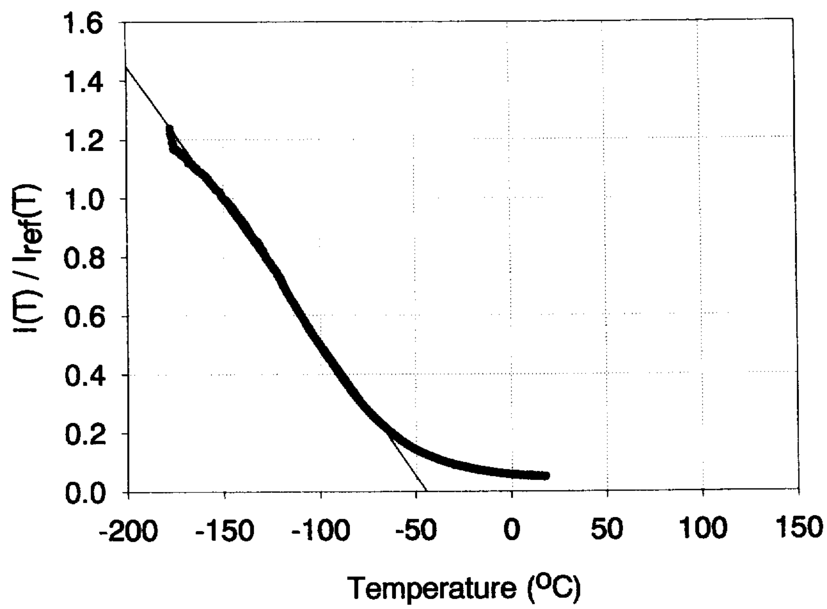


Figure A.12: $[Ru(trpy)(4'\text{-}NC\text{-}trpy)](NO_3)_2$ in CC



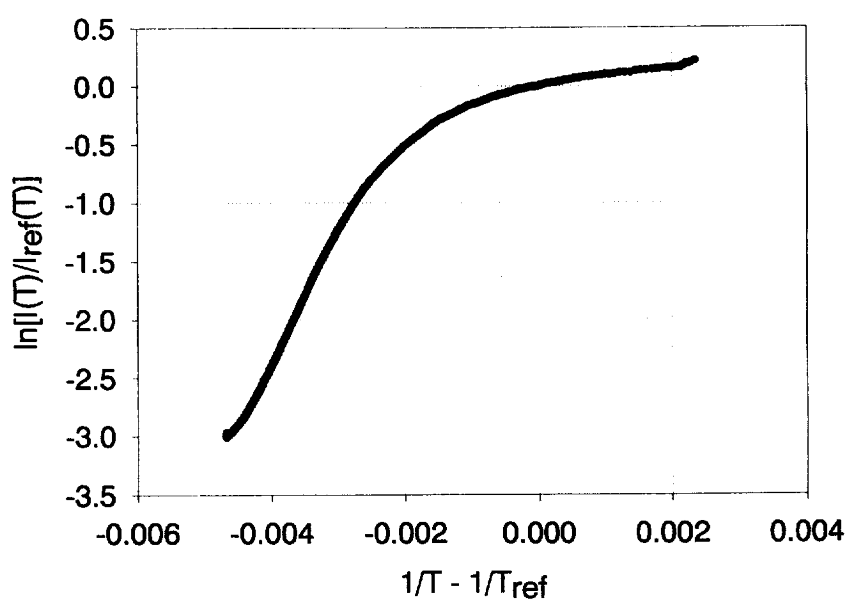


Figure A.13: [Ru(phtrpy)(Cltrpy)]$(NO_3)_2$ in CC

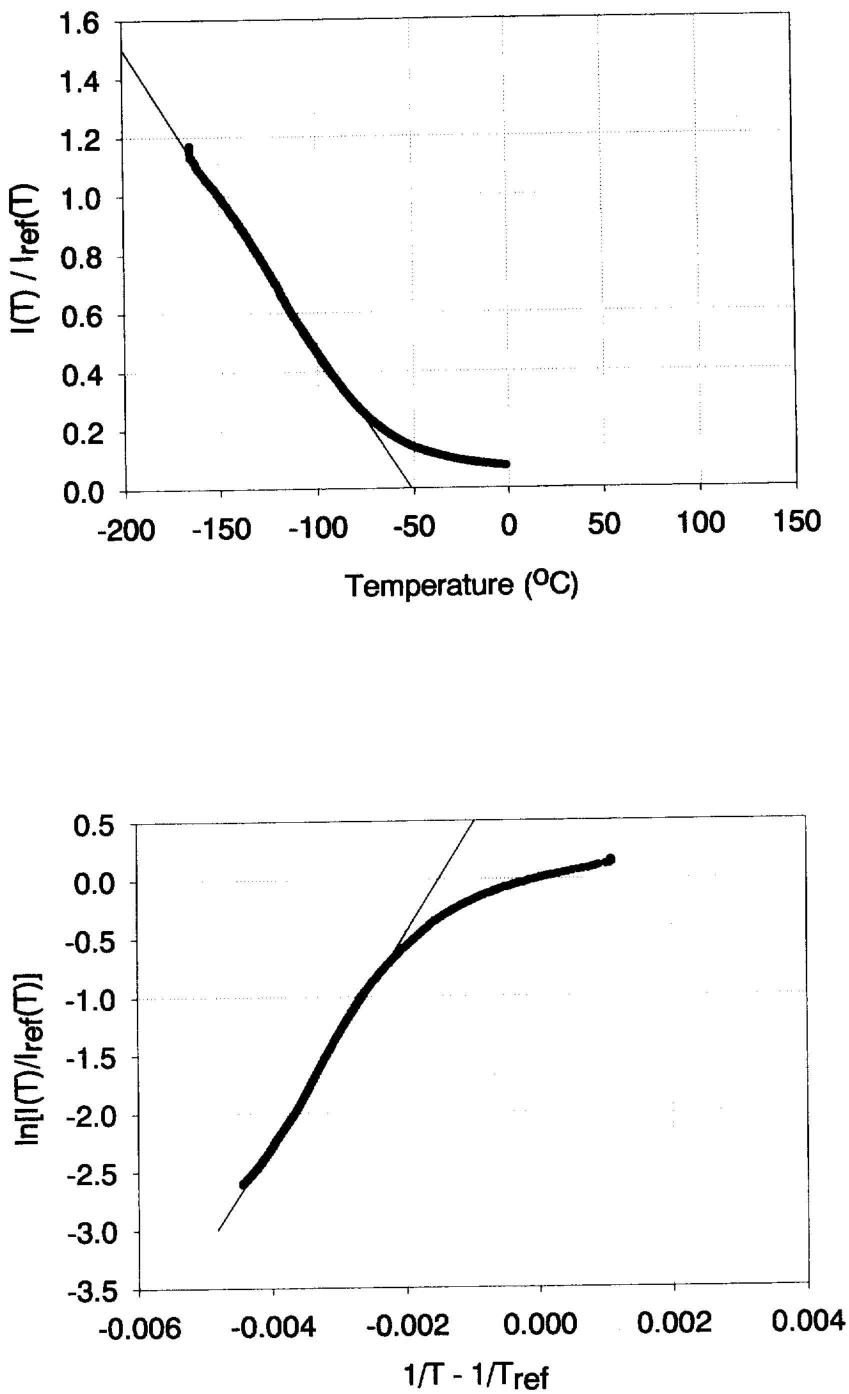
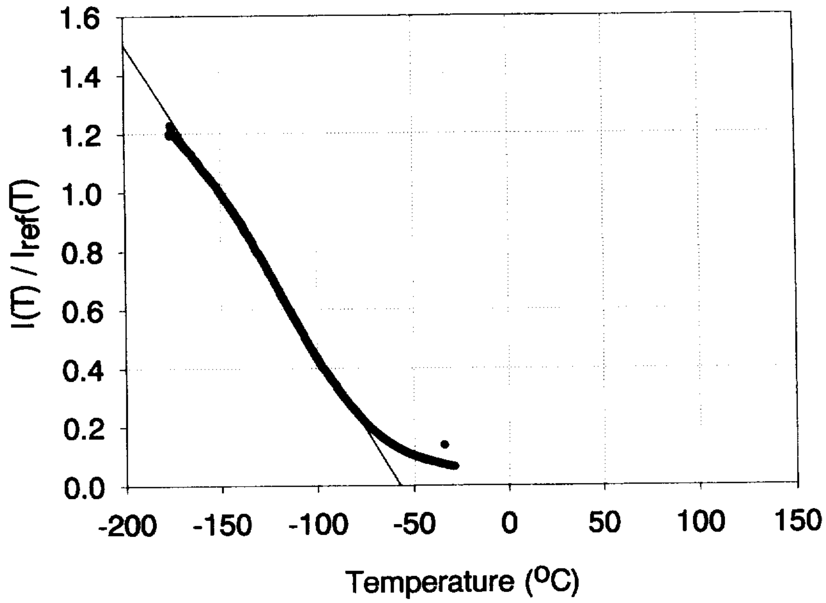


Figure A.14: $[Ru(trpy)(4'\text{-}TfO\text{-}trpy)](NO_3)_2$ in CC



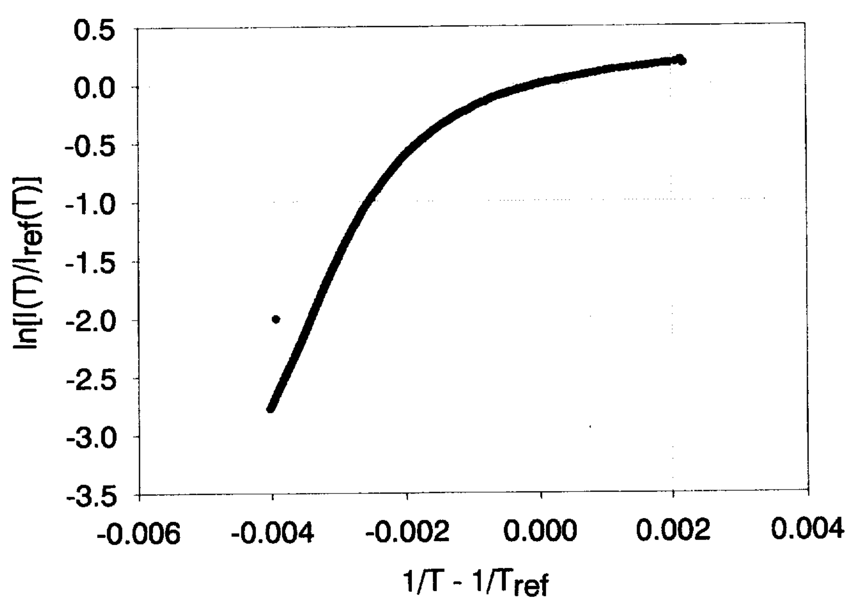
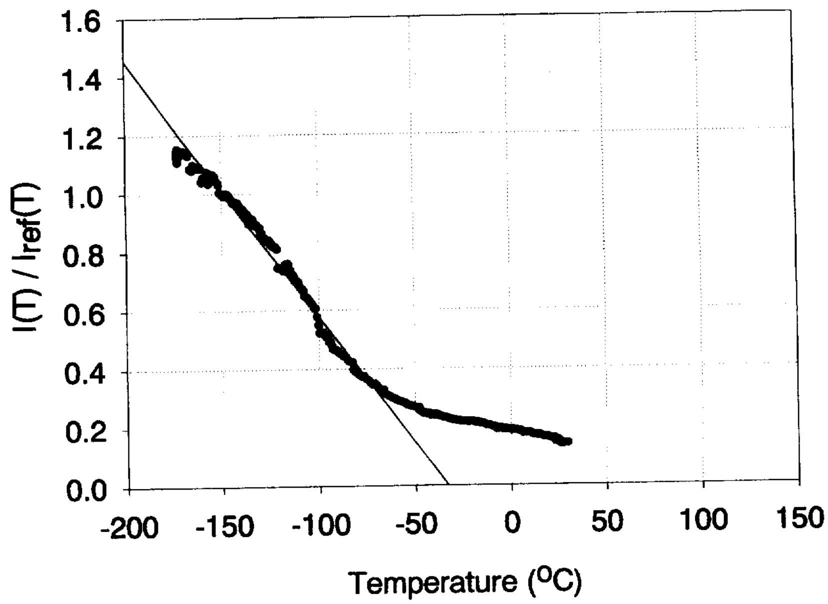


Figure A.15: $[Ru(trpy)(MeStrpy)](NO_3)_2$ in CC



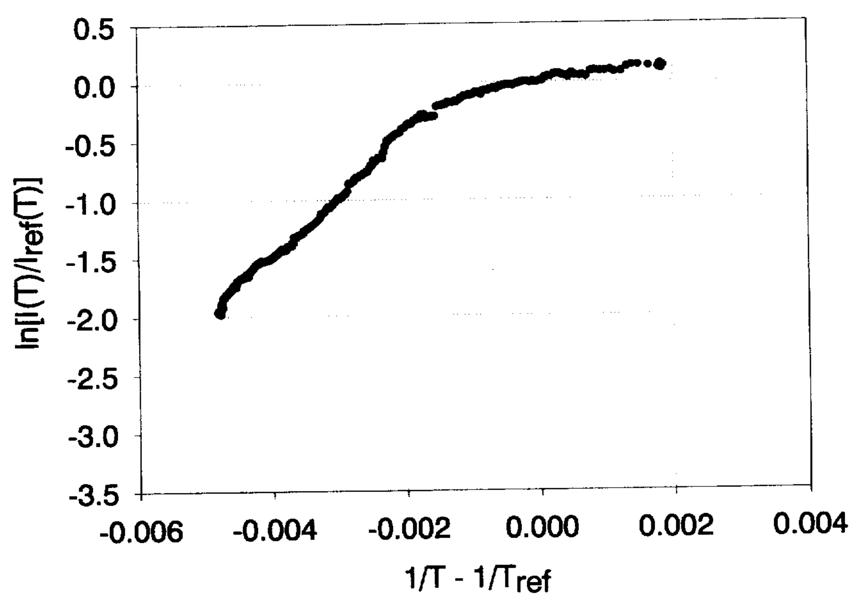
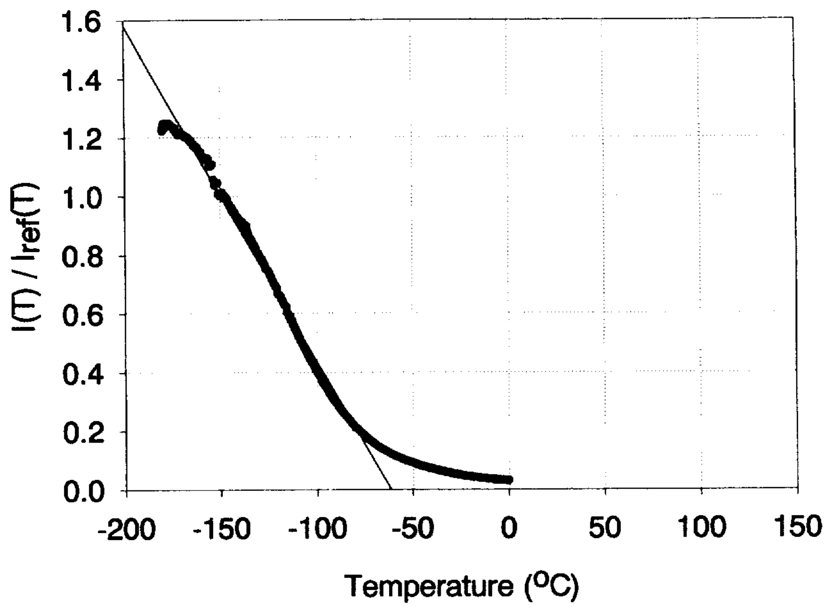


Figure A.16: [Ru(trpy$_2$)(NO$_2$(Phtrpy)](PF$_6$) in CC



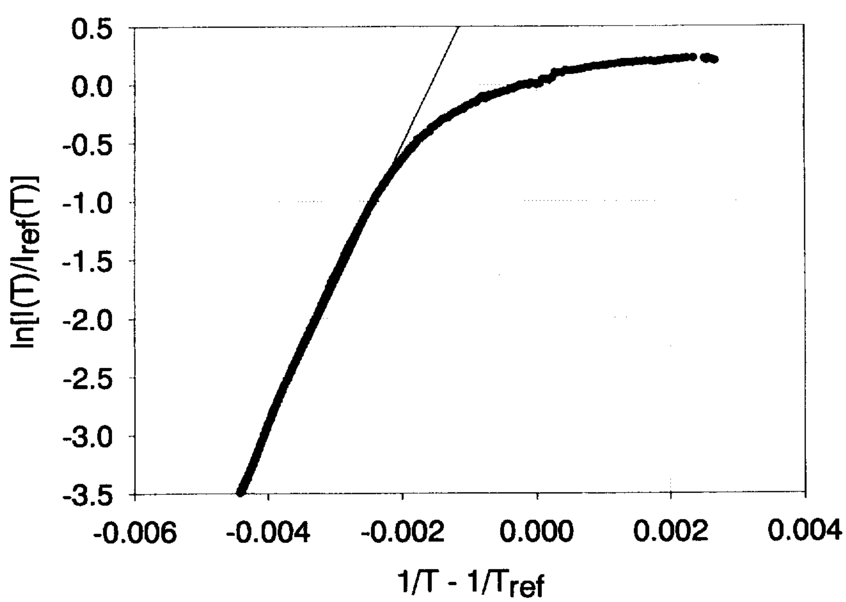
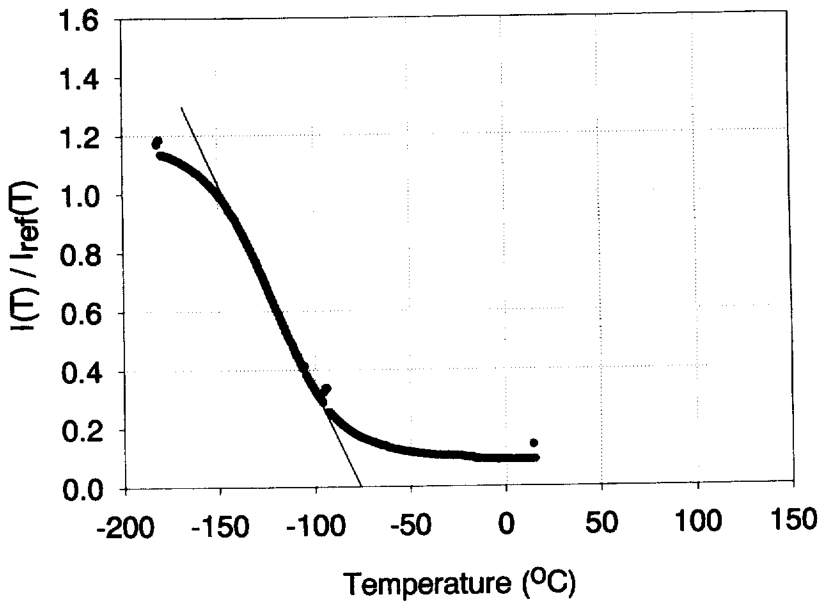


Figure A.17: $[Ru(trpy)(phtrpy)](PF_6)_2$ in GP-197



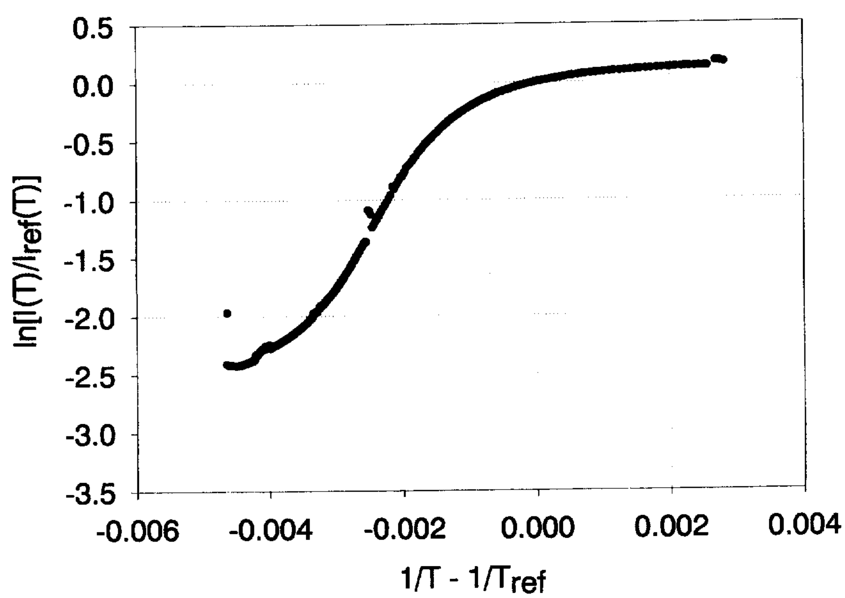
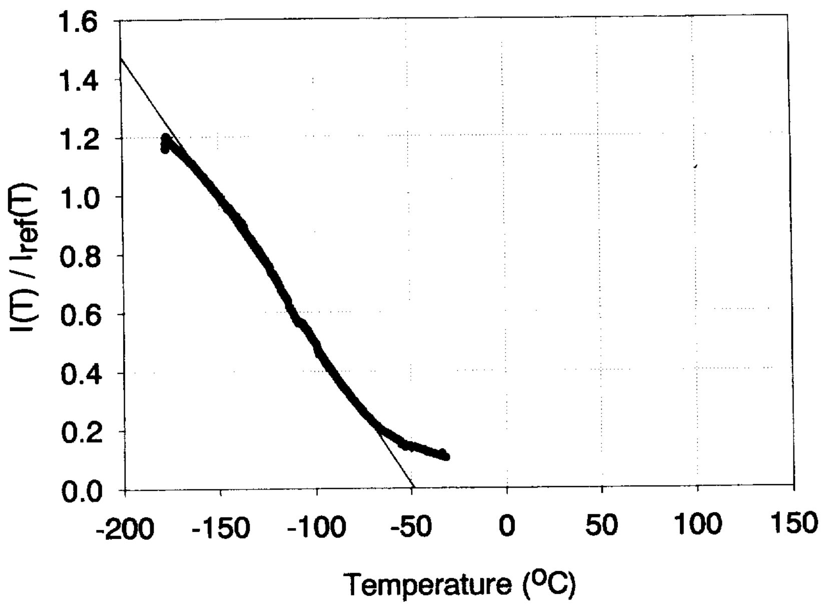


Figure A.18: $[Ru(trpy)(phtrpy)](PF_6)_2$ in CC



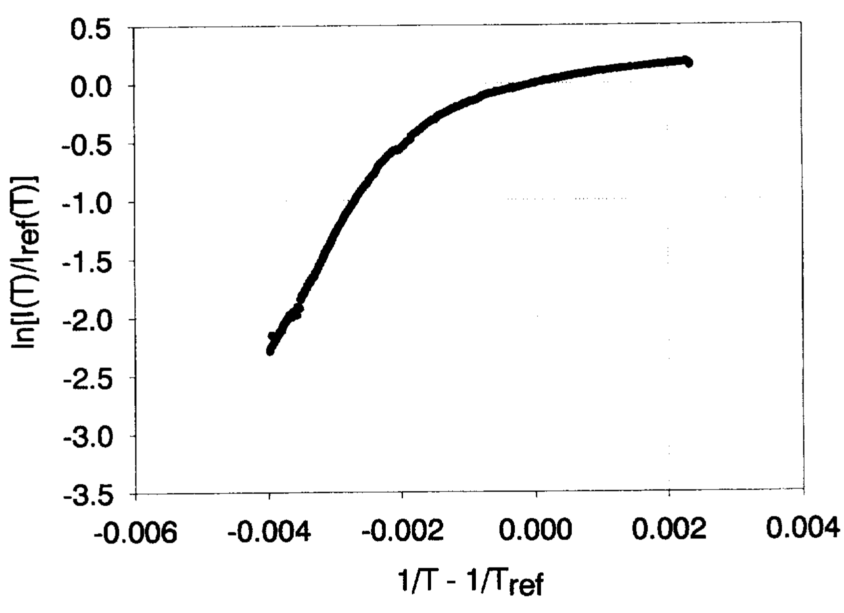
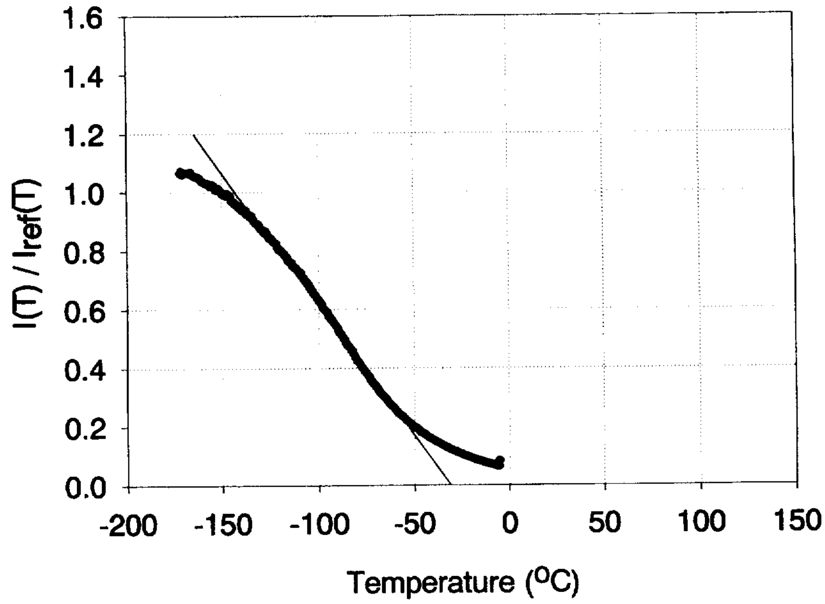


Figure A.19: $[Ru(trpy)(ppd\text{-}trpy)](TFPB)_2$ in CC



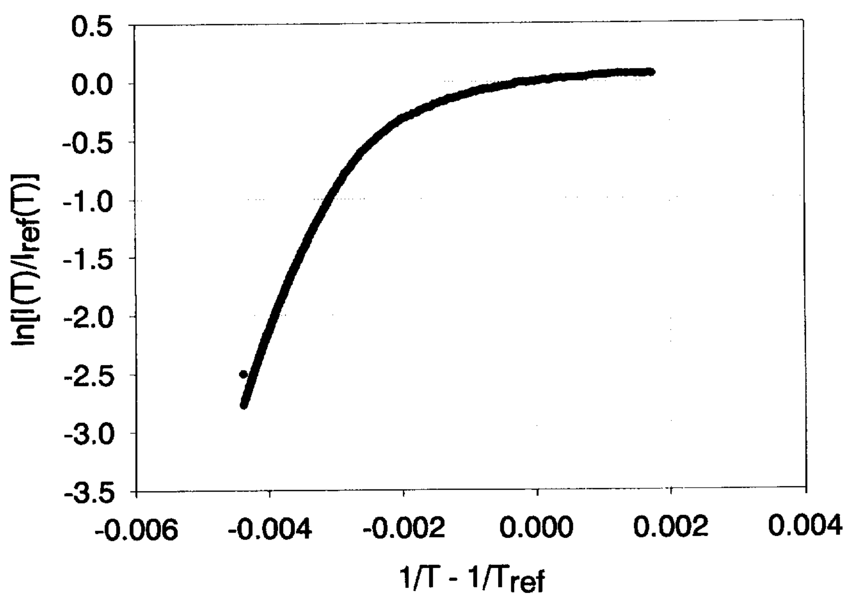
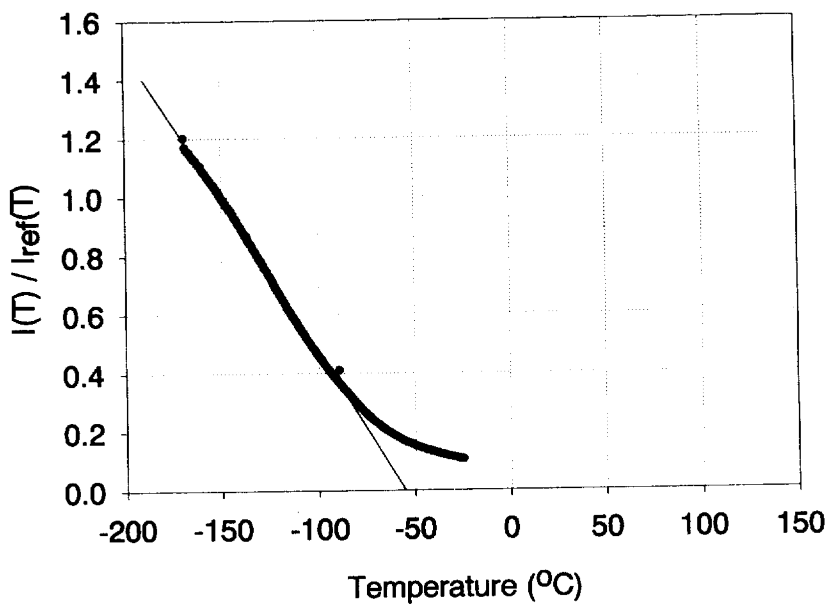


Figure A.20: $[Ru(trpy)(phyphen)](TFPB)_2$ in CC



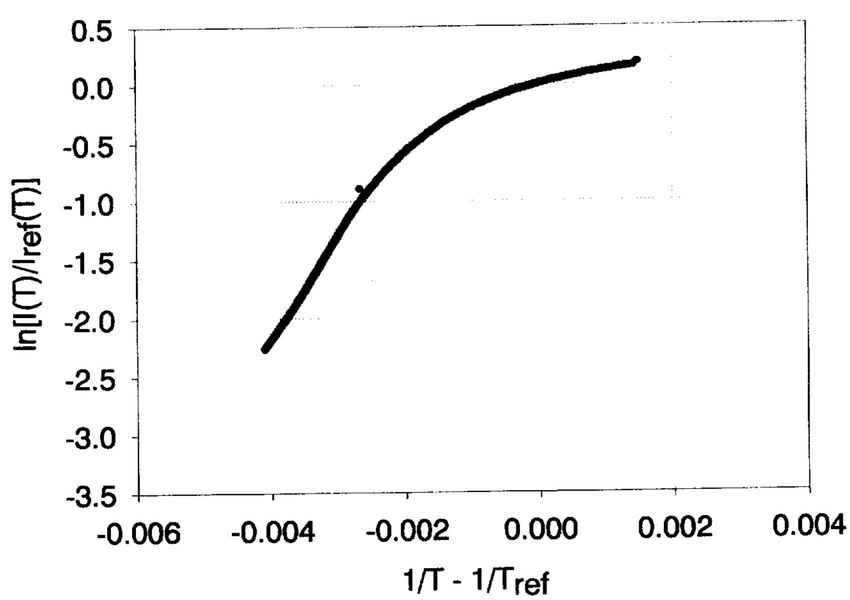


Figure A.21: [Ru(trpy)(SO_2Me-trpy)](PF_6)$_2$ in CC

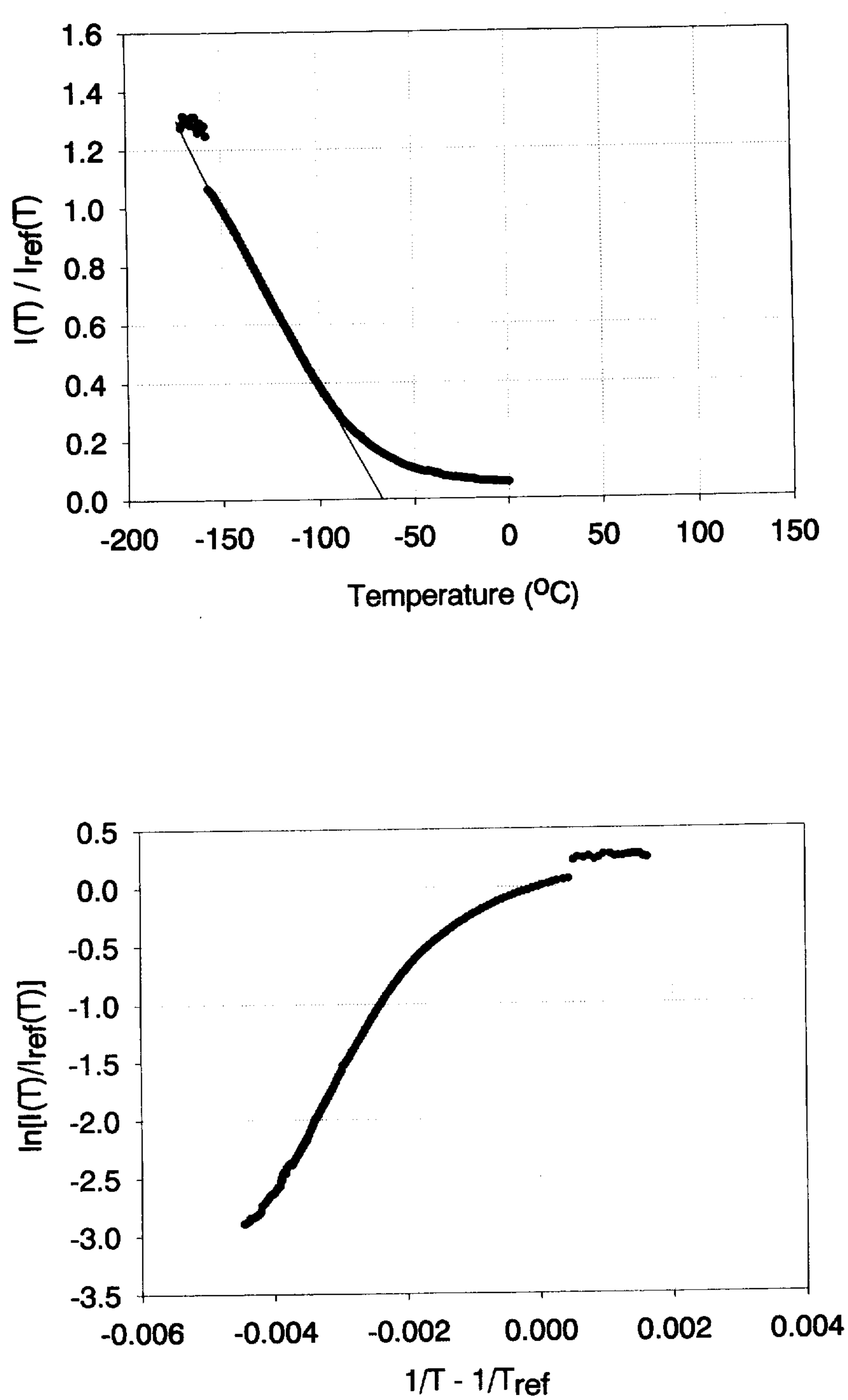
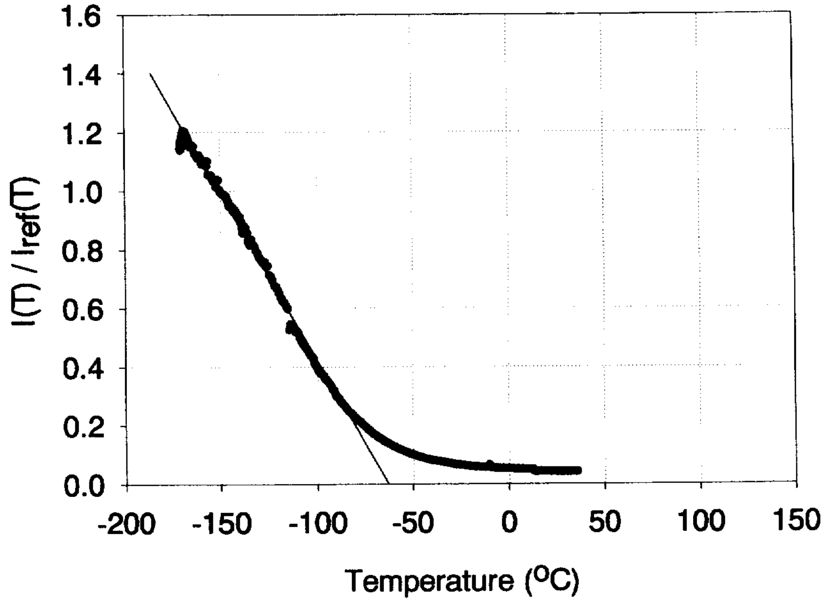


Figure A.22: $[Ru(trpy)_2](DS)_2$ in CC



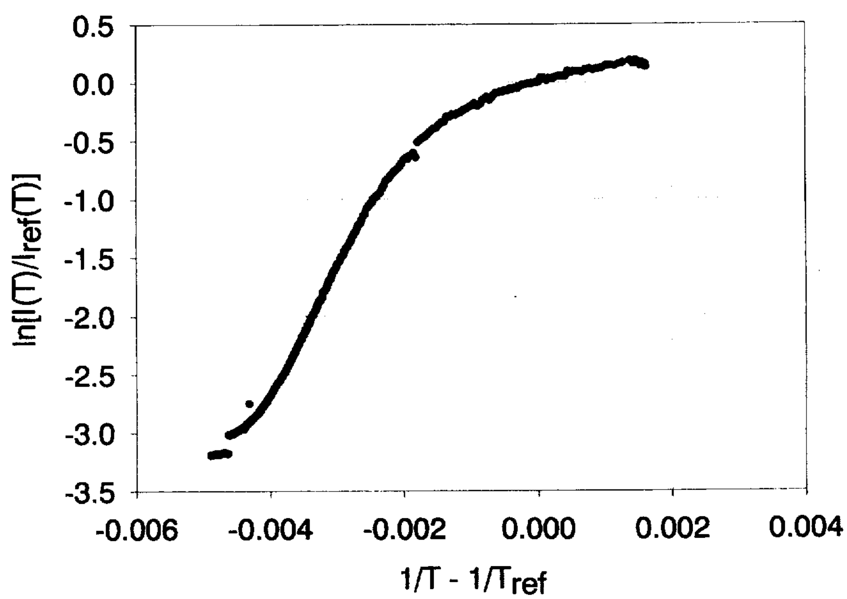
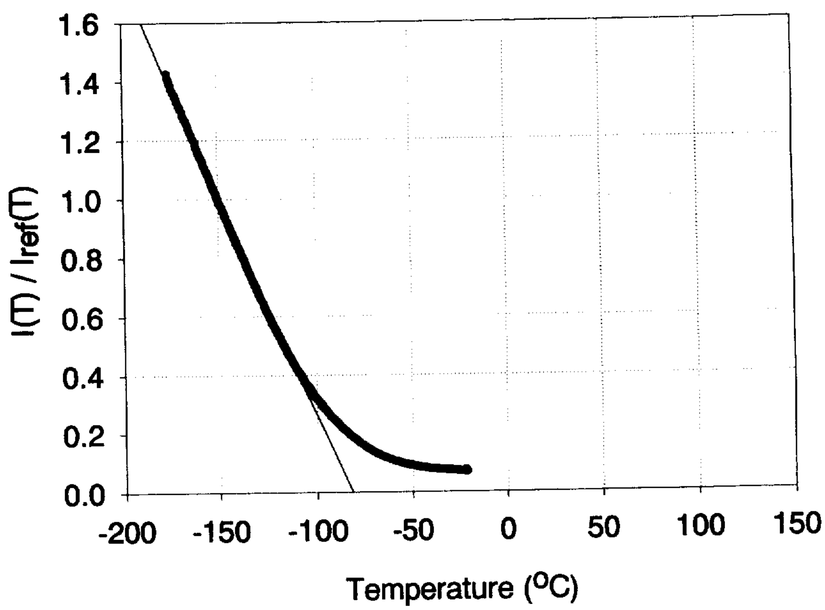


Figure A.23: [Ru(trpy$_2$)](TFPB)$_2$ in CC



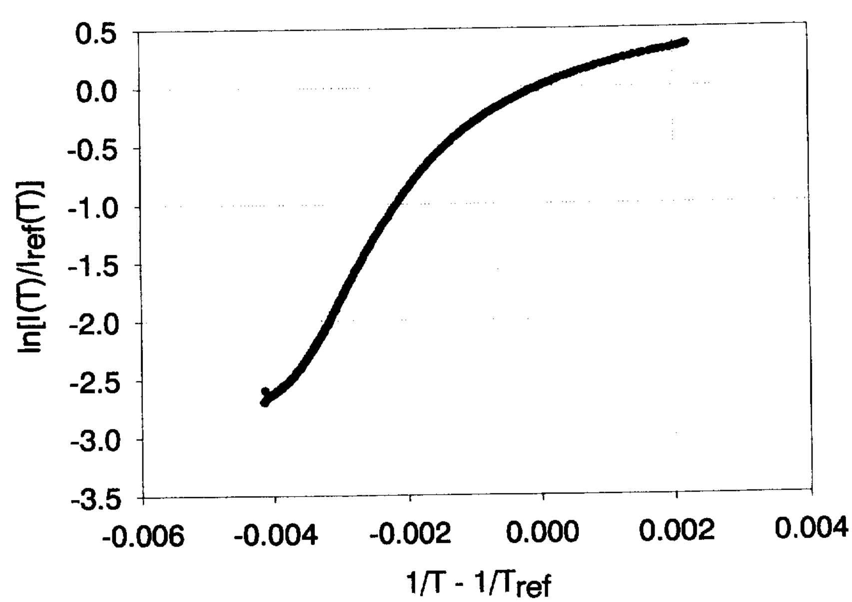
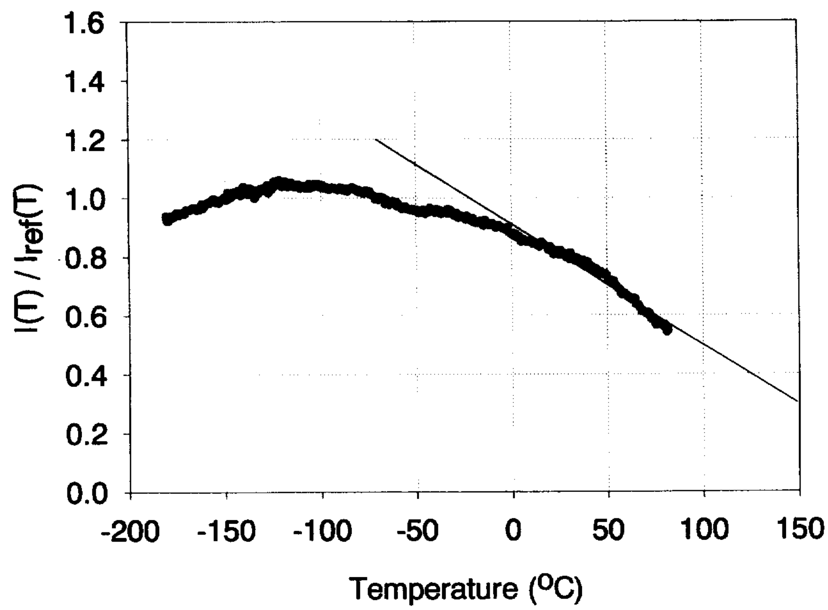


Figure A.24: $[Ru(ppd\text{-}trpy)_2](TFPB)_2$ in CC



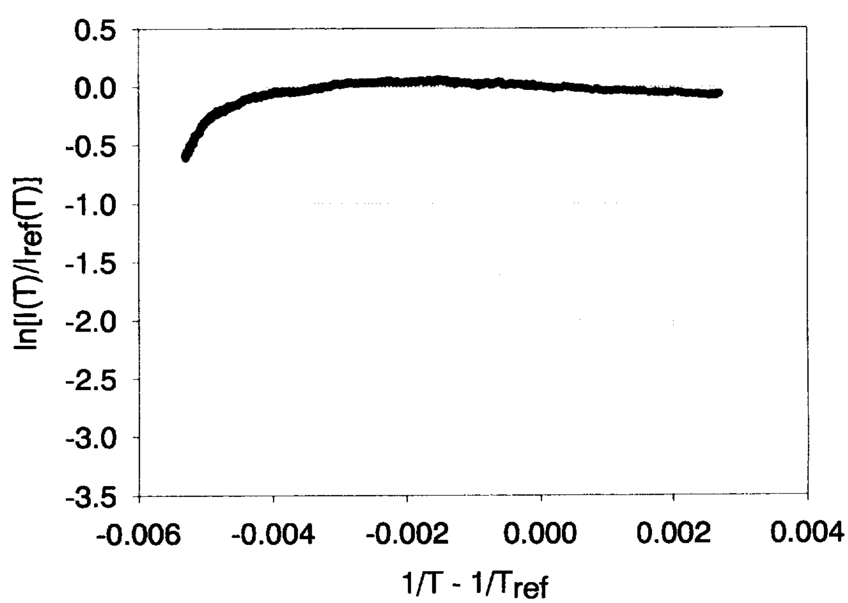
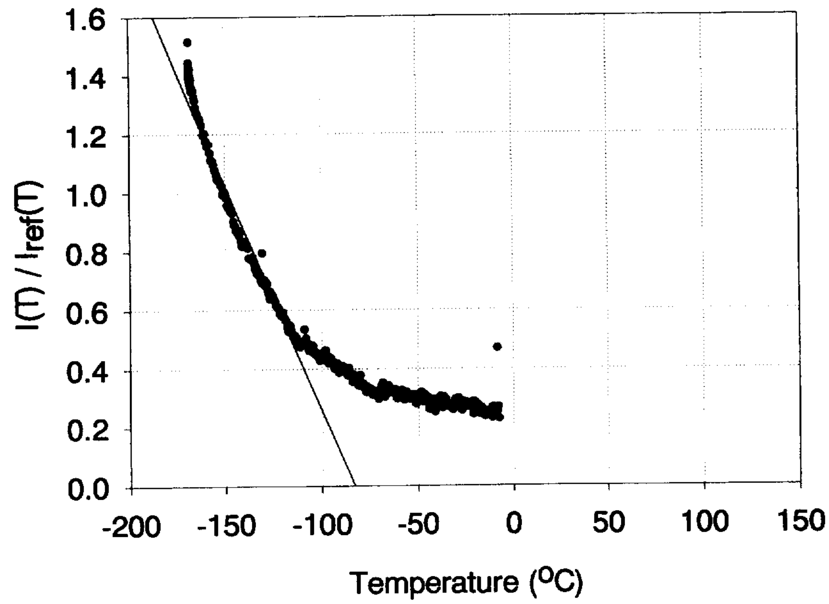


Figure A.25: $[Os(trpy)_2](PF_6)_2$ in CC



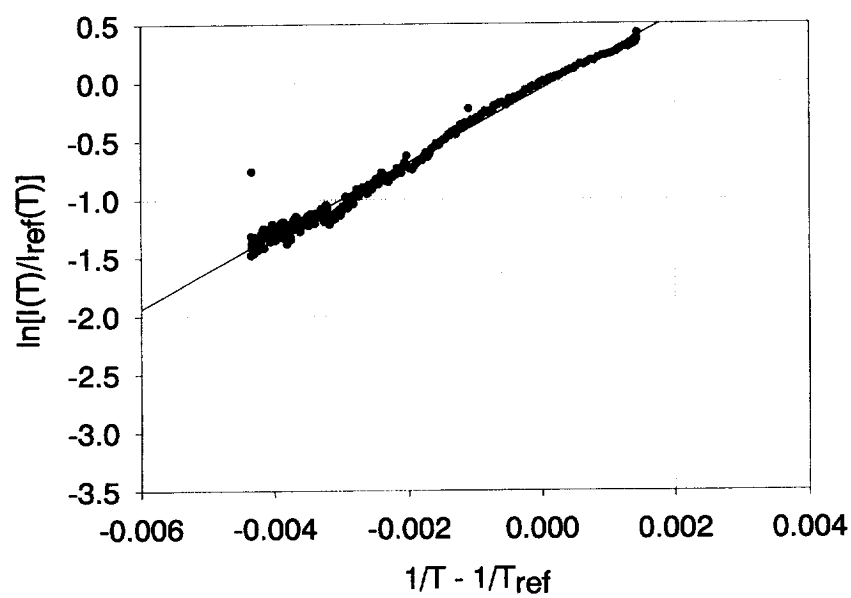


Figure A.26: $[Ru(trpy)(Vh127)](PF_6)_2$ in GP-197

APPENDIX B: ADDITIONAL PRESSURE CALIBRATION DATA

This appendix is a compilation of cryogenic pressure-sensitive paint calibration data. Data is presented in Stern-Volmer form. In all room temperature cases, reference conditions are taken at a static pressure of 14.7 psi with air as the test gas. All cryogenic data is normalized to reference conditions at O_2 partial pressure of 14.0 Pa.

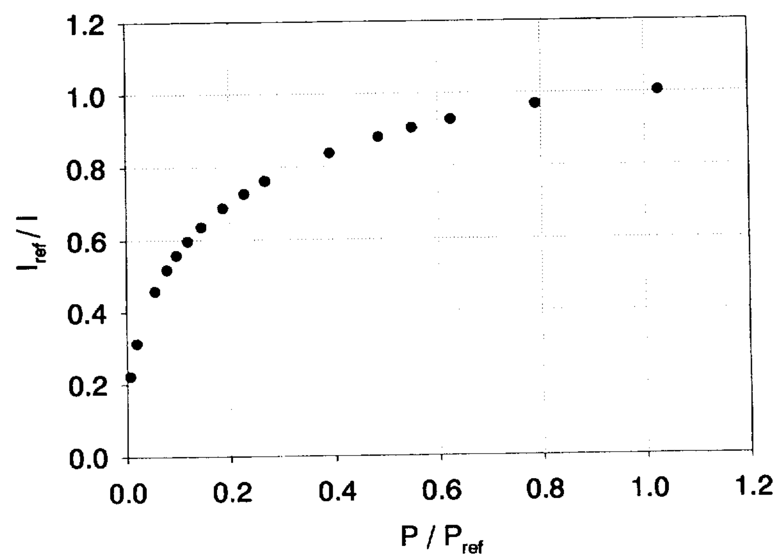


Figure B.1: Stern-Volmer for [Ru(ph$_2$-phen)$_3$] on Anodized Aluminum – 25 °C

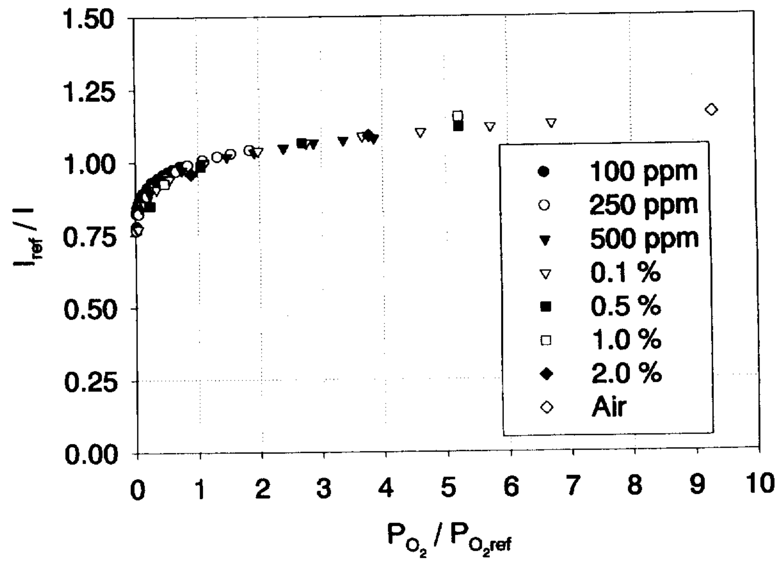


Figure B.2: [Ru(ph$_2$-phen)$_3$] on Anodized Aluminum – 150 K

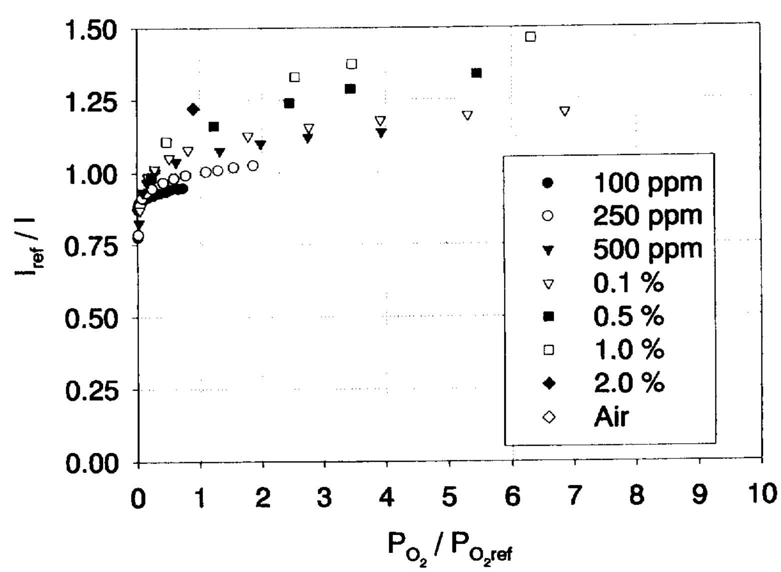


Figure B.3: [Ru(ph$_2$-phen)$_3$] on Anodized Aluminum – 100 K

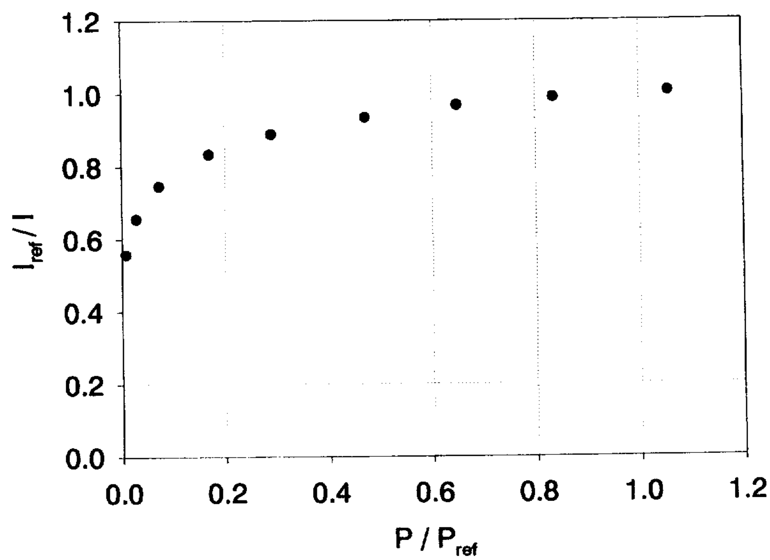


Figure B.4: Stern-Volmer for [Ru(ph$_2$-phen)$_3$] on Anodized 2024 Al Alloy – 25 °C

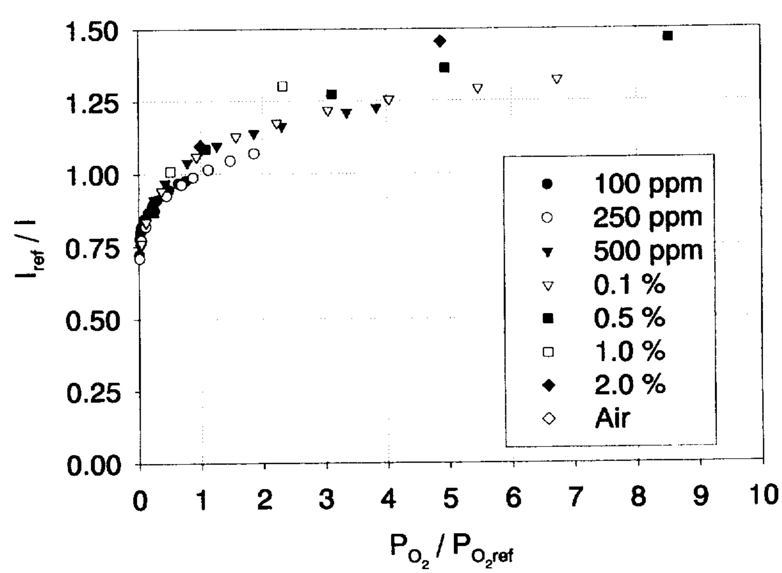


Figure B.5: [Ru(ph$_2$-phen)$_3$] on Anodized 2024 Al Alloy – 150 K

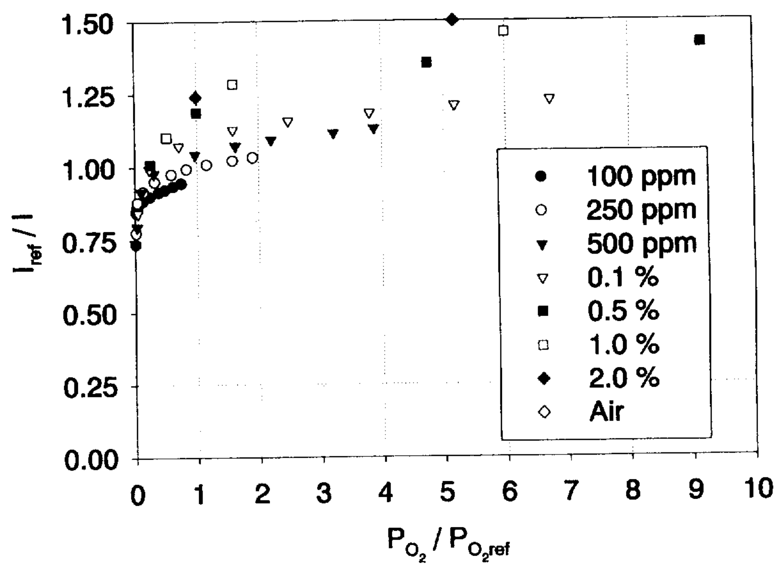


Figure B.6: [Ru(ph$_2$-phen)$_3$] on Anodized 2024 Al Alloy – 100 K

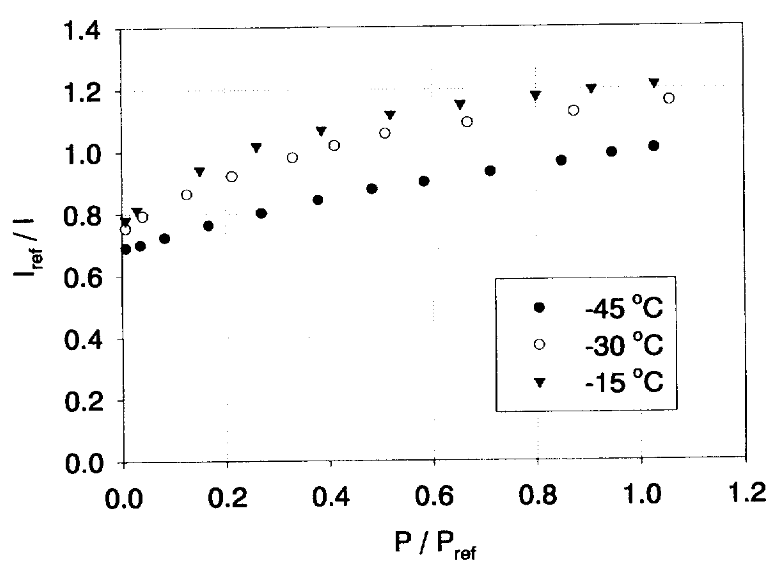


Figure B.7: Matrix Calibration for [Ru(ph$_2$-phen)$_3$] in RTV

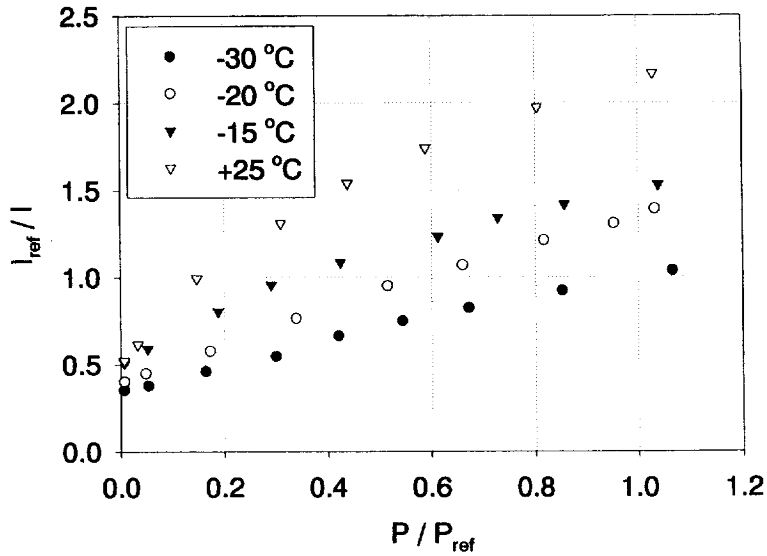


Figure B.8: Matrix Calibration for [Ru(ph$_2$-phen)$_3$] in RTV + 0.5 g Silica Gel

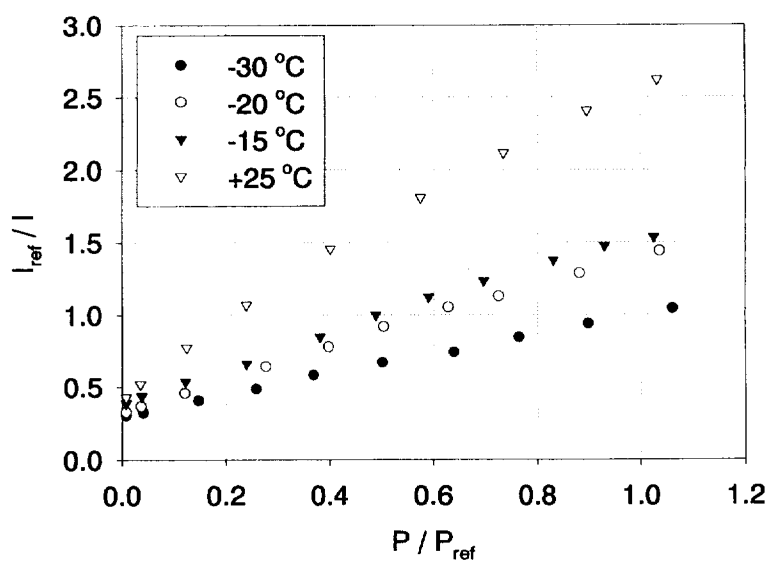


Figure B.9: Matrix Calibration for [Ru(ph$_2$-phen)$_3$] in RTV + 1.0 g Silica Gel

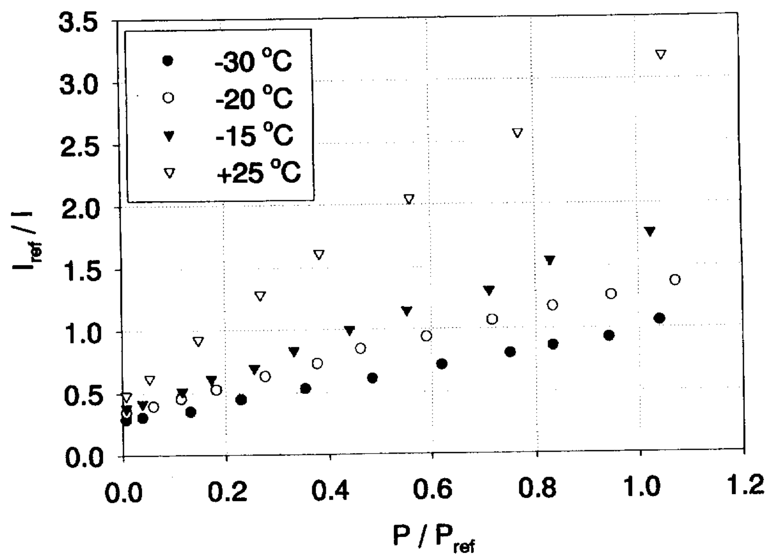


Figure B.10: Matrix Calibration for [Ru(ph$_2$-phen)$_3$] in RTV + 2.5 g Silica Gel

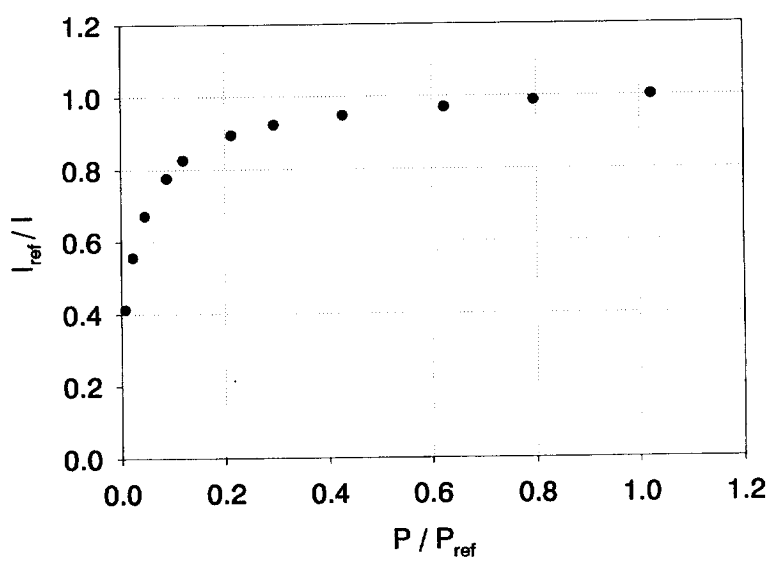


Figure B.11: Stern-Volmer for PtTFPP in RTV + 2.0 g RTV – 25 °C

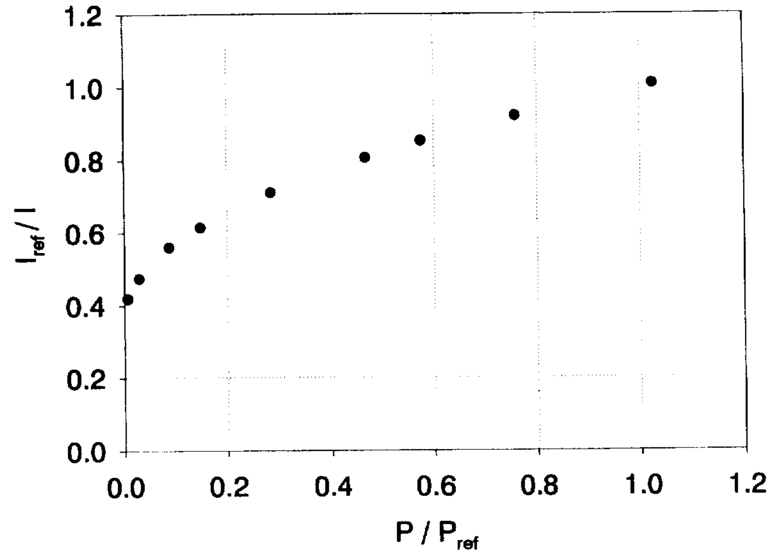
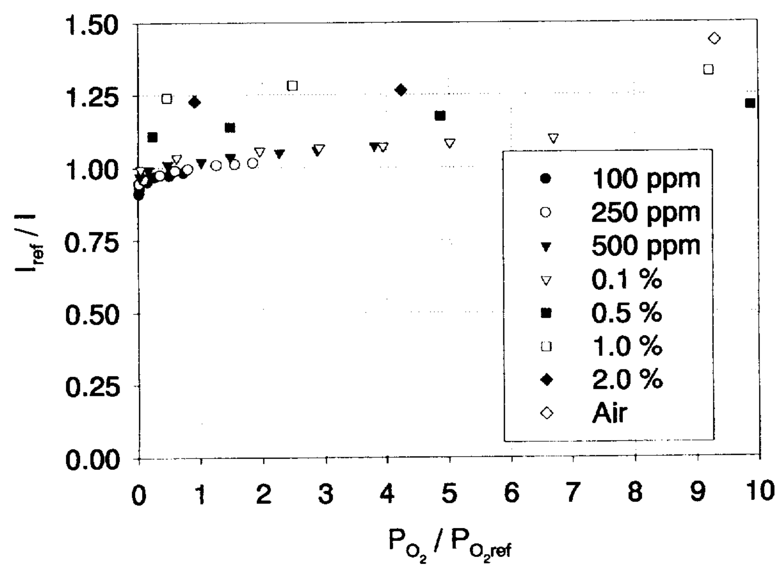


Figure B.12: Stern-Volmer for [Ru(ph$_2$-phen)$_3$] in GP-197 + 1.0g Silica Gel – 25 °C



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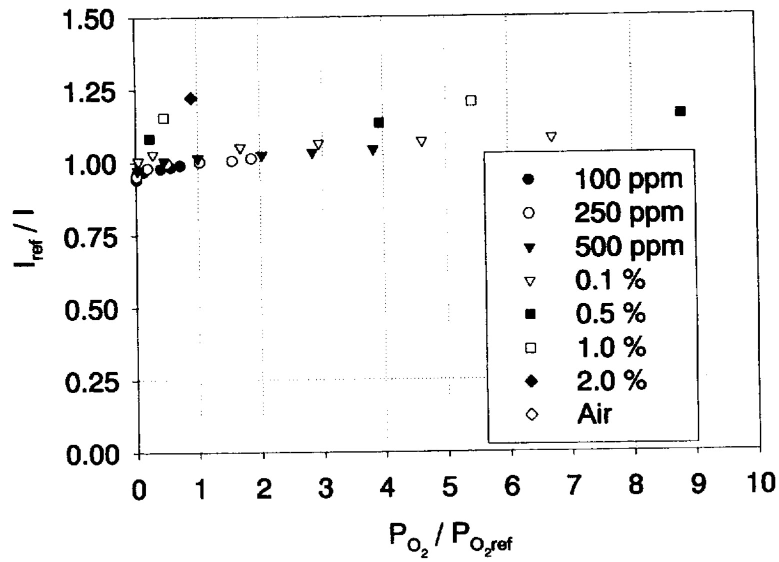

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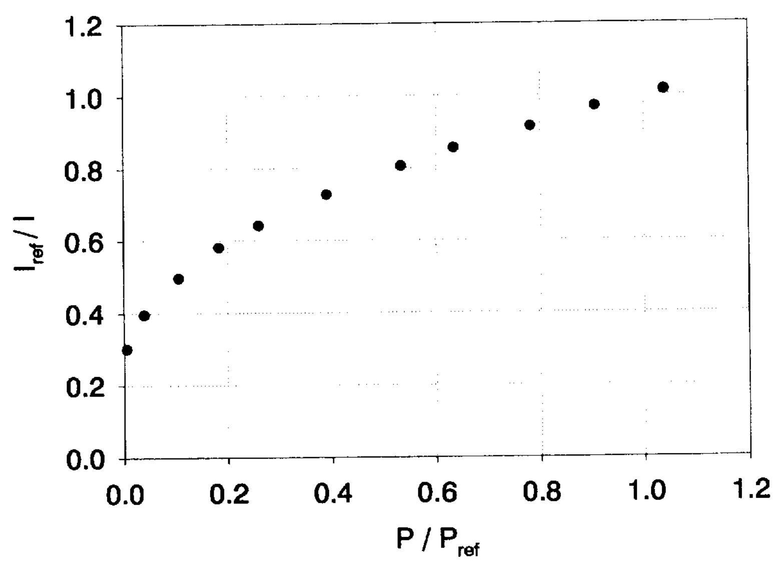

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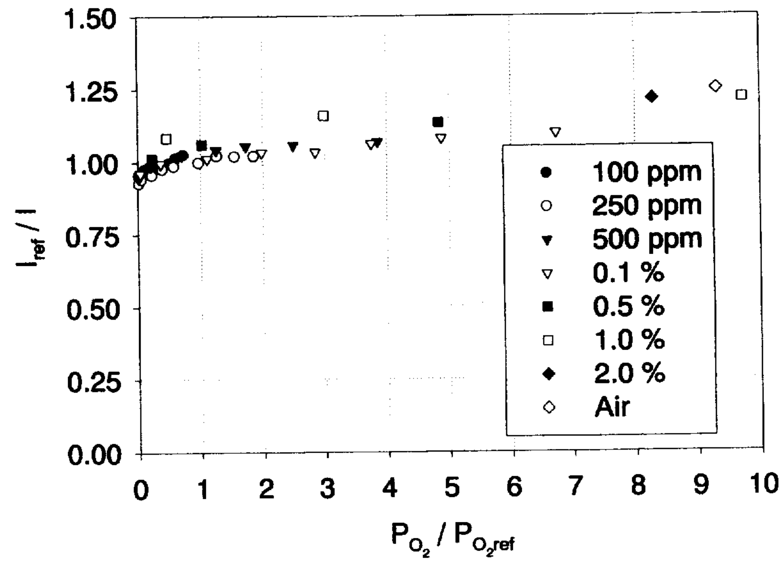

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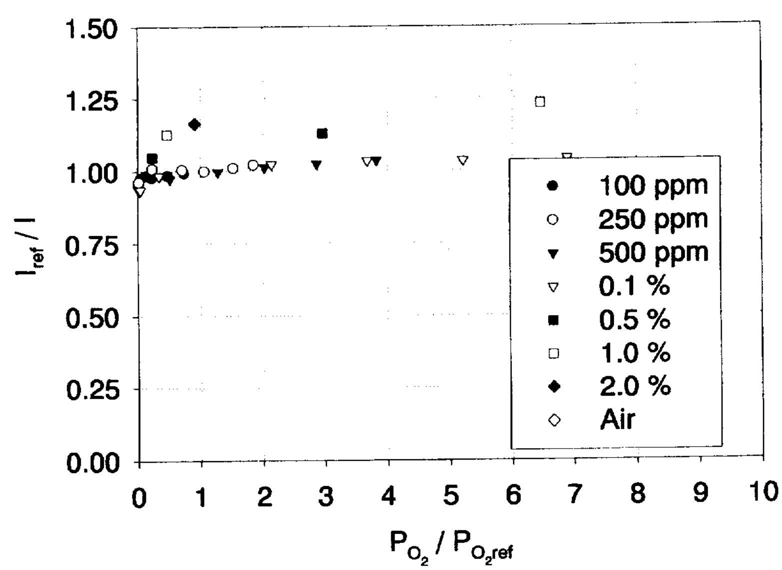

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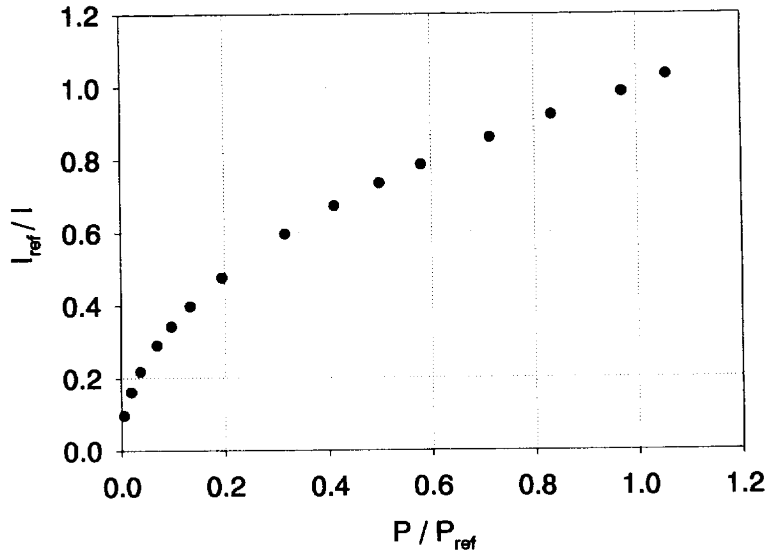

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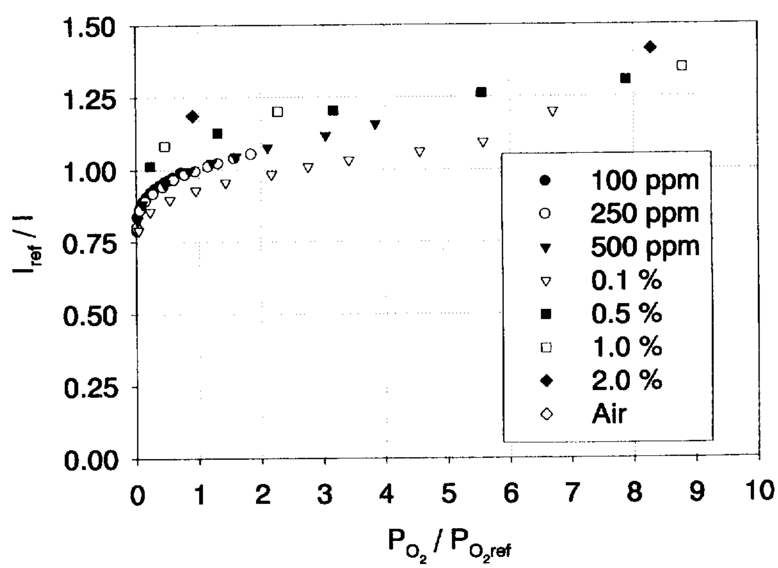

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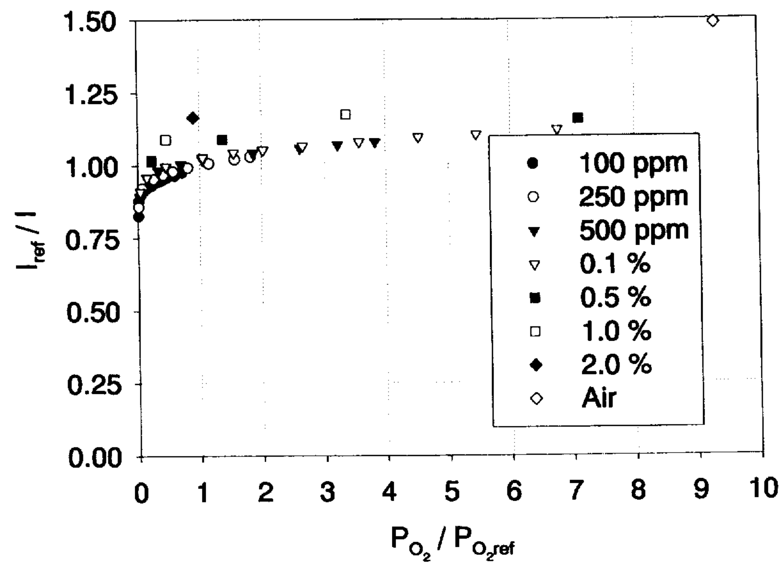

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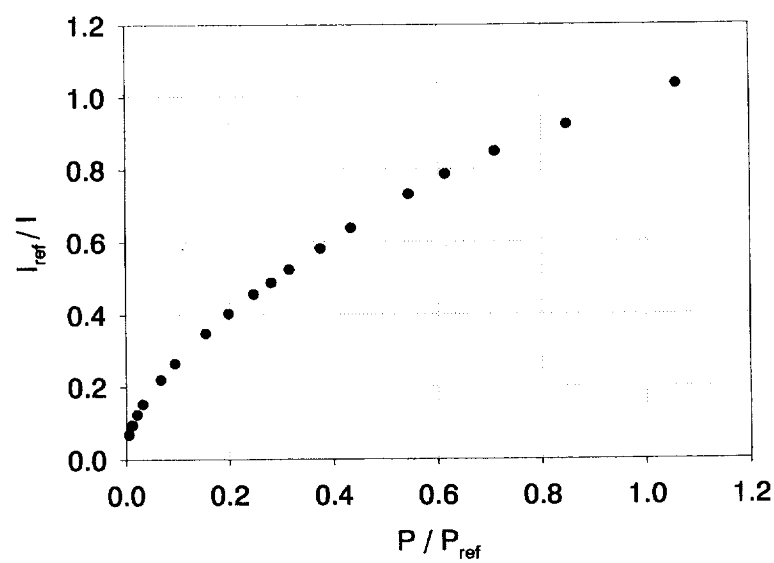

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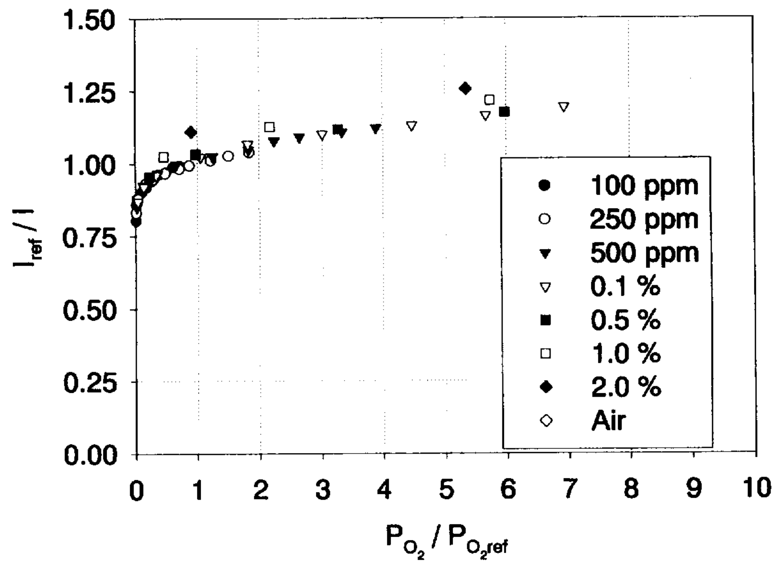

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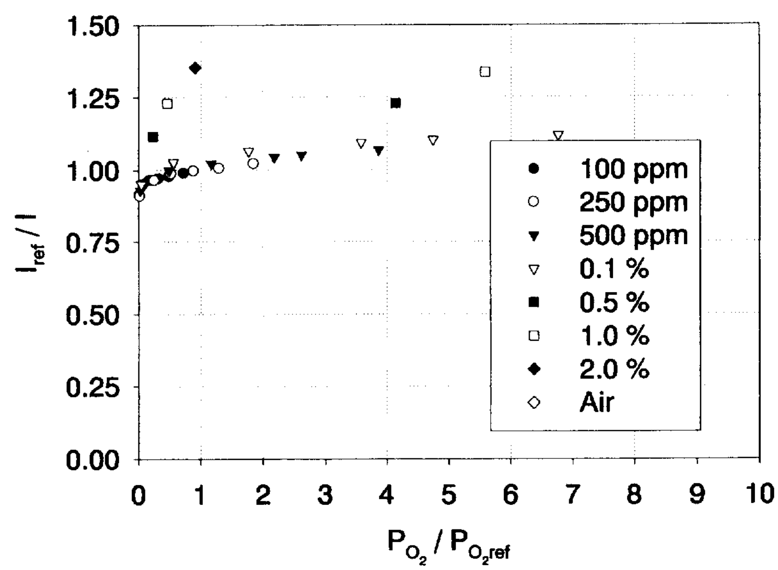

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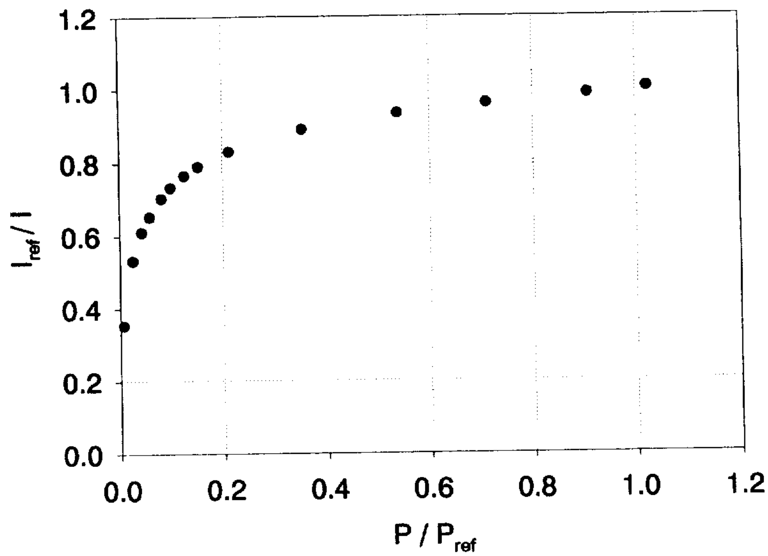

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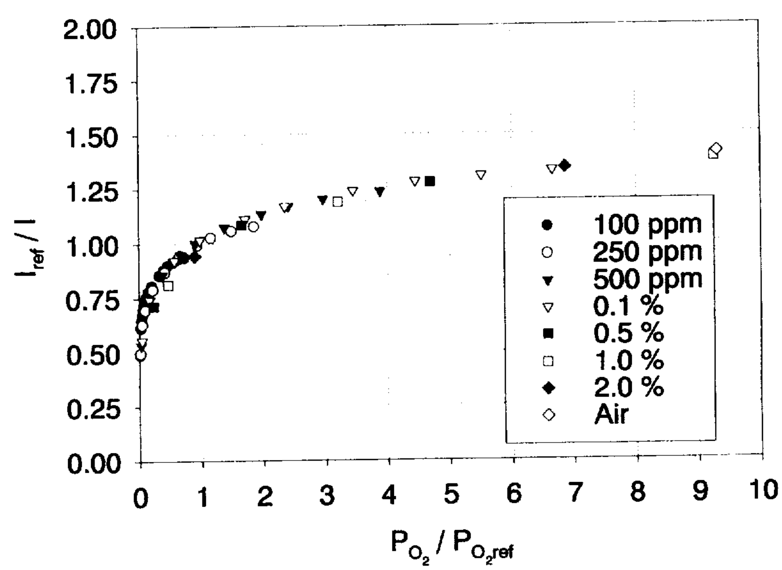

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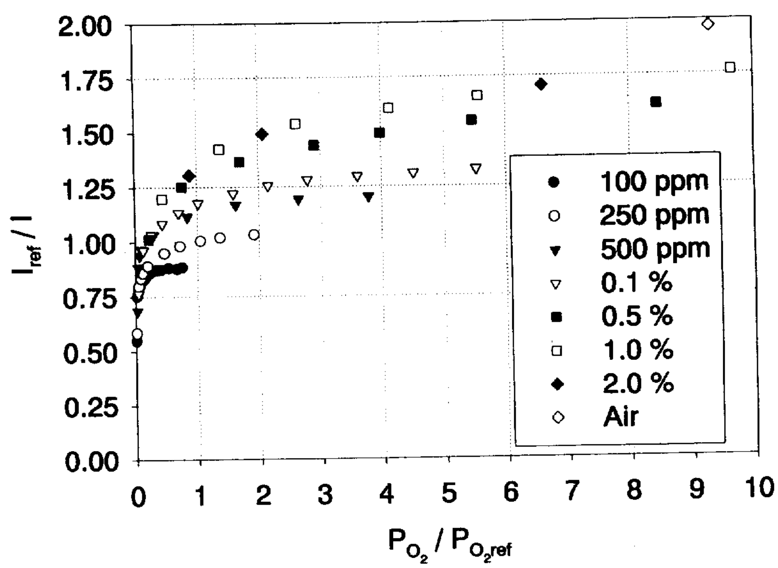

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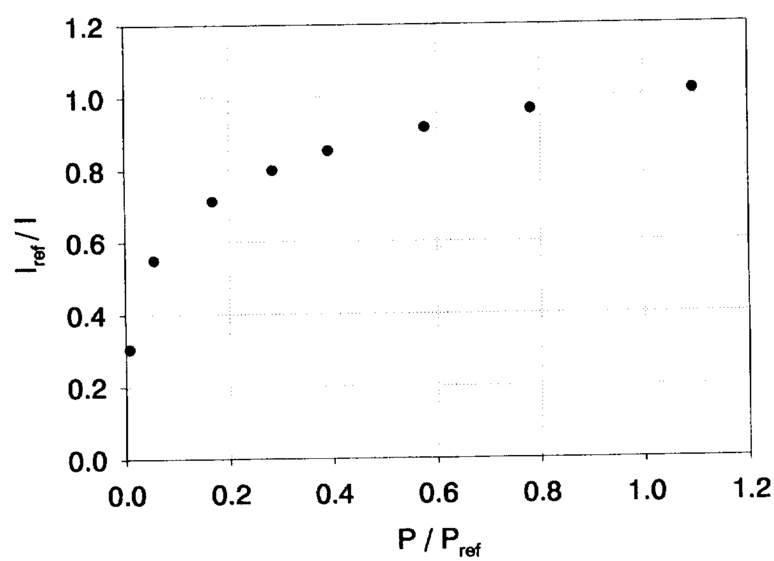

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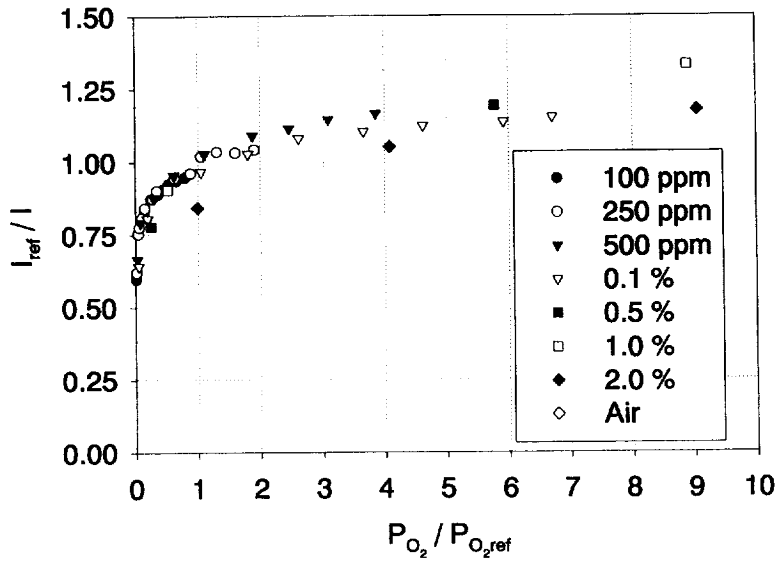

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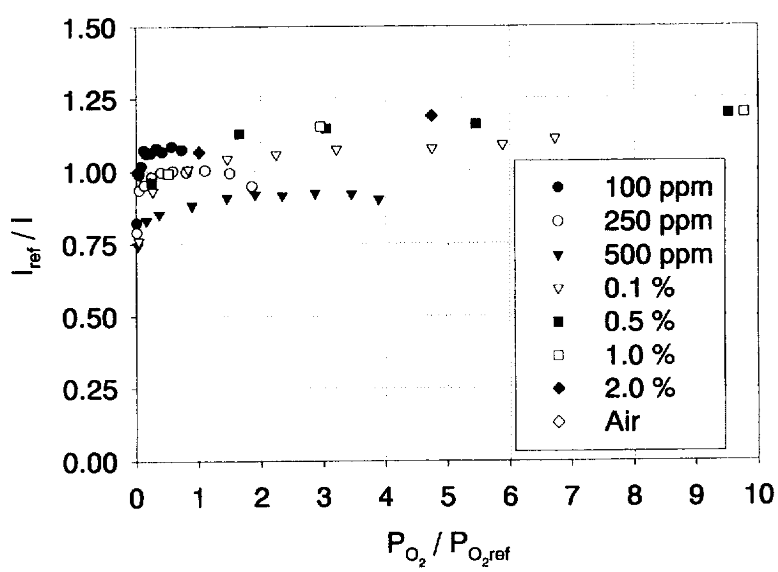

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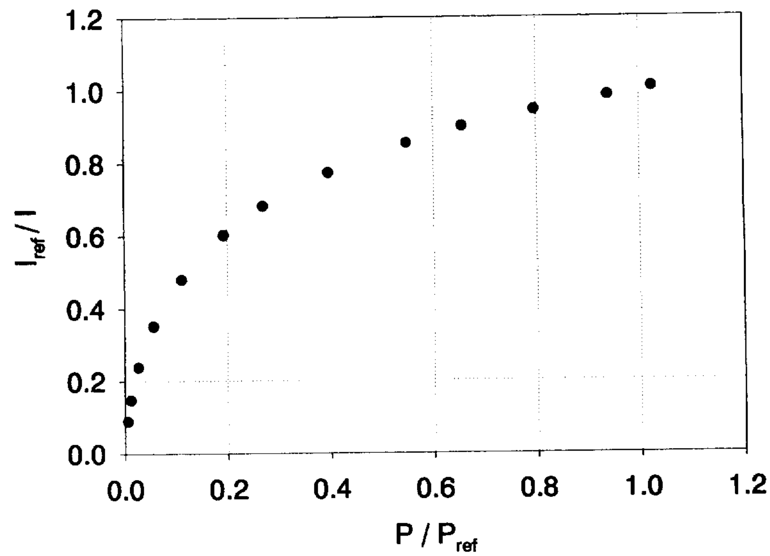

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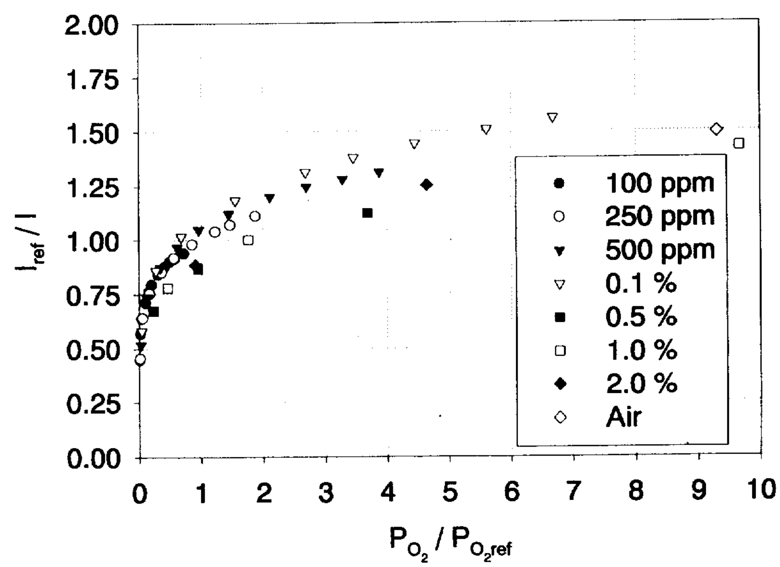

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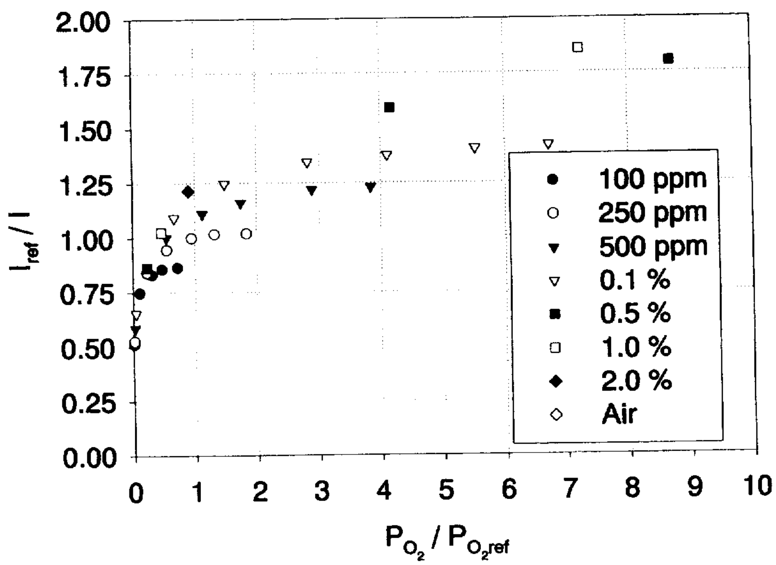

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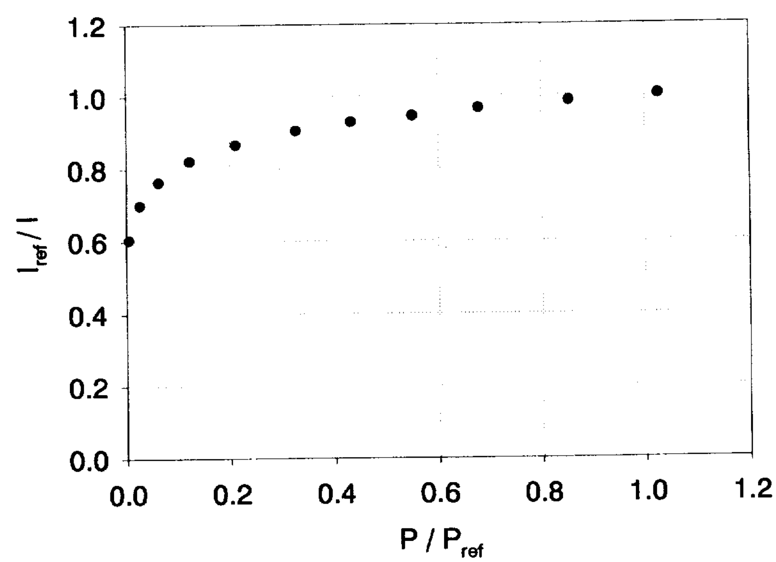

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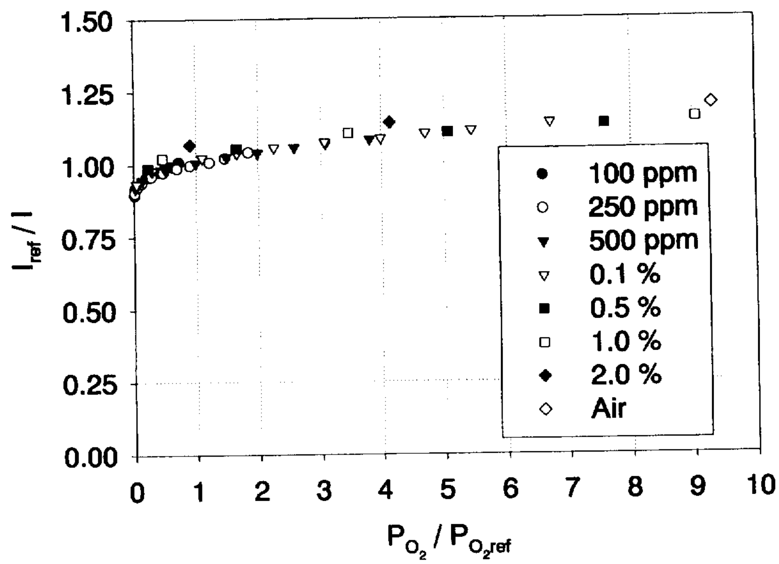

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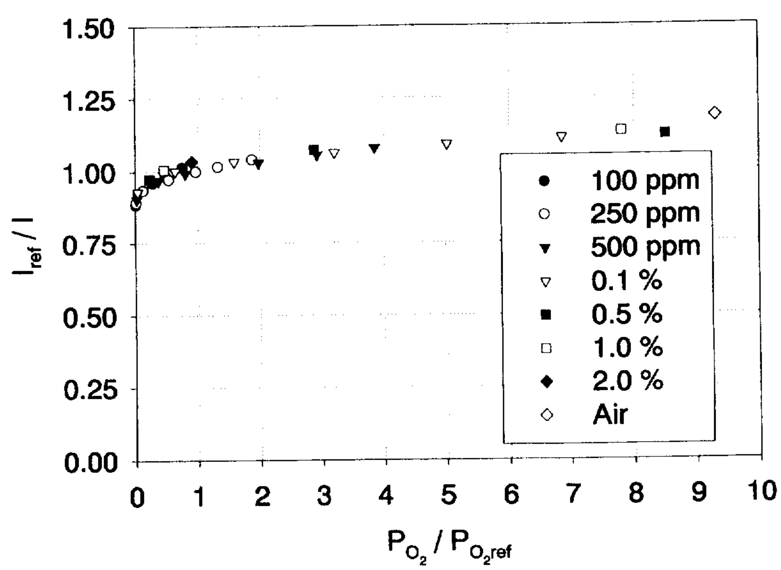

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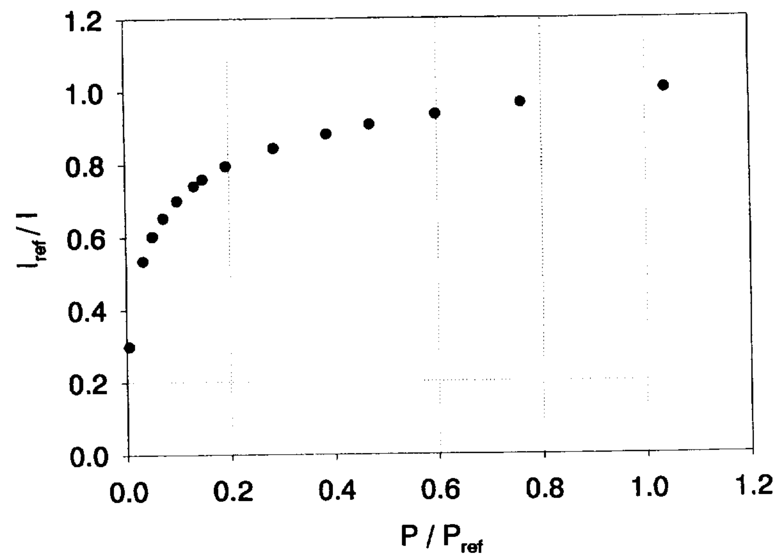

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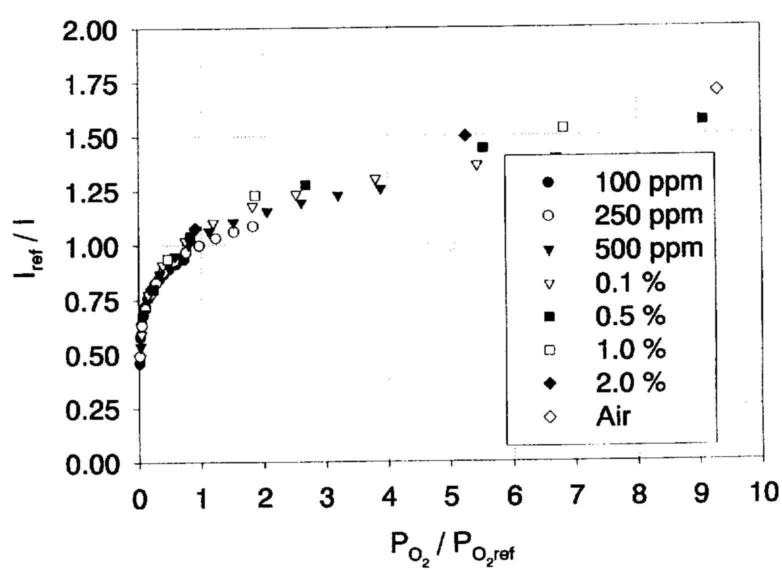

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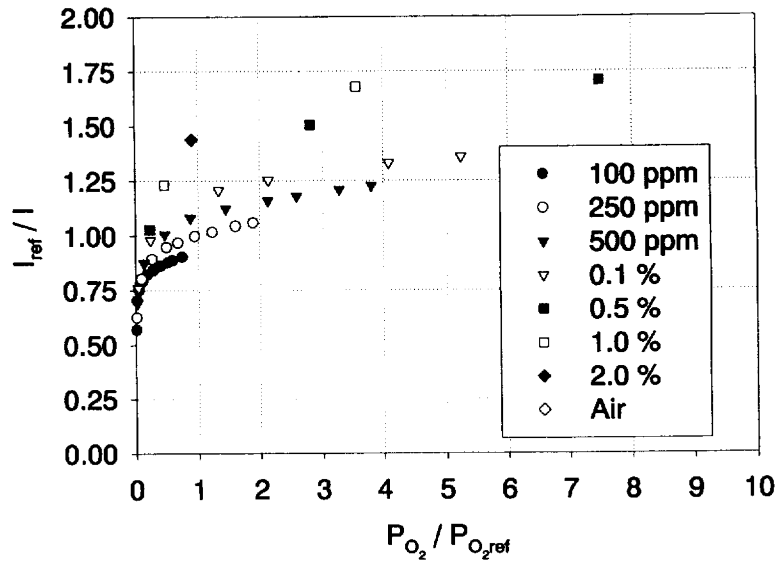

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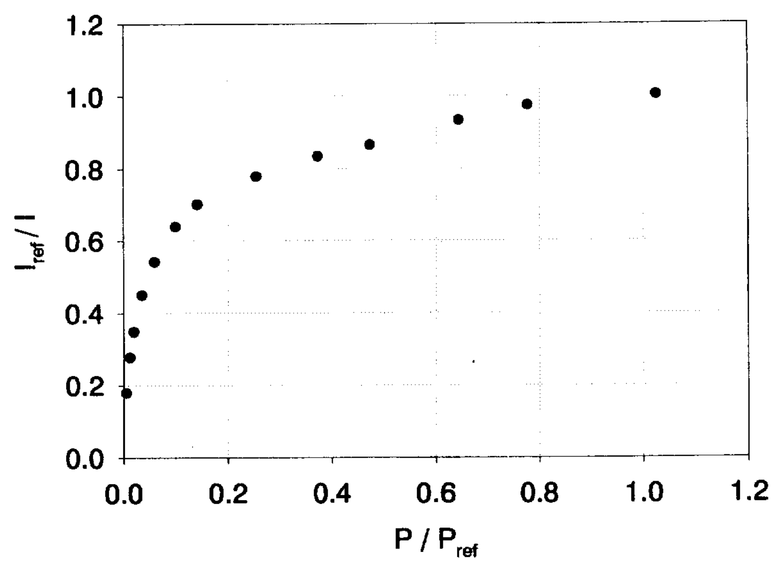

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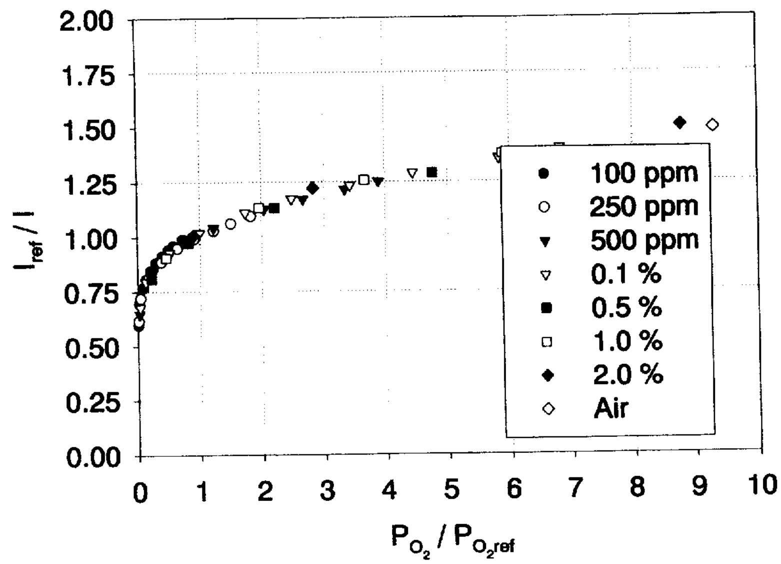

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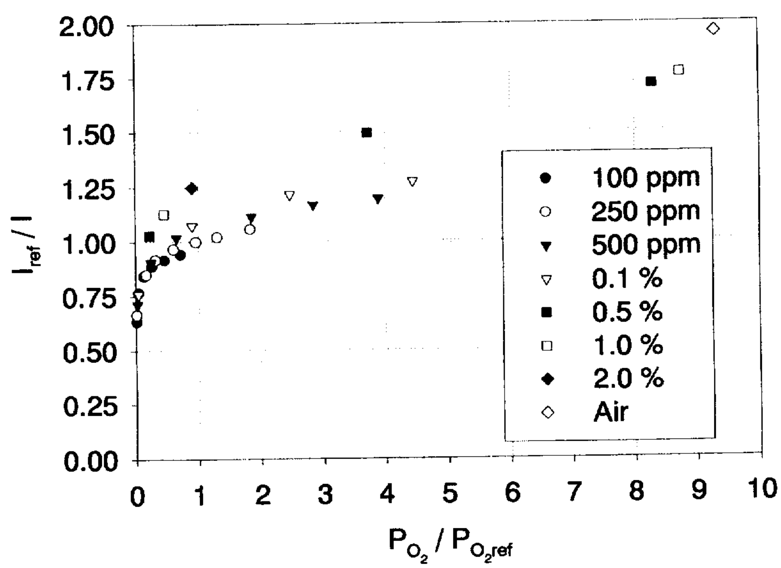

Figure B.41: PtOEP in Filter Paper – 100 K

SYNTHETIC AND GEOMETRIC PERTURBATIONS OF THE EXCITED STATES OF METAL-POLYPYRIDINE SYSTEMS

A Thesis

Submitted to the Faculty

of

Purdue University

by

Corey Thomas Cunningham

In Partial Fulfillment of the

Requirements for the Degree

of

Doctor of Philosophy

December 1998

To ALL of my family; my loving wife Kari;

Miss Moneypenny and the one and only Satan Dog

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The first person I must acknowledge is Dr. Dave McMillin. I came to Dave the summer after my sophomore year as an undergrad and asked him for summer employment (because I knew all his other undergrads had graduated). Dave reluctantly said yes and much to his dismay I'm sure, I've been here ever since. Dave has always been there when I had a question and his knowledge of photochemistry is impressive to say the least. He has taught me how to be a good scientist and a better researcher.

I would also like to thank Dr. John Sullivan for showing me how to apply chemistry to real-world applications and for giving me some excellent opportunities to travel, learn, and collaborate. He also taught me some aerodynamics in the process.

The first person to turn me on to science was my high school chemistry teacher, Mr. Steve Williams. He not only taught me chemistry, but he showed me that hot rods and science nerds do mix. And to coach Dorrell, "Don't to eat the yellow snow".

Of course, I could never have reached this point in my life without the support of a great (big) family. Ever since I could remember, every member of my family was always there with an encouraging joke about my grades. To all of you guys, thank you very much. To say the least, you always make coming home interesting. And a special thanks to my parents for letting me be as weird as I wanted and for letting me make my own choices. To my surrogate family, the Brunes', thanks for teaching this city boy what work is. And to my new in-laws, you fit in well with the rest of the bunch.

There have been many people whom I have met during my tenure at Purdue and a few of them deserve special recognition. The first person is Scott Hart. Scott was about the only chemistry person I associated with as an undergrad. Scott helped me harass many a lab TA and suffered the black eyes and bloody noses of PChem with me.

To him I wish the very best. And I could not forget the best two roommates in the world, Chuck and Porter. I lived with Chuck for 4 years and have known Porter since 8th grade. These guys made my stay at Purdue very, very enjoyable, 460 N. Grant.

Some of the first, and best, grad students I met were Dr. Cathern Miller and Dr. Michele Eggleston. They are two of the greatest women I know. Thanks for all the laughs, all the music, and most of all, the food. And to Dr. Denise Crites, even though I beat you into the group, you ducked out before I did. Your treats were always excellent and Mike was a nice addition to everything, especially golf. Thanks for being the same person I was and for the open bar at your wedding.

There were not many males in the McMillin lab in the early days, but we finally found a sucker in Joe Michalec. Joe has always been there to take my constant abuse and name calling and for some reason he keeps coming back for more. It has been a riot working with him and it gets better when I am kicking his sorry carcass all over the screen in Quake. Keep on fraggin. Jeff Moore, the new little monkey boy in our lab. Jeff can suck the work out of a computer. He can shoot the breeze like no one I have ever seen and if it was not such a good time I'd have to strangle him. I hope your house gets built on time and thanks for all the laughs. To Keith Thomas, I never thought I would enjoy being around a republican, but you do make it interesting. Keep on fraggin, but ditch the Mac.

I didn't meet too many people outside of the group, but one person I did spend a lot of time with, on the football field, was Murphy. Murph always had an organic b.s. answer for me when I needed one and he usually had a CD I needed to hear. Thanks for the mechanisms and music.

The last person I want to thank is my wife, Kari. Kari has taught me a lot. She showed me what grad school was all about and she has shown me what life outside the lab is all about. She has made my life complete and to her I will be eternally grateful.

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ABBREVIATIONS

Å	Angstrom
bcp	2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline
bipy	2,2-bipyridine
BPh_4	tetraphenylborate anion
p-Br-ph-trpy	4'-*p*-bromophenyl-2,2':6',2"-terpyridine
C_6F_5-trpy	4'-pentafluorophenyl-2,2':6',2"-terpyridine
p-Cl-ph-trpy	4'-*p*-chlorophenyl-2,2':6',2"-terpyridine
CT	charge-transfer
dap	2,9-di-*p*-anisolyl-1,10-phenanthroline
dbdmp	2,9-di-*n*-butyl-4,7-dimethyl-1,10-phenanthroline
dbp	2,9-di-*n*-butyl-1,10-phenanthroline
dbtmp	2,9-di-*n*-butyl-3,4,7,8-tetramethyl-1,10-phenanthroline
dcyp	2,9-dicyclohexyl-1,10-phenanthroline
dipp	2,9-di-*iso*-propyl-1,10-phenanthroline
dmbp	6,6'-dimethyl-2,2'-bipyridine
DMF	*N,N'*-dimethylformamide
dmp	2,9-dimethyl-1,10-phenanthroline
dnpp	2,9-di-*neo*-pentyl-1,10-phenanthroline

dnpentp	2,9-di-*n*-pentyl-1,10-phenanthroline
dsbp	2,9-di-*sec*-butyl-1,10-phenanthroline
dpdmp	2,9-diphenyl-4,7-dimethyl-1,10-phenanthroline
dpp	2,9-diphenyl-1,10-phenanthroline
dptmp	2,9-diphenyl-3,4,7,8-tetramethyl-1,10-phenanthroline
ε	molar extinction coefficient, $M^{-1}cm^{-1}$
EH	Extended Hückel
Em	emission
EtO-trpy	4'-ethoxy-2,2':6',2''-terpyridine
ϕ	emission quantum yield
HMPA	hexamethylphosphoramide
HOMO	highest occupied molecular orbital
IR	infrared
K	Kelvin
k_o	excited state decay, s^{-1}
k_1	formation of the exciplex, $M^{-1}s^{-1}$
k_{-1}	decomposition of the exciplex into starting materials, $M^{-1}s^{-1}$
k_Q	quenching of the exciplex, s^{-1}
k_q	overall quenching constant, $M^{-1}s^{-1}$
λ	wavelength
λ_{abs}	absorbance maximum
λ_{em}	emission maximum

LUMO	lowest unoccupied molecular orbital
M	Molar, moles/liter
MeS-trpy	4'-methylthio-2,2':6',2"-terpyridine
$MeSO_2$-trpy	4'-methylsulfonyl-2,2':6',2"-terpyridine
Me_2N-trpy	4'-dimethylamino-2,2':6',2"-terpyridine
mL	milliliter
MLCT	metal-to-ligand charge transfer
mmp	2-methyl-1,10-phenanthroline
NB	notebook
NC-trpy	4'-cyano-2,2':6',2"-terpyridine
nm	nanometers
NN	generic phenanthroline ligand
p-NO_2-ph	4'-*para*-nitrophenyl-2,2':6',2"-terpyridine
ppd-trpy	4'-*N*-piperidinyl-2,2':6',2"-terpyridine
ns	nanoseconds
ph-trpy	4'-phenyl-2,2':6',2"-terpyridine
phen	1,10-phenanthroline
pK_a	proton acidity
PM3	Perturbation Method 3
pmp	2,3,4,7,8-pentamethyl-1,10-phenanthroline
ppm	parts per million
PSP	pressure sensitive paint

4-py-trpy	4'-(4-pyridyl)-2,2':6',2"-terpyridine
3-py-trpy	4'-(3-pyridyl)-2,2':6',2"-terpyridine
2-py-trpy	4'-(2-pyrdiyl)-2,2':6',2"-terpyridine
SHOMO	second highest occupied molecular orbital
SLUMO	second lowest occupied molecular orbital
τ	excited state lifetime
τ_o	excited state lifetime in the absence of quencher
Θ_Z	dihedral angle between two opposing phen ligands
TfO-trpy	4'-trifluoromethylsulfonato-2,2':6',2"-terpyridine
TFPB	tetrakis[3,5-bistrifluoromethyl-phenyl]borate anion
THF	tetrahydrofuran
TLC	thin layer chromatography
trpy	2,2':6',6"-terpyridine
tmbp	4,4',6,6'-tetramethyl-2,2'-bipyridine
tmp	3,4,7,8-tetramethyl-1,10-phenanthroline
TSP	temperature sensitive paint
UV	ultraviolet
Vis	visible
zyz	2,6-bis-pyrazinyl-pyridine

ABSTRACT

Cunningham, Corey T. Ph.D., Purdue University, December, 1998.
Synthetic and Geometric Perturbations of the Excited States of Metal-Polypyridine Systems. Major Professor: David R. McMillin.

This work encompasses three chapters investigating modifications to the excited states of ruthenium(II) and copper(I) polypyridine systems. The main emphasis is on understanding what changes occur when the polypyridine ligands surrounding the metal center are modified. The synthetic modifications are those done in order to create new ligands with specialized steric and electronic characteristics. The geometric modifications refer to environmental changes placed on the coordination complex. The photophysical properties that are a result of the changes are studied, characterized, and discussed in order to better understand the governing factors of the excited states.

Chapter 1 focuses on electronic modifications of ruthenium(II) bis-terpyridine. The new compounds are then employed as luminescent molecular temperature sensors. The research was done in conjunction with Dr. John Sullivan of the Aerospace Engineering Department at Purdue University and the sensors were evaluated in a cryogenic wind tunnel at the National Aerospace Laboratory in Japan. This project has lead to the development of luminescent sensors that are effective at sensing shock waves at cryogenic temperatures. This is the first time a shock wave has been visualized at cryogenic temperatures. This method of detection is an improvement over existing methods as it is cheaper, easier, and gives a complete map of the wind tunnel model.

The second and third chapters deal with copper(I) bis-phenanthroline complexes. In chapter 2, synthetic modifications to some phenanthroline ligands lead to new complexes that resist quenching by Lewis bases. The third chapter studies the

photophysics of the copper complexes in the solid state. In this chapter, the solid state geometry, dictated by the crystal structure, is shown to have a dramatic effect on the photochemistry of the copper compounds. Also in this chapter is the first reported emission from a copper phenanthroline, with no substituent in the 2,9 positions.

PUBLICATIONS

3952 *Inorg. Chem.* 1997, *36*, 3952–3956

Luminescence Properties of Salts of the $[Pt(trpy)Cl]^+$ and $[Pt(trpy)(MeCN)]^{2+}$ Chromophores: Crystal Structure of $[Pt(trpy)(MeCN)](SbF_6)_2$

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The crystal structure of $[Pt(trpy)(MeCN)](SbF_6)_2$, where trpy denotes 2,2':6',2''-terpyridine, shows that the platinum complex packs as a monomer; however, the $^3\pi-\pi^*$ emission of the solid occurs at surprisingly long wavelengths at room temperature. At lower temperatures new, shorter-wavelength maxima appear. Of the known salts with the composition [Pt(trpy)Cl]A, the $A = SbF_6^-$ system is the lone example that exhibits a temperature-independent emission maximum. In these platinum(II) terpyridines, energy migration to defects or trap sites is one of the phenomena responsible for the temperature dependence of the solid-state emission spectrum. If trap emission is evident, the low-temperature spectral data are most representative of the bulk material.

Introduction

Luminescent square-planar complexes of Pt(II) containing α,α'-diimine ligands have intriguing spectroscopic and photophysical properties.[1] In a monomeric environment, such as in a dilute glass solution, the complexes may exhibit emission from intraligand[2] (IL), metal-to-ligand-charge-transfer[3] (MLCT), or ligand-field[3] (LF) states. Because these states are of similar energy, the relative ordering is sensitive to factors such as ligand field strength, diimine substituents, and the nature of the coligands. In the solid state, Pt–Pt or $\pi-\pi$ interactions between chromophores often have a strong influence on the emission. Three idealized solid-state structure types occur: *monomeric* structures in which the Pt–Pt distances are all greater than 4.5 Å; *linear-chain structures* in which the Pt(II) complexes are stacked equidistantly (Pt–Pt separations of 3.2–3.4 Å) along an axis that is usually, but not always, perpendicular to the plane of the complex; and *dimer* structures in which the Pt complexes segregate into pairs.[1] Compounds with monomeric structures display luminescence properties similar to those observed in dilute solutions. On the other hand, those with linear-chain structures typically exhibit $\pi^*(L) - d\sigma^*$ emissions from metal–metal-to-ligand-charge-transfer (MMLCT) excited states.[1] With these systems, the emission undergoes a characteristic red shift at lower temperatures due to a decrease in the mean Pt–Pt spacing.[4] Compounds with dimer structures also typically exhibit MMLCT emissions, but less information is available about the temperature-dependent properties. However, one study reported that the emissions from a series of ligand-bridged dimers blue-shift when the temperature drops from ambient to 77 K.[5]

By and large, Pt(II) complexes of the tridentate 2,2':6',2''-terpyridine (trpy) ligand possess luminescence properties much like those of the corresponding α,α'-diimine complexes. For example, Yip et al. have reported the properties of the $[Pt(trpy)Cl]CF_3SO_3$ salt at room temperature as well as 77 K, and they found that the emission maximum red-shifted at the lower temperature.[6] More recently, Bailey et al. examined the photophysical properties of a series of salts containing the $[Pt(trpy)Cl]^+$ moiety.[7] They assigned the low-temperature solid-state luminescence of these salts to ^{3}MMLCT states, and they concluded that the emission energy varied with the counterion (ClO_4^-, Cl^-, $CF_3SO_3^-$, or PF_6^-) because of differences in the Pt–Pt and $\pi-\pi$ interactions in the lattice.[7] Contrary to the results of Yip et al., however, for all except the red perchlorate salt, Bailey et al. reported that the emission narrowed and exhibited a blue shift with a decrease in temperature.

The present report deals with the temperature dependence of the emissions from $[Pt(trpy)Cl]SbF_6$ and $[Pt(trpy)Cl]CF_3SO_3$ in the solid state as well as the crystal structure and emission spectrum of $[Pt(trpy)(MeCN)](SbF_6)_2$. The acetonitrile adduct exhibits a triplet emission (^{3}IL parentage) from the solid, but the energy varies with temperature due to the participation of various trap centers.

Experimental Section

Materials and Syntheses. The purity of all reagent grade materials was adequate as received. The $Pt(PhCN)_2Cl_2$ starting complex and 2,2':6',2''-terpyridine (trpy) were obtained from Strem Chemicals, while the salts $AgSbF_6$ and $AgCF_3SO_3$ were from Fluka AG. Successive fractional distillations over sodium octanoate and sulfuric acid served

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to purify acetonitrile, but analytical grade solvents sufficed in all other cases.

[Pt(trpy)Cl]A ($A = SbF_6^-$, or $CF_3SO_3^-$). The preparation began with the addition of an equimolar amount of AgA (0.146 g for $A = SbF_6^-$, 0.109 g for $A = CF_3SO_3^-$; 0.424 mmol) in MeCN (5−7 cm³) to a suspension of $Pt(PhCN)_2Cl_2$ (0.200 g, 0.424 mmol) in MeCN (15 cm³). After a 15 h reflux and a filtration step, came the addition of a 5% excess of 2,2':6',2''-terpyridine (0.104 g, 0.445 mmol) and another 15 h reflux. A second filtration removed any additional AgCl precipitate prior to the removal of solvent. Finally, treatment with hot MeCN provided for the extraction of the [Pt(trpy)Cl]A salt. Slow cooling of the MeCN solution resulted in the precipitation of a crystalline solid of bright orange ($A = SbF_6^-$) or orange ($A = CF_3SO_3^-$) material. Washing the bright orange SbF_6^- salt with acetone effected a color change to bright yellow but did not alter the color of the other salt. Yield: 70−80%. Anal. Calcd (for $A = SbF_6^-$): C, 25.75; H, 1.58; N, 6.00. Found: C, 25.88, H, 1.67; N, 6.05. Calcd (for $A = CF_3SO_3^-$): C, 31.36; H, 1.81; N, 6.86. Found: C, 30.97; H, 1.67; N, 7.27. IR (KBr, cm⁻¹): ν(trpy) 1606s, 1480m, 1456s, 1442m, 1400m, 1317m, 1035m, 773s; ν(SbF_6^-): 656s; (ν($CF_3SO_3^-$)): 1256s, 1158s, 1030s.

[Pt(trpy)(MeCN)](SbF₆)₂. A vapor-extraction apparatus facilitated the continuous extraction of solid [Pt(trpy)Cl]SbF_6 (0.300 g, 0.318 mmol) into refluxing acetonitrile containing an excess of $AgSbF_6$ (0.291 g, 0.848 mmol). When all the [Pt(trpy)Cl]SbF_6 had dissolved (after ca. 4 h) and the solution had cooled to room temperature, filtration removed the precipitated AgCl. The precipitation of unreacted [Pt(trpy)Cl]SbF_6 occurred as the volume decreased. After filtration, further evaporation led to the deposition of the desired product. The final purification steps involved a wash with acetone and diethyl ether and then exposure to a vacuum. After dissolution in acetonitrile, the crystallization of [Pt(trpy)(MeCN)]$(SbF_6)_2$ as light-yellow block-shaped crystals occurred as the solvent evaporated. Yield: 45%. Anal. Calcd: C, 21.70; H, 1.50; N, 5.95. Found: C, 21.61; H, 1.39; N, 5.93. IR (KBr, cm⁻¹): ν(C≡N) 2332m, 2304w; ν(trpy) 1611s, 1574m, 1510m, 1510w, 1458m, 1455s, 1408m, 1322m, 1250m, 1036m, 785s; ν(SbF_6^-) 656s.

Methods. For luminescence measurements of solutions, a series of freeze−pump−thaw cycles served to remove dissolved dioxygen. During the steady-state emission studies and the lifetime experiments, a 400 nm long-wave-pass filter protected the detector from scattered light. For the lifetime studies, there was a 337 nm notch filter between the sample and the laser. In the course of the variable-temperature studies, all samples equilibrated at least 1 h after the sensor reached the desired temperature. A standard method of analysis yielded the lifetimes from the emission-decay data as before.[8]

Instrumentation. A Shimadzu FTIR-4300 spectrophotometer provided infrared spectra of samples in KBr disks, and a Perkin-Elmer Lambda 4C and a Hewlett Packard 8452A diode-array spectrophotometer provided the absorbance data. An SLM Aminco SPF-500 instrument yielded the emission results, and a previously described apparatus[9] provided the lifetime data, except that the excitation source was a Laser Science, Inc., Model 337ND-S nitrogen laser. For the variable-temperature emission measurements, the cryostat was an Oxford Instruments Model DN1704 liquid-nitrogen-cooled system complete with an Oxford Instruments temperature controller. For the 77 K data, the sample holder was a quartz finger dewar filled with liquid nitrogen. The diffractometer was an Enraf−Nonius CAD4.

Crystal Structure Determination. The crystal of [Pt(trpy)(MeCN)]$(SbF_6)_2$ used for the diffraction study was a nearly cube-shaped block with dimensions 0.12 × 0.15 × 0.12 mm. The ω−θ scan method in conjunction with monochromated Mo Kα radiation yielded cell dimensions and diffraction intensities. A total of 25 reflections with $6 < \theta < 12°$ sufficed for determining cell dimensions. The data out to $2\theta = 46°$ (a total of 3708 reflections) showed monoclinic symmetry and exhibited systematic absences characteristic of the space group $P2_1/c$ (14). Of the 2708 unique reflections, there were 1988 with $I > 3\sigma(I)$

Table 1. Crystal Parameters at 295 K for [Pt(trpy)(MeCN)]$(SbF_6)_2$

empirical formula	$C_{17}H_{14}F_{12}N_4PtSb_2$
fw	940.39
space group (No.)	$P2_1/c$ (14)
temp, °C	22
a, Å	13.705(6)
b, Å	12.524(4)
c, Å	14.507(4)
β, deg	98.27(3)
Z	4
V, Å³	2425.0(16)
ρ_{calc}, g cm⁻³	2.58
λ, Å	0.710 73
μ, cm⁻¹	54.18
transm coeff	0.678−0.998
R ($I > 3\sigma(I)$)[a]	0.043 for 1988 reflcns
R_w[a]	0.050 for 1988 reflcns

[a] $R = \sum||F_o| - |F_c||/\sum|F_o|$; $R_w = \sum w^{1/2}||F_o| - |F_c||/\sum w^{1/2}F_o$.

that were useful for the solution and refinement of the structure. The solution of the Patterson function gave the location of the Pt and Sb atoms, and the remaining non-H atoms appeared in a difference Fourier map phased on the heavy atoms. The H atoms appeared in calculated positions. For the purposes of refinement, all atoms, except the H atoms, were assigned anisotropic temperature parameters. The refinement utilized the full-matrix least-squares method and the weighting scheme $w = 1/[\sigma^2(F) - 0.00580F^2]$. Table 1 gives a summary of the crystal parameters and other details of the refinement.

Results

The approach used for the synthesis of the chloro-containing derivatives [Pt(trpy)Cl]A ($A = SbF_6^-$, $CF_3SO_3^-$) was different from that employed by Yip et al.[6] or Bailey et al.[7] in that the neutral compound $Pt(PhCN)_2Cl_2$, rather than the ionic species [Pt(trpy)Cl]Cl, served as the starting material. Thus, treatment of the benzonitrile complex with 1 equiv of the appropriate silver salt in refluxing acetonitrile, followed by addition of a slight excess of terpyridine, afforded an analytically pure product after workup and crystallization from acetonitrile. Interestingly, the SbF_6^- salt separated from acetonitrile as bright orange crystals that converted to yellow crystals over a period of ca. 10 min after the removal of the mother liquor. An instantaneous conversion from the metastable orange modification to the yellow form occurred with an acetone wash. For the synthesis of the acetonitrile salt [Pt(trpy)(MeCN)]$(SbF_6)_2$, [Pt(trpy)Cl]SbF_6 was the starting material. Treatment of a boiling solution of the latter with 2 equiv of $AgSbF_6$ led to the formation of the desired product, along with AgCl and unreacted [Pt(trpy)Cl](SbF_6); the latter selectively precipitated from a cooled acetonitrile solution, allowing the isolation of [Pt(trpy)(MeCN)]$(SbF_6)_2$ as light yellow block-shaped crystals. The solid-state infrared spectrum, measured in a KBr disk, exhibited two peaks in the C−N stretching region at 2330 and 2302 cm⁻¹, each attributable to the MeCN ligand. A similar C−N stretching peak pattern has been observed for $Pt(MeCN)_2Cl_2$.[10] Attempts to synthesize the BF_4^- and $CF_3SO_3^-$ salts of $[Pt(trpy)(MeCN)]^{2+}$ from [Pt(trpy)Cl]A ($A = CF_3SO_3^-$, BF_4^-) were unsuccessful, largely because of the difficulties incurred in the separation of the starting material from the desired product.

Crystal Structure of [Pt(trpy)(MeCN)](SbF₆)₂. The structure shows that the platinum adopts a planar coordination geometry; see Figure 1 for a perspective view of the cation. The positional and thermal parameters as well as the calculated interatomic distances and angles for [Pt(trpy)(MeCN)]$(SbF_6)_2$ appear in Tables 2 and 3. The maximum deviation from the

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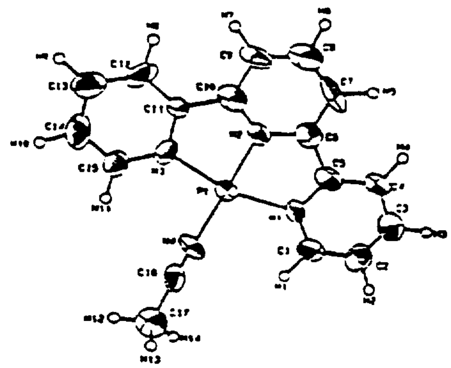

Figure 1. The molecular geometry and atom-numbering scheme employed for the [Pt(trpy)(MeCN)]$^{2+}$ cation. Atom designators are 50% probability ellipsoids except for those of the H atoms, which appear as spheres of arbitrary radius.

Table 2. Positional (×10^4) and Thermal Parameters (Å^2 × 10^3) for [Pt(trpy)(MeCN)](SbF$_6$)$_2$

atom	x	y	z	U_{eq}[a]
Pt	2394	2116(1)	4000	42
N1	2983(9)	1172(12)	3058(10)	50(3)
N2	2853(9)	3269(11)	3262(9)	43(3)
N3	1939(10)	3403(10)	4678(11)	53(4)
N4	1906(10)	929(13)	4751(10)	54(4)
C1	3043(14)	106(16)	3024(14)	65(5)
C2	3467(17)	−430(17)	2330(16)	85(7)
C3	3857(13)	147(19)	1709(15)	69(6)
C4	3842(14)	1321(17)	1736(14)	66(5)
C5	3384(12)	1771(15)	2439(13)	52(4)
C6	3322(12)	2963(16)	2546(12)	53(4)
C7	3693(13)	3793(25)	2044(14)	84(7)
C8	3539(17)	4852(21)	2295(18)	81(7)
C9	3062(15)	5091(16)	3004(12)	65(5)
C10	2710(12)	4274(16)	3507(11)	55(5)
C11	2163(11)	4367(13)	4305(12)	44(4)
C12	1889(14)	5311(16)	4648(17)	73(6)
C13	1376(15)	5363(18)	5390(17)	76(6)
C14	1154(14)	4372(21)	5754(17)	86(7)
C15	1446(12)	3413(16)	5419(13)	56(5)
C16	1654(12)	281(13)	5164(13)	57(5)
C17	1314(14)	−673(15)	5700(13)	71(5)
Sb1	4240(1)	−2792(1)	166(1)	58
F1	3589(1)	−4063(1)	150(1)	133(5)
F2	5288(1)	−3468(1)	−188(1)	216(10)
F3	3744(1)	−2567(1)	−1032(1)	198(9)
F4	4897(1)	−1521(1)	195(1)	234(10)
F5	3197(1)	−2110(1)	526(1)	188(9)
F6	4740(1)	−3013(1)	1371(1)	159(7)
Sb2	350(1)	6991(1)	7767(1)	65
F7	−13(1)	6484(1)	6607(1)	221(11)
F8	1549(1)	7322(1)	7490(1)	148(6)
F9	−95(1)	8317(1)	7400(1)	232(11)
F10	701(1)	7489(1)	8937(1)	144(6)
F11	−856(1)	6657(1)	8052(1)	149(6)
F12	785(1)	5661(1)	8144(1)	186(8)

mean plane through the Pt and four bonded N atoms is 0.012 Å for the metal atom. As a consequence of the geometric constraints imposed by the trpy ligand, the angles subtended at the Pt atom deviate from the idealized values of 90 and 180°; the relevant angles are 81.8(6) (N1−Pt−N2), 162.5(6) (N1−Pt−N3), 98.3(6) (N1−Pt−N4), 80.8(6) (N2−Pt−N3), 179.3(5) (N2−Pt−N4), and 99.1(6)° (N3−Pt−N4). The Pt−N distances are also typical of metal−terpyridine complexes.[6,7,11,12] in that the distance to the inner N atom (Pt−N2, 1.938(13) Å) is significantly shorter than those to the two outer N atoms (Pt−N1, 2.047(14) Å; Pt−N3, 2.013(13) Å). The trpy ligand is only slightly ruffled, the mean planes of the outer pyridine rings defining angles of 2.1 (N1 ring) and 3.2° (N3 ring) with that of the central pyridine ring. The Pt−N4 distance is 1.996(14) Å. This value is similar to the Pt−N (N of MeCN) distances of 1.977 and 1.981 Å for Pt(MeCN)$_2$Cl$_2$[10] and 1.94(2) Å for [Pt(phbpy)(MeCN)]PF$_6$ (Hphbpy = 6-phenyl-2,2'-bipyridine).[13]

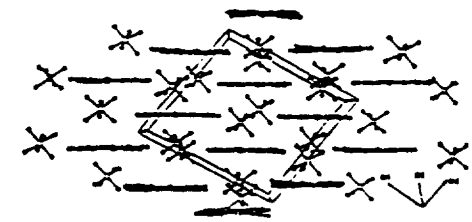

Figure 2. Packing diagram for [Pt(trpy)(MeCN)](SbF$_6$)$_2$.

Table 3. Selected Interatomic Distances (Å) and Angles (deg) for [Pt(trpy)(MeCN)](SbF$_6$)$_2$

Distances			
Pt−N1	2.047(14)	Pt−N2	1.938(13)
Pt−N3	2.013(13)	Pt−N4	1.996(14)
N1−C1	1.32(2)	N1−C5	1.34(2)
N2−C6	1.35(2)	N2−C10	1.31(2)
N3−C11	1.36(2)	N3−C15	1.35(2)
N4−C16	1.08(2)	C1−C2	1.40(3)
C2−C3	1.32(3)	C3−C4	1.45(3)
C4−C5	1.39(3)	C5−C6	1.48(3)
C6−C7	1.39(3)	C7−C8	1.38(3)
C8−C9	1.33(3)	C9−C10	1.37(3)
C10−C11	1.47(2)	C11−C12	1.34(2)
C12−C13	1.37(3)	C13−C14	1.38(3)
C14−C15	1.36(3)	C16−C17	1.52(1)
Angles			
N1−Pt−N2	81.8(6)	N1−Pt−N3	162.5(6)
N1−Pt−N4	98.3(6)	N2−Pt−N3	80.8(6)
N2−Pt−N4	179.3(5)	N3−Pt−N4	99.1(6)
Pt−N1−C1	128.6(13)	Pt−N1−C5	112.0(12)
Pt−N2−C6	116.6(12)	Pt−N2−C10	118.1(12)
Pt−N3−C11	113.0(11)	Pt−N3−C15	128.5(13)
Pt−N4−C16	179(2)	N4−C16−C17	177(2)

The crystal lattice consists of parallel sheets of cations and anions: Figure 2 gives a view of the packing parallel to these sheets. Within a sheet, the [Pt(trpy)(MeCN)]$^{2+}$ and SbF$_6^-$ moieties reside in alternating rows of cations and anions which extend along the b axis. Since the planar cations lie side-by-side, there are no $\pi-\pi$ or metal−metal interactions along a row of cations. A c-glide plane relates successive sheets such that a row of anions lies directly above a row of cations. Thus, there are no extended interactions involving cations in a direction perpendicular to the sheets either. Specifically, the Pt−Pt distances between neighboring cations from adjacent sheets are all greater than 4.90 Å. Similarly, the intermolecular C(trpy)−C(trpy) distances are all greater than 3.5 Å and close to the upper limit of 3.8 Å for π aromatic interactions.[14] We conclude that the [Pt(trpy)(MeCN)]$^{2+}$ chromophore resides in a monomeric environment in the SbF$_6^-$ salt and that this is a consequence of the cation:anion ratio of 1:2. Such a conclusion requires further verification, however, since this is the first

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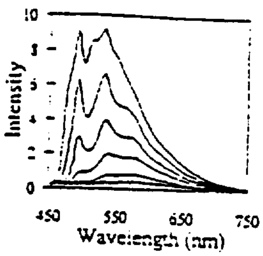

Figure 3. Solid-state emission spectra of [Pt(trpy)(MeCN)](SbF$_6$)$_2$ recorded at 40 K intervals over the range 30–280 K. The emission intensity increases as the temperature decreases. The excitation wavelength was 350 nm.

reported crystal structure determination of a terpyridyl salt of Pt(II) of 1:2 cation:anion stoichiometry.

Emission from [Pt(trpy)(MeCN)](SbF$_6$)$_2$. In the solid state, the emission from [Pt(trpy)(MeCN)](SbF$_6$)$_2$ clearly reflected different components at different temperatures (Figure 3). Thus, above ca. 240 K the principal emission maxima occurred at around 540 and 575 nm, respectively, and there were weaker emission maxima at ca. 495 and ca. 465 nm. From 200 K down to about 120 K, the overall intensity increased, but there was a change in the band shape. In this temperature regime, the band at 495 nm evolved into a dominant spectral feature along with the band at 530 nm, and both maxima shifted to somewhat shorter wavelengths. At the same time, the relative intensity of the band at 575 nm decreased, and it became a shoulder. Finally, at the lowest accessible temperature, ca. 30 K, the spectrum sharpened further and new shoulders appeared at about 480, 515, and 550 nm, respectively. At each temperature, the vibrational structure within the emission spectrum is consistent with a $^3\pi-\pi^*$ orbital parentage. Parenthetically, we may note that the apparent emission maximum at 465 nm in the room-temperature spectrum of Figure 3 could represent $^3\pi-\pi^*$ emission from coordinated trpy as well. However, it could also be an artifact, since the signal intensity changes very little at this wavelength over the entire temperature range investigated. A reviewer pointed out that reabsorption of the emission could be a factor influencing the observed band shape. However, experiments showed that, in the room-temperature, solid-state reflectance spectrum, the longest wavelength absorption band with any appreciable intensity had a maximum at about 390 nm and a tail that extended to only ca. 450 nm.

For comparison, we measured the emission from Pt(trpy)-(MeCN)$^{2+}$ in a butyronitrile glass at 77 K. The spectrum of the glass yielded well-resolved vibronic maxima, and the onset of the spectrum fell at a shorter wavelength. For a 150 μM solution, the emission maxima occurred at 457, 491, 529, and 565 nm.

Physical Data for the [Pt(trpy)Cl]A Solids. Like Bailey et al.,[7] we found that the emission spectrum of [Pt(trpy)Cl]$^+$ varied markedly with the counterion in the solid state as well as with the temperature. However, we often observed qualitatively different kinds of behavior. In our studies with SbF$_6^-$ as the counterion, the compound was yellow and the maximum in the uncorrected emission spectrum occurred at 552 nm. Although the wavelength maximum of the emission was essentially independent of the temperature (Figure 4), the intensity increased as the temperature decreased. The room-temperature decay was not monoexponential, but the emission lifetime was about 750 ns in the tail of the decay curve. On the other hand, the decay was essentially monophasic at 77 K and had a lifetime of about 3 μs. Although Bailey et al. studied

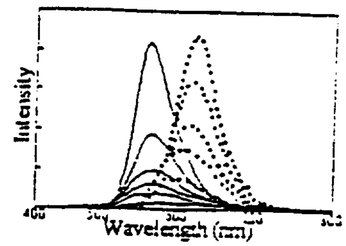

Figure 4. Emission spectra from solid-state samples of [Pt(trpy)Cl]-SbF$_6$ (left) and [Pt(trpy)Cl]CF$_3$SO$_3$ (right). In each case, the intensity increases as the temperature decreases. The temperatures are 100, 130, 160, 190, 220, and 280 K; there is no 220 K spectrum for the triflate compound. The excitation wavelength was 350 nm.

ostensibly the same chromophore as part of a yellow solid with PF$_6^-$ as the counterion,[7] they found that the room-temperature emission maximum occurred at a much longer wavelength, ca. 630 nm. Moreover, at lower temperatures, emission occurred at shorter wavelengths and there was a decrease in the bandwidth. By around 100 K, the emission maximum stopped shifting and stabilized at about 565 nm.[7] Our preparation of the triflate salt gave an uncorrected emission maximum at 585 nm at 280 K. At lower temperatures, the emission maximum shifted to longer wavelengths, out to 613 nm at 100 K (Figure 4), in line with the results of Yip et al.[9]

Discussion

The [Pt(trpy)(MeCN)](SbF$_6$)$_2$ System. The structured emission shown by the nitrile complex in the low-temperature glass or the solid state clearly represents ligand-centered $^3\pi-\pi^*$ emission. However, for the solid state, the emission appears at longer wavelengths and the spectrum is quite temperature dependent. At low temperature, new shorter-wavelength emission maxima appear in the solid-state spectrum, but even at 30 K, the emission does not attain the energy found from the glass. In principle, a phase transition could account for the temperature dependence of the emission spectrum; however, this is unlikely. One reason is that the data would require a series of phase changes at different temperatures. The other problem with this model is that the lowest energy emission occurs at room temperature, where the structure shows there are no significant neighbor–neighbor interactions, at least in the bulk material.

The most likely explanation of the data is that the emission originates from different trap sites depending on the temperature. The trap centers could be either defect sites or sites where the excitation itself generates a locally modified structure.[15] When energy transfer is facile in the solid, the chromophores in the bulk simply act as antennae that efficiently take up the energy which then flows into lower energy trap sites. Of course, the energy-distribution processes are temperature dependent and, at a sufficiently low temperature, the population of particular traps may no longer be feasible. Under these conditions, new, higher energy emission spectra appear at lower and lower temperatures. This model nicely accounts for the data, but the crucial assumption is that energy transfer occurs readily in the solid state. There are, however, good precedents for this behavior, particularly when the excitation involves IL excited states of aromatic ligands.[4,16–18] With IL excitation, the extent

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of structural reorganization and the barrier to energy transfer are frequently minimal. Regarding the structure of the trap center, some type of intermolecular interaction such as trpy–trpy stacking is very likely to be responsible for the red shift in the solid-state emission spectrum. Miskowski and Houlding have proposed that interligand interactions of this type can give rise to very large red shifts as well as the loss of vibrational structure.[7] On the other hand, in their studies of platinum(II) isobiquinolines, Kato et al. reported finding much smaller red shifts and emission with residual vibrational structure.[19] Kato et al. also found that the ^{3}IL emission from a mixed-ligand, dicyanide derivative exhibited multiple origins, consistent with the possible participation of trap centers.

The [Pt(trpy)Cl]A Systems in the Solid State. Extended interactions often have a profound influence on the optical and electrical properties of platinum(II) complexes in the solid state.[20] In the [Pt(trpy)Cl]A systems, this is evident from the influence the anion A has on the color of the material, as the energy of the MMLCT absorption varies with the metal-metal separation.[20-22] In particular, the effective intermolecular separation is clearly larger in the case of the yellow SbF_6^- derivative compared with the orange $CF_3SO_3^-$ compound. Figure 4 shows that the same effect is evident in the emission spectra, where the emission appears at significantly longer wavelengths when triflate is the anion. Moreover, the shift increases at lower temperatures almost certainly because of a further decrease in the mean platinum–platinum separation.[23] In contrast, the emission from what is probably a monomeric platinum center in the SbF_6^- salt occurs at significantly higher energy, and the maximum is effectively temperature independent. In this context, it is worth noting that Bailey et al. found that the apparently very similar, yellow PF_6^- salt exhibited a much longer wavelength emission maximum at room temperature.[7] However, they also reported that the emission underwent a blue shift at lower temperatures, down to about 160 K, and that at still lower temperatures a new emission signal emerged with a maximum at ca. 565 nm. The important point is that their low-temperature emission signal paralleled the signal we observed from the SbF_6^- analogue. The simplist way to reconcile the data for the PF_6^- system is to assume that the longer-wavelength emission, which was no longer evident at 100 K, originated at a trap site. This phenomenon provides another explanation for the fact that similar platinum(II) materials, or even different preparations of the same material, may exhibit distinct emissions. As a further illustration, consider the [Pt(trpy)Cl]CF_3SO_3 system. We observed a red shift in the emission maximum at lower temperatures whereas Bailey et al. reported a blue shift for the same compound. However, both groups observed similar emission spectra at the lowest temperatures.

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Supporting Information Available: Tables of complete atomic coordinates and isotropic thermal parameters, non-hydrogen anisotropic temperature factors, bond distances, and bond angles (7 pages). Ordering information is given on any current masthead page.

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Remarkable substituent effects on the photophysics of $Pt(4'\text{-}X\text{-}trpy)Cl^+$ systems (trpy = 2,2′:6′,2″-terpyridine)

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Abstract

In view of the interest in probing the binding interactions that occur between platinum complexes and biological macromolecules, the aim of this work has been to develop systems that exhibit enhanced excited-state lifetimes and emission yields in fluid solution. The investigation focuses on a series of complexes of the type $Pt(4'\text{-}X\text{-}T)Cl^+$ where 4′-X-T denotes a 4′-substituted derivative of 2,2′:6′,2″-terpyridine. In all cases the counterion is the non-coordinating ion tetrakis[3,5-bis(trifluoromethyl)phenyl]borate. The substituents employed include electron-withdrawing groups like CN and SO_2Me as well as electron-donating groups like SMe and NMe_2. Within the series of complexes, the first reduction wave ranges over about 0.7 V in DMF. Although the process probably entails ligand reduction, the acceptor orbital appears to have some platinum 6p, character. Even though electron-donating substituents destabilize the reduced form of the ligand, all substituents induce a red-shift in the charge-transfer (CT) absorption band system that occurs around 400 nm. Furthermore, there is generally an increase in the CT absorption intensity, the emission lifetime and the emission quantum yield in methylene chloride. Thus, at room temperature, the complex with the terpyridine ligand itself is a very poor emitter with an emission lifetime of 10 ns or less, while the $Pt(4'\text{-}SMe\text{-}T)Cl^+$ and $Pt(4'\text{-}NMe_2\text{-}T)Cl^+$ systems exhibit lifetimes of 140 ns and 1.9 μs, respectively. With the electron-donating substituents in particular, the lifetime enhancement reflects a configuration interaction between the original CT state and an intraligand charge-transfer excited state. Substituents also influence a thermally activated pathway to radiationless decay.

Keywords: Luminescence; Photophysics; Platinum complexes; Terpyridine complexes

1. Introduction

The binding interactions that complexes of platinum(II) with polypyridine ligands undergo with DNA [1–5] and globular proteins [6] have helped fuel interest in these systems. In addition, the platinum(II) materials themselves show interesting electronic properties in the solid state including photoluminescence [7–10]. The observation of photoluminescence in fluid solution is a rarer phenomenon, but there are some recent reports of emission from monomeric platinum(II) polypyridine complexes [11–15]. In the present context, the most relevant systems are $Pt(trpy)OH^+$, where trpy denotes the 2,2′:6′,2″-terpyridine ligand [13], and a $Pt(4'\text{-}R\text{-}trpy)Cl^+$ series, where R = C_6H_4OMe-*p*, C_6H_4Me-*p*, C_6H_4Br-*p* or C_6H_4CN-*p* [15]. When the emission originates in a metal-to-ligand charge-transfer (CT) excited state, the intensity and the lifetime vary dramatically with the solvent probably in large part because of the availability of open coordination sites at the metal center [13]. Reductive quenching of the CT state is also common [5,15]. For $Pt(trpy)L^{n+}$ systems, the luminescence properties are particularly sensitive to the nature of ligand L [13,15], due perhaps to a variation in the efficiency of radiationless decay via a thermally accessible d–d excited state [13,16]. In the case of the $Ru(trpy)_2^{2+}$ system, which shares some properties in common with platinum(II) terpyridines, the systematic exploration of substituent effects has provided useful insights into the photochemistry and photophysics [17–19]. Those reports provided the impetus for the following spectroscopic and electrochemical studies of a series of complexes of the type $Pt(4'\text{-}X\text{-}T)Cl^+$, where 4′-X-T denotes the trpy derivative with substituent X in the 4′ position. The most intriguing finding is that the introduction of an electron-donating group

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can dramatically enhance the emission yield and the lifetime as a consequence of the admixture of intraligand excited state character that occurs in the emitting state.

2. Experimental

2.1. Materials

Aldrich supplied 2,2':6',2"-terpyridine, 4'-chloro-2,2':6',2"-terpyridine, potassium tert-butoxide, 2-acetyl pyridine, carbon disulfide, methyl iodide, ammonium acetate, methyl magnesium bromide, selenium dioxide, potassium cyanide, *m*-chloroperoxybenzoic acid, 4-morpholineethanesulfonic acid (MES), 3,5-bis(trifluoromethyl)bromobenzene, hexamethylphosphoramide (HMPA) and tetrabutylammonium hexafluorophosphate (TBAH). The $ZnCl_2$ came from Mallinckrodt. Janssen Chimica supplied boron trifluoroetherate. Baxter supplied B&J brand high purity solvents for spectroscopic measurements (acetonitrile, *N,N*-dimethylformamide and methylene chloride). Other solvents were reagent grade. The K_2PtCl_4 was a gift from Johnson Matthey. The purity of most materials was satisfactory as received. In the case of TBAH, a series of three recrystallizations from ethanol gave a pure compound.

2.2. Methods

The methods reported by Potts et al. provided routes to the trpy derivatives 4'-thiomethyl-2,2':6',2"-terpyridine (4'-SMe-T), 4'-methylsulfonyl-2,2':6',2"-terpyridine (4'-SO_2-Me-T), 4'-methyl-2,2':6',2"-terpyridine (4'-Me-T) and 4'-cyano-2,2':6',2"-terpyridine (4'-CN-T) [20,21]. An adaptation of the procedure of Gupton et al. gave 4'-dimethylamino-2,2':6',2"-terpyridine (4'-NMe_2-T) [22]. For the synthesis of each [Pt(4'-X-T)Cl]Cl form, the reaction of Pt(COD)Cl_2 with the appropriate trpy derivative (4'-X-T ligand) gave the desired product in ~75% yield [23,24]. The preparation of the counter ion tetrakis[3,5-bis(trifluoromethyl)phenyl]borate (TFPB) followed the procedure published by Nishida et al. [25]. Finally, the addition of an ethanolic solution of the sodium salt of TFPB to an aqueous solution of the chloride salt of $Pt(4'\text{-X-T})Cl^+$ yielded the desired material [Pt(4'-X-T)Cl]TFPB. Microanalysis and proton NMR data showed that recrystallization from toluene/methylene chloride typically yielded a hemisolvate containing toluene. Microanalysis of [Pt(4'-X-trpy)Cl]TFPB·Y, where Y = toluene: (X = NMe_2·0.5 toluene): *Anal.* Calc.: C, 44.53; H, 2.28; N, 3.95%. Found: C, 44.25; H, 2.32; N, 3.73%. (X = CN·0.75 toluene): *Anal.* Calc: C, 45.0; H, 1.98; N, 3.9. Found: C, 44.85; H, 1.98; N, 3.84%. (X = SO_2Me·0.5 toluene): *Anal.* Calc: C, 42.62; H, 1.98; N, 2.89. Found: C, 42.92; H, 2.06; N, 2.88%. (X = SMe): *Anal.* Calc: C, 41.98; H, 1.83; N, 3.06. Found: C, 41.59; H, 1.80; N, 2.90%. The procedure of Hill et al. yielded the Zn(4'-X-T)Cl_2 derivatives without need for further purification [26].

A three electrode cell served to obtain the cyclic voltammetry data. In particular, the working electrode was a gold disc, the auxiliary electrode was a Pt wire and the reference electrode was a AgCl/Ag electrode in contact with 3 M NaCl(aq.). For reporting purposes ferrocene served as an internal reference and exhibited a potential of 0.57 V versus AgCl/Ag. The electrolyte solution was 0.1 M TBAH in DMF. This was the solvent of choice because the platinum complexes gave relatively clean waves in this medium, and the zinc complexes showed good solubility. A simple purge with dinitrogen gas sufficed to remove dissolved dioxygen from the sample. The scan rate was usually 50 mV s^{-1}.

For the luminescence studies, a stream of Ar gas acted as the deoxygenating agent. During spectral measurements, the slit settings were 10 nm for both the excitation and emission beams. For emission spectra a 400 nm long-wave-pass filter removed the scattered light, usually at an excitation wavelength of 375 nm. In the case of the lifetime studies the excitation wavelength was either 440 or 420 nm, and the long-wave-pass filter had a cutoff of 475 nm. The laser dye was Coumarin 440 or Stilbene 420, and the solvent for NMR spectra was $CDCl_3$. Dr H. Daniel Lee of Purdue University carried out the microanalyses.

2.3. Instrumentation

The spectrophotometer was a Perkin-Elmer Lambda 4C, and the spectrofluorometer was a SLM-Aminco SPF-500C. For variable temperature measurements the cryostat was an Oxford Instruments model DN1704 system with controller. Descriptions of the procedure and equipment for measuring lifetimes are in the literature [27]. The sweep unit for the electrochemical measurements was a model CV-27 cyclic voltammograph from Bioanalytical Systems.

3. Results

3.1. Electrochemistry

In accord with other platinum(II) complexes of heteroaromatic ligands, the $Pt(4'\text{-X-T})Cl^+$ systems show two ligand reduction waves separated by about 0.6 V in DMF [26,28,29], whereas anodic scans out to the solvent limit gave no indication of platinum oxidation. The potential of the first reduction varies by as much as 0.7 V with the change in the 4' substituent, whereas the effect on the second reduction is somewhat smaller (Table 1). The second wave is chemically less reversible in that it shows a greater difference in the cathodic and anodic currents. The Zn(4'-X-T)Cl_2 analogues also give well-resolved reduction waves that are substituent dependent. In line with the results of Hill et al. who studied the two parent complexes [26], the potential of the

Table 1
Reduction potentials in DMF vs. ferrocene [a]

X	E_1 (V)	E_2 (V)
Zn(4'-X-T)Cl₂		
CN	−1.43 (60, 1.0) [b]	
SO_2Me	−1.45 (100, 1.4)	
H	−1.86 (70, 1.7)	
SMe	−1.89 (60, 1.4)	
Me	−1.91 (60, 4.0)	
NMe_2	−2.12 (70, 1.5)	
Pt(4'-X-T)Cl⁺		
CN	−0.92 (60, 1.2) [b]	−1.56 (60, 1.4) [b]
SO_2Me	−0.98 (60, 1.3)	−1.58 (60, 1.3)
H	−1.24 (70, 1.2)	−1.82 (70, 1.6)
SMe	−1.28 (60, 1.2)	−1.79 (60, 1.5)
Me	−1.30 (70, 1.2)	−1.87 (70, 1.9)
NMe_2	−1.53 (70, 1.2)	−1.97 (60, 2.5)

[a] From cyclic voltammetry scans at 50 mV s^{-1} in DMF containing 0.1 M TBAH at 23°C.
[b] $E_{pc} - E_{pa}$ (mV), i_c/i_a.

first ligand reduction is ~0.5 V more negative for the zinc complex than it is for the corresponding platinum system.

3.2. Spectroscopy and photophysics

Solutions of the [Pt(4'-X-T)Cl]TFPB compounds are stable in methylene chloride for short periods of time; however, decreases in the near-UV absorption intensity begin to be apparent after 5–6 h. All reported data refer to freshly prepared solutions, except for the low-temperature data where the course of the experiment required ~6 h. As reported previously for the parent trpy complex [9,13], and for the 4'-phenyl-substituted complexes [15], the $Pt(4'\text{-}X\text{-}T)Cl^+$ systems exhibit one series of intraligand π–π^* absorptions centered around 280 nm and another around 320 nm (Fig. 1). Fig. 2 shows that $Zn(4'\text{-}X\text{-}T)Cl_2$ systems exhibit a similar series of UV absorption bands. Table 2 contains a compilation of absorbance data for the $Pt(4'\text{-}X\text{-}T)Cl^+$ complexes in two solvents. In addition to the π–π^* absorptions, the platinum systems exhibit lesser intensity CT absorption bands in the vicinity of 400 nm. Due to a net reduction of the dipole moment in the CT excited state [13,30], the CT transitions occur at shorter wavelengths in polar solvents like acetonitrile. With the exception of the methyl group, which has almost no effect, the introduction of a substituent in the 4' position of the trpy ligand induces a bathochromic shift in the CT absorption network (Table 2). This is true whether the substituent group is electron withdrawing or electron donating. As the results in Table 2 show, the presence of the substituent can greatly enhance the intensity of the CT absorption as well. Similar effects are evident in the spectra of 4'-phenyl-substituted $Pt(trpy)Cl^+$ systems [15].

At room temperature, the emission intensity and the lifetime vary dramatically with the nature of the 4' substituent as well as the solvent. Apart from the 4'-NMe_2-T derivative, none of the complexes listed in Table 2 gives a significant emission signal in the room temperature acetonitrile. For the most part, the complexes are emissive in methylene chloride, although the signal is extremely weak for $Pt(trpy)Cl^+$ itself and virtually non-detectable for the closely related 4'-Me-T system. In accordance with the CT absorption data, the introduction of a substituent at the 4' carbon of the trpy ligand generally causes the emission spectrum to shift to lower energy; however, the emission spectra all appear at rather similar wavelengths. For each system the emission shows well resolved vibrational structure, mono-exponential emis-

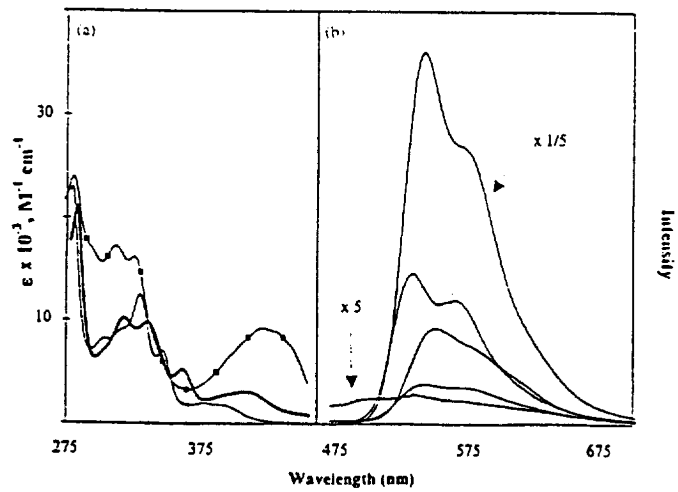

Fig. 1. (a) Near-UV absorption spectra of selected $Pt(4'\text{-}X\text{-}T)Cl^+$ complexes in MeCN at 23°C: X = NMe_2 (–■–), X = CN (–, thick trace), X = H (–, thin trace). (b) Uncorrected emission spectra of $Pt(4'\text{-}X\text{-}T)Cl^+$ systems in CH_2Cl_2 at 23°C. The samples all had the same absorbance at the excitation wavelength of 375 nm. In order of increasing intensity at 550 nm the spectra correspond to X = H, SO_2Me, CN, SMe and NMe_2, respectively.

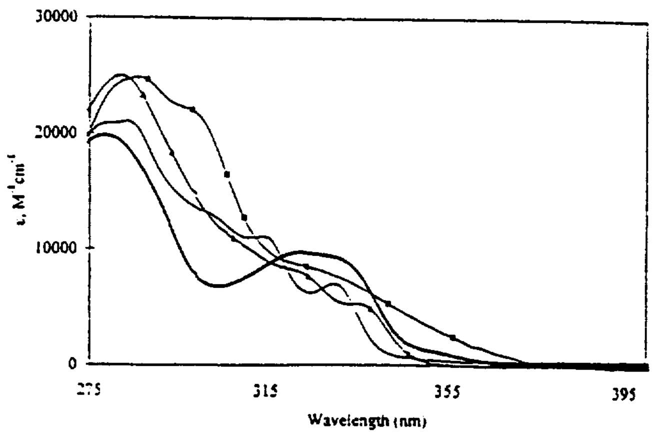

Fig. 2. Near-UV absorption spectra of Zn(4'-X-T)Cl_2 compounds in DMF at 23°C. The samples have X = NMe_2 (–■–), X = SMe (–▲–), X = Me (–, thin trace) and X = CN (–, thick trace).

sion decay and an excitation spectrum that matches the absorption spectrum. See Fig. 1(b) for some representative spectra. Except for the 4'-Me-T system, the introduction of an electron-withdrawing group or an electron-donating group at the 4' position of the trpy ligand enhances the lifetime and the emission quantum yield (Table 2). The most dramatic instance is the 4'-NMe_2-T derivative which has an emission lifetime in the microsecond regime. In view of the emission

Table 2
Absorption and emission data from Pt(4'-X-T)Cl^+ systems at 23°C

X	λ_{abs} (nm)		Emission data [a]		
	MeCN	CH_2Cl_2	λ_{max} (nm)	Φ_{em}	τ (ns)
CN		311sh			
	316	323	550	0.005	116
	335	345	590sh		
	(13 800) [b]				
	361	366			
	394	405sh			
	409 (3920)	428			
SO_2Me	316	325	542	0.002	21
	336 (15 200)		577		
	358	348			
	385	380			
	403 (3650)	430			
H	303	305	500	0.0004	< 10
	316	320	535		
	330 (14 200)	340	590		
	346				
	377 (2200)	390			
	390sh	403			
SMe	320	305	542	0.006	142
	333 (17 900)	330	575		
	388	400	625sh		
	409 (7750)	425			
Me	282	284			
	302	308			
	316 (10 100)	322			
	329	336			
	343 (6530)	352			
	374	386			
	390 (2240)	404			
NMe_2	280	282	535	0.08	1920
	311 (17 000)	316	570		
	324 (16 000)	346sh	635sh		
	340sh	420			
	419 (9290)	444			

[a] Emission measurements in CH_2Cl_2.
[b] Molar absorptivity (M^{-1} cm^{-1}).

lifetimes there is little doubt but that in all cases the emission originates from a state with triplet multiplicity. The presence of the well resolved vibronic structure is quite striking and contrasts with the broad emission attributed to metal-to-ligand ^{3}CT excited states of related platinum(II) terpyridine complexes [13,15]. It is entirely possible that the vibronic structure reflects the fact that the emission emanates from states that have significant intraligand excited-state character, vide infra.

Temperature-dependent lifetime measurements were only possible over a limited temperature range since methylene chloride is a non-glassing medium. The lack of long-term sample stability was another complication. The complexes selected for detailed studies were Pt(4'-SMe-T)Cl^+ and Pt(4'-CN-T)Cl^+. For each complex the data satisfies the following phenomenological equation for the temperature dependence of the lifetime:

$$1/\tau = k_0 + A\exp[-\Delta E/(RT)] \tag{1}$$

The best fit of the data for the 4'-SMe-T complex has a limiting lifetime (k_0^{-1}) of 2.5 μs, a frequency factor (A) of 1.3×10^{10} s^{-1} and an apparent activation energy (ΔE) of 1640 cm^{-1}. The corresponding parameters for the 4'-CN-T complex are 0.25 μs, 1.8×10^{8} s^{-1} and 730 cm^{-1}.

4. Discussion

The goals of this investigation have been to understand the electronic structure of the platinum(II) terpyridine complexes and to develop systems with longer excited state lifetimes. The parent complex $Pt(trpy)Cl^{+}$ shows no significant photoluminescence intensity in room temperature acetonitrile, although the mixed-ligand trpy complexes that have thiocyanate or hydroxide in place of the chloride ligand are emissive [13]. The systems selected for the present studies involve modified trpy ligands and are freely soluble with TFPB as the counterion in the non-coordinating medium methylene chloride. Although not the principal focus of this work, the electrochemistry of the complexes is germane to the interpretation of the CT spectra. The most important point to recognize is the strong influence substituents have on the first ligand reduction. Electron-donating substituents like SMe or NMe_2 shift the potential in the negative direction, while electron-accepting substituents like CN have the opposite effect.

4.1. Intramolecular charge transfer

As noted above, the absorption bands with $\lambda_{max} > 350$ nm and $\epsilon > 1000$ M^{-1} cm^{-1} normally correspond to platinum-to-trpy MLCT transitions and therefore involve a type of ligand reduction [13,30]. These band assignments are consistent with the shifts that occur with a change in solvent polarity or the spectator ligand. Comparisons with the low-temperature emission from systems like $Ru(trpy)_2^{2+}$ also reveal that the lifetime and the Stokes shift are compatible with photoluminescence from a corresponding ^{3}CT state [13,31]. Finally, the population of a metal-to-ligand CT state can account for the pronounced emission quenching that occurs in donor solvents like acetonitrile. Due to the increase in the metal's formal oxidation state and the availability of open coordination sites, solvent-induced exciplex quenching is likely to be a very efficient process for such CT states [32–34].

One problem with the concept of a low energy metal-to-ligand CT excited state is the absence of a well defined wave corresponding to the oxidation of the metal center. However, a compensating effect is the fact that the first trpy reduction occurs at an unusually positive potential. Previous investigators have attributed this to a mixing interaction involving the relatively low-lying $6p_z$ orbital of platinum and an empty π^* orbital of the polypyridine ligand [26]. This requires that the redox-active π^* orbital (assumed also to be one in the same as the spectroscopically active π^* orbital) be antisymmetric with respect to a rotation about the two-fold axis that passes through the ligand. In the notation of Orgel, the symbols ψ and χ designate orbitals that are respectively antisymmetric and symmetric with respect to the two-fold rotation operation [35,36]. Extended Huckel calculations show that the LUMO of the trpy ligand has ψ symmetry [37], and mixing with the higher energy $6p_z$(Pt) orbital would tend to drive the energy of the corresponding molecular orbital of the complex to even lower energy. The fact that the first ligand reduction is so sensitive to substitution at the 4' position of trpy is certainly consistent with this interpretation. Thus, mesomeric interactions with donor groups like NMe_2 or acceptor groups like CN depend upon overlap with the $p\pi$ orbital of the 4' carbon atom, and this requires an orbital with ψ symmetry. Table 1 reveals that the potential of the second ligand reduction is less sensitive to 4' substituents. This could mean that the electron enters a ligand orbital with a different symmetry or that this reduction involves a metal-centered orbital [26]. In terms of the spectroscopy, the fact that the introduction of a 4' CN or SO_2Me group induces a bathochromic shift in the CT absorption and emission maxima is easy to appreciate because formation of the excited state at least formally entails a ligand reduction. It is no surprise that an electron-withdrawing group would facilitate the process. However, electron-donating groups like NMe_2 and SMe also shift the CT maxima to lower energy, so there are obviously other factors involved. Indeed, a number of recent studies have made the point that CT processes are not just one-electron, center-to-center charge transfers [38,39].

For the platinum(II)–trpy systems at hand, particularly those with electron-donating substituents, the following analysis suggests that a configuration interaction with another CT state has a major influence on the state energies. The literature dealing with substituent effects and the absorption spectrum of benzene illustrate the phenomenon and serve as a useful basis for comparison [40,41]. The important point is that the introduction of either an electron-withdrawing or an electron-releasing substituent induces a red shift in the low energy π–π^* absorption of benzene. For example, the lowest energy $^1\pi$–π^* transition, the so-called α band, occurs around 250 nm in the spectrum of benzene whereas for aniline the corresponding band falls around 285 nm. The reason is clear if one views aniline as a composite molecule containing a benzene ring and a peripheral nitrogen center with an active lone pair [40]. In essence, a configuration interaction with a higher lying nitrogen-to-ring CT state drives down the energy of the π–π^* state that is the terminus of the α transition and, at the same time, enhances the oscillator strength. The same kind of effect is evident in the $Pt(4'\text{-SMe-T})Cl^{+}$ and $Pt(4'\text{-NMe}_2\text{-T})Cl^{+}$ systems which exhibit anomalously intense, but relatively low energy CT transitions. Note that the red shifts occur despite the fact that the 4' substituents are electron donating and destabilize the reduced forms of the respective ligands. The UV spectra of the $Zn(4'\text{-X-T})Cl_2$ analogues

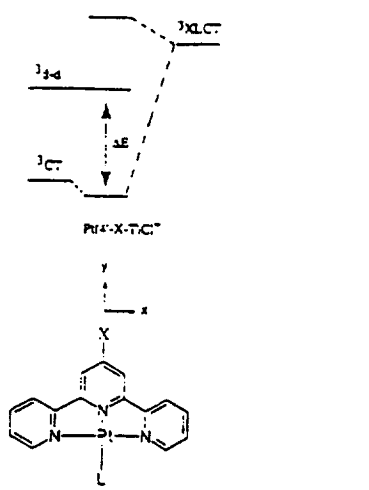

Fig. 3. Axis system and scheme for a configuration interaction between the emitting ^{3}CT state and a ^{3}XLCT intraligand excited state of Pt(4'-X-T)Cl$^+$. The relative energy of the ^{3}d–d state is uncertain, but it may be the thermally accessible state that mediates decay.

are useful for the identification of the participating substituent-to-trpy (XLCT) transitions since there are no interfering MLCT phenomena. Indeed, Fig. 2 shows that, by comparison with Zn(4'-Me-T)Cl$_2$, both the 4'-SMe and the 4'-NMe$_2$ complexes exhibit extra absorption intensity in the region of 290 nm that plausibly reflects XLCT excitation.

The structure given in Fig. 3 is useful for assessing the CT coupling phenomenon. Although the two-fold axis normally defines the z-direction in C_{2v} symmetry, the connections with archetypical D_{4h} complexes are more evident with the proposed choice of axes. However, apart from $d(x^2-y^2)$, the relative order of the d orbitals is unclear in these polypyridine complexes [13,42]. Fortunately, intensity considerations are of some help in making band assignments. According to a simple model, the CT transitions that benefit from the charge-transfer term usually exhibit the bulk of the absorption intensity [43–45], and here these correspond to the y-polarized $d(zy) \rightarrow \psi$ and $d(xz) \rightarrow \chi$ transitions to $^1A_1$ excited states [13]. In view of the voltammetry data, the transition to the ψ orbital should occur at lower energy. Despite our earlier reservations [13], the CT absorption that occurs in the vicinity of 380 nm for Pt(trpy)Cl$^+$ appears to be intense enough to represent, or include, the $d(zy) \rightarrow \psi$ transition. For comparison, the reported values of the molar absorptivity of the corresponding visible band of Ru(trpy)$_2^{2+}$, which contains twice as many acceptor ligands, range from 10 000 to 16 000 M^{-1} cm^{-1} [19,31,46]. Thus, the CT absorption intensity is of the same order of magnitude for the platinum system. Since the y-polarized XLCT transition from the lone pair of the NMe$_2$ group also gives rise to a $^1A_1$ excited state, the interaction between the two zero-order $^1A_1$ states produces the state with the absorption maximum at 420 nm in the spectrum of Pt(4'-NMe$_2$-T)Cl$^+$. A simple vector coupling argument based on the collinear transition moments accounts for the increase in the absorption intensity [40]. Exactly the same argument applies to the SMe analogue. By analogy with aniline, there is likely to be further mixing with a π–π^* state with $^1A_1$ symmetry. In principle, the same kind of coupling is possible with a ligand-to-metal or a ligand-to-ligand CT state involving the ligand L opposite trpy [1,12]. And when X is electron-withdrawing, coupling to a trpy-to-X state can be important. However, a simple inductive argument is capable of explaining the absorption and the emission data pertaining to the 4'-CN-T and 4'-SO$_2$-T systems, and the absorption spectra of the corresponding Zn(4'-X-T)Cl$_2$ systems do not show any indication of that kind of a CT transition. Nevertheless, the emission from Pt(4'-CN-T)Cl$^+$ occurs at a lower energy than that of the Pt(4'-NMe$_2$-T)Cl$^+$ system. This is not a cause for concern because configuration interaction undoubtedly has a weaker influence on the energy of the triplet state of the 4'-NMe$_2$-T complex. For sure, the dipole–dipole coupling between the two excitations is negligible in the triplet manifold due to the spin forbidden character of each of the CT processes.

4.2. Emission intensities and lifetimes

Contrary to the energy-gap law [47], the unsubstituted trpy complex has the highest energy emission but practically the shortest excited-state lifetime in the whole series. The only system that appears to have a shorter lifetime is the 4'-Me-T complex, and it, too, has a high energy CT absorption. These results are incompatible with direct relaxation from a homologous series of metal-to-ligand CT states [48], but they make sense if another state influences the decay. Suppose that an interaction with another state alters the orbital parentage to differing degrees within the series. Then, the intrinsic lifetimes vary in a way that does not simply depend on the excited state energy. Alternatively, there may be substituent-dependent deactivation through a thermally accessible excited state. The preliminary lifetime-versus-temperature results suggest that both effects are probably important. Although there is clear evidence of thermally activated decay, the nature of the state mediating decay is uncertain. In principle, the state involved could reside within the same potential energy surface. With certain copper(II) and zinc(II) porphyrins, for example, thermal population of vibrationally excited levels of the emitting state fosters decay [49–51]. The same effect can operate in the Pt(4'-X-T)Cl$^+$ systems if the resonance with the intra-ligand excited state alters the shape and/or the equilibrium geometry of the excited-state potential energy surface [52]. Although this mechanism is plausible, the presence of the vibrational structure in the emission spectra suggests that the excited-state surface nests within that of the ground state. If so, vibrationally induced relaxation is unlikely to be of great consequence.

In view of other reports dealing with emissive ^{3}CT states of platinum(II) polypyridines and related systems [13,16,19], it seems more likely that the systems deactivate via a short-lived ^{3}d–d state. The fact that electron-donating substituents could hinder such a pathway is interesting. In the course of their studies of the related Ru(4'-X-T)$_2^{2+}$ systems, Maestri et al. have reported that an electron-donating substituent lowers the energy of the first ^{3}d–d state and thereby reduces the barrier to quenching [19]. This makes sense in terms of the orbitals involved. While the lowest unoccupied orbital of the ruthenium system is a dσ^* orbital, the highest occupied orbital is a dπ orbital. The inductive effect of an electron-donating group should destabilize the dσ^* orbital, but the substituent can destabilize the dπ orbital even more because of direct conjugation via the trpy π orbital. With two trpy ligands involved, the upshot is that the deactivating ^{3}d–d state drops to lower energy relative to the ^{3}CT state so that quenching is more efficient. For platinum(II) polypyridines the relative energies of the d orbitals are less certain, but the filled d(z^2) orbital is probably the next highest energy level in these planar systems, in keeping with the importance metal–metal interactions have on packing and the electronic properties [7,8]. Thus, the HOMO and the LUMO of the metal center appear to have dσ^* character so that an electron-donating substituent destabilizes both. If so, the effect on d(x^2-y^2) is likely to be greater due to better overlap with the nitrogen-donor orbitals of the ligand. The upshot would be an increase in the energy of the d–d state as well as ΔE, the activation energy for radiationless decay. However, in view of the uncertain influence that other factors such as configuration interaction with the intraligand excited state have, the diagram in Fig. 3 assumes that the energy of the lowest energy ^{3}d–d state remains essentially constant. Due to the drop in the energy of the emitting CT state, there is still a net increase in the energy required for deactivation via the metal-centered excited state. By the same kind of reasoning, the inductive effect associated with an electron-withdrawing substituent should stabilize the ^{3}d–d state. The effect on the emitting ^{3}CT state is also stabilizing, but even if there is a net increase in ΔE, the effect will not be as dramatic as it is in the case of an electron-donating substituent. The results in Table 2 are obviously in accord with these qualitative predictions based on the assumption of a thermally accessible ^{3}d–d state. On the other hand, the analyses of the temperature-dependent lifetime data yield modest frequency factors. The values obtained are indicative of nested surfaces or perhaps reversible population of the deactivating state [18,53]. Surer identification of the state that mediates the decay will require a great deal more experimental work.

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Cooperative Substituent Effects Influence the Excited States of Copper Phenanthrolines

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ABSTRACT

Although copper systems are attractive as potential photosensitizers because of the ready availability of the metal, efficient nonradiative decay and solvent-induced quenching phenomena ordinarily limit their utility. Emission studies show that methyl substituents in the 3,8 positions constrain bulky groups in the 2,9 positions of 1,10-phenanthroline so as to enhance the lifetime of the reactive charge-transfer excited state of bis-ligand copper(I) complexes. Whereas, photoexcited $Cu(dbtmp)_2^+$ has a lifetime of 330 ns in dichloromethane, the parent complex without the 3,8 methyl substituents has a lifetime of only 150 ns under the same conditions. (dbtmp = 2,9-di(*n*-butyl)-3,4,7,8-tetramethyl-1,10-phenanthroline) Even in a strongly donating solvent like dimethylformamide, the dbtmp complex exhibits an excited-state lifetime of 140 ns. In dichloromethane the complex with the 2,9-diphenyl-3,4,7,8-tetramethyl-1,10-phenanthroline ligand exhibits a lifetime of 480 ns, the longest decay time yet reported for a bis-phenanthroline copper(I) complex in room temperature, fluid solution.

INTRODUCTION

Substituent effects have come to the fore in the development of the chemistry of copper(I) with 1,10-phenanthroline derivatives. (In the following phen denotes the 1,10-phenanthroline ligand itself, and NN designates a generic derivative.) A seminal finding was that the presence of moderately bulky substituents in the 2,9 ring positions enhances the selectivity for copper(I) binding and stabilizes the copper(I) oxidation state.[1,2] Subsequent work has shown that incorporation of bulky substituents in the 2 and 9 positions also enhances the energy, the intensity and the lifetime of the emission from the lowest energy metal-to-ligand charge-transfer (CT) excited state.[3,4,5] One reason is that bulky substituents inhibit a flattening distortion that often occurs in the excited state and promotes nonradiative decay.[3,4,6] Bulky substituents also suppress ligand-addition reactions of the excited state, and formation of a fifth coordinate-covalent bond to the (formally) copper(II) center of the excited state initiates a novel type of exciplex quenching.[7,8,9] In 1983 Dietrich-Buchecker et al. showed that the reactive CT state of $Cu(dpp)_2^+$ is much less susceptible to exciplex formation than that of the less hindered complex $Cu(dmp)_2^+$.[10] (dpp denotes 2,9-diphenyl-1,10-phenanthroline, and dmp denotes 2,9-dimethyl-1,10-phenanthroline.) Subsequent work involving alkyl substituents has shown that the importance of exciplex quenching decreases as follows with a change of substituent:[4]

methyl > *n*-butyl > neo-pentyl > sec-butyl.

However, if the substituents are too bulky, the ground-state complex itself becomes unstable as a result of interligand steric interactions. Thus, attempts to isolate the $Cu(NN)_2^+$ complex carrying tert-butyl or mesityl substituents in the 2 and 9 positions have proved unsuccessful.[11,12] Recently, however, Karpishin and co-workers characterized the complex with the 2,9-bis(trifluoromethyl)-1,10-phenanthroline ligand.[13]

The present report shows that the coexistence of methyl substituents in the 3,8 positions and bulky substituents in the 2,9 positions of the phenanthroline produces a more crowded coordination sphere and dramatically extends the excited-state lifetime. The motivation for the investigation came from a recent study which showed that reductive quenching of the $Cu(tptap)_2^+$ system is extremely facile.[14] (tptap is 2,3,6,7-tetraphenyl-1,4,6,7-tetraazaphenanthroline.) The implication was that juxtapositioning the phenyl substituents lent rigidity to the system and reduced the Franck-Condon barrier to electron-transfer quenching. The ligands employed below are 2,9-di(*n*-butyl)-3,4,7,8-tetramethyl-1,10-phenanthroline (dbtmp) and 2,9-diphenyl-3,4,7,8-tetramethyl-1,10-phenanthroline (dptmp). The emitting CT states of the resulting $Cu(NN)_2^+$ complexes exhibit remarkably long lifetimes even in donor media; indeed, the dptmp system has the longest excited-state lifetime ever measured for a $Cu(NN)_2^+$ system in fluid solution.

EXPERIMENTAL

Materials. Scientific Products was the source of Burdick and Jackson high-purity, distilled-in-glass-grade acetonitrile, N,N-dimethylformamide (DMF), dichloromethane (DCM), and tetrahydrofuran (THF). The laser dye Coumarin 440 came from Laser Science. The phen, dmp, 3,4,7,8-tetramethyl-1,10-phenanthroline (tmp), $CuCl_2 \cdot 2H_2O$, KPF6, 2.0 M solutions of *n*-butyl lithium in hexanes and phenyl lithium in diethyl ether were from Aldrich Chemical Co. G. F. Smith provided the 4,7-dimethyl-1,10-phenanthroline (4,7-dmp). The complexes $[Cu(dbp)_2]PF_6$ and $[Cu(dpp)_2]PF_6$ were on hand from previous studies.[15] (dbp = 2,9-di(*n*-butyl)-1,10-phenanthroline) .

Methods. The general method for the addition of the 2,9 substituents to the appropriate ligand precursor was that of Pallenburg and co-workers.[11] The desired product was typically the first fraction that eluted from an alumina column with DCM as the mobile phase. A published method sufficed for the preparation of all $[Cu(NN)_2]PF_6$ compounds.[16]

2,9-di(n-butyl)-4,7-dimethyl-1,10-phenanthroline (dbdmp). Recrystallization of a pale yellow fraction off the alumina column yielded a white solid. Here and in all subsequent tabulations the chemical shifts are relative to TMS. ^1H NMR ($CDCl_3$, δ in ppm): 7.92 (s, 2H), 7.34 (s, 2H), 3.19 (quartet, 4H), 2.74 (s, 6H), 1.88 (pentet, 4H), 1.51 (sextet, 4H), 1.00 (t, 6H).

2,9-di(n-butyl)-3,4,7,8-tetramethyl-1,10-phenanthroline (dbtmp). The final product was a white solid. ^{1}H NMR ($CDCl_3$, δ in ppm): 7.92 (s, 2H), 3.18 (quartet, 4H), 2.67 (s, 6H), 2.50 (s, 6H), 1.90 (pentet, 4H), 1.55 (sextet, 4H), 1.07 (t, 6H).

2,9-diphenyl-4,7-dimethyl-1,10-phenanthroline (dpdmp). The final product was a pale yellow solid. ^{1}H NMR ($CDCl_3$, δ in ppm): 8.49 (s, 4H), 8.00 (m, 4H), 7.55 (m, 6H), 2.85 (s, 6H).

2,9-diphenyl-3,4,7,8-tetramethyl-1,10-phenanthroline (dptmp). The final product was a cream-colored crystalline solid. ^{1}H NMR ($CDCl_3$, δ in ppm): 8.09 (s, 2H), 7.70 (d, 4H), 7.45 (t, 2H), 7.15 (t, 4H), 2.78 (s, 6H), 2.50 (s, 6H)..

$[Cu(dbdmp)_2]PF_6$•½H_2O. This compound crystallized as an orange solid. Calculated: 61.56% C, 6.58% H, 6.53% N. Found: 61.52% C, 6.55% H, 6.46% N. The ^{1}H-NMR spectrum confirmed the presence of the lattice water.

$[Cu(dbtmp)_2]PF_6$. After recrystallization from water and ethanol, the solid was orange brown. Calculated: 63.67% C, 7.12% H, 6.19% N. Found: 63.60% C, 6.81% H, 6.17% N.

$[Cu(dpdmp)_2]PF_6$·$(CH_3C(O)CH_3)$. Recrystallization of a wine-red material from water and ethanol yielded dark red crystals. Calculated: 63.25% C, 4.08% H, 5.67% N. Found: 63.01% C, 4.15% H, 5.48% N. The ^{1}H-NMR spectrum confirmed the presence of acetone.

$[Cu(dptmp)_2]PF_6$•½H_2O. Precipitation from water and ethanol yielded red needles. Calculated: 67.63% C, 4.97% H, 5.66% N. Found: 67.37% C, 4.74% H, 5.63% N. The ^{1}H-NMR spectrum confirmed the presence of the lattice water.

Prior to luminescence, lifetime, or quenching studies, a series of freeze-pump-thaw cycles removed dioxygen from the samples. A 525 nm long-pass filter protected the photomultiplier tube from stray light, while a 450 nm notch filter helped isolate the excitation wavelength. A user-written program provided fits to the luminescence decay curves, and in all cases, the residual plots justified the use of a single exponential. The internal reference for the NMR spectra was the residual proton signal of the $CDCl_3$ solvent.

Instrumentation. The absorption and emission spectra came from Perkin-Elmer Lambda 4C and SLM SPF 500C spectrophotometers, respectively. A description of the lifetime apparatus is in the literature.[15] The ^{1}H-NMR spectrometer was a 200 MHz Gemini unit. H. Daniel Lee performed the microanalyses at Purdue University.

RESULTS

Table 1 contains absorbance data for the CT transitions of a number of $Cu(phen)_2^+$ derivatives. With or without other substituents present, the introduction of alkyl substituents in the 2,9 positions induces a distinct bathochromic shift in the CT maximum. The length of the carbon chain is not especially critical because $Cu(dmp)_2^+$ absorbs at almost the same wavelength as $Cu(dbp)_2^+$.[4] Substituent effects are smaller at other ring positions. Upon introduction of methyl substituents at the 4,7 or the 3,8 positions, the principal CT absorption band shifts to slightly shorter wavelengths. Combinations of substituents at the 2,3,8,9 positions do, however, strongly impact the emission spectrum. Whereas the dbdmp and the dbp systems exhibit almost the same emission maximum and lifetime in DCM solution, the emission from $Cu(dbtmp)_2^+$ occurs at a shorter wavelength and has a significantly longer lifetime (Table 1).

The dptmp system shows a similar effect in the emission spectrum and is no less interesting from the point of view of absorption. Figure 1 reveals that the absorption spectrum exhibits a maximum at 467 nm in DCM as well as a rather weak shoulder at longer wavelengths. In contrast, the spectrum of the dpp or the dpdmp analogue has a maximum at ca. 440 nm and prominent shoulder at around 560 nm (Figure 1).

Independent of the ligand, the absorption maximum remains constant, but the emission maximum shifts to lower energy in polar solvents like DMF or acetonitrile (Table 2). The emission lifetime is also sensitive to the solvent, but it does not correlate with the polarity. Thus, the emission lifetime of $Cu(dbtmp)_2^+$ or $Cu(dptmp)_2^+$ is about the same in DCM or acetonitrile but much shorter in DMF. Most notably, the lifetime of the dptmp system in DCM is the longest yet reported for a $Cu(NN)_2^+$ system in room-temperature, fluid solution.

DISCUSSION

Absorption spectra. The shape of the visible absorption spectrum provides important insights into the structure present in solution. Characteristically, $Cu(NN)_2^+$ systems with approximate D_{2d} symmetry exhibit an intense CT maximum in the neighborhood of 450 nm along with a weak shoulder at longer wavelengths. Both transitions relate to terms associated with the same HOMO → LUMO excitation.[17,18] However, in order to account for the existence and the polarization of the low-energy shoulder, it is necessary to invoke a static or dynamic flattening distortion.[17,18] The data in Table 1 show that all complexes with *n*-butyl substituents in the 2,9 positions as well as $Cu(dptmp)_2^+$ exhibit spectra that conform to this classic pattern. In contrast, the anomalous intensity of the shoulder in the spectrum of the dpp or the dpdmp complex (Figure 1) reveals that some systems assume a highly flattened structure in solution. Crystallographic reports establish that a significant distortion is possible. Thus, in the solid state the dihedral angle between the two phenanthroline cores of the dpp system deviates 10 - 20° from the ideal value of 90° (D_{2d} symmetry), depending on the counterion.[19,20] Even larger distortions are possible because the dihedral angle of the copper(II) analogue is 118.9°.[20] The balance of forces includes steric effects and π conjugation between the phenyl substituents and the attached phenanthroline.[19] Such resonance is not possible in the D_{2d} structure which requires a 90° torsion angle for the two phenyl substituents. In the case of the dptmp complex the 3,8 methyl substituents should certainly promote the D_{2d} structure as they tend to enforce a 90° torsion angle for each phenyl substituent.

The wavelength of the CT absorption maximum varies markedly with the substituents present at the 2,9 positions of the phenanthroline. However, the basis for the variation is not clear.[21] The fact that the transition tends to shift to longer wavelength as the size of the substituent increases seems surprising. One might expect larger substituents to lead to longer Cu-N distances and higher-energy CT absorptions. The reason is that the excited state formally involves copper(II), an oxidation state that favors shorter Cu-N bond distances.[20] The CT absorption energy is not solvent dependent because the $Cu(NN)_2^+$ system does not have a ground-state dipole moment that can specifically polarize the medium.

Photophysical data. The marked influence the 3,8 methyl substituents have on the luminescence is undoubtedly a steric effect. Whereas methyl substituents in the 4,7 positions have relatively little impact, methyl substituents in the 3,8 positions significantly restrict the conformational freedom of groups in the 2,9 positions. In the case of the dbtmp complex, for example, this is equivalent to increasing the effective size of the *n*-butyl groups. Consequently, the emission energy and the excited-state lifetime increase due to a reduction in structural relaxation. With phenyl groups in the 2,9 positions, the dptmp system exhibits an even longer excited-state lifetime. Till now, the dsbp complex had the longest reported lifetime (400 ns) for a photoexcited $Cu(NN)_2^+$ system in fluid solution.[4] (dsbp denotes 2,9-di(sec-butyl)-1,10-phenanthroline.) Aside from having a longer lived excited-state, the dptmp system is a better benchmark because the dsbp complex exists as a mixture of optical isomers.

Unlike the absorption, the emission is quite sensitive to the solvent medium. One obvious effect is the decrease in the emission energy as the dielectric constant increases. The probable explanation is that the CT state develops a dipole moment and Cu^{2+}-$(NN)^-$ character as the excitation localizes in the π^* orbital of one of the ligands.[22] Consequently, polar media more effectively solvate the relaxed CT state, and this produces a decrease in the emission energy. However, the same effect is not responsible for the trend in lifetimes because the emission from $Cu(dbtmp)_2^+$ occurs at the same wavelength in acetonitrile and DCM, yet the lifetime is much shorter in DMF. Solvent-induced exciplex quenching is evidently also a significant factor. As the Gutmann donor numbers reveal,[23] DMF is a much stronger Lewis base than acetonitrile and is therefore a more effective quencher. The results in Table 2 demonstrate that the addition of the 3,8 methyl groups also inhibits exciplex quenching. Inhibition occurs because the increase in interligand steric interactions destabilizes the five-coordinate form of copper.[4,5,10] Thus, the $Cu(dbtmp)_2^+$ system has a much longer excited-state lifetime than the analogous dbp complex in acetonitrile. For the same reason the emissive state of $Cu(dbtmp)_2^+$ has a lifetime of 320 ns in acetonitrile, whereas the lifetime of dsbp complex is only 130 ns.[4] This is despite the fact that the 2,9 substituents, themselves, are larger in the case of the dsbp ligand.

CONCLUSIONS

In combination with adjacent *n*-butyl or phenyl groups, methyl substituents in the 3,8 positions of bis-phenanthroline copper(I) complexes have a dramatic influence on the photochemical and photophysical properties. For the 2,9-diphenyl derivative, the presence of the 3,8 methyl groups destabilizes the flattened tetrahedral structure and forces the ground state to adopt a D_{2d}-like geometry. Likewise, the same tetragonal distortion is less favorable in the CT excited state, and the emission therefore occurs at a higher energy. In dichloromethane the emission lifetime increases to 480 ns, the longest yet reported for a $Cu(NN)_2^+$ system. Finally, the back-to-back substituents combine to destabilize five-coordinate forms of the copper center and thereby suppress solvent-induced exciplex quenching. As a result, the dptmp complex exhibits a lifetime upwards of 100 ns even in donor media.

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Table 1. Room-Temperature Absorption and Emission Data for $Cu(NN)_2^+$ Systems in CH_2Cl_2.

Ligand	λ_{max}(abs), nm	λ_{max}(em)[a], nm	τ, ns
phen	440	-	-
4,7-dmp	434	-	-
tmp	430	-	-
dbp	457	670	150
dbdmp	456	670	145
dbtmp	453	635	330
dpp	440	685	270
	560sh		
dpdmp	440	685	310
	550sh		
dptmp	467	670	480

[a]From uncorrected spectrum.

Table 2. Solvent Dependence of Room-Temperature Emission from $Cu(NN)_2^+$ Systems[a]

	MeCN		THF		DMF	
NN	λ_{max}, nm	τ, ns	λ_{max}, nm	τ, ns	λ_{max}, nm	τ, ns
dbp	690	35	680	50	690	<10ns
dbtmp	650	320	640	330	650	140
dpp	715	120	710	190	700	70
dptmp	690	255	685	365	685	70

[a]All emission maxima from uncorrected spectra

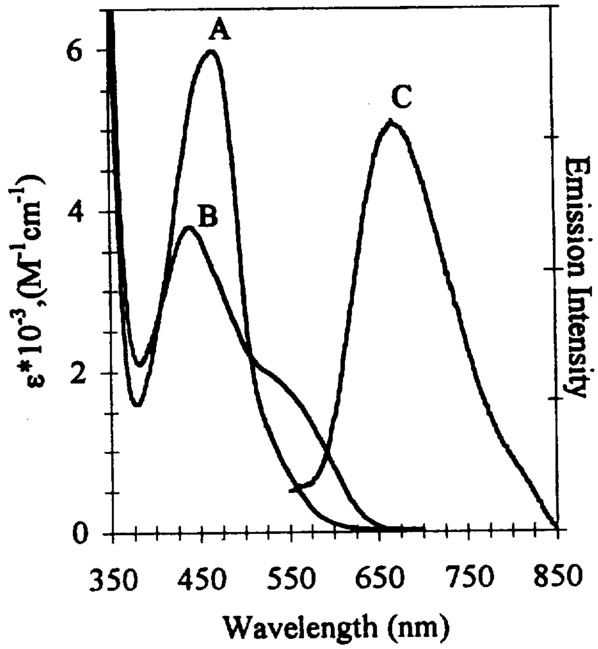
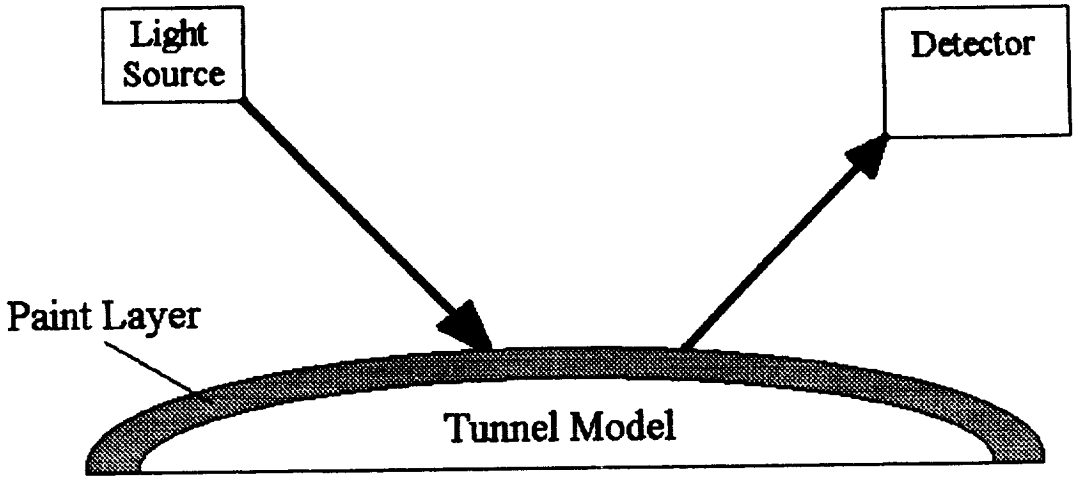


Figure 1. Absorption spectra of A: $Cu(dptmp)_2^+$, B: $Cu(dpdmp)_2^+$ and emission spectrum of $Cu(dptmp)_2^+$ (C) in DCM at room temperature.

CHAPTER 1
LUMINESCENT MOLECULAR TEMPERATURE SENSORS

Introduction

The synthesis of paint additives that have the ability to sense changes in temperature and or pressure is an area that is rapidly expanding.[1, 2, 3] The application of this kind of technology falls into two major categories, aerodynamics and biology. Applying this to aerodynamics involves mixing the desired compounds into a polymer and applying this paint on wind tunnel models, turbine blades, even airplane wings.[2] The information these sensors give back can be used to measure temperature, pressure, air flow, etc. Scheme 1.1 shows a schematic of the experimental setup for application of this type of sensor. This kind of sensor (thin surface film) is very desirable because it is a very non-destructive and non-invasive way to characterize a system. The pressure taps and thermocouples primarily used today do not allow for complete surface mapping, nor do they allow for testing without incorporating the sensors and the appropriate cables into the model.[1] In other words, a pressure tap or thermocouple requires the model to be structurally modified to hold the sensor, which can change the properties of the model. Mounting these sensors into a model could disrupt strength, increase stress, and can disrupt air flow, not to mention the cost involved in machining. By using a luminescent, thin film sensor that covers the surface, optical data can be sent to remote detectors located outside the wind tunnels with essentially no modification to the model. Also, since the entire model can be coated and measured, the data collected allows the entire model to be mapped, giving surfaces instead of data points.[1-3] There are two main types of luminescent chemical sensors in use today; pressure sensing paints (PSP)[1, 2] and temperature sensing paints (TSP).[1, 3]



Scheme 1.1. Schematic showing the experimental setup for a luminescent molecular sensor in a wind tunnel.

For the PSP's, an intense emission under anaerobic conditions that decreases dramatically as oxygen is introduced is desired. To date, several different types of compounds have been tested and it seems that tris(4,7-diphenyl-1,10-phenanthroline) ruthenium(II), as well as several porphyrins and laser dyes, work well here.[1] These compounds all have very intense room temperature emission that is adversely affected when oxygen is introduced. One difficulty in creating a very effective PSP is the juggling act that must be performed with the many factors that can affect the response of a PSP. For instance, if the sensor is a cationic coordination compound, the anion plays a major role in determining the solubility of the sensor in both the solvent and the paint.[4] Probably the most important factor is the polymer binder, since the oxygen molecule must travel through the binder to reach the sensor.[5] These and many other factors have been investigated and reported by others and will not be the focus of this project.[1-5]

For TSP's, there are several factors that figure in. The first is the temperature range of interest.[3] This is mostly determined by the facility since most wind tunnels are designed for use at specific temperatures. The lowest temperature range is approximately 100K to 150K, used in cryogenic wind tunnels. The paints that work in this temperature region are called cryogenic TSP's, and are the focus of this research report. To date, the best sensors have been based on $[Ru(trpy)_2]^{2+}$ (where trpy = 2,2':6',2"-terpyridine).[3] An effective temperature sensor will be one which shows a dramatic change in luminescence intensity over a small temperature range and is consistent data in more than one binder.

Starting with the $[Ru(trpy)_2]^{2+}$ base, the easiest way to make changes is to add functional groups to one of the terpyridine ligands. Based on the response of the new sensors, it should be apparent which combination of ligands gives the best sensor. This report deals with the design and synthesis of terpyridine ligands and their use in creating new cryogenic sensors.

Experimental

Materials

All of the aldehydes and acetyl compounds, along with the NaH, ammonium acetate, paraformaldehyde, dimethylammonium chloride, iodine, triflic anhydride, $RuCl_3$, KPF_6, $NaBPh_4$, terpyridine, and 4'-chloro-terpyridine (Cl-trpy) were purchased from Aldrich and used as is. All solvents, except THF, were of reagent grade unless noted. The THF was distilled over Na metal and benzophenone under nitrogen to remove trace water. The deuterated solvents were purchased from Cambridge Isotope Laboratories. The ligands 4'-methylthio-2,2':6',2"-terpyridine (MeS-trpy) and 4'-methylsulfonyl-2,2':6',2"-terpyridine ($MeSO_2$-trpy) were available from a previous study.[14]

Instrumentation

NMR spectra were recorded on a Gemini 200 MHz spectrometer and referenced to the residual proton of the solvent. Infrared spectra were recorded on a Perkin-Elmer IR spectrometer as nujol mulls. UV-Visible and emission spectra were measured on Perkin-Elmer Lambda 4C and SLM SPF 500C spectrophotometers, respectively. A description of the lifetime apparatus is in the literature.[14] Luminophores were calibrated on the bench setup in the literature.[3] These calibrations were ran by Rick Erausquin. Wind tunnel measurements were performed by Dr. Keisuke Asai and his support staff at the National Aerospace Laboratory in Japan.

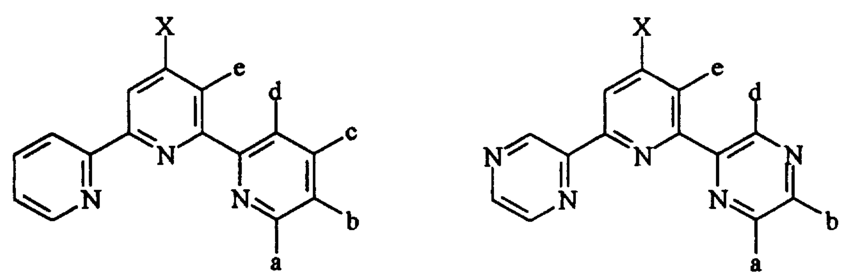
Preparations

The ligands 4'-phenyl-2,2':6'-2"-terpyridine (ph-trpy),[6] 4'-(4-pyridyl)-2,2':6'-2"-terpyridine (4-py-trpy),[7] 4'-(3-pyridyl)-2,2':6'-2"-terpyridine (3-py-trpy),[7] 4'-(2-pyridyl)-2,2':6'-2"-terpyridine (2-py-trpy),[7] 4'-pentafluorophenyl-2,2':6'-2"-terpyridine (C_6F_5-trpy),[6] 4'-*p*-bromophenyl-2,2':6'-2"-terpyridine (*p*-Br-ph-trpy),[6] 4'-*p*-chlorophenyl-2,2':6'-2"-terpyridine (*p*-Cl-ph-trpy),[6] 4'-*p*-nitrophenyl-2,2':6'-2"-terpyridine (*p*-NO_2-ph-trpy),[7-10] 2,6-bis(pyrazinyl)-pyridine (zyz),[11] 2,6-bis(2-pyridyl)-4-pyridone (HO-trpy),[12, 13] 2,6-bis(pyrazinyl)-4-pyridone (HO-zyz),[12, 13] 4'-triflato-2,2':6'-2"-terpyridine (TfO-trpy),[12] 2,6-bis(pyrazinyl)-4-triflato-pyridine (TfO-zyz),[12] 4'-dimethylamino-2,2':6'-2"-terpyridine (Me_2N-trpy),[14, 15] 4'-ethoxy-2,2':6'-2"-terpyridine (EtO-trpy),[13] 2,4,6-triphenyl-pyridine,[7-10] 4,6-diphenyl-2,2'-bipyridine,[7-10] and 6,6"-diphenyl-2,2':6'-2"-terpyridine[16-18] were all prepared by literature methods using the appropriate starting materials. Tables 1.1 and 1.2 list the UV-Vis absorption and proton NMR data on all the prepared ligands, respectively.

Table 1.1. UV-Vis data for selected terpyridine ligands, in CH_3CN, unless noted.

Ligand	λ_{max} (nm)
trpy	310, 274, 251[a]
4'-HO-trpy	278, 248
4'-TfO-trpy	277, 238
4'-phenyl-trpy	307, 275, 250
4'-*p*-NO_2-phenyl-trpy	284, 249, 241[a]
4'-(4-pyridyl)-trpy	312, 275, 240
4'-(3-pyridyl)-trpy	307, 275, 245
4'-(2-pyridyl)-trpy	316, 277, 243
zyz	284, 241, 229

[a] in diethyl ether



Scheme 1.1. Labeling scheme for NMR data.

Table 1.2. ^1H NMR data for terpyridine ligands, in $CDCl_3$.

Ligand	a	b	c	d	e	other	NB-ref
trpy	8.73	7.36	7.86	8.64	8.47	8.0	III-73
4'-HO-trpy	8.75	7.4	7.85	7.93	7.34		III-8, 28
4'-TfO-trpy	8.73	7.4	7.9	8.63	8.43		III-18
4'-Cl-trpy	8.7	7.35	7.85	8.6	8.48		III-63
4'-EtO-trpy	8.7	7.34	7.87	8.63	8.2	4.3, 1.5	III-134
4'-Me_2N-trpy	8.67	7.3	7.83	8.62	7.78	3.2	III-53
4'-*N*-piperidinyl-trpy	8.67	7.3	7.83	8.62	7.93	3.55, 1.69	III-106
4'-*N*-piperazinyl-trpy	8.66	7.29	7.82	8.62	7.94	4.13, 3.56, 2.68	III-121
4'-ph-trpy	8.74	7.37	7.9	8.69	8.77	7.9, 7.5	III-74
4'-*p*-Cl-ph-trpy	8.74	7.37	7.89	8.65	8.70	7.85, 7.48	IV-1
4'-*p*-Br-ph-trpy	8.73	7.37	7.89	8.67	8.7	7.79, 7.64	III-83
4'-*p*-NO_2-ph-trpy	8.72	7.37	7.88	8.66	8.73	8.35, 8.02	II-124
4'-C_6F_5-trpy	8.72	7.36	7.89	8.67	8.55		III-58
4-py-trpy	8.74	7.39	7.9	8.69	8.77	8.77, 7.8	III-59
3-py-trpy	8.75	7.38	7.9	8.69	8.75	9.14, 8.75, 8.18, 7.45	III-74
2-py-trpy	8.74	7.35	7.87	8.66	9.1	8.8, 8.66, 7.83, 7.35	III-70
zyz	8.63	8.63		9.8	8.44	7.99	II-150
4-HO-zyz	8.17	8.17		9.3	7.47		III-45
4-TfO-zyz	8.73	8.73		9.83	8.43		IV-26
6,6"-diphenyl-trpy		7.82	7.98	8.64	8.72	7.51, 7.98, 8.21	V-11, 15
4,6-diphenyl-bipy	8.23	7.35	7.96	8.7	8.0	7.52	III-143
2,4,6-triphenyl-pyridine					7.93	7.52, 7.78, 8.25	III-133

All of the ruthenium compounds were synthesized and purified by following literature methods.[19] Metathesis reactions, when necessary, were performed by dissolving the ruthenium complex in acetone and adding the desired anion as a concentrated solution in water or in a mixture of acetone and water. Evaporation of the acetone resulted in precipitation of the ruthenium complex with the desired anion.

1,5-bis(2-pyridyl)-3-phenyl-1,5-pentanedione (II-72).[6] White solid, yield: 1.934 g (5.85 mmol) 66%. UV-Vis in Et_2O: 266 nm, 227 nm. IR $\nu_{C=O}$ in nujol oil: 1689 cm^{-1}. ^1H NMR in $CDCl_3$: 3.7 ppm (m, 4H), 4.15 ppm (p, 1H), 7.15 ppm (d, 1H), 7.24 ppm (t, 2H), 7.37 ppm (d, 2H), 7.43 ppm (ddd, 2H), 7.67 ppm (dt, 2H), 7.94 ppm (d, 2H), 8.63 ppm (d, 2H).

1-(2-pyridyl)-3-(*p*-nitrophenyl)-propenone (II-113).[6] Pale yellow solid, yield: 6.290 g (24.74 mmol) 92%. UV-Vis in Et_2O: 314 nm. IR $\nu_{C=O}$ in nujol oil: 1653 cm^{-1}, $\nu_{N=O}$: 1636 cm^{-1}. ^1H NMR in $CDCl_3$: 7.51 ppm (ddd, 1H), 7.86 ppm (m, 4H), 8.18 ppm (d, 1H), 8.25 ppm (d, 2H), 8.41 ppm (d, 1H), 8.74 ppm (d, 1H).

N-{1-(2'-pyridyl)-1-oxo-2-ethyl}pyridinium iodide (II-111).[20, 21] Yellow product. IR$\nu_{C=O}$ in nujol oil: 1627 cm^{-1}. ^1H NMR in DMSO-d_6: 6.50 ppm (s, 2H), 7.84 ppm (dt, 1H), 8.10 ppm (m, 2H), 8.27 ppm (t, 2H), 8.73 ppm (t, 1H), 8.87 ppm (d, 1H), 9.00 ppm (d, 2H).

1-pyrazinyl-3-dimethylaminopropanone (II-132).[11] White product, yield: 98 mg of white solid, only 64.3 % pure by NMR, 63 mg (0.352 mmol) 4.3%. ^1H NMR in $CDCl_3$: 2.86 ppm (s, 6H), 3.51 ppm (brd. s, 2H), 3.92 ppm (brd s, 2H), 8.64 ppm (s, 1H), 8.78 ppm (s, 1H), 9.20 ppm (s, 1H).

N-{1-(2'-pyrazinyl)-1-oxo-2-ethyl}pyridinium iodide (II-146).[20, 21] Light beige product. IR $\nu_{C=O}$ in nujol oil: 1699 cm^{-1}. ^1H NMR in DMSO-d_6: 6.49 ppm (s, 2H), 8.29 ppm (t, 2H), 8.75 ppm (t, 1H), 8.98 (m, 3H), 9.07 ppm (d, 1H), 9.25 (d, 1H).

1,5-bis(2-pyridyl)pentane-1,3,5-trione (III-4, III-26).[12, 13] Light mustard yellow solid. ^1H NMR in $CDCl_3$: 8.65 ppm (d, 2H), 8.05 ppm (q, 2H), 7.8 ppm (t, 2H), 7.38 ppm (d, 2H), 6.78 ppm (s, 1.75H), 4.4 ppm (s, 0.75 H). IR in nujol: $\nu_{C=O}$ 1619 cm^{-1}, 1558 cm^{-1}. UV-Vis in CH_3CN: 379 nm, 315 nm, 231 nm.

1,5-bis(pyrazinyl)pentane-1,3,5-trione (III-43).[12, 13] Orange solid, yield: 1.4 g (5.18 mmol) 60%. ^{1}H NMR in $CDCl_3$: 8.90 ppm (s), 8.5 ppm (d), 8.45 ppm (d), 7.25 ppm (s), 6.58 ppm (s). UV-Vis in CH_3CN: 382 nm, 321 nm, 268 nm, 220 nm.

4'-(*N*-piperidinyl)-2,2':6'-2"-terpyridine (III-106). 541 mg (2.02 mmol) 4'-chloro-terpyridine was brought to reflux in a 25 mL rb flask containing 10 mL piperidine. This mixture was allowed to reflux overnight, whereupon a white ppt. had formed. After cooling to room temperature, this yellow-brown solution was poured onto 100 mL of ice and water. Lots of white solid formed immediately. This was filtered off and washed with ample amounts of water. Proton NMR of this material (in $CDCl_3$) showed residual protons from the starting material so the product was treated a second time, in the same manner, with piperidine. Following the same work-up, this material gave a pure NMR spectrum, with the proper integration. Yield: 560 mg (1.8 mmol) 89%. ^{1}H NMR in $CDCl_3$: 8.68 ppm (d, 2H), 8.66 ppm (d, 2H), 7.93 ppm (s, 2H), 7.83 ppm (t, 2H), 7.3 ppm (q, 2H + $CHCl_3$), 3.55 ppm (broad s, 4H), 1.70 ppm (broad s, 6H).

4'-(*N*-piperazinyl)-2,2':6'-2"-terpyridine (III-121). Same procedure as for 4'-(*N*-piperidinyl)-terpyridine, utilizing 407 mg (1.52 mmol) 4'-chloro-terpyridine and 15 g (174 mmol) solid piperazine. Heating at ~140°C overnight followed by the same workup provided a pure (by NMR) sample. Yield: 473 mg (1.49 mmol) 98%. ^{1}H NMR in $CDCl_3$: 8.65 ppm (m, 4H), 7.93 ppm (s, 2H), 7.84 ppm (t, 2H), 7.3 ppm (q, 2H + $CHCl_3$), 4.1 ppm (broad, ~1H), 3.55 ppm (broad t, 4H), 3.08 ppm (broad t, 4H).

1-(2-pyridyl)-3-phenyl-propenone (II-177).[6] Yellow product. ^{1}H NMR in $CDCl_3$: 7.42 ppm (m, 3H), 7.49 ppm (ddd, 1H), 7.74 ppm (m, 2H), 7.88 ppm (dt, 1H), 7.95 ppm (d, 1H), 8.20 ppm (d, 1H), 8.32 ppm (d, 1H), 8.75 ppm (d, 1H).

N-{1-(2'-phenyl)-1-oxo-2-ethyl}pyridinium iodide (III-130).[20, 21] Pale brown powder, yield: 36.7 g (113.2 mmol) 94%. ^{1}H NMR in DMSO-d_6: 6.6 ppm (s, 2H), 7.67 ppm (t, 2H), 8.1 ppm (m, 4H), 8.63 ppm (t, 1H), 8.78 ppm (t, 1H), 9.07 ppm (d, 2H).

Bis-β-(dimethylamino)vinyl-2,6-pyridyl ketone (V-13).[16-18] Pale brown solid. ^{1}H NMR in $CDCl_3$: 8.22 ppm (d, 2H), 7.9 ppm (m, 3H), 6.6 ppm (d, 2H), 3.2 ppm (s, 6H), 3.0 ppm (s, 6H).

Results

Synthesis

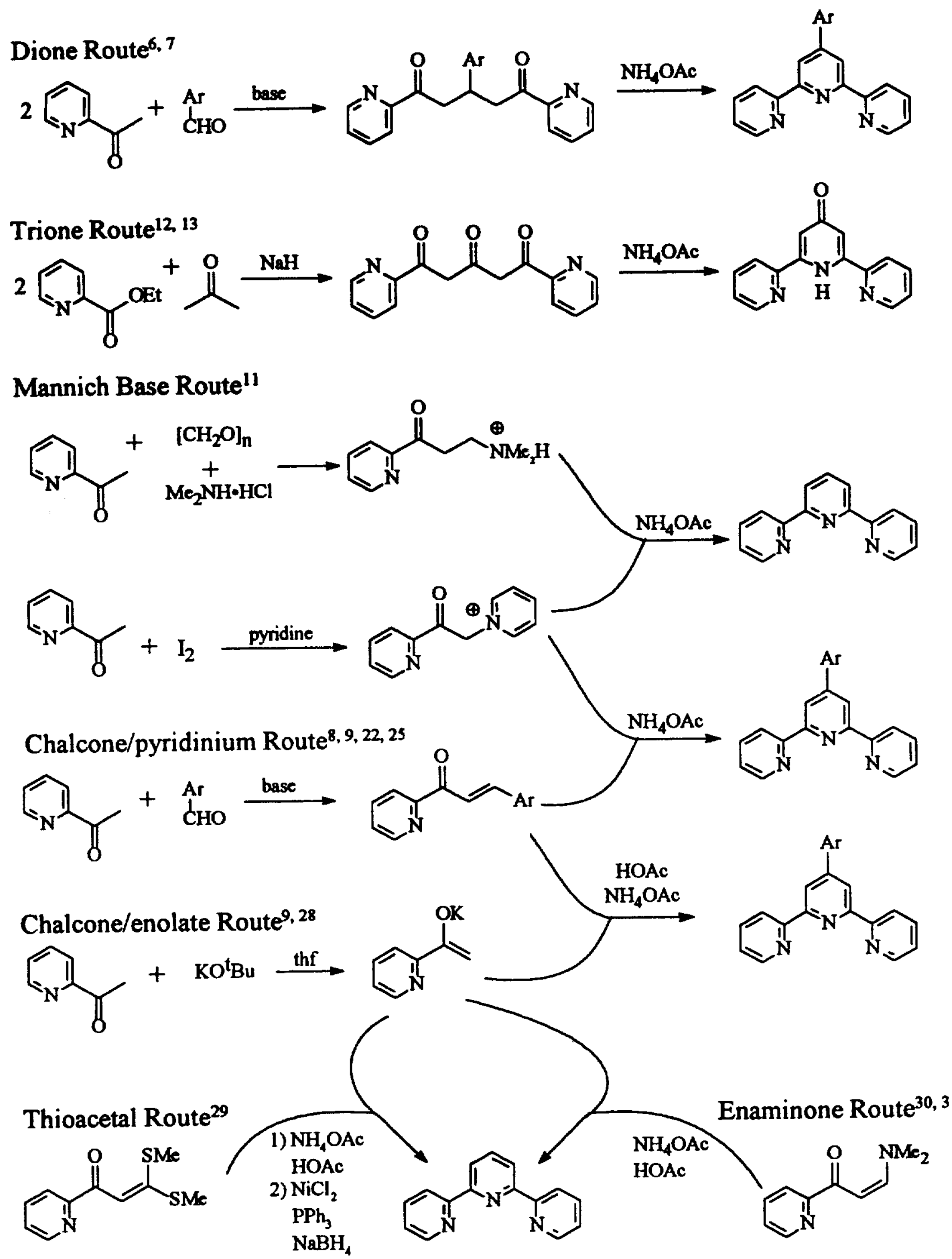
Ring-forming condensation (RFC) reactions make up the bulk of trpy synthesis.[22] These types of reaction schemes are usually based on the idea of taking the outer pieces, with the appropriate functional groups, and bringing them together while forming the central pyridine ring. The main RFC routes are shown in Scheme 1.2.

The dione route is the simplest of all the RFC reactions and works fairly well, when it is applicable. This pathway involves an Aldol condensation followed by a Michael addition, creating the 1,5-dione intermediate,[6] which then undergoes a RFC reaction, forming the central pyridine ring. This type of reaction was one of the first non-metal-mediated coupling pathways utilized to prepare 4'-aryl-terpyridines.

This route leads to 4'-aryl terpyridines in a relatively good yield under very simple reaction conditions. However, this route is not applicable to all aryl aldehydes. Unsubstituted to mildly substituted aldehydes work best. For example, benzaldehyde,[6] 2-, 3-, and 4-pyridine[7] carboxaldehyde all work very well and both the intermediate and final product are relatively pure, straight from the reaction mixture. The presence of a *para* Br, Cl, or CH_3 usually led to a gum-like dione product, which can be used directly in the next step, but does present some problems in characterizing the intermediate.

The exact reason for the gooey product is unclear. Different solvents (*iso*-propanol and butanols) and different ethanol concentrations have no effect on its formation. Regardless, the RFC reaction will still proceed on the gooey material and a pure terpyridine ligand is isolable without any extra work. E. C. Constable claims[7] that methanol titration of the gooey product will give a white precipitate, but it was unclear exactly how this is done and was therefore not investigated further since the goo produces a pure product.

In addition to the gooey product, if acetyl-pyrazine is used instead of acetyl-pyridine, a nice white powder is formed, which analyzes as some kind of oligomer that



Scheme 1.2. Summary of ring-forming condensation (RFC) reactions.

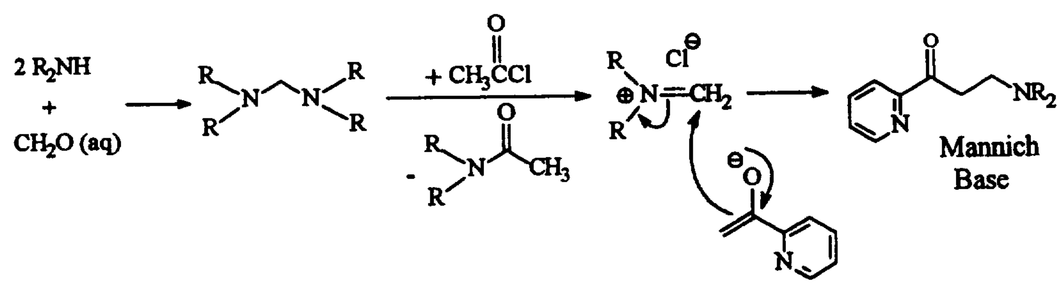
has well defined ^{1}H NMR peaks from 1 ppm to 9 ppm almost continuously. This material is formed, regardless of the conditions, consistently in the reaction between acetyl-pyrazine and benzaldehyde.

The presence of strong functional groups (nitro, amino, methoxy) leads to the formation of highly colored precipitates. These precipitates analyze to be the corresponding chalcones (α,β-ene-one product) and not the diones as was expected. These were not anticipated initially, but literature searches confirmed them as products and also how they could be converted to the corresponding terpyridine ligands.[7-10]

The trione route is based on the dione route, and leads, with decent yield, to 2,6-bis(2-pyridyl)-4-pyridone.[12, 13] Synthesis of the pyridone is based on a crossed Claisen condensation between the pyridyl ethyl ester and acetone, creating the trione product. Condensation of the two outer ketones with one equivalent of ammonium acetate creates the pyridone ring, which can tautomerize to give the 4'-hydroxyl-trpy derivative. This is facilitated by the presence of metal ions.[13] This reaction scheme also works on acetyl-pyrazine, creating 2,6-bis(pyrazinyl)-4-pyridone in excellent yield.

The Mannich base route offers a pathway to create unsubstituted central ring derivatives and has been used to synthesize several new ligands.[11] It utilizes the Mannich base generated in the reaction between an acetyl-pyridine derivative, dimethylammonium chloride, and paraformaldehyde. This then undergoes a Michael-type reaction, forming a non-isolable 1,5-dion-2-ene intermediate, which undergoes a RFC reaction to form the central ring. Formation of the Mannich base can be done in either acidic or basic conditions.[23] Alternatively, the Mannich base may be prepared by addition of the acetyl-derivative to an iminium reagent, as shown in Scheme 1.3.[24]

In our hands, for both pyrazine and pyridine, the corresponding Mannich bases were extremely difficult to synthesize, regardless of the conditions. Mostly a brown tar would be formed that had a strong amine stench to it. This material would not chromatograph well and TLC analysis showed a mixture of products. Synthesis via the Mannich base route was scrapped.

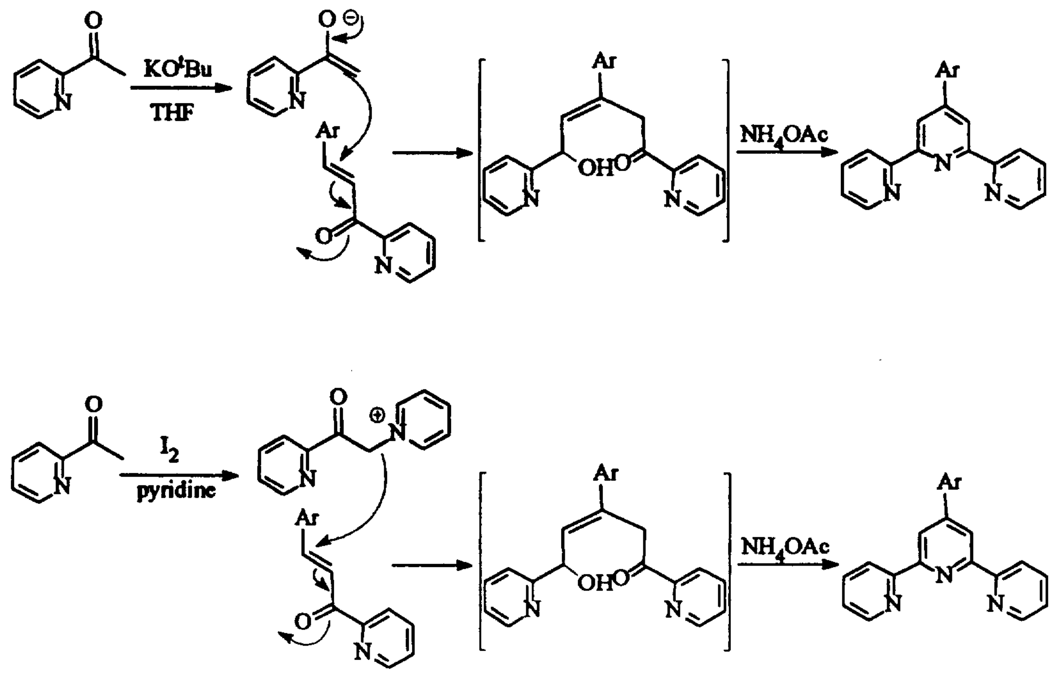


Scheme 1.3. Mannich base synthesis using an iminium reagent.

The chalcone/pyridinium and chalcone/enolate pathways are both used quite frequently to synthesize trpy derivatives.[22, 25] They work well for trpy derivatives that do not form the dione, due to solubility reasons, etc. In both cases the first step of the synthesis is the Aldol condensation of the acetyl-derivative with an aromatic aldehyde to form the chalcone. The second step is the Michael addition of an activated acetyl-derivative, either a preformed enolate or a stabilized enolate, to presumably create a 1,5-dion-2-ene intermediate.[8] This then condenses to form the central ring. Overall, this reaction scheme is more commonly referred to as the Kröhnke synthesis[8] and has been exploited very effectively by E.C. Constable et al,[9] see Scheme 1.4.

The chalcone/pyridinium route was the first route examined in converting chalcones to terpyridines. The preparation of the pyridinium iodide salt was the first step. This reaction was in the literature,[20] but the purification and spectroscopic data (other than $\nu_{C=O}$) was unavailable. Correspondence with Grant Summerton, of Dr. John Field's group in Natal, South Africa, lead to a simple purification involving a short reflux in ethanol with decolorizing charcoal.[21]

The pyridinium reagent is fairly interesting in itself. Based on the reaction and inductive arguments, it would seem that this reagent is a stabilized carbocation. This is very unlikely since the carbonyl carbon is already electrophilic in nature and the presence of two adjacent partial positive charges seems rather unlikely.[26] A better way of viewing this compound is by treating it as a stabilized enolate. In this case, even though the α-methylene is bound to a quaternary nitrogen, the hydrogens are still acidic and the carbon is therefore nucleophilic in nature and will undergo Michael-type reactions.[27]

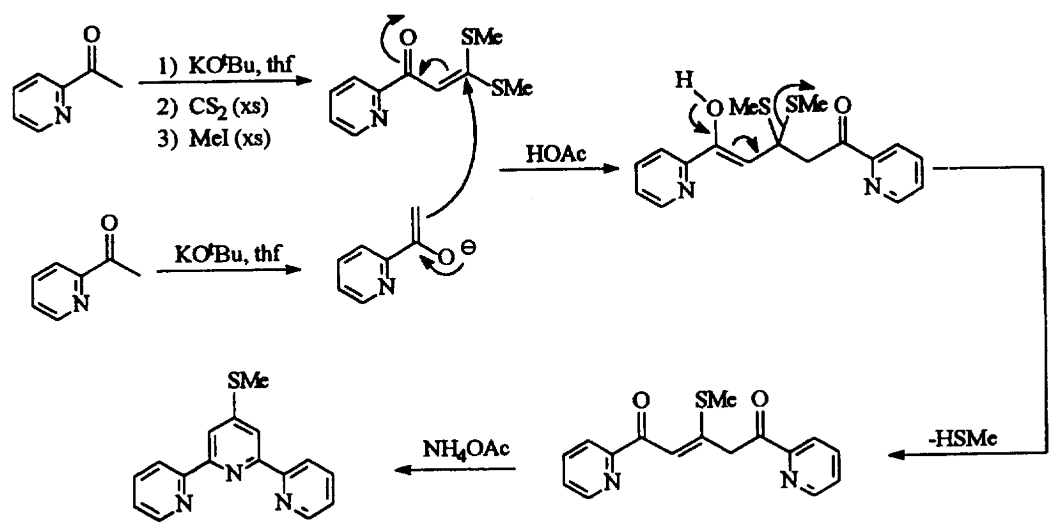


Scheme 1.4. Summary of the Kröhnke synthesis.

Once a pure pyridinium salt was obtained, examination of the literature revealed several different experimental conditions for the formation of terpyridines from chalcones and pyridinium salts.[7-10] With electron withdrawing groups, the reactions seemed to work best with just an ethanol reflux and ammonium acetate overnight. With electron donating groups present on the benzene ring, nothing seemed to work. It is not clear why, as there are literature reports of terpyridine ligand synthesis bearing electron donating substituents performed in this fashion. A solution to this problem was referred to in a review article[22] which turned out to be useful in synthesizing electron donating terpyridines as well as some sterically demanding terpyridines. This method has been utilized very effectively by Michalec et al[28] as well as E. C. Constable and co-workers.[9] This method is the chalcone/enolate route.

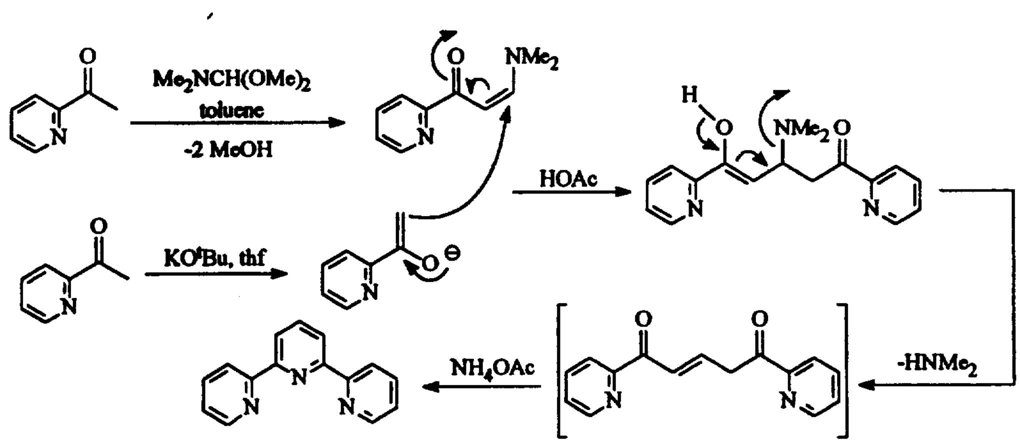
The chalcone/enolate route involves treating the chalcone with a preformed potassium enolate of acetyl-pyridine followed by treatment with acetic acid and ammonium acetate. The reaction itself works pretty well but the best method of purification is yet to be determined.

The thioacetal route has been pioneered by K.T. Potts et al.[29] This synthetic scheme produces 4'-methylthio-trpy, in which the MeS group can be converted to several different functional groups, including hydrogen.[29] This route is based on the chalcone/enolate pathway to some degree. In this case the bis(methylthioether)-eneone is synthesized, then treated with an enolate species, followed by condensation to give the corresponding trpy derivative in a Michael-type reaction, see Scheme 1.5. The bis(methylthioether) functionality activates the alkene for attack to create a 1,5-dione-2-ene intermediate that is usually not isolated. This method has relatively good yields, but the release of methylthiol, which never seems to leave the product,[16] makes this pathway somewhat unpleasant. Also, the remaining methylthioether functionality is somewhat difficult to remove.[16]



Scheme 1.5. Summary of the thioacetal method.

The last route has very recently crept into the forefront of trpy synthesis.[6, 17] This reaction is similar to the thioacetal route, except it uses an enaminone to react with the enolate. This reaction most likely, again, forms a 1,5-dione-2-ene intermediate that condenses to form the central ring, see Scheme 1.6. This method has been used to prepare unsubstituted terpyridine in 2 steps, with excellent yield.[16] It has also been used to prepare some trpy derivatives and is a very straightforward route to these ligands.[17]

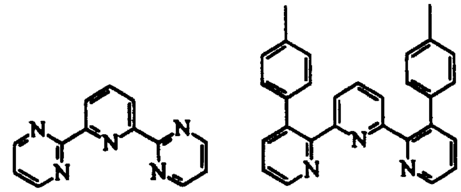


Scheme 1.6. Summary of the enaminone method.

One appealing feature of this preparation is the fact that it leaves the central ring unsubstituted. Until now, this was not an easy task, see the Mannich base discussion above. Other notable characteristics about this reaction are the rather high yield it offers and its applicability.

One of the main reasons for the high yield is the ability to obtain an almost quantitative yield of the starting enaminone. Reaction of acetyl-pyridine with dimethylformamide dimethyl acetal produces the enaminone and methanol. If the methanol is distilled off during the reaction,[16] the equilibrium is forced towards the product side. Purification is accomplished by precipitating the product and filtering. Analysis of the filtrate indicates it is mostly unreacted acetyl-pyridine with some product. By treating the mother liquor with another equivalent of dimethylformamide acetal, more enaminone is formed and the reaction nears 100% yield.

Another interesting point is that this route seems to be the only one so far that is completely applicable to all the nitrogen heterocycles. Terpyridine derivatives based on pyridine and pyrimidine have already been synthesized,[17] see Scheme 1.7, and there is no reason to suggest that pyrazine, quinolines, and other diazines would not work. This reaction also works with 2,6-diacetyl-pyridine, which makes it ideal for synthesizing 6,6"-disubstituted terpyridines.



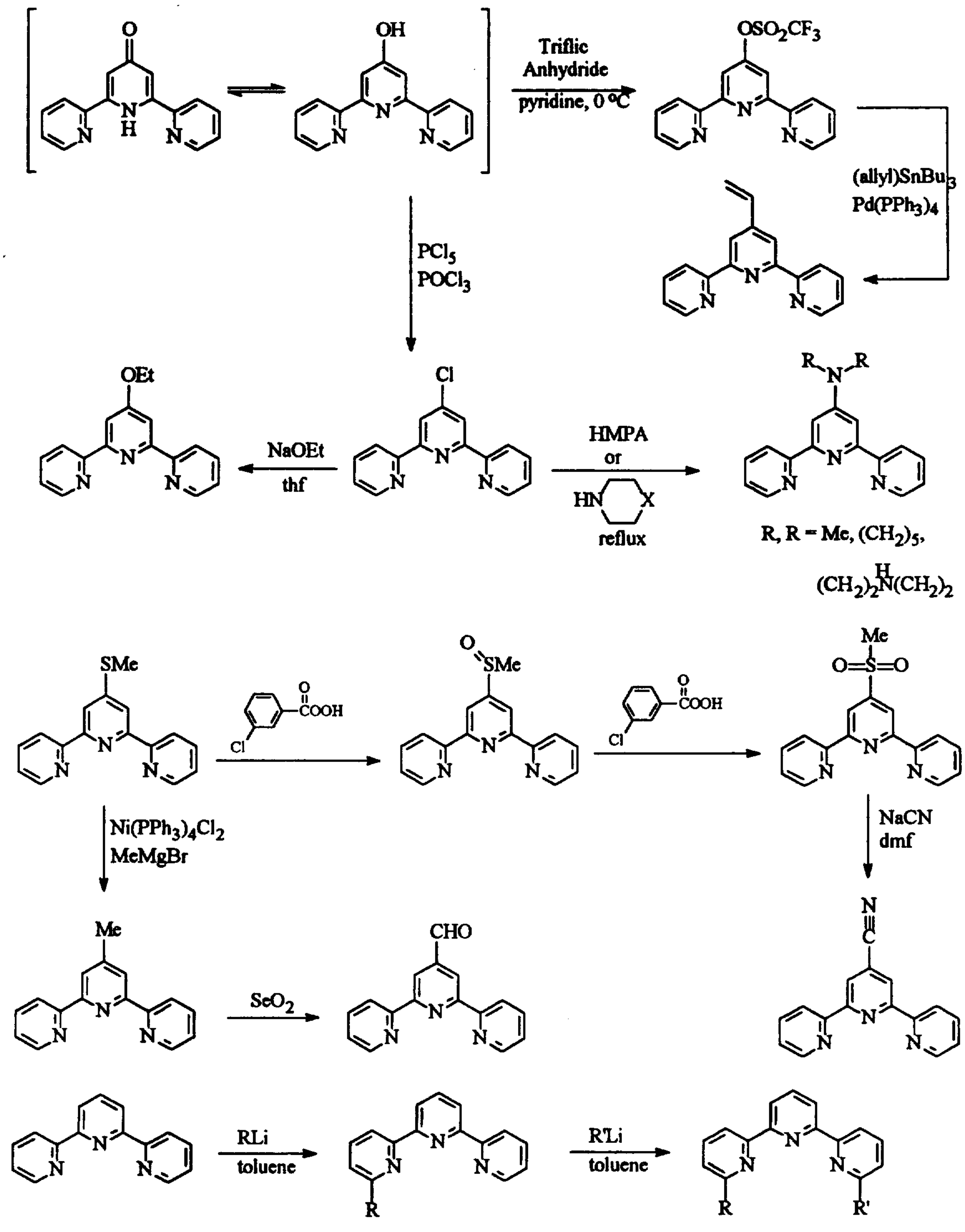
Scheme 1.7. Terpyridine ligands synthesized using acetyl-pyridine derivatives.

Functional Group Transformation Reactions

There are many examples of synthetic functional group transformations in terpyridine chemsitry, see Scheme 1.8. For the most part these reactions work as reported in the literature. The one exception is the conversion of 4'-chloro-terpyridine into 4'-dimethylamino-terpyridine.[30] Constable claims that chelation of 4'-Cl-trpy around Fe(II), refluxing in ethanol with dimethylammonium chloride and KOH, then oxidation of the iron produces the desired product in good yield.[30] In our work, no such reaction occurred with dimethylammonium chloride, diethyl amine, or piperidine. The chloride derivative could be converted, however; by simple reflux in the neat amine (to give the piperidine and piperazine derivatives) or HMPA[15] (to give the dimethylamine derivative). This type of reaction is much more straightforward and the work-up is simple. The yields of these reactions also were higher than the reported values. These types of reactions did not work on converting *p*-halogen-phenyl-terpyridine derivatives into their corresponding amino derivatives.

Potts and co-workers have done extensive work with the methylthioether functionality.[29] They have shown how to convert the alkyl thiol into a sulfonyl, alkyl, even an aldehyde. They have also shown how to synthesize a 4'-triflato-terpyridine derivative which allows for palladium catalyzed coupling reactions to be investigated.[12]

Electronically and sterically tuned terpyridines represent the next wave of these ligands and promise to hold some very interesting chemistry. The limiting reagent is the fact that terpyridine chemistry has only some similarities to pyridine chemistry and even fewer to benzene chemistry. This limited understanding is growing everyday and soon very elaborate ligands should be available with only limited synthetic effort.



Scheme 1.8. Summary of substitution reactions.

NMR Data

All the terpyridine ligands synthesized in this project have similar chemical shifts for the outer ring protons, which is not surprising based on the limited interaction the three rings would have, in the metal-free case. The *e* proton (3' and 5' hydrogens) shows the most change in the chemical shift. This proton shifts to a higher field (lower chemical shift) as the π-donating ability of the 4' substituent increases. For example, the chemical shift decreases in the order H, TfO, EtO, *N*-piperidinyl, Me_2N. This is consistent with the idea that the stronger π-donating amines can conjugate with the ring π-system more, thus decreasing the amount of shielding of the ring hydrogens by placing more electron density on the protons.[31] Conversely, with the electron withdrawing Cl group, the *e* proton is shielded more and the chemical shift moves to a slightly lower field (higher chemical shift) since it pulls electron density away from the proton.[31] These effects are also seen with substituted benzene complexes.[31] If the terpyridine is substituted in the 4' position with a phenyl ring, the *e* proton shift does not change as much when the phenyl ring is substituted. The main differences in these compounds are the locations of the phenyl protons, due to their proximity to the functional groups.

Ruthenium Terpyridines

The photophysical properties of the ruthenium(II) terpyridines synthesized with the aforementioned ligands are tabulated below in Table 1.3, and some representative spectra are shown in Figure 1.1. Previously reported compounds agree with reported values, and the new compounds seem to follow the same trends.[19] One of the new compounds, $[Ru(trpy)(NC\text{-}trpy)]^{2+}$, proved difficult to purify. The impurity seemed to be $[Ru(trpy)_2]^{2+}$, which only shows up during low temperature emission scans. The impurity seemed traceable back to the starting material $Ru(trpy)Cl_3$. Boiling ethanol extractions and synthesis of $Ru(trpy)Cl_3$ in the presence of excess NaCl seemed to help considerably. The room temperature lifetime value for $[Ru(trpy)(NC\text{-}trpy)]^{2+}$ is one of the longest for simple bis-terpyridine ruthenium complexes.

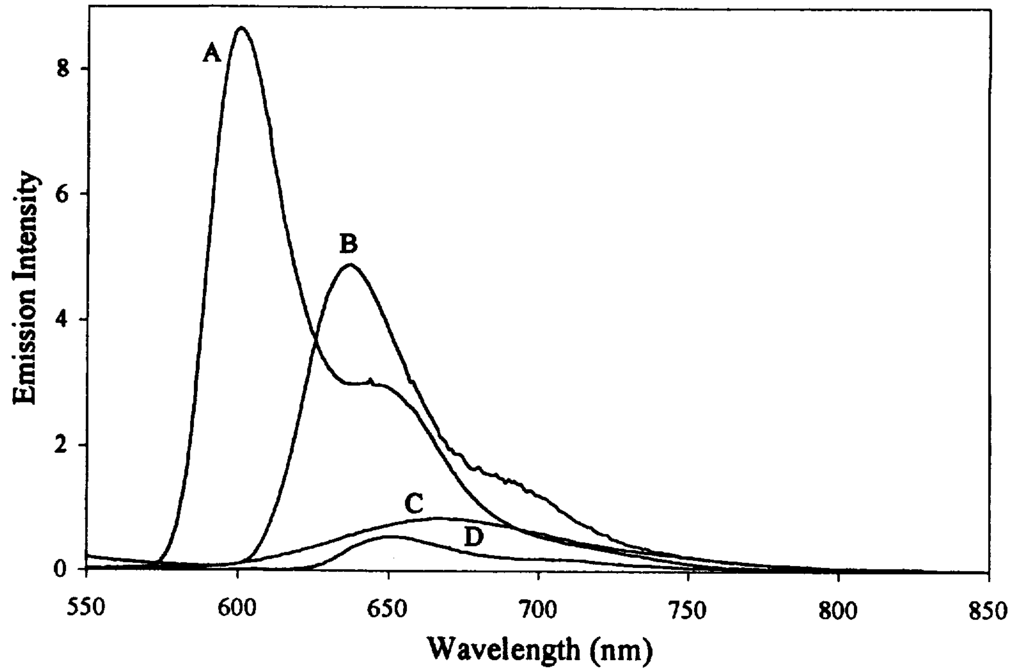


Figure 1.1. Representative emission spectra of $[Ru(X\text{-}trpy)(Y\text{-}trpy)]^{2+}$ complexes at room temperature and 77K. A) $[Ru(trpy)_2]^{2+}$ in butyronitrile glass at 77K. B) $[Ru(NC\text{-}trpy)_2]^{2+}$ in butyronitrile glass at 77K. C) $[Ru(NC\text{-}trpy)_2]^{2+}$ in acetonitrile at room temperature. D) $[Ru(ppd\text{-}trpy)_2]^{2+}$ in butyronitrile glass at 77K.

Sensor Calibrations

Calibration of the ruthenium complexes as temperature sensors was handled very effectively by the bench setup designed by Rick Erausquin of Dr. John Sullivan's laboratory. The emission intensity was monitored from 100K up to 300K. The faster the emission intensity drops as the temperature increases, the more sensitive the paint. Figure 1.2 shows the response of some of the new terpyridine complexes along with the benchmark sensor, VH-127, which was donated to the Sullivan laboratory by Prof. R. Thummel. The steep slope of the VH-127 compound makes it a very desirable compound, while its elaborate and involved synthesis makes it a very undesirable compound.

Table 1.3. Room temperature photophysical data for $[Ru(X\text{-}trpy)(Y\text{-}trpy)]^{2+}$ complexes.

X	Y	Abs (nm)[a]	Em (nm)[b]	τ (ns)[b]
H	H	475	---	---
H	Cl	478	~635	<10
H	MeS	483	---	---
H	TfO	475		
H	$MeSO_2$	479	672	44
H	NC	482	665	55
H	ppd	492	~700	<10
H	ph	480	---	
H	*p*-NO_2-ph	475	---	
H	C_6F_5	481	---	
H	4-py			
NC	NC	489	666	
ppd	ppd	502	---	---
TfO-zyz	TfO-zyz	495	---	---
TfO	TfO	480	---	---

a in CH_3CN
b in CH_3CN, not deoxygenated

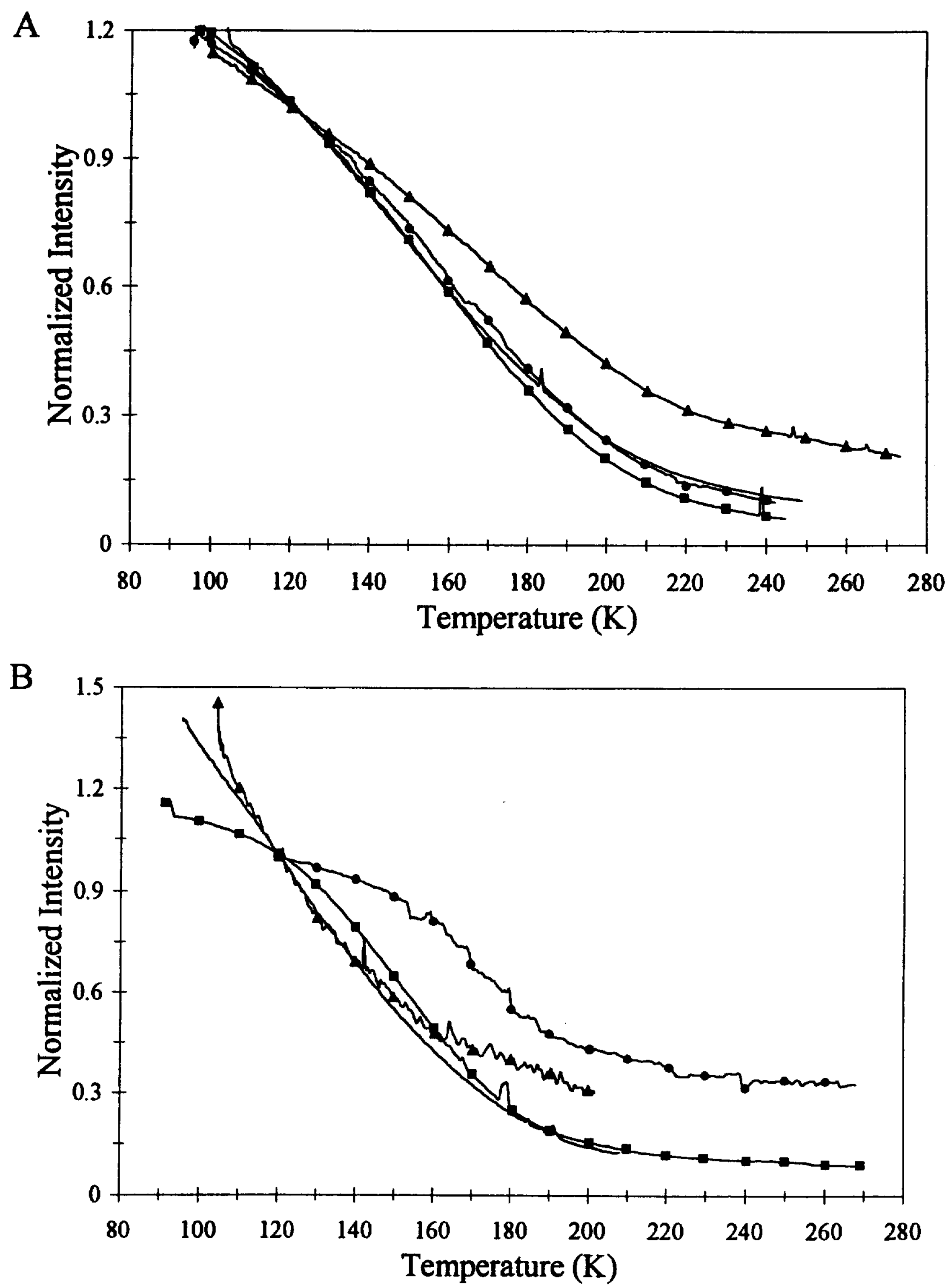


Figure 1.2. Intensity versus temperature calibration plots. In A, the triangle is HNC, the line is $HMeSO_2$, the square is HMeS, and the circle is Hppd. In B, the triangle is HVH-127, the line is ppdppd, the square is Hph, and the circle is HH.

Wind Tunnel Evaluation

Some of the new terpyridine compounds were tested in the cryogenic wind tunnel at the National Aerospace Laboratory (NAL) in Japan by Dr. Keisuke Asai. However, none of the new compounds were able to generate the emission signal that $[Ru(trpy)_2]^{2+}$ can at temperatures between 100 and 150K. Figure 1.3 shows the response of a $[Ru(trpy)_2]^{2+}$ based paint in the NAL cryogenic wind tunnel. This data was taken by Dr. John Sullivan, Dr. Keisuke Asai, and the cryogenic wind tunnel support staff at NAL. The model was a circular arc bump and the tunnel temperature was 150K. The picture is generated by taking a reference picture at Mach 0.25, then another picture at Mach 0.75. The ratio of the second photo to the first gives the image shown. The faint line about 3/4 of the way back is a shock wave. The temperature difference across the shock wave is ~5°C. The dot followed by a triangular region is a small "bump" placed at the front of the model to induce turbulent flow as a test to see if the paint will in fact respond to such a small change in temperature. The gray scale is artificial.

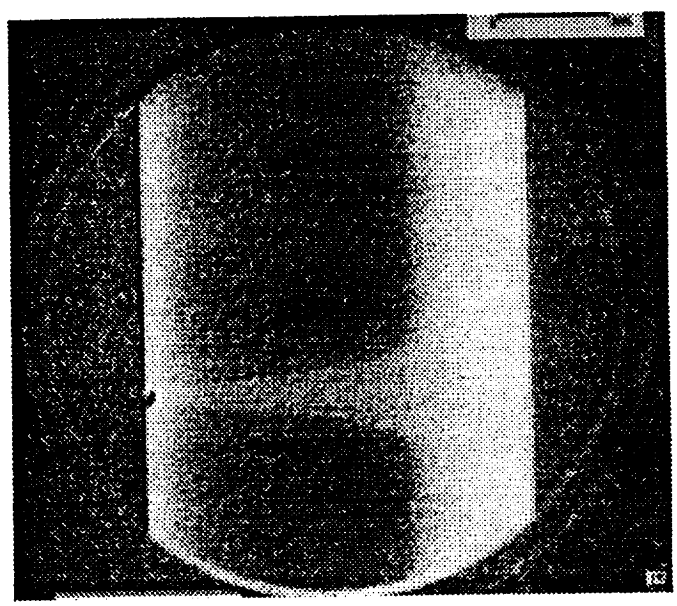


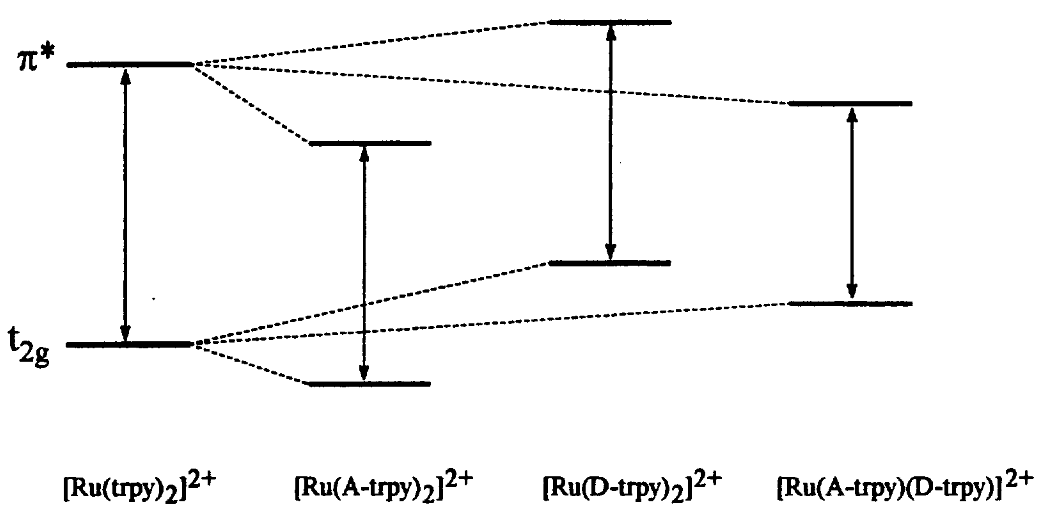
Figure 1.3. $[Ru(trpy)_2]^{2+}$ in GP-197 binder in NAL's cryogenic wind tunnel.

Discussion

Photophysics

The photophysical data reported here for this series of $[Ru(X\text{-}trpy)(Y\text{-}trpy)]^{2+}$ complexes agrees with the literature data and these compounds follow the same trends.[19] The compounds all show a decrease in emission energy, relative to $[Ru(trpy)_2]^{2+}$, regardless of the 4' substituent and an increase in room temperature excited state lifetime when the 4' substituent is strongly electron withdrawing.

The photophysical trends are explained by examining the effects the substituents have on the π^* orbital of the trpy ligand and on the lower energy t_{2g} orbitals of the metal center. The two types of functionalities placed on the trpy ligands are electron withdrawing (referred to as A) and electron donating (referred to as D). The π^* and t_{2g} orbitals are important because the absorption responsible for emission is metal-to-ligand charge transfer (MLCT) in origin. The MLCT takes a t_{2g} electron and places it in the ligand π^* orbital, thus, they are the two most important orbitals used in predicting changes in electronic structure. Scheme 1.9 shows an energy level diagram showing the π^* and t_{2g} orbitals for a generic bis-trpy ruthenium compound.



Scheme 1.9. Schematic of energy levels and the changes due to the presence of functional groups on the terpyridine ligands. This scheme is adapted from ref. 19.

As far as electron withdrawing groups are concerned, they will stabilize the ligand LUMO more than the metal orbitals simply because the metal is further away. Further, in the excited state, the electron withdrawing group can help to stabilize the anionic ligand, while the now Ru(III) metal center becomes more Lewis acidic. It receives no stabilization from the functional group in the excited state. The net result is a slight lowering of the energy gap between the LUMO and the metal orbitals.

Electron donating groups work in very much the opposite direction. In the ground state an electron donating group will place more electron density on the chelating nitrogen atoms, thus destabilizing the ligand LUMO. More importantly, the metal t_{2g} orbitals are destabilized more in the excited state by the donor group not directly involved in the MLCT. The donor group not involved in the transition places excess electron density on the metal center. Again, the net result is a slight lowering of the energy gap between the two orbitals.

When it comes to making a heteroleptic complex with both an electron withdrawing group and an electron donating group, both of the functional groups do what they do best. That is to say that the withdrawing group helps to stabilize the LUMO (and the anionic ligand in the excited state) and the donor group destabilizes the metal orbital, except in the excited state where it soothes the Ru(III) center. The net result for a heteroleptic complex is a lowering of the energy gap between the t_{2g} and π^* orbitals. Only this time the difference is more dramatic.

This discussion focuses on the energy levels involved in the MLCT only, since they are directly responsible for absorption and emission. There is a d-d transition that lies close in energy to the MLCT, which competes as a non-radiative pathway for relaxation. Even though the sharp temperature dependence has been attributed to this energy gap, it has been shown to be much less of a factor when not in the solution state.[32] Therefore, the effect on the d-d by donors and acceptors has been ignored.

Sensor Effectiveness

From the data shown in Figure 1.3, it is fairly clear that the addition of donor groups increases the response to temperature much better than acceptor groups. The drawback is that with the addition of donor groups comes a decrease in intensity. Regardless, luminescent molecular sensors are very effective on wind tunnel models, and have been used, for the first time, to effectively visualize shockwaves at cryogenic temperatures. The application of these paints will make the testing of wind tunnel models much easier and will reduce the cost tremendously.

There are some bugs still to be worked out, however. First, these paints, especially the substituted terpyridine complexes, need to be brighter. It seems that for all the increase in slope that can be gained, the intensity falls off in some proportion. In order to make the detecting and analyzing easier and more precise, the intensity needs to be improved. It would be nice to use the much brighter tris-phen based sensors, but they have only a fraction of the temperature response as the trpy derivatives.

And secondly, there needs to be some more work done as to the best binder/complex/application method combination. These complex interactions can make or break a sensors effectiveness, and have proven quite the troublesome beast, especially in the PSP area.

Conclusion

Through the use of rational design and understanding of the photophysics of a series of ruthenium(II) bis-terpyridine complexes, a set of luminescent molecular sensors have been developed and used to visualize a shock wave at cryogenic temperatures. Once this technology becomes more refined, it is hoped that it can be expanded to warmer temperatures and then used in other fields outside the world of aerodynamics.

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CHAPTER 2
PERIPHERAL METHYL GROUPS:
A LOCK ON THE FLATTENING DISTORTION

Introduction

Since the discovery of luminescence from $[Cu(dmp)_2]^+$ in methylene chloride solution,[1] where dmp represents 2,9-dimethyl-1,10-phenanthroline, a lot of research has been focused on the photophysics of copper phenanthrolines. Specifically, studies have shown that both aryl and alkyl substituents in the 2 and 9 positions of the phenanthroline ligand have a dramatic effect upon the photophysics and photochemistry of the corresponding copper complexes.[2, 4, 5] One reason is that these substituents limit the extent of the D_2 flattening distortion that occurs in the oxidized form of the complex.[1, 2] In addition, these substituents inhibit the addition of a fifth ligand that tends to occur when the excited state is created in donor media.[3-5]

Quenching of excited states has been studied for many years. The data obtained from quenching experiments help to understand both the energies of the excited state[6] and its reactivity.[7] McMillin and co-workers have investigated the quenching processes of copper phenanthrolines and they have proposed a model[2] in which the pseudo-tetrahedral bis-phenanthroline complex first absorbs light, then releases this excess energy by twisting (or flattening). They have also shown that deactivation is further facilitated by the presence of Lewis base quenchers such as CH_3CN, THF, and DMF.[8]

The Lewis bases facilitate the quenching by forming an excited state complex (exciplex) with the metal compound.[8, 9] Exciplex quenching has been known for years in organic chemistry,[9, 10] but is much more rare in inorganic chemistry.[11] The main reason is that much of inorganic photochemistry is dominated by systems like $[Ru(bipy)_3]^{2+}$, which are coordinatively saturated and do not have enough physical space to add another ligand to the metal center. The case is quite the opposite for Cu(I) bis-phenanthrolines, since their excited states involve the creation of a formal copper(II) center that is four coordinate. Since Cu(II) is Jahn-Teller active, if the flattening distortion is large enough, a fifth ligand can enter the coordination sphere around the copper center. This new five coordinate complex is the exciplex. Formation of the exciplex (or addition of a fifth ligand) is favored due to the stabilization of the more Lewis acidic Cu(II) metal center with more electron density from a fifth ligand. The exciplex then dissipates the excited state energy in returning to the ground state and thus has deactivated the excited state. Although the flattening occurs without a Lewis base present, the Cu(II)...Lewis base interaction is necessary for exciplex formation. Unfortunately, the exciplex only exists for the briefest amount of time and has yet to be observed directly.

Sakaki and coworkers have shown,[12] via ab initio calculations, that the preferred geometry for a copper(I) phenanthroline bis phosphine complex is pseudo-tetrahedral (by ca.16.5 kcal/mol). Their computations predict a metal-to-ligand charge transfer absorbance low in energy that gives rise to a more Lewis acidic metal center. The computational data also predict that the excited state is not nearly as discerning in its structure. The difference between a pseudo-tetrahedral structure and a nearly planar one is only ca. 4.1 kcal/mol. When they factor in coordination by a water molecule, the nearly planar (now 5 coordinate) geometry is favored by ca.19.2 kcal/mol over a trigonal bipyramidal structure. This data supports the previous hypothesis that it is not the excited state energy but rather the attack by a Lewis base that drives exciplex quenching. This data also agrees well with the models proposed by McMillin et al[2, 8] and also the fact that the sterics of the ligands and the strength of the base dictate the rate of quenching.

By increasing the steric bulk at the 2 and 9 positions on the phenanthroline backbone, the rate of attack by the Lewis base slows which allows the excited state to exist longer.[1, 5, 8, 13, 14] The increase in excited state lifetime suggests that the formation of the exciplex is less favored energetically. This type of response is intuitive if the structure of the exciplex is considered.[1, 5, 8, 13, 14] Since its structure will be trigonal bipyramidal in nature, if the phenanthroline ligands cannot approach one another due to steric interactions, the approach and/or docking of the base will be blocked and the exciplex will not form.[1, 5, 8, 13, 14]

To date, many systems have been developed, using substituents such as methyl,[1, 5, 8, 13, 14] *n*-octyl,[13] *sec*-butyl,[15] *iso*-propyl,[16] *neo*-pentyl,[13, 17] and phenyl.[3, 5, 14] All of these systems have focused on steric bulk at the 2 and 9 positions and what effect it has on the photophysics. In this study, the addition of methyl groups at positions 3, 4, 7 and 8 has been investigated. These new ligands also have *n*-butyl or phenyl groups at the 2 and 9 positions. The effects of the methyl groups will be discussed with regard to absorption energies and excited state structure and reactivity.

Experimental

Materials

Acetonitrile, N,N'-dimethylformamide, methylene chloride, and tetrahydrofuran were obtained as Burdick and Jackson high-purity distilled in glass-grade chemicals from Scientific Products. The laser dye Coumarin 440 came from Laser Science, while Aldrich Chemical Co. supplied the 1,10-phenanthroline (phen), 2,9-dimethyl-1,10-phenanthroline (2,9-dmp), 3,4,7,8-tetramethyl-1,10-phenanthroline (tmp), 2,9-diphenyl-1,10-phenanthroline (dpp), $CuCl_2{\cdot}2H_2O$, KPF_6, 2.0 M *n*-butyl lithium in hexanes, and 2.0 M phenyl lithium in diethyl ether. G. F. Smith provided the 4,7-dimethyl-1,10-phenanthroline (4,7-dmp). The ligands 2,9-di(*n*-butyl)-1,10-phenanthroline (dbp), 2,9-di(*n*-butyl)-4,7-dimethyl-1,10-phenanthroline (dbdmp), 2,9-di(*n*-butyl)-3,4,7,8-tetramethyl-1,10-phenanthroline (dbtmp), 2,9-diphenyl-4,7-dimethyl-1,10-phenanthroline (dpdmp), 2,9-diphenyl-3,4,7,8-tetramethyl-1,10-phenanthroline (dptmp) were all prepared by modifications of the procedure of Pallenberg et al.[15] Copper complexes were prepared by literature methods.[18] 2,9-diphenyl-3,4,7,8-tetramethyl-phenanthroline (dptmp), $[Cu(dbp)_2]PF_6$, and $[Cu(dpp)_2]PF_6$ were available from a previous study.[16]

Methods

For luminescence, lifetime, and quenching studies, solutions were degassed using a series of freeze-pump-thaw cycles. A 525 nm long pass filter was used to keep stray light from the photomultiplier tube, while a 450 nm notch filter was used to filter stray light from the 440 nm excitation beam. The lifetime decays were analyzed with a user-written program. In all cases, the residual plots justified the use of a single exponential.

Quenching data was analyzed using a Stern-Volmer relationship[19] between the quencher concentration and the lifetime, as shown below:

$$1/\tau = 1/\tau_o + k_q[Q]$$

where τ_o is the lifetime of the complex in the absence of quencher, or in this case, pure CH_2Cl_2 and [Q] is the concentration of the quencher, DMF in this case. Linear regression of the data yielded the second order quenching constant k_q. The data was also analyzed using the integrated emission intensity with the following relationship:

$$I_o/I = \tau_o k_q[Q] + b$$

Here, again, τ_o is the lifetime in the absence of quencher, [Q] is the concentration of quencher, I_o is the emission intensity in the absence of quencher, and b is taken to be 1. Linear regression of the data yielded the second order quenching constant k_q.

In both cases, the quencher concentration varied from 0 to 1 M, while the copper complex concentration remained constant. Linear regression was done on two sets of the same data. The first set spanned the range 0 to 1 M DMF, while the second only covered 0 to 0.1 M DMF.

pK_a values were taken from references 20a, 20b, and 20c. Following the discussion in reference 20d, values for the new phenanthrolines were extrapolated. Butyl groups were considered to have the same effect as a methyl or ethyl group, based on data in references 20a, 20b, and 20d.

Instrumentation

Absorption and emission spectra were recorded on Perkin-Elmer Lambda 4C and SLM SPF 500C spectrometers, respectively. A description of the lifetime apparatus is in the literature.[7] Microanalyses were performed by H. Daniel Lee at the Purdue University Microanalysis Laboratory.

Computational Methodology

All computations were performed using HyperChem software, version 5.1 Pro, from HyperCube Inc., running on a Pentium II 166 MHz personal computer. The ligands were constructed using idealized bond distances and angles. This idealized geometry was used and no attempts were made to minimize the geometry of the ligand structure. Both molecular mechanics and semi-empirical computations were performed using the standard parameter sets included with the software.

For the molecular mechanics computations, ligand models were constructed using ethyl groups instead of butyl to isolate the rotation contribution to the β carbon. Also, only one "active" substituent was used, the remaining substituent was a methyl group. For example, to model the dbtmp ligand, computations were performed on 2-ethyl-3,4,7,8,9-pentamethyl-1,10-phenanthroline. Along a similar vein, to model the dptmp ligand, 2-phenyl-3,4,7,8,9-pentamethyl-1,10-phenanthroline was used. Only one "active" substituent was used to isolate the contribution of only one group and to minimize the number of conformations. The actual computations were single point calculations based on the idealized geometry, after adjusting the torsion angle between the nitrogen atom and the substituent of interest. Single point calculations were performed every 10 degrees.

For the semi-empirical computations, all butyl groups were replaced with methyl groups to minimize any conformational effects caused by the butyl chain. For example, the data reported for the dbp ligand was calculated using 2,9-dimethyl-1,10-phenanthroline as a model. Data for the phenyl derivatives was calculated with the phenyl rings having the same torsion angle. Calculations were performed at torsion angles of 0, 30, 45, 52, 60, and 90 degrees. An average of the values is reported as the data. The crystal structure of dpp shows a torsion angle of 0 degrees, while crystal structures of copper(I) complexes with dpp show an average torsion angle of approximately 52 degrees.

Preparations

2,9-di(*n*-butyl)-4,7-dimethyl-1,10-phenanthroline (dbdmp) [V-3]. This ligand was prepared by following the procedure of Pallenberg et al[15] using a 2.0 M n-butyl lithium solution in ether and 4,7-dimethyl-1,10-phenanthroline as starting materials. The product was purified on alumina and eluting with methylene chloride, collecting the first, faster moving fraction. The pale yellow material was recrystallized from ethanol to yield a white solid. ^{1}H NMR in $CDCl_3$ (in ppm): 7.92 (s, 2H), 7.34 (s, 2H), 3.19 (quartet, 4H), 2.74 (s, 6H), 1.88 (pentet, 4H), 1.51 (sextet, 4H), 1.00 (t, 6H).

2,9-di(*n*-butyl)-3,4,7,8-tetramethyl-1,10-phenanthroline (dbtmp) [IV-67]. This ligand was prepared as above[15] using a 2.0 M n-butyl lithium solution in ether and 3,4,7,8-tetramethyl-1,10-phenanthroline as starting materials and purified in the same fashion. The final product was a white solid. ^{1}H NMR in $CDCl_3$ (in ppm): 7.92 (s, 2H), 3.18 (quartet, 4H), 2.67 (s, 6H), 2.50 (s, 6H), 1.90 (pentet, 4H), 1.55 (sextet, 4H), 1.07 (t, 6H).

2,9-diphenyl-4,7-dimethyl-1,10-phenanthroline (dpdmp) [V-5]. This ligand was prepared as above[15] using a 1.6 M phenyl lithium solution in hexanes and 4,7-dimethyl-1,10-phenanthroline as starting materials and purified in the same manner. The final product was a pale yellow solid. ^{1}H NMR in $CDCl_3$ (in ppm): 8.49 (s, 4H), 8.00 (m, 4H), 7.55 (m, 6H), 2.85 (s, 6H).

$[Cu(dbdmp)_2]PF_6$ [V-55]. This compound was prepared by previous methods.[18] The orange material was recrystallized from water and ethanol to yield orange crystals. Calculated:(based on the hemihydrate $[Cu(dbdmp)_2]PF_6{\cdot}\frac{1}{2}H_2O$) 61.56% C, 6.58% H, 6.53% N. Found: 61.52% C, 6.55% H, 6.46% N. The presence of water was confirmed by proton NMR spectroscopy in $CDCl_3$.

$[Cu(dbtmp)_2]PF_6$ [IV-111, IV-187]. This compound was prepared by previous methods.[18] The orange material was recrystallized from water and ethanol to yield orange brown crystals. Calculated: 63.67% C, 7.12% H, 6.19% N. Found: 63.60% C, 6.81% H, 6.17% N.

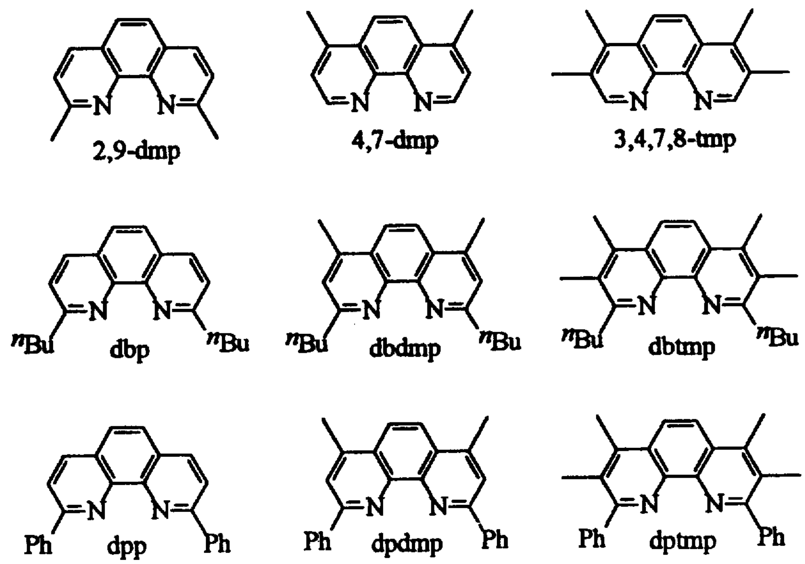
$[Cu(dpdmp)_2]PF_6$ [V-57]. This compound was prepared by previous methods.[18] The wine red material was rectrstallized from water and acetone to yield dark red crystals. Calculated:(based on the acetone monosolvate) 63.25% C, 4.08% H, 5.67% N. Found: 63.01% C, 4.15% H, 5.48% N. The presence of acetone was confirmed by proton NMR spectroscopy in $CDCl_3$.

$[Cu(dptmp)_2]PF_6$ [IV-188]. This compound was prepared by literature methods[18] and recrystallized from water and ethanol to yield red needles. Calculated:(based on the hemihydrate $[Cu(dptmp)_2]PF_6{\cdot}\frac{1}{2}H_2O$) 67.63% C, 4.97% H, 5.63% N. Found: 67.37% C, 4.74% H, 5.63% N. The presence of water was confirmed by proton NMR spectroscopy in $CDCl_3$.

Results

Synthesis

A schematic diagram showing the ligands of interest is shown in Scheme 2.1. All of the ligands, except for 2,9-dmp, that have substituents in the 2 and 9 positions, were synthesized by addition of organolithium reagents to the parent phenanthroline backbone. The method of Pallenberg et al[15] was employed and worked very nicely for the synthesis of the substituted phenanthroline ligands.



Scheme 2.1. The ligands and abbreviations used in this study.

Absorption Data

Table 2.1 shows all of the absorption data for both the butyl and phenyl derivatives as well as for the complexes with the parent phenanthroline backbones. None of the complexes show any appreciable solvatochromism in their absorption maxima.

Inspection of the absorption data suggests that the compounds can be divided into three groups. The first group is made of compounds with no substituents in the 2,9 positions. The second group has alkyl substituents in the 2,9 positions and the third group has aryl substituents in the 2,9 positions. These groups will be referred to as the parent group, the alkyl group, and the aryl group, respectively. The differentiation between the parent group and the alkyl group is necessary as substitution in the 2,9 positions of a phenanthroline drastically change its properties.[22]

Table 2.1. Absorption data for $[Cu(NN)_2]PF_6$ complexes.

Ligand	λ_{max} (nm), CH_2Cl_2	ε ($M^{-1}cm^{-1}$)	λ_{max} (nm), THF	λ_{max} (nm), CH_3CN
phen	440	7000[21]	441	442
4,7-dmp	434		435	435
tmp	430		430	431
2,9-dmp	454	7800[13]	456	457
dbp	457	7000[13]	457	457
dbdmp	456	9900	456	457
dbtmp	453	9300	452	452
dpp	440, 560	3200[5]	440, 560	440, 560
dpdmp	440, 550	3800	440, 550	441, 560
dptmp	467	6000	467	467

The absorption maxima, for the parent and alkyl groups, correlate well with the pK_a values for the ligands and also the calculated LUMO energies. This data is shown in Table 2.2 and Figure 2.1. This result is not surprising since the absorbance corresponds to placing an electron into a π^* orbital of the ligand, whose energy will be directly affected by the presence of electron donating functionalities. Therefore, the presence of additional electron donating methyl substituents on the ligand should make this process more difficult. The methyl groups also place more electron density on the nitrogen atoms in the free ligand, making them stronger bases.

The correlation of the parent and alkyl data indicates that within a group, the ground state structure, which is responsible for the absorbance energy, is not changing with addition of the peripheral methyl groups. This was not the case in the paper by Eggleston et al[13] in which the change in absorbance maxima was attributed to the changing steric bulk of the alkyl substituents in the 2,9 positions. The switching of substituents was causing a change in the ground state structure, as reflected in the absorption spectra. For the alkyl and parent groups, they should have a similar structure since they are substituted the same, within their respective series, at the 2,9 positions.

Table 2.2. Calculated orbital energies and pK_a values.

Ligand	pK_a	EH LUMO[d]	PM3 LUMO[d]	EH SLUMO[d]	PM3 SLUMO[d]
phen	4.88[b]	-9.726260	-1.043975	-9.574359	-0.728441
4,7-dmp	5.95[b]	-9.613302	-0.998210	-9.499872	-0.656965
tmp	6.48[b]	-9.576261	-0.929885	-9.479396	-0.601576
dbp[a]	~6.15[c]	-9.680675	-0.963496	-9.456161	-0.652240
dbdmp[a]	~6.81[c]	-9.568657	-0.920969	-9.379386	-0.583770
dbtmp[a]	~7.37[c]	-9.525309	-0.857133	-9.380155	-0.525717
dpp[e]	~5.00[f]	-12.0104	-8.679496		
dpdmp[e]	~6.1[g]	-11.8961	-8.574135		
dptmp[e]	~6.6[g]	-11.8409	-8.523982		

a calculations were performed on the methyl derivatives.

b pK_a values were taken from ref. 20a, 20b, 20c.

c data from ref. 20a, 20b, & 20c and estimations from discussions in ref. 20d

d energies in eV

e single point calculations were performed with the torsion angle between the phenyl group and the phenanthroline at 0, 30, 45, 52, 60 and 90 degrees and the reported data reflects an average value

f the pK_a is for 2,9-di(*p*-anisolyl)-1,10-phenanthroline, as reported in ref. 23

g data from ref. 23 and estimations from discussions in ref. 20d

Chart A

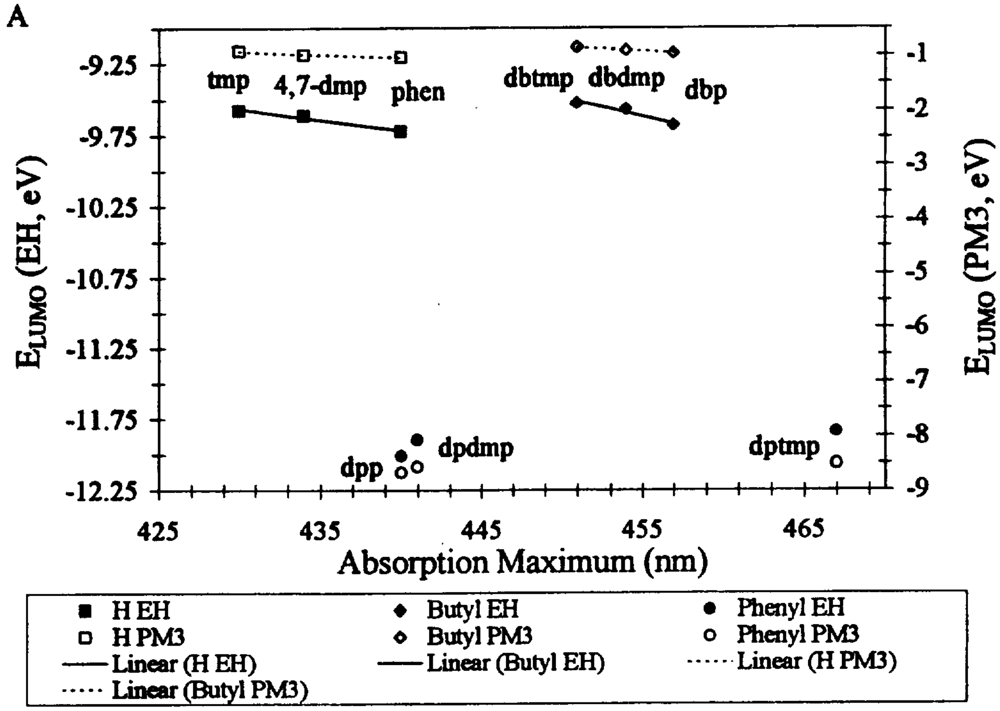


Chart B

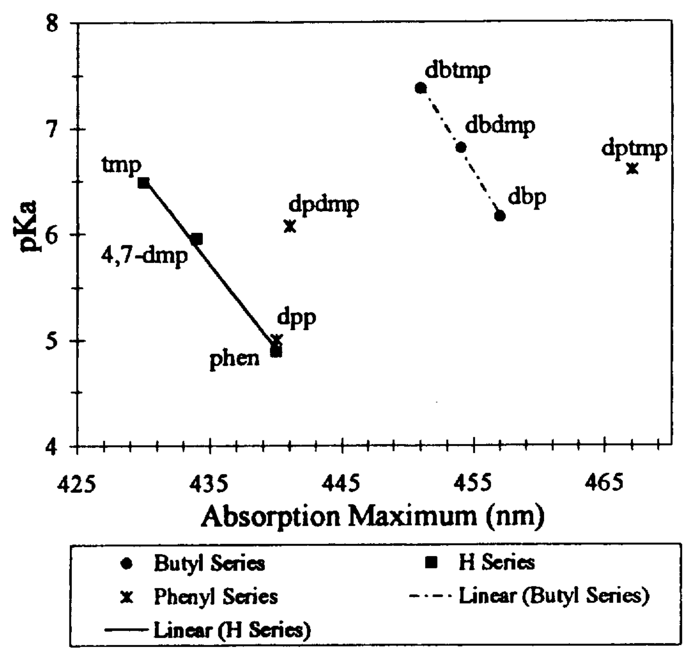


Figure 2.1. Correlation of the absorption of the copper complex with properties of the free ligand. Chart A is the correlation of the calculated orbital energies of the free ligand and the absorption maxima of the copper complexes. Chart B is the correlation of the free ligand pK_a and the absorption maxima of the copper complex.

Also shown in Table 2.2 and Figure 2.1 is the corresponding data for the aryl group. It is clear that this group does not correlate as well. The data for the dptmp complex does not seem to conform to the same trends when compared to the dpp and dpdmp complexes.

The dpp and dpdmp complexes show small changes in their pK_a and calculated LUMO energies compared to the changes with the corresponding butyl derivatives. Consequently, there is no apparent change in the absorption maximum to accompany the change in pK_a and LUMO energy. This is very different behavior compared to the parent and alkyl groups and most likely reflects a considerably different ground state structure.

As for the dptmp complex, it stands out from the other phenyl compounds as it has no low energy shoulder present in the absorption spectrum. In fact, the absorption spectrum of the dptmp complex resembles that of an alkyl-substituted phenanthroline more than it does and aryl-substituted phenanthroline, see Figure 2.2. Again this is indicative of a change in the ground state structure. In this case, the change is quite dramatic and seems to indicate a change back from an aryl-like to an alkyl-like structure.

A similar result was observed by McMillin et al using a derivative of phenanthroline containing 1-naphthyl groups in the 2 and 9 positions.[14] The steric bulk of the naphthyl groups keeps it from being in conjugation with the phenanthroline backbone. This lack of π-conjugation may also be occurring with the dptmp derivative since the 3,8 methyl groups should keep the phenyl ring approximately perpendicular to the phenanthroline backbone. A perpendicular phenyl ring will not conjugate in the π sense and thus is merely a σ donor.[21] However, a perpendicular phenyl ring will be able to stack, or interact, with the opposite phenanthroline backbone that it extends over.[23] This type of stacking may be responsible for the bathochromic shift observed in the absorption maxima relative to alkyl substituents.

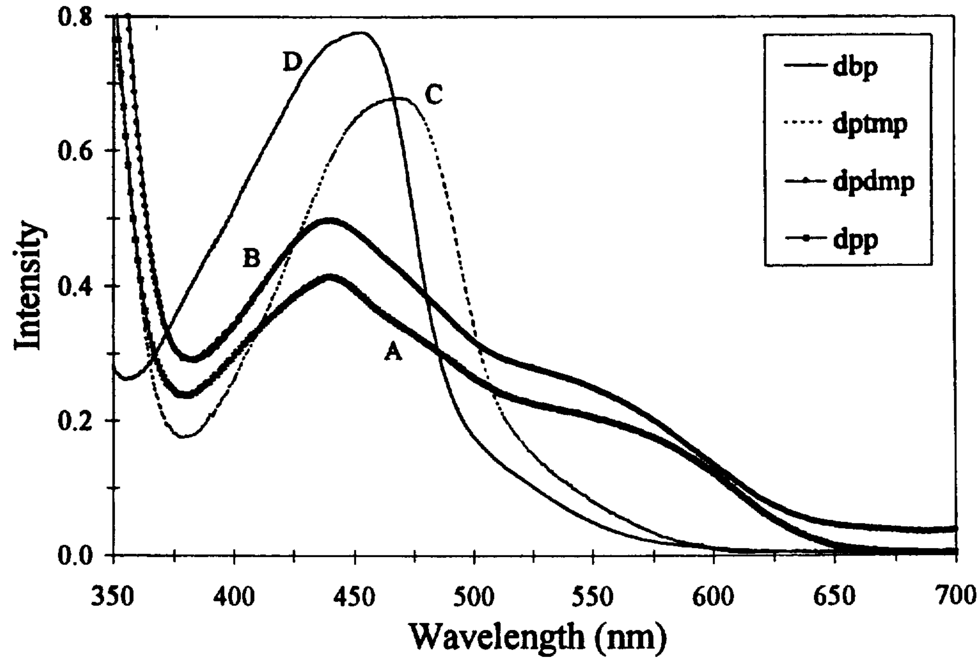


Figure 2.2. Absorption spectra for $[Cu(NN)_2]PF_6$ in CH_2Cl_2. Line A) NN = dpp, B) NN = dpdmp, C) NN = dptmp, D) NN = dbp.

Luminescence Data

Table 2.3 shows all of the luminescence data for both the butyl and phenyl derivatives. None of the complexes containing the parent phenanthroline backbones shows any emission in solution. All of the remaining complexes exhibit a bathochromic shift in their emission maxima with increasing polarity of the solvent.

For example, the dbp complex shifts from 670 nm to 685 nm to 690 nm as the solvent changes from CH_2Cl_2 to THF to CH_3CN. The presence of aryl substituents also lowers the emission energy, relative to alkyl substituents. On the other hand, for both series of complexes, the addition of 3,8 methyl groups causes a hypsochromic shift in the emission energy, whereas 4,7 methyl groups have little effect.

The lifetimes for all of the compounds listed in Table 2.3 increase with addition of the 3,8 methyl groups. In the butyl series, the non-methylated complex has a lifetime in CH_2Cl_2 of 136 ns, while the dbtmp complex has a lifetime of 330 ns. Addition of methyl groups in the 4 and 7 positions, again, has little effect. The lifetime data also shows that the 3,8 methylated ligands add a resistance to exciplex quenching. For instance, the dbp complex has a lifetime of 136 ns in CH_2Cl_2 while the lifetime is less than 10 ns in CH_3CN. The dbtmp complex has a lifetime of 330 ns in CH_2Cl_2 and a lifetime of 320 ns in CH_3CN. This is the first copper phenanthroline that has shown a definite resistance to quenching by donor solvents. The dptmp complex has the longest-lived excited state in methylene chloride, but still shows considerable quenching by acetonitrile.

The quantum yield for emission follows a similar trend as the lifetimes and emission maxima; a small increase with addition of the 4,7 methyl groups and a significant increase with addition of the 3,8 methyl groups, for both series. A comparison of quantum yields in the different solvents also shows a dramatic loss of intensity for the non- and di-methylated ligand complexes, whereas the tetra-methylated ligand complexes show a resiliency to addition of a fifth ligand.

Table 2.3. Luminescence data for $[Cu(NN)_2]PF_6$ complexes.[a]

Ligand	CH_2Cl_2	THF	CH_3CN
	Em λ_{max}[b], [τ[c]], (10^4 x ϕ)	Em λ_{max}[b], [τ[c]], (10^4xϕ)	Em λ_{max}[b], [τ[c]], (10^4xϕ)
2,9-dmp	690, [90], (4)	~700	~700
dbp	670, [140], (9)	685, [45], (3)	690, [25], (1)
dbdmp	670, [145], (15)	685, [105], (7)	690, [45], (4)
dbtmp	635, [330], (125)	640, [330], (124)	650, [320], (44)
dpp	685, [270], (10)	710, [190], (4)	715, [120], (3)
dpdmp	685, [310], (26)	700, [155], (13)	710, [125], (9)
dptmp	670, [480], (57)	685, [365], (29)	690, [255], (24)

a in deoxygenated methylene chloride from uncorrected spectra
b in nanometers
c in nanoseconds

Lewis Base Quenching

Analysis of the data in Table 2.4 reveals two major trends. First of all, for the non-methylated and 4,7-dimethyl series of compounds, the aryl containing compounds have a smaller quenching rate. For example, the quenching rate of $[Cu(dbp)_2]^+$ is $2.1*10^7$ $M^{-1}s^{-1}$ whereas $[Cu(dpp)_2]^+$ has a quenching constant of $6.7*10^6$ $M^{-1}s^{-1}$. This is no doubt due to the larger steric bulk of the phenyl ring relative to the butyl group.[5] The phenyl ring inhibits the approach of quencher molecules and limits the amount of flattening that can occur.

The second trend conveyed in the quenching data is that addition of the 3,8 methyls retards the quenching rate to a limiting value. For the phenyl series, the rate slows by about a factor of 3, whereas for the butyl series the rate is slowed by almost a full order of magnitude, which gives both $[Cu(dbtmp)_2]^+$ and $[Cu(dptmp)_2]^+$ a k_q of $2*10^6$ $M^{-1}s^{-1}$. This means that the 3,8 methyl groups are somehow hindering the attack of Lewis bases and causing the formation of the five coordinate to be much more difficult.

One other interesting observation was the fact that all four of the complexes measured showed some degree of downward curvature in their Stern-Volmer curves, see Figure 2.3 for an example. The data shown in Figure 2.3 is for the transient analysis of the dptmp complex. As the concentration of the DMF increases, the rate constant decreases. This is not a new phenomenon, and most likely stems from the fact that as the DMF concentration increases, the compound is being solvated differently, thus changing the τ_o that is used as the Y-intercept. The changing Y-intercept gives the appearance of a non-linear quenching rate. This is a pre-equilibrium association and has been seen in other systems that are sensitive to the solvent.[25]

Table 2.4. Quenching constants, k_q in $M^{-1}s^{-1}$, for DMF in deoxygenated CH_2Cl_2. The data has been separated into low DMF concentration (up to .1M) and high DMF concentration (up to 1M) to show the variation due to solvent polarity change.

Ligand	Transient, up to 1M	Transient, up to .1M	Intensity, up to 1 M	Intensity, up to .1 M
dbp	$2.1*10^7$	$2.0*10^7$	$3.6*10^7$	$2.4*10^7$
dbtmp	$1.7*10^6$	$2.9*10^6$	$7.0*10^6$	$1.2*10^6$
dpp	$6.7*10^6$	$8.3*10^6$	$7.6*10^7$	$6.1*10^6$
dptmp	$2.1*10^6$	$2.9*10^6$	$1.5*10^7$	$1.8*10^6$

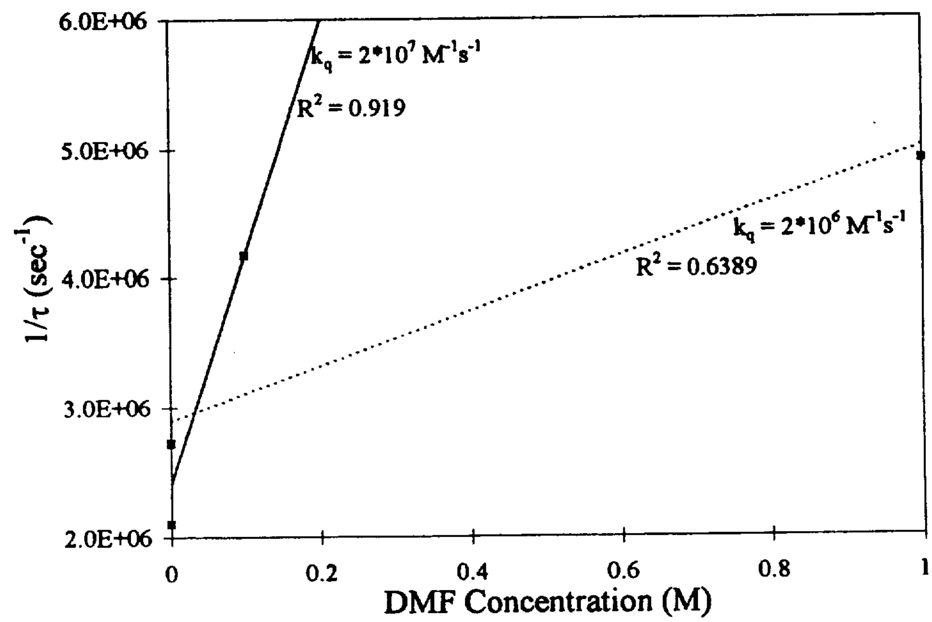


Figure 2.3. Stern-Volmer curve for $[Cu(dptmp)_2]PF_6$. The solid line represents the fit of the data up 0.1M DMF while the dotted line is the fit of the data up to 1M DMF.

Discussion

The addition of the methyl groups in the 3 and 8 positions of the phenanthroline backbone adds some interesting characteristics to the copper compounds. These methyl groups affect the absorption spectra, the emission spectra, and the resistance to exciplex quenching by oxygen or Lewis base solvents. The ability to alter these three phenomena indicates that these methyl groups modify both the ground state and the excited state.

Absorption Spectra

As mentioned previously, for the alkyl group, the addition of more methyl groups causes an increase in the energy of the charge-transfer absorbance for electronic reasons only. The ground state structure should be very similar within the series.

However, for the aryl series this is not the case. The spectrum of the dptmp complex does not look like other aryl-substituted phenanthroline complexes, indicative of a change in the ground state structure. Most aryl-substituted phenanthroline complexes show a maxima around 440 nm with a broad shoulder extending out past 600 nm. This is the case for dpp, dpdmp, and also agrees with the spectrum of $[Cu(tpp)_2]^+$, where tpp is 2,4,7,9-tetraphenyl-1,10-phenanthroline.[14] With dptmp, the spectrum seems to look more like an alkyl-substituted derivative with one intense absorbance and a very weak shoulder (or tail).

The presence of shoulders on the CT spectra of aryl-substituted complexes has been ascribed to the D_2 flattening distortion that is common to copper phenanthrolines.[24] For the usual aryl derivatives, the exceptionally broad shoulder is a result of the ease of rotation of the phenyl rings which allows for the flattening.[5] One of the main driving forces for flattening would be to increase conjugation between the aryl ring and the phenanthroline moiety it is bonded to.[21]

In the dptmp case this is assumed not to occur since the presence of the peripheral methyl groups should "lock" the geometry in a more rigid D_{2d} configuration thus limiting the contribution of the flattened geometry. Since the absorbance spectrum of the dptmp complex resembles that of an alkyl complex, where conjugation is not possible, it should have a similar more D_{2d}-like structure. The bathochromic shift exhibited by the dptmp complex relative to the alkyl-substituted phenanthroline complexes may be attributed to π-π interactions between a phenyl ring and the π-orbitals of the opposite phenanthroline backbone.[23]

Molecular modeling studies on the free phenanthroline ligands reveal that rotation of either the butyl or the phenyl group with a locking methyl group present is very difficult. Figures 2.4 and 2.5 show the total molecular mechanics energy as well as the Van der Waals component for both ligands. The computations were performed on model ligands that contained only one rotating group and used an ethyl group instead of a butyl group. These changes were done in order to isolate the rotational barrier for only one functional group and in the case of the butyl series, minimize conformational effects of the longer chain.

These figures indicate that it is approximately six times more difficult to rotate a butyl (ethyl) group with the 3,8 methyl groups present. Similarly, for the phenyl derivatives, the difference is roughly seven times as large. This data helps to support the idea that the phenyl groups remain perpendicular to the phenanthroline moiety and thus help to keep the geometry of the dptmp complex more D_{2d} and severely hamper the flattening distortion so common to copper phenanthrolines.

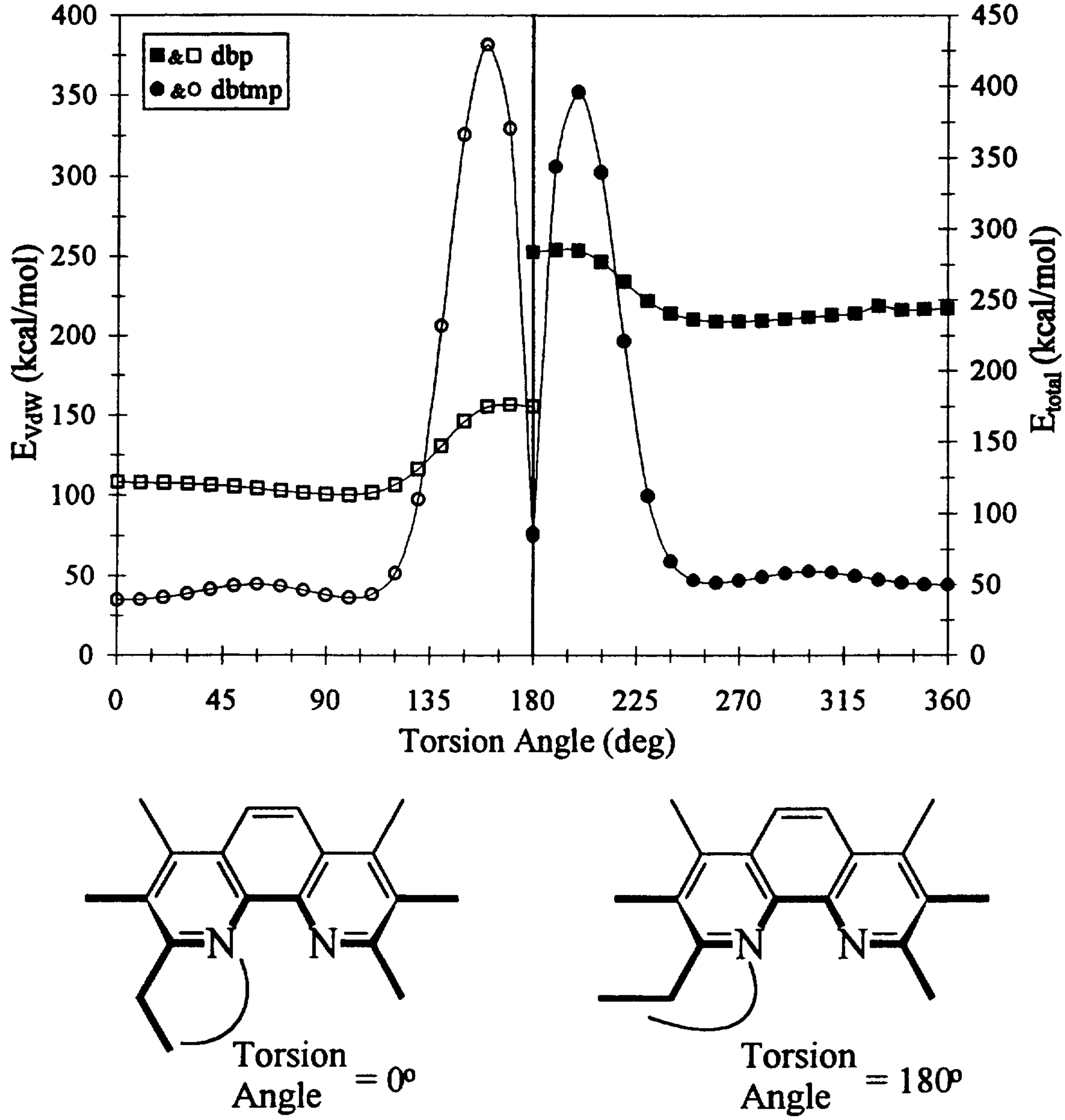
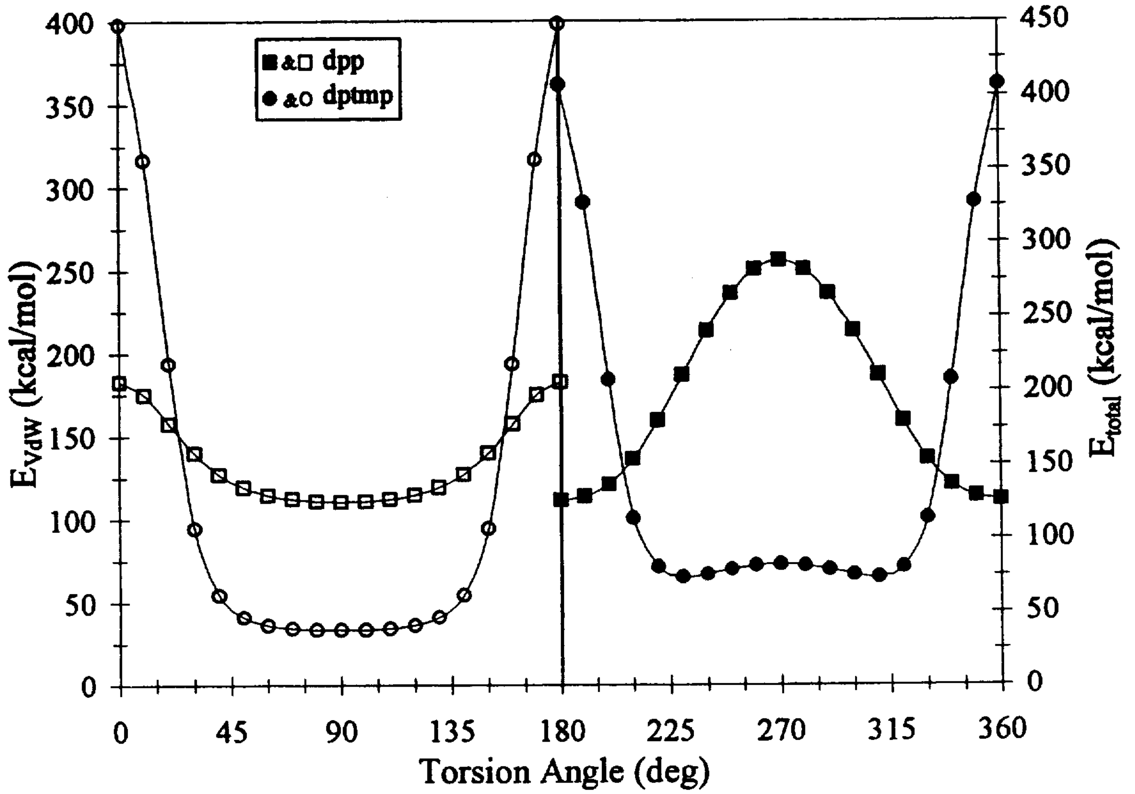


Figure 2.4. Molecular mechanics data for the free ligands dbp and dbtmp. The left side of the graph represents the Van der Waals component of the total energy, while the right side shows the total molecular mechanics energy of the free ligand. Circles are for data on the dbtmp ligand and squares are for data on the dbp ligand. The figures represent the torsion angles of interest at their extremes.



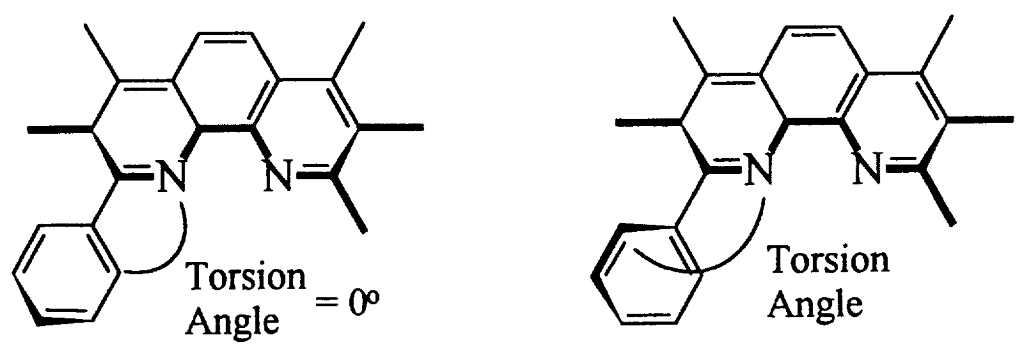


Figure 2.5. Molecular mechanics data for the free ligands dpp and dptmp. The left side of the graph represents the Van der Waals component of the total energy, while the right side shows the total molecular mechanics energy of the free ligand. Circles are for data on the dptmp ligand and squares are for data on the dpp ligand. The figures represent the torsion angles of interest, at their extremes.

Luminescence Data

As mentioned above, the addition of the methyl groups in the 3 and 8 positions is expected to rigidify the 2,9 substituents and therefore lock the copper complex into a more tetrahedral-like geometry. What is known about copper(I) phenanthrolines is that upon excitation of the metal electron into the ligand π^*, the now formal copper(II) complex undergoes a twisting or flattening distortion to form a complex that can accept a fifth ligand.[2, 8] This distortion is due to the steric flexibility of most phenanthrolines and the Jahn-Teller distortion that Cu(II) is famous for.[2, 24] With the tetra-methyl ligand series, the induced rigidity keeps the structure of the excited state close to that of tetrahedral. Since the major deactivation pathway is energy lost due to nuclear motion during the twisting processes, the lack of movement in this case results in a longer lived excited state and higher energy luminescence. The increase in emission energy is due to a larger energy difference between the more tetrahedral and more stable Cu(I) ground state and the more tetrahedral and destabilized Cu(II) excited state.[2, 8]

Quenching Phenomena

Exciplex quenching is a common type of quenching exhibited by copper(I) phenanthrolines and these new compounds are no different. The two tetra-methyl compounds do, however, exhibit a much slower rate of quenching when compared to other copper phenanthrolines.

A minimal kinetic scheme[3, 8] is presented in equations 1 through 3, where Cu* and Cu refer to the excited, emissive metal complex and the ground state metal complex, respectively. Q denotes the Lewis base quencher and [Cu*–Q] denotes the complex formed between Cu* and Q. These equations indicate that kq is not a simple rate constant but a combination of several rates. In this scheme, all deexcitation processes are assumed to be irreversible.

$$Cu^* \xrightarrow{k_0} Cu \tag{1}$$

$$Cu^* + Q \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} [Cu^*\text{-}Q \tag{2}$$

$$[Cu^*\text{-}Q] \xrightarrow{k_Q} Cu + Q \tag{3}$$

The complex [Cu*–Q] is not a simple encounter complex as can be the case,[25] but rather an exciplex that takes energy to dissociate. Since direct spectroscopic observance of the exciplex has yet to occur,[26] the concentration of the exciplex is assumed not to build up.[3, 8] This allows for the assumption of a steady-state concentration of [Cu*–Q]. With this assumption, kq is predicted to be second order, and takes to form of equation 4.

$$k_q = \frac{k_1}{1+k_{-1}/k_Q} \tag{4}$$

This model predicts that when k_{-1}, dissociation of the exciplex, competes with k_Q, quenching of the excited state, the observed rate of quenching will slow. In the cases presented here involving the tetra-methyl derivatives, k_{-1} is not a factor. In this case it is actually k_1, the formation of the exciplex that is the rate limiting step. Due to the increased steric repulsions between the bulkier ligands and the quencher, formation of the exciplex is slow and therefore the overall quenching rate is reduced. The addition of the steric locks slows the quenching of the excited state by making it a much less stable species.

Conclusion

The data presented in this paper show that the geometry of copper(I) phenanthrolines can not only be controlled by the size of the substituents in the 2,9 positions, but also by placing "locks" at the 3,8 positions of the ring. These locks help to restrict the mobility of the 2,9 substituents which inhibit the flattening distortion usually associated with copper(I) phenanthrolines. This increased rigidity leads to complexes with longer lived excited states with more efficient quantum yields and with less susceptibility towards exciplex quenching. This series of compounds has provided the longest lived copper(I) phenanthroline in methylene chloride solution and also a copper(I) phenanthroline that is resistant to quenching by all except the strongest Lewis bases.

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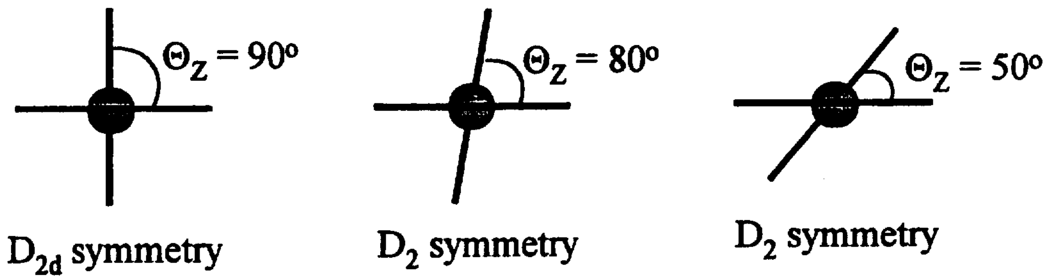
CHAPTER 3
SOLID STATE STRUCTURE CORRELATIONS IN COPPER(I) PHENANTHROLINES

Introduction

Crystal structures have long been used to predict the structures of molecules in solution; however, with copper(I) phenanthroline compounds the crystal structure can differ greatly from the solution structure.[1] Copper(I) phenanthrolines are psuedo-tetrahedral molecules with D_{2d} symmetry in solution. This symmetry is apparent from the solution absorption data and even complexes with rather large substituents on the phenanthroline backbone still conform to this assignment.[2] When these molecules crystallize, however; they no longer keep their neat D_{2d} symmetry, as evident by the range of absorption maxima from the solid state absorbance data.[1]

In perfect D_{2d} symmetry, the angle defined by the planes of the two phenanthroline ligands, denoted Θ_Z, is 90°.[3] Scheme 3.1 shows a schematic representation of the dihedral angle and its effect on structure. In the solid state, most copper(I) phenanthrolines show major departure from the ideal value. Θ_Z's have been reported anywhere from 50° to ~90°. The flattening observed in the crystal structures has been attributed to the packing forces of the lattice.[4, 25] This is not unreasonable to assume since Cu(I) is stable with a coordination number of 3,[10] coupled with the fact that the same cation shows different dihedral values with different anions. For example, $[Cu(dmp)_2]^+$, where dmp denotes 2,9-dimethyl-1,10-phenanthroline, has a dihedral angle of 72.4° with NO_3 as the anion[6] and 88.8° when $TCNQ^-$ is the anion.[7] In solution, the dihedral angle is assumed to be 90° since there are no outside forces distorting the geometry.[1]



Scheme 3.1. Schematic of Θ_Z and its effect on structure and symmetry.

From the limited number of crystal structures published on copper(I) phenanthrolines, it seems that the dihedral angle can be controlled by either changing the anion or by altering the steric bulk of the substituents in the 2 and 9 positions of the phenanthroline ring. For instance, of the 5 crystal structures of $[Cu(dmp)_2]^+$, none of them have the same dihedral angle, presumably due to the differing anions.[3, 5-7] Also, as the steric bulk, in the 2 and 9 positions, changes from H to CH_3 to *n*-pentyl, the dihedral angle changes by 40°.[3, 8, 9] However, the comparison is somewhat artificial, as these compounds also have different anions.

Correlation of the photophysical properties of copper phenanthrolines with their dihedral angles is another area that has not been fully explored. Kaizu and Shinozaki [1] have previously shown, computationally, that for $[Cu(ethanediimine)_2]^+$, the energy levels of the highest occupied and the lowest unoccupied molecular orbitals are dependant on the dihedral angle. Their DV-Xα calculations predict that the lowest energy allowed metal-to-ligand charge transfer absorbance will decrease in energy as the dihedral angle between the diimine ligands becomes smaller. Experimentally, the solid state absorbance of some $[Cu(dmp)_2]X$ salts, where the dihedral angle was known, were shown to follow this prediction. However, only two of the solids measured had defined dihedral angles. Further absorption analysis of solids with known dihedral angles along with their luminescent properties in the solid state should lead to a more clear understanding of what impact the dihedral angle has on the spectrum.

Another interesting aspect of copper phenanthroline solution chemistry is emission. Copper phenanthrolines with substituents in the 2,9 positions show emission in CH_2Cl_2 at room temperature.[10] If there are no substituents in positions 2 and 9, then the complexes are non-emissive in solution, as well as in a frozen glass.[1, 10] The main reason is due to a large geometry change that accompanies excitation.[10] Since the absorption is a metal-to-ligand charge transfer, a formal d^9 Cu(II) metal center is created. Since d^9 is Jahn-Teller active, tetrahedral geometry is not the preferred geometry for d^9. The excited compound undergoes a flattening distortion to alleviate the excess energy and return to the ground state.[10] McMillin and co-workers have shown many ways around this distortion,[10, 11] but perhaps one of the simplest is to examine the salts in the solid state. The solid state should severely retard the flattening distortion and lead to longer lived excited states. The examination and correlation of copper phenanthroline structure with absorption and emission properties will be the focus of this work.

Experimental

Materials

All solvents were of reagent grade unless otherwise stated. The 1,10-phenanthroline (phen), 3,4,7,8-tetramethyl-1,10-phenanthroline (tmp), 2,9-dimethyl-1,10-phenanthroline (dmp), 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline (bcp), 2,2'-bipyridine (bipy), 4,4'-dimethyl-2,2'-bipyridine (dmbp), KPF_6, $NaBPh_4$, 2.0 M *n*-butyl lithium solution in ether, and 1.6 M phenyllithium in hexanes were purchased from Aldrich and used as is. The ligands 2,9-di-*n*-butyl-1,10-phenanthroline (dbp), 2,9-diphenyl-1,10-phenanthroline (dpp), 6,6'-dimethyl-2,2'-bipyridine (dmbp), and 4,4',6,6'-tetramethyl-2,2'-bipyridine (tmbp) were prepared by modifying the prep by Pallenberg et al[9] to include the necessary starting materials. The ligands 2,9-di-*n*-butyl-4,7-dimethyl-1,10-phenanthroline (dbdmp), 2,9-di-*n*-butyl-3,4,7,8-tetramethyl-1,10-phenanthroline (dbtmp), 2,9-diphenyl-4,7-dimethyl-1,10-phenanthroline (dpdmp), and 2,9-diphenyl-3,4,7,8-tetramethyl-1,10-phenanthroline (dptmp) were available from a previous study.[11]

Methods

Solid state absorbance measurements were made using the opal-glass method.[12] Whatman filter paper grades 1 and 6 were used with paraffin oil. The spectrometer was backgrounded with a blank filter paper and oil sample. The data was corrected by dividing the intensity at each wavelength by the intensity at the starting wavelength of the scan, then subtracting 1. The new intensity value was then used in all the spectral plots.

Solid state emission measurements were made by packing a melting point capillary with ~1.75 cm (0.5 in.) of sample. The open end of the capillary was then sealed over a flame. During emission and lifetime measurements, a 452 nm notch filter was placed on the excitation beam to isolate the 440 nm excitation light. A 525 nm cutoff filter was used to protect the photomultiplier tube and both the excitation and emission bandpasses were set at 10 nm.

Excited state lifetimes were measured on the same capillary samples as for the emission measurements. The same filter setup was used except for an additional 575 nm filter that was placed in front of the photomultiplier tube. Data was taken from a digital oscilloscope and fit to an exponential decay with a user-written program.

Lorentz and polarization corrections were applied to the crystal structure data. The linear absorption coefficient is 5.2/cm for Mo K radiation. An empirical absorption correction using SCALEPACK [14] was applied. The structure was solved using the structure solution program PATTY in DIRDIF92,[15a] or by the direct methods using SIR97.[15b] The remaining atoms were located in succeeding difference Fourier syntheses. Hydrogen atoms were included in the refinement but restrained to ride on the atom to which they are bonded. The structure was refined in full-matrix least-squares where the function minimized was $\Sigma w(|F_o|^2-|F_c|^2)^2$ and the weight w is defined as

$$w=1/[\sigma^2(F_o^2)+(0.0996P)^2+0.0000P]$$

where $P=(F_o^2+2F_c^2)/3$. Scattering factors were taken from the "International Tables for Crystallography".[16] The space group was determined by the program ABSEN.[17] Refinement of the crystal data was performed with SHELX-97.[18]

Instrumentation

Absorbance measurements were made on a Perkin-Elmer Lambda 4C spectrophotometer, while emission measurements were recorded on a SLM SPF-500 spectrofluorometer. Excited state lifetime measurements were made on the laser setup described in the literature.[13] Preliminary examination of the crystals and subsequent data collection were performed with Mo K_α radiation ($\lambda = 0.71073$Å) on a Nonius KappaCCD. Structure refinement was performed on a AlphaServer 2100 computer.

Crystal Structure Determinations

$[Cu(tmp)_2]BPh_4$. An orange plate of $C_{56}H_{52}CuBN_4$ having approximate dimensions of 0.30 x 0.18 x 0.10 mm was grown from vapor diffusion of toluene into a methylene chloride solution of the complex. The crystal was mounted on a glass fiber in a random orientation. Cell constants and an orientation matrix for data collection were obtained from least-squares refinement, using the setting angles of 57010 reflections in the range $2 < \theta < 32°$. Data were collected to a maximum 2θ of 66.0°. A total of 57010 reflections were collected, of which 12948 were unique. Transmission coefficients ranged from 0.770 to 0.949 with an average value of 0.905. Intensities of equivalent reflections were averaged. The agreement factor for the averaging was 8.8% based on intensity. 12948 reflections were used in the refinements. However, only reflections with $F_o^2 > 2\sigma(F_o^2)$ were used in calculating R. The final cycle of refinement included 567 variable parameters and converged (largest parameter shift was 0.03 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma |F_o - F_c| / \Sigma F_o = 0.065$$

$$R2 = SQRT (\Sigma w (F_o^2 - F_c^2)^2 / \Sigma w (F_o^2)^2) = 0.157$$

The standard deviation of an observation of unit weight was 1.03. The highest peak in the final difference Fourier had a height of 0.51 e/A^3. The minimum negative peak had a height of -0.72 e/A^3. Table 3.1 gives a summary of the crystal parameters and other details of refinement.

Table 3.1. Crystallographic data for $[Cu(C_{32}H_{32}N_4)]BC_{24}H_{20}$.

$CuN_4C_{56}BH_{52}$	formula weight 855.42
a = 17.4883(4)Å	space group $P2_1/n$ (No. 14)
b = 9.86860(10)Å	T = 296. K
c = 26.3747(6)Å	λ = 0.71073Å
β = 97.7021(8)°	ρ_{calc} = 1.260g cm^{-3}
V = 4510.8(3)$Å^3$	μ = 0.525mm^{-1}
Z = 4	transmission coeff = 0.770-0.949
$R(F_o)^a$ = 0.065	$R_w(F_o^2)^b$ = 0.157

a $R = \Sigma \,||F_o| - |F_c|| / \Sigma |F_o|$ for $F_o^2 > 2\sigma(F_o^2)$
b $R_w = [\Sigma\, w\, (|F_o^2| - |F_c^2|)^2 / \Sigma\, w\, |F_o^2|^2]^{1/2}$

$[Cu(dipp)_2]$TFPB. A yellow-orange plate of $C_{68}H_{52}CuBF_{24}N_4$ having approximate dimensions of 0.25 x 0.22 x 0.10 mm was grown by slow evaporation of an aqueous alcoholic solution of the compound. The crystal was mounted on a glass fiber in a random orientation. Cell constants and an orientation matrix for data collection were obtained from least-squares refinement, using the setting angles of 43343 reflections in the range $4 < \theta < 30°$. Data were collected to a maximum 2θ of 61.0°. A total of 43343 reflections were collected, of which 8774 were unique. Transmission coefficients ranged from 0.706 to 0.958 with an average value of 0.894. Intensities of equivalent reflections were averaged. The agreement factor for the averaging was 6.2% based on intensity. 8774 reflections were used in the refinements. However, only reflections with $F_o^2 > 2\sigma(F_o^2)$ were used in calculating R. The final cycle of refinement included 891 variable parameters and converged (largest parameter shift was 0.04 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma\, |F_o - F_c| \,/\, \Sigma\, F_o = 0.093$$

$$R2 = SQRT\, (\, \Sigma\, w\, (\, F_o^2 - F_c^2\,)^2 \,/\, \Sigma\, w\, (F_o^2)^2\,) = 0.253$$

The standard deviation of an observation of unit weight was 1.03. The highest peak in the final difference Fourier had a height of 0.86 e/A^3. The minimum negative peak had a height of -0.71 e/A^3. Table 3.2 gives a summary of the crystal parameters and other details of refinement.

Table 3.2. Crystallographic data for $[Cu(C_{44}H_{40}N_4)]BC_{24}H_{12}F_{24}$.

$CuF_{24}N_4C_{68}BH_{52}$	formula weight 1455.51
a = 14.2523(3)Å	space group $P\bar{1}$ (No. 2)
b = 16.0496(4)Å	T = 296. K
c = 17.5801(3)Å	λ = 0.71073Å
α = 112.4150(13)°	ρ_{calc} = 1.418g cm^{-3}
β = 105.7480(13)°	μ = 0.425mm^{-1}
γ = 99.6078(11)°	transmission coeff = 0.706-0.958
V = 3408.7(3)Å^3	$R(F_o)^a$ = 0.093
Z = 2	$R_w(F_o^2)^b$ = 0.253

a $R = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$ for $F_o^2 > 2\sigma(F_o^2)$
b $R_w = [\Sigma w (|F_o^2| - |F_c^2|)^2 / \Sigma w |F_o^2|^2]^{1/2}$

$[Cu(dptmp)_2]PF_6$•THF. An orange chunk of $C_{60}H_{56}CuF_6N_4OP$ having approximate dimensions of 0.25 x 0.20 x 0.18 mm was grown by slow diffusion of toluene into a THF solution of the compound. The crystal was mounted on a glass fiber in a random orientation. Cell constants and an orientation matrix for data collection were obtained from least-squares refinement, using the setting angles of 33837 reflections in the range $3 < \theta < 31°$. Data were collected to a maximum 2θ of 63.9°. A total of 33837 reflections were collected, of which 13753 were unique. Transmission coefficients ranged from 0.751 to 0.911 with an average value of 0.875. A secondary extinction correction was applied.[18] The final coefficient, refined in least-squares, was 0.0240000 (in absolute units). Intensities of equivalent reflections were averaged. The agreement factor for the averaging was 5.5% based on intensity. 13753 reflections were used in the refinements. However, only reflections with $F_o^2>2\sigma(F_o^2)$ were used in calculating R. The final cycle of refinement included 666 variable parameters and converged (largest parameter shift was 0.04 times its esd) with unweighted and weighted agreement factors of:

$$R1 = \Sigma\ |F_o - F_c| / \Sigma\ F_o = 0.074$$

$$R2 = SQRT\ (\Sigma\ w\ (F_o^2 - F_c^2)^2 / \Sigma\ w\ (F_o^2)^2) = 0.190$$

The standard deviation of an observation of unit weight was 1.03. The highest peak in the final difference Fourier had a height of 0.67 e/A^3. The minimum negative peak had a height of -0.56 e/A^3. Table 3.3 gives a summary of the crystal parameters and other details of refinement.

Table 3.3. Crystallographic data for $[Cu(C_{56}H_{48}N_4)]PF_6{\cdot}C_4H_8O$.

$CuPF_6ON_4C_{60}H_{56}$	formula weight 1057.65
a = 12.8486(4)Å	space group $P\bar{1}$ (No. 2)
b = 13.7341(4)Å	T = 296. K
c = 15.1678(3)Å	λ = 0.71073Å
α = 99.5819(14)°	ρ_{calc} = 1.355g cm^{-3}
β = 96.7263(13)°	μ = 0.516mm^{-1}
γ = 97.3311(12)°	transmission coeff = 0.751-0.911
V = 2591.3(2)Å^3	$R(F_o)^a$ = 0.074
Z = 2	$R_w(F_o^2)^b$ = 0.190

a $R = \Sigma\ ||F_o| - |F_c|| / \Sigma\ |F_o|$ for $F_o^2>2\sigma(F_o^2)$
b $R_w = [\Sigma\ w\ (|F_o^2| - |F_c^2|)^2 / \Sigma\ w\ |F_o^2|^2]^{1/2}$

Preparations

Copper complexes were prepared following literature methods[19] and were recrystallized from ethanol and water. Metathesis reactions were done in a mixture of ethanol and water and the compound was isolated sacrificially, meaning that the isolated yields were on the order of 75%. This was done to insure conversion without contamination.

Results

Crystal Structure Analysis

$[Cu(tmp)_2]BPh_4$

Figure 3.1 gives a view of the copper complex along with the atom labels. The positional and thermal parameters, along with bond lengths and bond angles are given in Tables 3.4, 3.5, and 3.6, respectively. The geometry around the copper center is best described as psuedotetrahedral with molecular symmetry closer to D_{2d} than D_2. The average chelate-bite angle is 81.25°, which is a typical value for copper phenanthrolines.[3, 20] All of the Cu-N bond distances are similar in value, so there is no "rocking" distortion as is present in 2,9-diaryl substituted phenanthroline complexes.[21, 22] The average Cu-N bond distance is 2.044 Å. This value is close to other non-2,9-substituted phenanthroline complexes. For example, the average Cu-N distance in $[Cu(phen)_2]ClO_4$ is 2.049 Å,[8] while for $[Cu(phen)_2]CuBr_2$ the average value is 2.039 Å.[8] The one geometrical characteristic that sets $[Cu(tmp)_2]BPh_4$ apart is its rather large dihedral angle. $[Cu(tmp)_2]BPh_4$ has a dihedral angle of 81.8°, while the dihedral angles (Θ_Z) for $[Cu(phen)_2]ClO_4$, $[Cu(phen)_2][Cu(OAc)_2]$, and $[Cu(phen)_2]CuBr_2$ are 49.9°,[8] 68.6°,[8] and 76.8°,[23] respectively. In fact, this dihedral angle is larger than the Θ_Z of some $[Cu(dmp)_2]X$ complexes. $[Cu(dmp)_2]Br$ and $[Cu(dmp)_2]NO_3$ have dihedral angles of

79.9° and 72.4°, respectively.[3, 6] Figure 3.2 shows the $[Cu(tmp)_2]^+$ cation from behind one of the phenanthroline ligands. The almost perpendicular arrangement of the two tmp ligands is indicative of the large Θ_Z.

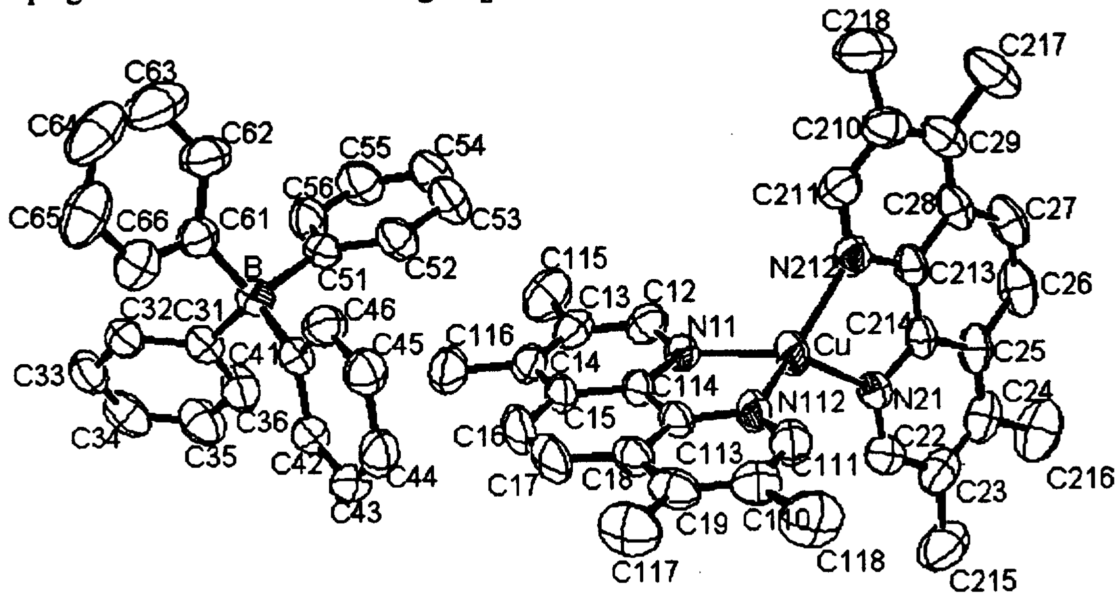


Figure 3.1. ORTEP drawing of $[Cu(tmp)_2]BPh_4$ with labeling scheme and 50% ellipsoids. Hydrogen atoms have been omitted for clarity.

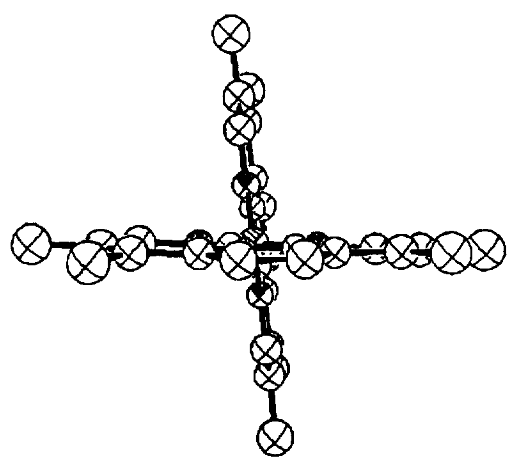


Figure 3.2. ORTEP drawing of the $[Cu(tmp)_2]^+$ cation from behind one phenanthroline ligand. The angle between the two phenanthroline lignds is Θ_Z (81.8°).

Table 3.4. Positional and temperature parameters (Å^2) for $[Cu(tmp)_2]BPh_4$.

Atom	x	y	z	U(Å^2)[a]
Cu	0.253358(19)	0.06729(4)	0.274371(15)	0.06220(14)
N(11)	0.18432(12)	0.1880(2)	0.31252(8)	0.0479(7)
N(21)	0.34472(13)	0.1290(2)	0.23961(9)	0.0517(7)
N(112)	0.14921(13)	0.0173(2)	0.23484(9)	0.0502(7)
N(212)	0.33801(13)	-0.0455(2)	0.31586(9)	0.0507(7)
C(12)	0.20183(17)	0.2720(3)	0.35194(11)	0.0554(9)
C(13)	0.14855(19)	0.3512(3)	0.37416(11)	0.0592(9)
C(14)	0.07192(18)	0.3393(3)	0.35543(12)	0.0557(9)
C(15)	0.05009(15)	0.2467(3)	0.31503(11)	0.0495(8)
C(16)	-0.02781(17)	0.2174(3)	0.29423(14)	0.0674(12)
C(17)	-0.04626(17)	0.1275(4)	0.25627(14)	0.0676(11)
C(18)	0.01154(15)	0.0562(3)	0.23309(12)	0.0514(8)
C(19)	-0.00541(18)	-0.0378(3)	0.19275(13)	0.0585(9)
C(22)	0.34804(19)	0.2165(3)	0.20183(12)	0.0633(10)
C(23)	0.4158(2)	0.2577(3)	0.18300(13)	0.0668(12)
C(24)	0.4848(2)	0.2056(3)	0.20613(14)	0.0670(10)
C(25)	0.48395(16)	0.1112(3)	0.24617(13)	0.0580(9)
C(26)	0.55179(17)	0.0497(4)	0.27391(17)	0.0772(12)
C(27)	0.54802(18)	-0.0411(4)	0.31152(16)	0.0746(12)
C(28)	0.47664(16)	-0.0813(3)	0.32707(13)	0.0567(9)
C(29)	0.4698(2)	-0.1775(3)	0.36633(13)	0.0633(10)
C(31)	-0.23565(15)	0.3798(3)	0.43421(11)	0.0464(8)
C(32)	-0.29496(17)	0.4278(3)	0.45997(11)	0.0519(8)
C(33)	-0.31154(19)	0.5657(3)	0.46317(13)	0.0647(10)
C(34)	-0.2702(2)	0.6609(3)	0.44075(14)	0.0701(12)
C(35)	-0.21201(19)	0.6182(3)	0.41510(15)	0.0701(12)
C(36)	-0.19498(18)	0.4810(3)	0.41197(13)	0.0621(9)
C(41)	-0.22485(14)	0.1543(3)	0.37489(10)	0.0446(7)
C(42)	-0.23328(16)	0.2281(3)	0.32956(11)	0.0518(8)
C(43)	-0.24297(16)	0.1646(4)	0.28160(11)	0.0609(9)
C(44)	-0.24423(16)	0.0265(4)	0.27746(12)	0.0606(9)
C(45)	-0.23670(17)	-0.0502(3)	0.32147(12)	0.0568(9)
C(46)	-0.22728(17)	0.0128(3)	0.36839(11)	0.0529(9)
C(51)	-0.11567(15)	0.2115(2)	0.45375(10)	0.0447(7)
C(52)	-0.06418(17)	0.1233(3)	0.43470(12)	0.0551(9)
C(53)	0.01366(18)	0.1190(3)	0.45359(14)	0.0672(10)
C(54)	0.04453(19)	0.2027(3)	0.49220(13)	0.0649(10)
C(55)	-0.0040(2)	0.2922(3)	0.51196(13)	0.0689(10)
C(56)	-0.08184(18)	0.2955(3)	0.49320(11)	0.0588(9)
C(61)	-0.25896(17)	0.1261(3)	0.46828(11)	0.0500(8)
C(62)	-0.2267(2)	0.0565(3)	0.51226(12)	0.0680(12)
C(63)	-0.2713(4)	-0.0246(4)	0.53970(16)	0.0995(18)
C(64)	-0.3484(4)	-0.0403(4)	0.52524(19)	0.1012(18)
C(65)	-0.3819(3)	0.0252(4)	0.48257(18)	0.0872(14)
C(66)	-0.3379(2)	0.1056(3)	0.45446(13)	0.0652(10)
C(110)	0.0558(2)	-0.0981(3)	0.17336(13)	0.0631(10)
C(111)	0.13080(19)	-0.0676(3)	0.19632(12)	0.0608(10)
C(113)	0.08919(14)	0.0817(3)	0.25270(11)	0.0445(7)
C(114)	0.10867(14)	0.1754(3)	0.29405(10)	0.0443(7)
C(115)	0.1788(3)	0.4424(4)	0.41808(15)	0.0895(14)
C(116)	0.0121(2)	0.4223(3)	0.37779(15)	0.0796(14)

Table 3.4, continued

Atom	x	y	z	U(Å^2)^a
C(117)	-0.0877(2)	-0.0736(4)	0.17136(16)	0.0845(14)
C(118)	0.0455(3)	-0.1970(4)	0.12931(14)	0.0916(15)
C(210)	0.3983(2)	-0.2019(3)	0.37970(12)	0.0652(10)
C(211)	0.33530(19)	-0.1310(3)	0.35433(12)	0.0595(9)
C(213)	0.40965(14)	-0.0200(3)	0.30211(11)	0.0449(8)
C(214)	0.41263(15)	0.0749(3)	0.26135(11)	0.0469(8)
C(215)	0.4091(3)	0.3575(4)	0.13935(15)	0.0992(17)
C(216)	0.5605(2)	0.2489(4)	0.18823(17)	0.1001(17)
C(217)	0.5408(2)	-0.2485(4)	0.39281(16)	0.0995(15)
C(218)	0.3835(3)	-0.2995(4)	0.42172(15)	0.0973(16)
B	-0.20917(18)	0.2192(3)	0.43287(12)	0.0452(9)

a $U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a^*_i a^*_j a_i \cdot a_j$

Table 3.5. Bond distances (Å) for $[Cu(tmp)_2]BPh_4$. Numbers in parentheses are estimated standard deviations in the least significant digits.

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
Cu	N(112)	2.034(2)	C(29)	C(210)	1.365(5)
Cu	N(21)	2.039(2)	C(29)	C(217)	1.512(4)
Cu	N(212)	2.048(2)	C(31)	C(32)	1.397(4)
Cu	N(11)	2.053(2)	C(31)	C(36)	1.399(4)
N(11)	C(12)	1.332(4)	C(31)	B	1.653(4)
N(11)	C(114)	1.353(3)	C(32)	C(33)	1.396(4)
N(21)	C(22)	1.326(4)	C(33)	C(34)	1.368(5)
N(21)	C(214)	1.357(3)	C(34)	C(35)	1.362(5)
N(112)	C(111)	1.323(4)	C(35)	C(36)	1.391(4)
N(112)	C(113)	1.364(3)	C(41)	C(42)	1.391(4)
N(212)	C(211)	1.326(4)	C(41)	C(46)	1.408(4)
N(212)	C(213)	1.373(3)	C(41)	B	1.647(4)
C(12)	C(13)	1.404(4)	C(42)	C(43)	1.401(4)
C(13)	C(14)	1.370(4)	C(43)	C(44)	1.367(5)
C(13)	C(115)	1.506(5)	C(44)	C(45)	1.377(4)
C(14)	C(15)	1.417(4)	C(45)	C(46)	1.375(4)
C(14)	C(116)	1.510(4)	C(51)	C(52)	1.394(4)
C(15)	C(114)	1.415(3)	C(51)	C(56)	1.398(4)
C(15)	C(16)	1.428(4)	C(51)	B	1.656(4)
C(16)	C(17)	1.345(5)	C(52)	C(53)	1.386(4)
C(17)	C(18)	1.434(4)	C(53)	C(54)	1.365(4)
C(18)	C(113)	1.409(4)	C(54)	C(55)	1.375(4)
C(18)	C(19)	1.412(4)	C(55)	C(56)	1.385(4)
C(19)	C(110)	1.381(5)	C(61)	C(66)	1.394(4)
C(19)	C(117)	1.515(4)	C(61)	C(62)	1.400(4)
C(22)	C(23)	1.405(4)	C(61)	B	1.641(4)
C(23)	C(24)	1.376(5)	C(62)	C(63)	1.386(5)
C(23)	C(215)	1.508(5)	C(63)	C(64)	1.360(7)
C(24)	C(25)	1.410(5)	C(64)	C(65)	1.360(6)
C(24)	C(216)	1.525(4)	C(65)	C(66)	1.387(5)
C(25)	C(214)	1.407(4)	C(110)	C(111)	1.401(5)
C(25)	C(26)	1.442(5)	C(110)	C(118)	1.509(5)
C(26)	C(27)	1.345(5)	C(113)	C(114)	1.436(4)
C(27)	C(28)	1.421(5)	C(210)	C(211)	1.398(4)
C(28)	C(213)	1.402(4)	C(210)	C(218)	1.516(5)
C(28)	C(29)	1.422(5)	C(213)	C(214)	1.432(4)

Table 3.6. Bond angles (deg.) for $[Cu(tmp)_2]BPh_4$. Numbers in parentheses are estimated standard deviations in the least significant digits.

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
N(112)	Cu	N(21)	122.94(10)	C(25)	C(24)	C(216)	120.9(4)
N(112)	Cu	N(212)	132.49(9)	C(214)	C(25)	C(24)	118.7(3)
N(21)	Cu	N(212)	81.29(9)	C(214)	C(25)	C(26)	116.7(3)
N(112)	Cu	N(11)	81.20(9)	C(24)	C(25)	C(26)	124.6(3)
N(21)	Cu	N(11)	126.49(9)	C(27)	C(26)	C(25)	122.4(3)
N(212)	Cu	N(11)	118.95(9)	C(26)	C(27)	C(28)	122.0(3)
C(12)	N(11)	C(114)	116.7(2)	C(213)	C(28)	C(29)	118.9(3)
C(12)	N(11)	Cu	130.87(19)	C(213)	C(28)	C(27)	117.1(3)
C(114)	N(11)	Cu	112.40(18)	C(29)	C(28)	C(27)	124.0(3)
C(22)	N(21)	C(214)	116.7(2)	C(210)	C(29)	C(28)	118.4(3)
C(22)	N(21)	Cu	130.43(19)	C(210)	C(29)	C(217)	121.5(3)
C(214)	N(21)	Cu	112.74(18)	C(28)	C(29)	C(217)	120.1(3)
C(111)	N(112)	C(113)	116.2(3)	C(32)	C(31)	C(36)	114.5(2)
C(111)	N(112)	Cu	131.0(2)	C(32)	C(31)	B	124.3(2)
C(113)	N(112)	Cu	112.80(19)	C(36)	C(31)	B	121.0(2)
C(211)	N(212)	C(213)	116.5(2)	C(33)	C(32)	C(31)	122.3(3)
C(211)	N(212)	Cu	131.1(2)	C(34)	C(33)	C(32)	121.2(3)
C(213)	N(212)	Cu	112.28(18)	C(35)	C(34)	C(33)	118.4(3)
N(11)	C(12)	C(13)	125.2(3)	C(34)	C(35)	C(36)	120.7(3)
C(14)	C(13)	C(12)	118.3(3)	C(35)	C(36)	C(31)	123.0(3)
C(14)	C(13)	C(115)	123.7(3)	C(42)	C(41)	C(46)	114.7(3)
C(12)	C(13)	C(115)	118.0(3)	C(42)	C(41)	B	125.5(2)
C(13)	C(14)	C(15)	118.6(2)	C(46)	C(41)	B	119.8(2)
C(13)	C(14)	C(116)	120.6(3)	C(41)	C(42)	C(43)	121.9(3)
C(15)	C(14)	C(116)	120.8(3)	C(44)	C(43)	C(42)	121.1(3)
C(114)	C(15)	C(14)	118.6(3)	C(43)	C(44)	C(45)	118.8(3)
C(114)	C(15)	C(16)	116.9(3)	C(46)	C(45)	C(44)	119.8(3)
C(14)	C(15)	C(16)	124.5(3)	C(45)	C(46)	C(41)	123.8(3)
C(17)	C(16)	C(15)	122.8(3)	C(52)	C(51)	C(56)	114.2(3)
C(16)	C(17)	C(18)	121.9(3)	C(52)	C(51)	B	124.4(2)
C(113)	C(18)	C(19)	119.2(3)	C(56)	C(51)	B	121.4(2)
C(113)	C(18)	C(17)	117.1(3)	C(53)	C(52)	C(51)	122.7(3)
C(19)	C(18)	C(17)	123.7(3)	C(54)	C(53)	C(52)	121.4(3)
C(110)	C(19)	C(18)	117.8(3)	C(53)	C(54)	C(55)	118.0(3)
C(110)	C(19)	C(117)	120.4(3)	C(54)	C(55)	C(56)	120.5(3)
C(18)	C(19)	C(117)	121.8(3)	C(55)	C(56)	C(51)	123.3(3)
N(21)	C(22)	C(23)	125.3(3)	C(66)	C(61)	C(62)	114.8(3)
C(24)	C(23)	C(22)	117.8(3)	C(66)	C(61)	B	121.0(3)
C(24)	C(23)	C(215)	123.8(3)	C(62)	C(61)	B	124.1(3)
C(22)	C(23)	C(215)	118.4(4)	C(63)	C(62)	C(61)	121.6(4)
C(23)	C(24)	C(25)	118.8(3)	C(64)	C(63)	C(62)	121.6(4)
C(23)	C(24)	C(216)	120.3(3)	C(65)	C(64)	C(63)	118.6(4)
C(64)	C(65)	C(66)	120.4(4)	C(211)	C(210)	C(218)	117.9(3)
C(65)	C(66)	C(61)	123.0(4)	N(212)	C(211)	C(210)	125.3(3)
C(19)	C(110)	C(111)	118.3(3)	N(212)	C(213)	C(28)	122.1(3)
C(19)	C(110)	C(118)	123.0(3)	N(212)	C(213)	C(214)	116.4(2)
C(111)	C(110)	C(118)	118.6(3)	C(28)	C(213)	C(214)	121.5(2)
N(112)	C(111)	C(110)	125.8(3)	N(21)	C(214)	C(25)	122.6(3)
N(112)	C(113)	C(18)	122.6(3)	N(21)	C(214)	C(213)	117.2(2)

Table 3.6, continued

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
======	======	======	=====	======	======	======	=====
N(112)	C(113)	C(114)	116.6(2)	C(25)	C(214)	C(213)	120.2(3)
C(18)	C(113)	C(114)	120.8(2)	C(61)	B	C(41)	106.0(2)
N(11)	C(114)	C(15)	122.5(3)	C(61)	B	C(31)	110.7(2)
N(11)	C(114)	C(113)	117.0(2)	C(41)	B	C(31)	112.4(2)
C(15)	C(114)	C(113)	120.5(2)	C(61)	B	C(51)	111.1(2)
C(29)	C(210)	C(211)	118.6(3)	C(41)	B	C(51)	109.0(2)
C(29)	C(210)	C(218)	123.5(3)	C(31)	B	C(51)	107.7(2)

$[Cu(dipp)_2]TFPB$

A view of the $[Cu(dipp)_2]^+$ cation, along with the atomic labeling scheme, is shown in Figure 3.3. The positional and thermal parameters, bond distances, and bond angles are shown in Tables 3.7, 3.8, and 3.9, respectively. In this case, the dihedral angle between the two phenanthroline ligands around the metal complex is almost 90°. All 4 isopropyl groups are oriented so that each methine hydrogen is pointing towards the copper center, to relieve steric congestion. A least-squares fit of the two ligand planes gives an angle of 88.92°, while calculation of Θ_Z from the bond angles gives a value of 88.8°. This large angle is in line with that of other phenanthroline complexes with large 2,9 substituents and therefore not surprising considering the steric bulk of the isopropyl substituents. For example, with either *n*-pentyl[9] or CF_3[24] groups in the 2,9 positions, Θ_Z approximately is 87°. If however, a perchlorinated phenanthroline ligand is used, Θ_Z is 89.5°.[25] The average chelate-bite angle for the ligands in $[Cu(dipp)_2]^+$ is 82.76°, in line with other phenanthroline complexes.[3, 20] What is surprising about this structure is the asymmetry of the Cu-N bond lengths. One of the ligands has average bond lengths (2.020 and 2.053 Å), while the other dipp ligand has one rather short (2.007 Å) and one rather long (2.068 Å) bond. This type of coordination is usually found in 2,9 aryl substituted phenanthrolines.[21, 22] In this case, however, the lack of conjugation with the 2,9 substituent has left the physical properties unaltered, unlike what occurs with aryl substitution, vida infra.

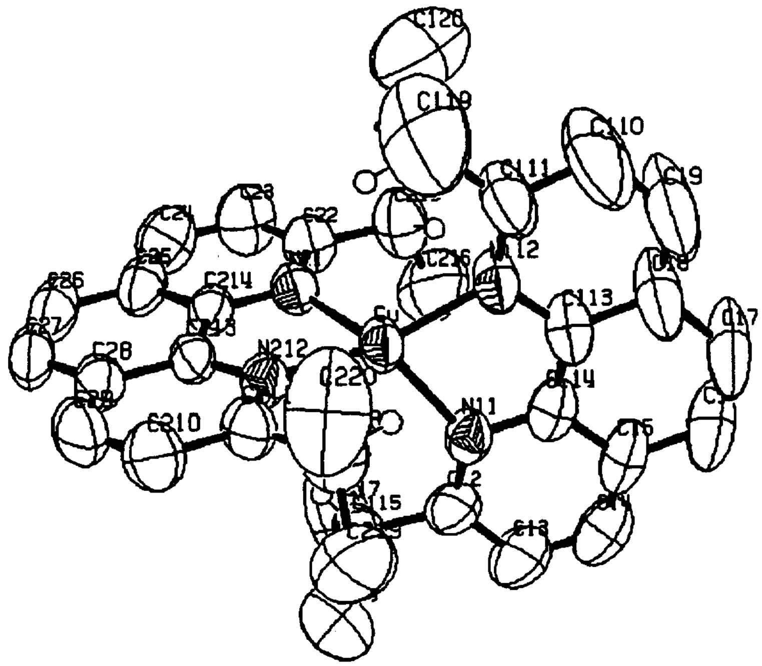


Figure 3.3. ORTEP drawing of the $[Cu(dipp)_2]^+$ cation with labeling scheme. All hydrogens, save the methine hydrogens, have been omitted for clarity. Ellipsoids are 50% except for the spheres representing hydrogen atoms.

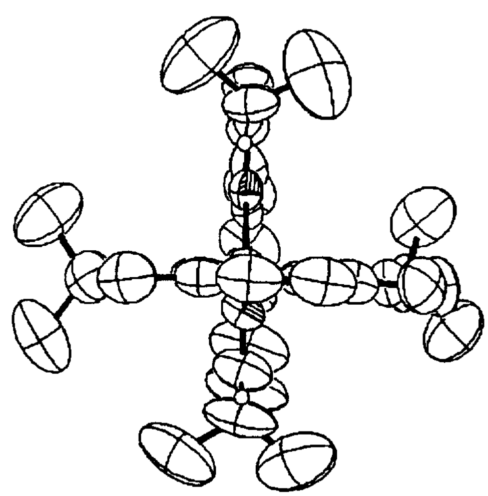


Figure 3.4. ORTEP drawing of the $[Cu(dipp)_2]^+$ cation from behind one phenanthroline ligand. The angle between the two phenanthroline lignds is Θ_Z (88.8°).

Table 3.7. Positional and temperature parameters ($Å^2$) for $[Cu(dipp)_2]TFPB$.

Atom	x	y	z	U(Å²)*
Cu	0.77055(6)	0.52667(5)	-0.29681(4)	0.0632(4)
N(11)	0.7266(4)	0.3865(4)	-0.3888(3)	0.063(2)
N(21)	0.8736(4)	0.5657(3)	-0.1728(3)	0.063(2)
N(112)	0.8120(4)	0.5486(4)	-0.3896(3)	0.073(2)
N(212)	0.6846(4)	0.5812(3)	-0.2281(3)	0.061(2)
C(12)	0.6842(5)	0.3077(5)	-0.3859(5)	0.079(3)
C(13)	0.6612(7)	0.2179(6)	-0.4572(6)	0.107(4)
C(14)	0.6863(7)	0.2118(6)	-0.5280(6)	0.104(4)
C(15)	0.7325(6)	0.2919(6)	-0.5321(4)	0.091(4)
C(16)	0.7607(10)	0.2893(9)	-0.6039(6)	0.128(6)
C(17)	0.8053(12)	0.3700(10)	-0.6036(6)	0.151(7)
C(18)	0.8252(10)	0.4625(8)	-0.5319(6)	0.128(6)
C(19)	0.8743(15)	0.5485(11)	-0.5252(10)	0.200(10)
C(22)	0.9688(5)	0.5614(5)	-0.1459(4)	0.078(3)
C(23)	1.0240(7)	0.5865(7)	-0.0574(6)	0.105(4)
C(24)	0.9797(7)	0.6154(6)	0.0039(5)	0.104(4)
C(25)	0.8808(7)	0.6223(5)	-0.0202(4)	0.081(3)
C(26)	0.8286(9)	0.6538(5)	0.0390(5)	0.097(4)
C(27)	0.7335(8)	0.6596(5)	0.0107(5)	0.094(4)
C(28)	0.6814(6)	0.6366(4)	-0.0791(4)	0.075(3)
C(29)	0.5852(7)	0.6454(5)	-0.1111(6)	0.097(4)
C(110)	0.8900(15)	0.6329(10)	-0.4553(10)	0.199(11)
C(111)	0.8552(9)	0.6304(6)	-0.3876(6)	0.113(5)
C(113)	0.7957(6)	0.4644(6)	-0.4606(4)	0.080(3)
C(114)	0.7508(5)	0.3794(5)	-0.4599(4)	0.069(3)
C(115)	0.6639(7)	0.3174(5)	-0.3030(6)	0.095(4)
C(116)	0.4438(11)	0.7328(13)	0.3212(11)	0.221(10)
C(117)	0.2649(15)	0.7170(16)	0.2499(11)	0.227(15)
C(118)	0.8725(12)	0.7229(7)	-0.3068(8)	0.143(7)
C(119)	0.1959(15)	0.2211(11)	0.3400(12)	0.210(12)
C(120)	0.0127(15)	0.2201(12)	0.2633(13)	0.230(12)
C(210)	0.5405(6)	0.6228(6)	-0.1974(6)	0.096(4)
C(211)	0.5917(5)	0.5906(5)	-0.2563(5)	0.073(3)
C(213)	0.7288(5)	0.6039(4)	-0.1413(4)	0.061(3)
C(214)	0.8293(5)	0.5964(4)	-0.1110(4)	0.062(2)
C(215)	1.0144(6)	0.5273(7)	-0.2167(5)	0.100(4)
C(216)	1.0037(10)	0.4221(9)	-0.2473(9)	0.170(8)
C(217)	0.1244(8)	0.5834(10)	0.8108(9)	0.161(8)
C(218)	0.5434(6)	0.5676(6)	-0.3524(5)	0.096(4)
C(219)	0.4479(10)	0.4796(11)	0.5979(8)	0.175(7)
C(220)	0.4813(12)	0.3491(11)	0.3650(9)	0.174(9)
F(331)	0.2798(8)	0.3426(5)	-0.3282(5)	0.195(5)
F(332)	0.2212(6)	0.3860(6)	-0.2346(8)	0.205(7)
F(333)	0.3562(5)	0.4715(4)	0.7854(5)	0.171(4)
F(351)	0.6467(8)	0.4497(7)	-0.0034(9)	0.309(8)
F(352)	0.3272(5)	0.6626(14)	0.0570(6)	0.357(12)
F(353)	0.6248(5)	0.3524(7)	0.0346(6)	0.211(5)
F(431)	0.0595(4)	0.8343(5)	0.2422(4)	0.138(4)
F(432)	0.1086(5)	0.8618(10)	0.1536(6)	0.235(8)
F(433)	0.1211(5)	0.9711(5)	0.2706(8)	0.268(7)
F(451)	0.1575(8)	0.1673(8)	0.0977(4)	0.214(7)
F(452)	0.1591(9)	0.0354(6)	0.0496(4)	0.255(6)

Table 3.7, continued

Atom	x	y	z	U(Å²)[a]
F(453)	0.2846(5)	0.1453(7)	0.0938(4)	0.192(5)
F(531)	0.2882(4)	-0.0351(5)	-0.6026(3)	0.140(3)
F(532)	0.4103(4)	0.0411(5)	-0.4845(3)	0.139(3)
F(533)	0.3047(7)	0.1074(6)	-0.5261(7)	0.213(7)
F(551)	-0.0648(4)	-0.1574(4)	-0.4853(4)	0.141(3)
F(552)	-0.0467(5)	-0.1715(5)	-0.6035(4)	0.185(4)
F(553)	0.0078(5)	-0.2492(4)	-0.5396(5)	0.157(3)
F(631)	0.3285(10)	-0.1547(8)	-0.0764(9)	0.295(11)
F(632)	0.3553(8)	-0.2572(5)	-0.1696(5)	0.194(5)
F(633)	0.4658(6)	-0.1707(7)	-0.0615(7)	0.208(6)
F(651)	0.3477(6)	0.0857(7)	0.2378(6)	0.183(6)
F(652)	0.4294(7)	0.0546(13)	0.3279(8)	0.286(13)
F(653)	0.3417(8)	0.9540(7)	0.2125(13)	0.318(13)
C(31)	0.3539(4)	0.1844(4)	-0.1894(3)	0.048(2)
C(32)	0.3106(4)	0.2397(4)	-0.2245(4)	0.057(2)
C(33)	0.3604(5)	0.3329(4)	-0.1994(4)	0.063(3)
C(34)	0.4592(5)	0.3755(4)	-0.1369(5)	0.074(3)
C(35)	0.5043(5)	0.3226(4)	-0.1002(4)	0.069(2)
C(36)	0.4522(4)	0.2291(4)	-0.1260(3)	0.056(2)
C(41)	0.2048(4)	0.0820(4)	-0.1741(3)	0.049(2)
C(42)	0.1074(4)	0.0880(4)	-0.2100(3)	0.056(2)
C(43)	0.0404(4)	0.1003(5)	-0.1653(4)	0.068(3)
C(44)	0.0682(5)	0.1050(5)	-0.0816(4)	0.073(3)
C(45)	0.1630(4)	0.1011(4)	-0.0435(4)	0.062(3)
C(46)	0.2306(4)	0.0915(4)	-0.0882(3)	0.056(2)
C(51)	0.2335(4)	0.0251(3)	-0.3331(3)	0.049(2)
C(52)	0.2855(4)	0.0495(4)	-0.3820(3)	0.056(2)
C(53)	0.2484(5)	0.0043(5)	-0.4739(4)	0.065(3)
C(54)	0.1555(5)	-0.0654(5)	-0.5213(4)	0.072(3)
C(55)	0.1017(4)	-0.0898(4)	-0.4754(4)	0.064(2)
C(56)	0.1406(4)	-0.0484(4)	-0.3836(4)	0.057(2)
C(61)	0.3607(4)	0.0110(4)	-0.2040(3)	0.050(2)
C(62)	0.3416(4)	-0.0525(4)	-0.1705(4)	0.057(2)
C(63)	0.4070(5)	-0.1063(4)	-0.1563(4)	0.066(3)
C(64)	0.4911(5)	-0.1008(5)	-0.1806(5)	0.076(3)
C(65)	0.5097(5)	-0.0405(5)	-0.2174(4)	0.071(3)
C(66)	0.4477(4)	0.0142(4)	-0.2273(4)	0.061(3)
C(331)	0.3099(6)	0.3850(5)	0.7576(7)	0.094(4)
C(351)	0.6094(6)	0.3660(7)	-0.0338(6)	0.098(4)
C(431)	0.0616(6)	0.8914(9)	0.2072(6)	0.109(5)
C(451)	0.1918(6)	0.1057(7)	0.0447(5)	0.089(4)
C(531)	0.3127(6)	0.0340(7)	-0.5209(5)	0.099(4)
C(551)	-0.0003(6)	-0.1655(6)	-0.5261(5)	0.088(3)
C(631)	0.3853(7)	-0.1685(6)	-0.1166(6)	0.091(4)
C(651)	0.4020(8)	0.0364(9)	0.2460(8)	0.116(6)
B	0.2869(4)	0.0743(4)	-0.2245(4)	0.049(2)

a $U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a^*_i a^*_j a_i \cdot a_j$

Table 3.8. Bond distances (Å) for [Cu(dipp)$_2$]TFPB. Numbers in parentheses are estimated standard deviations in the least significant digits.

Atom 1	Atom 2	Distance
Cu	N(112)	2.007(5)
Cu	N(212)	2.020(5)
Cu	N(21)	2.053(5)
Cu	N(11)	2.068(5)
F(331)	C(331)	1.301(11)
F(332)	C(331)	1.311(10)
F(333)	C(331)	1.267(9)
F(351)	C(351)	1.197(11)
F(352)	C(351)	1.178(12)
F(353)	C(351)	1.272(10)
F(431)	C(431)	1.283(11)
F(432)	C(431)	1.292(11)
F(433)	C(431)	1.279(12)
F(451)	C(451)	1.338(11)
F(452)	C(451)	1.189(10)
F(453)	C(451)	1.257(9)
F(531)	C(531)	1.342(9)
F(532)	C(531)	1.329(9)
F(533)	C(531)	1.237(11)
F(551)	C(551)	1.306(9)
F(552)	C(551)	1.299(9)
F(553)	C(551)	1.302(10)
F(631)	C(631)	1.205(9)
F(632)	C(631)	1.283(10)
F(633)	C(631)	1.300(10)
F(651)	C(651)	1.215(10)
F(652)	C(651)	1.284(13)
F(653)	C(651)	1.260(13)
N(11)	C(12)	1.333(8)
N(11)	C(114)	1.355(8)
N(21)	C(22)	1.334(8)
N(21)	C(214)	1.375(7)
N(112)	C(111)	1.336(9)
N(112)	C(113)	1.374(9)
N(212)	C(211)	1.337(8)
N(212)	C(213)	1.356(7)
C(12)	C(13)	1.412(10)
C(12)	C(115)	1.517(10)
C(13)	C(14)	1.359(13)
C(14)	C(15)	1.381(12)
C(15)	C(114)	1.410(9)
C(15)	C(16)	1.414(13)
C(55)	C(551)	1.505(9)
C(61)	C(62)	1.384(7)
C(61)	C(66)	1.405(8)
C(61)	B	1.643(8)
C(62)	C(63)	1.409(8)
C(63)	C(64)	1.378(9)
C(63)	C(631)	1.458(10)
C(16)	C(17)	1.341(15)
C(17)	C(18)	1.454(15)
C(18)	C(19)	1.385(16)
C(18)	C(113)	1.418(10)
C(19)	C(110)	1.369(17)
C(22)	C(23)	1.399(10)
C(22)	C(215)	1.520(10)
C(23)	C(24)	1.364(12)
C(24)	C(25)	1.394(12)
C(25)	C(26)	1.428(11)
C(25)	C(214)	1.421(9)
C(26)	C(27)	1.343(12)
C(27)	C(28)	1.417(11)
C(28)	C(29)	1.387(11)
C(28)	C(213)	1.417(8)
C(29)	C(210)	1.348(12)
C(31)	C(36)	1.388(7)
C(31)	C(32)	1.394(8)
C(31)	B	1.644(8)
C(32)	C(33)	1.381(8)
C(33)	C(34)	1.387(9)
C(33)	C(331)	1.475(10)
C(34)	C(35)	1.386(9)
C(35)	C(36)	1.392(8)
C(35)	C(351)	1.475(10)
C(41)	C(46)	1.394(7)
C(41)	C(42)	1.396(7)
C(41)	B	1.642(8)
C(42)	C(43)	1.386(8)
C(43)	C(44)	1.384(9)
C(43)	C(431)	1.495(10)
C(44)	C(45)	1.360(9)
C(45)	C(46)	1.391(8)
C(45)	C(451)	1.461(9)
C(51)	C(52)	1.397(7)
C(51)	C(56)	1.405(7)
C(51)	B	1.645(7)
C(52)	C(53)	1.389(8)
C(53)	C(54)	1.376(8)
C(53)	C(531)	1.522(9)
C(54)	C(55)	1.368(8)
C(55)	C(56)	1.387(8)
C(119)	C(118)	1.576(18)
C(120)	C(118)	1.54(2)
C(210)	C(211)	1.413(10)
C(211)	C(218)	1.508(10)
C(213)	C(214)	1.428(9)
C(215)	C(217)	1.513(13)
C(215)	C(216)	1.530(15)

Table 3.8, continued

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
C(64)	C(65)	1.382(9)	C(217)	C(215)	1.513(13)
C(65)	C(66)	1.368(8)	C(218)	C(220)	1.516(14)
C(65)	C(651)	1.478(10)	C(218)	C(219)	1.544(14)
C(110)	C(111)	1.421(13)	C(219)	C(218)	1.544(14)
C(111)	C(118)	1.536(13)	C(220)	C(218)	1.516(14)
C(113)	C(114)	1.413(10)	C(331)	F(331)	1.301(11)
C(115)	C(116)	1.494(14)	C(331)	F(332)	1.311(10)
C(115)	C(117)	1.508(16)	C(331)	C(33)	1.475(10)
C(116)	C(115)	1.494(14)	C(351)	F(352)	1.178(12)
C(117)	C(115)	1.508(16)	C(431)	C(43)	1.495(10)
C(118)	C(120)	1.54(2)	C(651)	F(653)	1.260(13)
C(118)	C(119)	1.576(18)	C(651)	C(65)	1.478(10)

Table 3.9. Bond angles (deg.) for $[Cu(dipp)_2]$TFPB.

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
N(112)	Cu	N(212)	132.8(2)	C(29)	C(28)	C(213)	116.6(7)
N(112)	Cu	N(21)	122.6(2)	C(29)	C(28)	C(27)	123.7(7)
N(212)	Cu	N(21)	82.76(19)	C(213)	C(28)	C(27)	119.7(7)
N(112)	Cu	N(11)	82.6(2)	C(210)	C(29)	C(28)	120.5(7)
N(212)	Cu	N(11)	123.09(19)	C(36)	C(31)	C(32)	115.6(5)
N(21)	Cu	N(11)	117.60(19)	C(36)	C(31)	B	125.4(5)
C(12)	N(11)	C(114)	119.1(5)	C(32)	C(31)	B	118.9(4)
C(12)	N(11)	Cu	130.5(4)	C(33)	C(32)	C(31)	123.4(5)
C(114)	N(11)	Cu	110.4(4)	C(32)	C(33)	C(34)	119.8(6)
C(22)	N(21)	C(214)	118.5(5)	C(32)	C(33)	C(331)	119.7(6)
C(22)	N(21)	Cu	131.4(4)	C(34)	C(33)	C(331)	120.4(6)
C(214)	N(21)	Cu	110.0(4)	C(35)	C(34)	C(33)	118.2(5)
C(111)	N(112)	C(113)	120.0(6)	C(34)	C(35)	C(36)	120.9(5)
C(111)	N(112)	Cu	128.8(5)	C(34)	C(35)	C(351)	119.4(6)
C(113)	N(112)	Cu	111.1(4)	C(36)	C(35)	C(351)	119.7(7)
C(211)	N(212)	C(213)	118.2(5)	C(31)	C(36)	C(35)	122.0(6)
C(211)	N(212)	Cu	130.3(4)	C(46)	C(41)	C(42)	114.5(5)
C(213)	N(212)	Cu	111.3(4)	C(46)	C(41)	B	122.2(4)
N(11)	C(12)	C(13)	120.8(7)	C(42)	C(41)	B	123.1(4)
N(11)	C(12)	C(115)	117.9(6)	C(43)	C(42)	C(41)	123.2(5)
C(13)	C(12)	C(115)	121.2(7)	C(42)	C(43)	C(44)	119.9(5)
C(14)	C(13)	C(12)	119.5(8)	C(42)	C(43)	C(431)	120.1(6)
C(13)	C(14)	C(15)	121.1(7)	C(44)	C(43)	C(431)	119.9(6)
C(14)	C(15)	C(114)	116.6(7)	C(45)	C(44)	C(43)	118.8(5)
C(14)	C(15)	C(16)	123.3(8)	C(44)	C(45)	C(46)	120.6(5)
C(114)	C(15)	C(16)	120.1(9)	C(44)	C(45)	C(451)	118.6(6)
C(17)	C(16)	C(15)	120.2(9)	C(46)	C(45)	C(451)	120.8(6)
C(16)	C(17)	C(18)	122.6(9)	C(45)	C(46)	C(41)	122.9(5)
C(19)	C(18)	C(113)	117.2(9)	C(52)	C(51)	C(56)	115.1(5)
C(19)	C(18)	C(17)	125.9(9)	C(52)	C(51)	B	120.0(4)
C(113)	C(18)	C(17)	116.8(10)	C(56)	C(51)	B	124.7(4)
C(110)	C(19)	C(18)	122.3(9)	C(53)	C(52)	C(51)	122.5(5)
N(21)	C(22)	C(23)	122.0(7)	C(54)	C(53)	C(52)	120.8(5)
N(21)	C(22)	C(215)	116.4(6)	C(54)	C(53)	C(531)	120.8(5)
C(23)	C(22)	C(215)	121.5(7)	C(52)	C(53)	C(531)	118.4(5)
C(24)	C(23)	C(22)	119.7(8)	C(55)	C(54)	C(53)	118.1(5)
C(23)	C(24)	C(25)	120.8(7)	C(54)	C(55)	C(56)	121.4(5)
C(24)	C(25)	C(26)	125.2(7)	C(54)	C(55)	C(551)	118.9(5)
C(24)	C(25)	C(214)	116.6(7)	C(56)	C(55)	C(551)	119.7(5)
C(26)	C(25)	C(214)	118.2(8)	C(55)	C(56)	C(51)	121.9(5)
C(27)	C(26)	C(25)	121.6(7)	C(62)	C(61)	C(66)	114.8(5)
C(26)	C(27)	C(28)	121.3(7)	C(62)	C(61)	B	125.5(5)
C(66)	C(61)	B	119.5(4)	F(333)	C(331)	F(331)	109.1(9)
C(61)	C(62)	C(63)	122.7(5)	F(333)	C(331)	F(332)	103.4(8)
C(64)	C(63)	C(62)	120.0(5)	F(331)	C(331)	F(332)	99.3(9)
C(64)	C(63)	C(631)	120.0(6)	F(333)	C(331)	C(33)	117.7(7)
C(62)	C(63)	C(631)	120.0(6)	F(331)	C(331)	C(33)	113.4(7)
C(63)	C(64)	C(65)	118.3(6)	F(332)	C(331)	C(33)	112.0(7)
C(66)	C(65)	C(64)	120.9(5)	F(352)	C(351)	F(351)	101.7(11)
C(66)	C(65)	C(651)	120.7(6)	F(352)	C(351)	F(353)	99.1(12)
C(64)	C(65)	C(651)	118.4(6)	F(351)	C(351)	F(353)	103.0(10)

Table 3.9, continued

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
======	======	======	=====	======	======	======	=====
C(65)	C(66)	C(61)	123.2(5)	F(352)	C(351)	C(35)	115.9(8)
C(19)	C(110)	C(111)	117.8(11)	F(351)	C(351)	C(35)	118.1(10)
N(112)	C(111)	C(110)	121.5(9)	F(353)	C(351)	C(35)	116.3(7)
N(112)	C(111)	C(118)	118.4(6)	F(433)	C(431)	F(431)	104.8(9)
C(110)	C(111)	C(118)	120.0(9)	F(433)	C(431)	F(432)	107.3(9)
N(112)	C(113)	C(114)	118.3(5)	F(431)	C(431)	F(432)	104.0(10)
N(112)	C(113)	C(18)	121.0(8)	F(433)	C(431)	C(43)	110.8(9)
C(114)	C(113)	C(18)	120.6(7)	F(431)	C(431)	C(43)	114.8(7)
N(11)	C(114)	C(15)	122.9(7)	F(432)	C(431)	C(43)	114.4(8)
N(11)	C(114)	C(113)	117.4(5)	F(452)	C(451)	F(453)	110.9(9)
C(15)	C(114)	C(113)	119.7(7)	F(452)	C(451)	F(451)	101.8(8)
C(116)	C(115)	C(117)	108.6(13)	F(453)	C(451)	F(451)	95.1(9)
C(116)	C(115)	C(12)	113.5(9)	F(452)	C(451)	C(45)	117.1(8)
C(117)	C(115)	C(12)	111.9(8)	F(453)	C(451)	C(45)	116.4(6)
C(111)	C(118)	C(120)	109.6(11)	F(451)	C(451)	C(45)	112.4(7)
C(111)	C(118)	C(119)	107.5(11)	F(533)	C(531)	F(532)	110.8(8)
C(120)	C(118)	C(119)	112.0(12)	F(533)	C(531)	F(531)	108.8(8)
C(29)	C(210)	C(211)	120.3(8)	F(532)	C(531)	F(531)	100.7(7)
N(212)	C(211)	C(210)	121.1(7)	F(533)	C(531)	C(53)	113.4(8)
N(212)	C(211)	C(218)	118.3(5)	F(532)	C(531)	C(53)	111.6(6)
C(210)	C(211)	C(218)	120.6(7)	F(531)	C(531)	C(53)	110.9(7)
N(212)	C(213)	C(28)	123.3(6)	F(552)	C(551)	F(553)	106.4(7)
N(212)	C(213)	C(214)	118.0(5)	F(552)	C(551)	F(551)	107.0(8)
C(28)	C(213)	C(214)	118.7(6)	F(553)	C(551)	F(551)	102.3(7)
N(21)	C(214)	C(25)	122.3(6)	F(552)	C(551)	C(55)	113.3(6)
N(21)	C(214)	C(213)	117.2(5)	F(553)	C(551)	C(55)	112.2(7)
C(25)	C(214)	C(213)	120.5(6)	F(551)	C(551)	C(55)	114.7(6)
C(217)	C(215)	C(22)	114.2(8)	F(631)	C(631)	F(632)	107.6(10)
C(217)	C(215)	C(216)	110.4(9)	F(631)	C(631)	F(633)	104.0(10)
C(22)	C(215)	C(216)	110.0(8)	F(632)	C(631)	F(633)	95.4(7)
C(211)	C(218)	C(220)	112.7(8)	F(631)	C(631)	C(63)	117.9(6)
C(211)	C(218)	C(219)	111.9(8)	F(632)	C(631)	C(63)	114.8(7)
C(220)	C(218)	C(219)	110.9(10)	F(633)	C(631)	C(63)	114.5(8)
F(651)	C(651)	F(653)	105.4(11)	C(41)	B	C(61)	113.4(4)
F(651)	C(651)	F(652)	104.6(11)	C(41)	B	C(31)	104.8(4)
F(653)	C(651)	F(652)	99.0(11)	C(61)	B	C(31)	111.5(4)
F(651)	C(651)	C(65)	120.4(8)	C(41)	B	C(51)	114.1(4)
F(653)	C(651)	C(65)	113.4(10)	C(61)	B	C(51)	104.7(4)
F(652)	C(651)	C(65)	111.5(9)	C(31)	B	C(51)	108.4(4)

$[Cu(dptmp)_2]PF_6$•THF

A view of the $[Cu(dptmp)_2]PF_6$•THF cation, along with the atomic labeling scheme, is shown in Figure 3.5. The positional and thermal parameters, bond distances, and bond angles are shown in Tables 3.10, 3.11, and 3.12, respectively. The crystal structure of this 2,9 aryl substituted phenanthroline complex looks on the surface like other aryl substituted phenanthrolines.[21, 22, 26] This compound shows a very distorted geometry around the copper center with one long, one short, and two average Cu-N bond distances. This type of arrangement has been seen in both of the crystal structures of $[Cu(dpp)_2]^+$,[21, 22] however, the dptmp complex shows the greatest difference between the long and the short bonds (0.157 Å for dptmp, 0.093 Å for $[Cu(dpp)_2]PF_6$,[22] and 0.137 Å for $[Cu(dpp)_2]CuCl_2$ [21]). This uneven bonding leads to chelate-bite angles that are uneven, as if one of the dptmp ligands was trying to back away. This type of distortion was not seen in the dpp structures.[21, 22] Another interesting feature of this crystal structure is its rather large dihedral angle, see Figure 3.6. This is most likely a steric consequence caused by the lock placed on the phenyl rings by the peripheral methyl groups.[11] Indeed, the torsion angles between the phenyl groups and the phenanthroline backbone are much larger for dptmp than any other aryl substituted phenanthroline. For dptmp, the phenyl-phenanthroline torsion angles are 73.38°, 99.53°, -52.30°, and 81.49°, whereas in the dpp structures, the phenyl torsion angles all lie in the range of 40-70°.[21, 22] The rather large angles indicate an almost perpendicular arrangement with the ligand backbone and a lack of π-conjugation. The smaller angles indicate some twisting and probably cause the larger distortions seen in the coordination geometry around the copper center.[21, 22] Figures 3.6, 3.7, and 3.8 show different views of the $[Cu(dptmp)_2]^+$ cation that show the phenyl torsion angles and the displacements present in the coordination geometry. For $[Cu(dpp)_2]^+$, the phenyl-phenanthroline torsion angles fall in the range of 50-60°, depending on the amount of interligand π-overlap and intraligand π-conjugation.[21, 22, 26]

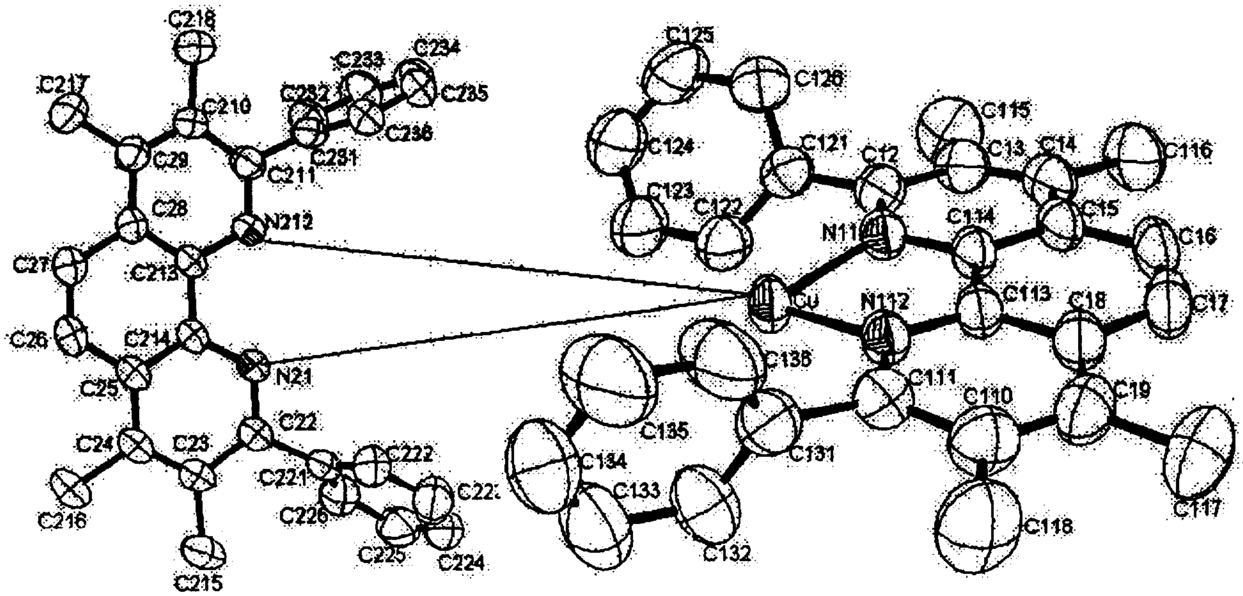


Figure 3.5. ORTEP drawing of the $[Cu(dptmp)_2]^+$ cation with atomic labeling scheme and 50% ellipsoids. One of the dptmp ligands has been pulled out from the metal center for ease of viewing. Additionally, the hydrogen atoms have been omitted for clarity.

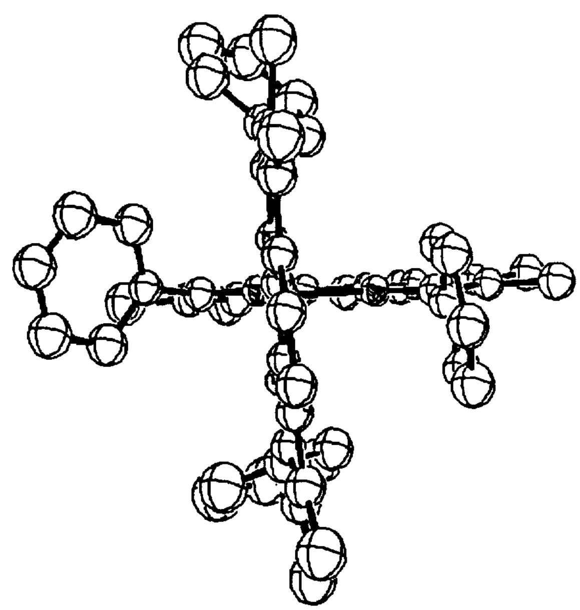


Figure 3.6. ORTEP drawing of the $[Cu(dptmp)_2]^+$ cation from behind one of the phenanthroline ligands.

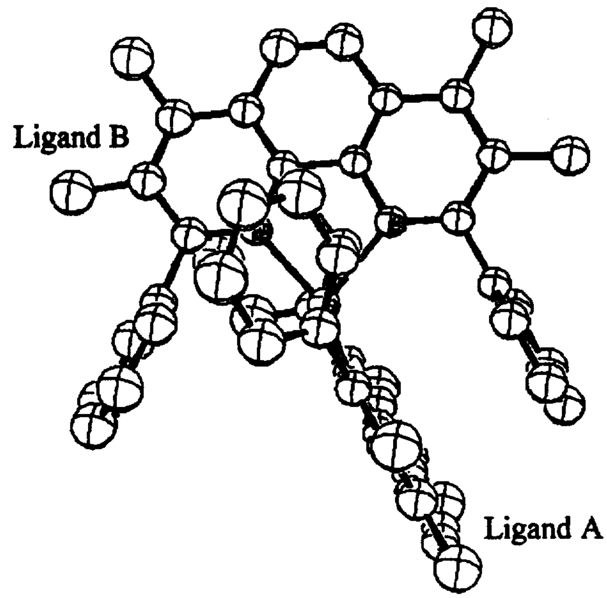


Figure 3.7. ORTEP drawing of the $[Cu(dptmp)_2]^+$ cation looking down onto one phenanthroline ligand.

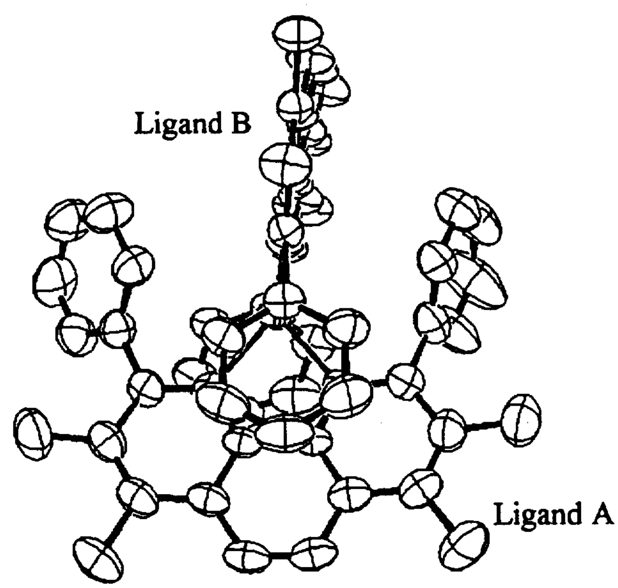


Figure 3.8. ORTEP drawing of the $[Cu(dptmp)_2]^+$ cation looking down onto one phenanthroline ligand.

Table 3.10. Positional and temperature parameters (Å^2) for $[Cu(dptmp)_2]PF_6 \cdot THF$.

Atom	x	y	z	U (Å^2)[a]
Cu	0.14447(3)	0.19769(3)	0.27160(3)	0.05238(16)
P(1)	0.51069(14)	-0.20560(13)	0.21604(13)	0.1007(6)
F(1)	0.4909(6)	-0.3152(4)	0.1802(7)	0.272(5)
F(2)	0.4216(7)	-0.1896(8)	0.1541(7)	0.332(6)
F(3)	0.5854(6)	-0.1864(9)	0.1531(5)	0.312(6)
F(4)	0.6104(6)	-0.2178(6)	0.2782(4)	0.233(4)
F(5)	0.4421(11)	-0.2245(6)	0.2845(8)	0.351(7)
F(6)	0.5258(5)	-0.0954(4)	0.2697(4)	0.194(3)
O(301)	0.2337(6)	0.4909(8)	0.8560(6)	0.208(4)
N(11)	0.0589(2)	0.1986(2)	0.14837(19)	0.0480(8)
N(21)	0.2832(2)	0.2580(2)	0.34572(19)	0.0497(8)
N(112)	0.0740(2)	0.0522(2)	0.24421(18)	0.0475(8)
N(212)	0.0868(2)	0.2723(2)	0.38816(18)	0.0463(8)
C(12)	0.0522(3)	0.2733(3)	0.1018(3)	0.0546(11)
C(13)	-0.0257(3)	0.2653(3)	0.0250(3)	0.0626(13)
C(14)	-0.0921(3)	0.1767(3)	-0.0065(3)	0.0624(13)
C(15)	-0.0837(3)	0.0962(3)	0.0401(2)	0.0546(10)
C(16)	-0.1509(3)	0.0016(3)	0.0154(3)	0.0651(13)
C(17)	-0.1468(3)	-0.0691(3)	0.0656(3)	0.0672(13)
C(18)	-0.0725(3)	-0.0571(3)	0.1462(3)	0.0583(11)
C(19)	-0.0672(3)	-0.1283(3)	0.2032(3)	0.0679(13)
C(22)	0.3800(3)	0.2464(3)	0.3256(2)	0.0581(12)
C(23)	0.4737(3)	0.2832(4)	0.3875(3)	0.0707(13)
C(24)	0.4655(3)	0.3342(3)	0.4727(3)	0.0654(13)
C(25)	0.3640(3)	0.3492(3)	0.4942(3)	0:0575(10)
C(26)	0.3469(3)	0.4033(4)	0.5785(3)	0.0707(13)
C(27)	0.2503(3)	0.4180(3)	0.5971(3)	0.0667(13)
C(28)	0.1559(3)	0.3756(3)	0.5334(2)	0.0505(10)
C(29)	0.0528(3)	0.3868(3)	0.5512(2)	0.0511(10)
C(110)	0.0105(4)	-0.1083(3)	0.2783(3)	0.0713(16)
C(111)	0.0813(3)	-0.0174(3)	0.2954(3)	0.0583(11)
C(113)	-0.0014(3)	0.0331(3)	0.1707(2)	0.0489(10)
C(114)	-0.0084(3)	0.1120(3)	0.1178(2)	0.0484(10)
C(115)	-0.0364(5)	0.3577(4)	-0.0171(4)	0.096(2)
C(116)	-0.1762(4)	0.1641(5)	-0.0881(3)	0.091(2)
C(117)	-0.1443(5)	-0.2238(4)	0.1824(5)	0.100(2)
C(118)	0.0202(5)	-0.1805(4)	0.3425(4)	0.103(2)
C(121)	0.1291(3)	0.3653(3)	0.1376(3)	0.0590(11)
C(122)	0.1395(4)	0.4111(3)	0.2269(3)	0.0695(14)
C(123)	0.2143(4)	0.4955(4)	0.2617(4)	0.088(2)
C(124)	0.2785(5)	0.5359(4)	0.2084(4)	0.098(2)
C(125)	0.2699(5)	0.4917(4)	0.1198(4)	0.098(2)
C(126)	0.1967(4)	0.4079(4)	0.0828(3)	0.0796(16)
C(131)	0.1711(3)	0.0065(3)	0.3723(3)	0.0669(13)
C(132)	0.1626(4)	0.0669(4)	0.4522(3)	0.0794(18)
C(133)	0.2465(5)	0.0907(5)	0.5211(4)	0.099(2)
C(134)	0.3370(5)	0.0539(7)	0.5113(5)	0.128(3)
C(135)	0.3458(6)	-0.0122(8)	0.4318(5)	0.157(4)
C(136)	0.2632(5)	-0.0327(6)	0.3634(4)	0.116(3)
C(210)	-0.0318(3)	0.3359(3)	0.4878(2)	0.0502(10)
C(211)	-0.0114(3)	0.2774(3)	0.4079(2)	0.0476(10)

Table 3.10, continued

Atom	x	y	z	U(Å²)[a]
C(213)	0.1701(3)	0.3206(2)	0.4506(2)	0.0456(9)
C(214)	0.2753(3)	0.3093(3)	0.4290(2)	0.0498(10)
C(215)	0.5803(4)	0.2650(5)	0.3597(4)	0.109(2)
C(216)	0.5634(3)	0.3727(5)	0.5420(3)	0.0895(19)
C(217)	0.0352(4)	0.4517(3)	0.6366(3)	0.0684(14)
C(218)	-0.1453(3)	0.3429(4)	0.5031(3)	0.0693(14)
C(221)	0.3865(3)	0.1978(3)	0.2310(3)	0.0596(12)
C(222)	0.3709(4)	0.2519(4)	0.1626(3)	0.0749(14)
C(223)	0.3852(4)	0.2139(5)	0.0753(3)	0.090(2)
C(224)	0.4135(4)	0.1202(5)	0.0560(4)	0.091(2)
C(225)	0.4264(4)	0.0642(5)	0.1217(4)	0.095(2)
C(226)	0.4131(4)	0.1033(4)	0.2099(3)	0.0816(18)
C(231)	-0.0993(3)	0.2150(3)	0.3415(2)	0.0512(10)
C(232)	-0.1448(3)	0.1237(3)	0.3582(3)	0.0693(14)
C(233)	-0.2278(4)	0.0652(4)	0.2974(4)	0.0795(16)
C(234)	-0.2660(3)	0.0972(4)	0.2219(3)	0.0783(15)
C(235)	-0.2226(3)	0.1876(4)	0.2052(3)	0.0775(15)
C(236)	-0.1391(3)	0.2465(3)	0.2642(3)	0.0621(13)
C(302)	0.2586(10)	0.5817(9)	0.8681(14)	0.298(13)
C(303)	0.3620(11)	0.6198(10)	0.8954(17)	0.348(13)
C(304)	0.4180(8)	0.5414(9)	0.8782(12)	0.240(10)
C(305)	0.3401(10)	0.4548(9)	0.8637(9)	0.184(6)

a $U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a^*_i a^*_j \mathbf{a}_i \cdot \mathbf{a}_j$

Table 3.11. Bond distances (Å) for [Cu(dptmp)$_2$]PF$_6$•THF. Numbers in parentheses are estimated standard deviations in the least significant digits.

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
Cu	N(21)	1.993(3)	C(28)	C(213)	1.396(5)
Cu	N(112)	2.039(3)	C(28)	C(29)	1.405(5)
Cu	N(11)	2.058(3)	C(29)	C(210)	1.390(5)
Cu	N(212)	2.150(3)	C(29)	C(217)	1.503(5)
P(1)	F(2)	1.457(6)	C(110)	C(111)	1.415(6)
P(1)	F(3)	1.461(6)	C(110)	C(118)	1.508(6)
P(1)	F(5)	1.472(7)	C(111)	C(131)	1.503(5)
P(1)	F(1)	1.491(6)	C(113)	C(114)	1.458(5)
P(1)	F(4)	1.543(6)	C(121)	C(122)	1.378(6)
P(1)	F(6)	1.570(5)	C(121)	C(126)	1.411(6)
N(11)	C(12)	1.345(5)	C(123)	C(124)	1.353(7)
N(11)	C(114)	1.355(4)	C(123)	C(122)	1.393(6)
N(21)	C(22)	1.337(5)	C(124)	C(125)	1.365(8)
N(21)	C(214)	1.362(4)	C(125)	C(126)	1.381(7)
N(112)	C(111)	1.334(5)	C(131)	C(136)	1.374(7)
N(112)	C(113)	1.355(4)	C(131)	C(132)	1.375(7)
N(212)	C(211)	1.339(4)	C(132)	C(133)	1.376(7)
N(212)	C(213)	1.362(4)	C(133)	C(134)	1.339(9)
C(12)	C(13)	1.423(5)	C(134)	C(135)	1.409(11)
C(12)	C(121)	1.481(5)	C(135)	C(136)	1.360(8)
C(13)	C(14)	1.371(6)	C(232)	C(231)	1.390(6)
C(13)	C(115)	1.528(6)	C(232)	C(233)	1.392(6)
C(14)	C(15)	1.416(6)	C(210)	C(211)	1.410(5)
C(14)	C(116)	1.517(5)	C(210)	C(218)	1.516(5)
C(15)	C(114)	1.402(5)	C(211)	C(231)	1.490(5)
C(15)	C(16)	1.432(6)	C(213)	C(214)	1.449(5)
C(16)	C(17)	1.332(6)	C(221)	C(226)	1.381(6)
C(17)	C(18)	1.433(6)	C(221)	C(222)	1.383(6)
C(18)	C(113)	1.408(5)	C(222)	C(223)	1.383(7)
C(18)	C(19)	1.412(6)	C(223)	C(224)	1.375(8)
C(19)	C(110)	1.388(6)	C(224)	C(225)	1.364(8)
C(19)	C(117)	1.503(6)	C(225)	C(226)	1.395(7)
C(22)	C(23)	1.417(5)	C(231)	C(236)	1.382(5)
C(22)	C(221)	1.495(5)	C(233)	C(234)	1.356(7)
C(23)	C(24)	1.387(6)	C(234)	C(235)	1.370(7)
C(23)	C(215)	1.517(6)	C(235)	C(236)	1.386(6)
C(24)	C(25)	1.412(6)	O(301)	C(302)	1.225(12)
C(24)	C(216)	1.518(5)	O(301)	C(305)	1.511(12)
C(25)	C(214)	1.405(5)	C(304)	C(303)	1.375(18)
C(25)	C(26)	1.424(6)	C(304)	C(305)	1.423(13)
C(26)	C(27)	1.336(6)	C(302)	C(303)	1.354(14)
C(27)	C(28)	1.450(5)			

Table 3.12. Bond angles (deg.) for $[Cu(dptmp)_2]PF_6{\bullet}THF$. Numbers in parentheses are estimated standard deviations in the least significant digits.

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
N(21)	Cu	N(112)	128.85(12)	C(114)	C(15)	C(14)	117.8(4)
N(21)	Cu	N(11)	140.15(12)	C(114)	C(15)	C(16)	118.1(4)
N(112)	Cu	N(11)	81.82(11)	C(14)	C(15)	C(16)	124.1(3)
N(21)	Cu	N(212)	81.23(11)	C(17)	C(16)	C(15)	122.2(4)
N(112)	Cu	N(212)	108.22(11)	C(16)	C(17)	C(18)	122.3(4)
N(11)	Cu	N(212)	116.18(11)	C(113)	C(18)	C(19)	118.1(3)
F(2)	P(1)	F(3)	92.1(6)	C(113)	C(18)	C(17)	117.3(4)
F(2)	P(1)	F(5)	91.9(7)	C(19)	C(18)	C(17)	124.5(4)
F(3)	P(1)	F(5)	175.9(7)	C(110)	C(19)	C(18)	118.7(4)
F(2)	P(1)	F(1)	91.5(5)	C(110)	C(19)	C(117)	121.0(4)
F(3)	P(1)	F(1)	93.0(6)	C(18)	C(19)	C(117)	120.3(4)
F(5)	P(1)	F(1)	87.8(5)	N(21)	C(22)	C(23)	123.0(3)
F(2)	P(1)	F(4)	175.9(6)	N(21)	C(22)	C(221)	116.6(3)
F(3)	P(1)	F(4)	84.1(5)	C(23)	C(22)	C(221)	120.3(3)
F(5)	P(1)	F(4)	91.8(7)	C(24)	C(23)	C(22)	118.9(4)
F(1)	P(1)	F(4)	90.4(5)	C(24)	C(23)	C(215)	121.5(4)
F(2)	P(1)	F(6)	92.5(4)	C(22)	C(23)	C(215)	119.6(4)
F(3)	P(1)	F(6)	96.2(5)	C(23)	C(24)	C(25)	118.8(3)
F(5)	P(1)	F(6)	82.8(4)	C(23)	C(24)	C(216)	120.8(4)
F(1)	P(1)	F(6)	169.8(5)	C(25)	C(24)	C(216)	120.4(4)
F(4)	P(1)	F(6)	86.2(4)	C(214)	C(25)	C(24)	118.5(3)
C(12)	N(11)	C(114)	118.0(3)	C(214)	C(25)	C(26)	118.2(3)
C(12)	N(11)	Cu	130.1(2)	C(24)	C(25)	C(26)	123.4(3)
C(114)	N(11)	Cu	111.5(2)	C(27)	C(26)	C(25)	122.5(3)
C(22)	N(21)	C(214)	118.0(3)	C(26)	C(27)	C(28)	121.6(4)
C(22)	N(21)	Cu	127.4(2)	C(213)	C(28)	C(29)	119.4(3)
C(214)	N(21)	Cu	114.3(2)	C(213)	C(28)	C(27)	117.3(3)
C(111)	N(112)	C(113)	118.6(3)	C(29)	C(28)	C(27)	123.4(3)
C(111)	N(112)	Cu	128.5(2)	C(210)	C(29)	C(28)	118.0(3)
C(113)	N(112)	Cu	112.0(2)	C(210)	C(29)	C(217)	121.3(3)
C(211)	N(212)	C(213)	118.3(3)	C(28)	C(29)	C(217)	120.7(3)
C(211)	N(212)	Cu	131.9(2)	C(19)	C(110)	C(111)	119.1(4)
C(213)	N(212)	Cu	109.7(2)	C(19)	C(110)	C(118)	121.6(4)
N(11)	C(12)	C(13)	122.0(4)	C(111)	C(110)	C(118)	119.3(4)
N(11)	C(12)	C(121)	115.4(3)	N(112)	C(111)	C(110)	122.6(4)
C(13)	C(12)	C(121)	122.5(4)	N(112)	C(111)	C(131)	115.5(3)
C(14)	C(13)	C(12)	119.5(4)	C(110)	C(111)	C(131)	121.9(4)
C(14)	C(13)	C(115)	121.8(4)	N(112)	C(113)	C(18)	122.8(3)
C(12)	C(13)	C(115)	118.6(4)	N(112)	C(113)	C(114)	116.8(3)
C(13)	C(14)	C(15)	119.1(3)	C(18)	C(113)	C(114)	120.4(3)
C(13)	C(14)	C(116)	121.6(4)	N(11)	C(114)	C(15)	123.5(3)
C(15)	C(14)	C(116)	119.3(4)	N(11)	C(114)	C(113)	116.9(3)
C(15)	C(114)	C(113)	119.6(3)	C(28)	C(213)	C(214)	121.0(3)
C(122)	C(121)	C(126)	117.3(4)	N(21)	C(214)	C(25)	122.8(3)
C(122)	C(121)	C(12)	121.1(4)	N(21)	C(214)	C(213)	117.7(3)
C(126)	C(121)	C(12)	121.6(4)	C(25)	C(214)	C(213)	119.5(3)
C(124)	C(123)	C(122)	120.8(5)	C(226)	C(221)	C(222)	118.7(4)
C(123)	C(124)	C(125)	118.9(5)	C(226)	C(221)	C(22)	122.6(4)
C(124)	C(125)	C(126)	122.0(5)	C(222)	C(221)	C(22)	118.6(4)

Table 3.12, continued

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
======	======	======	=====	======	======	======	=====
C(125)	C(126)	C(121)	119.7(5)	C(223)	C(222)	C(221)	120.9(5)
C(136)	C(131)	C(132)	119.0(4)	C(224)	C(223)	C(222)	119.4(5)
C(136)	C(131)	C(111)	120.0(4)	C(225)	C(224)	C(223)	120.8(5)
C(132)	C(131)	C(111)	121.1(4)	C(224)	C(225)	C(226)	119.6(5)
C(131)	C(132)	C(133)	120.5(5)	C(221)	C(226)	C(225)	120.5(5)
C(134)	C(133)	C(132)	120.2(6)	C(236)	C(231)	C(232)	118.6(4)
C(133)	C(134)	C(135)	120.4(6)	C(236)	C(231)	C(211)	121.7(3)
C(136)	C(135)	C(134)	118.6(7)	C(232)	C(231)	C(211)	119.7(3)
C(135)	C(136)	C(131)	121.2(6)	C(121)	C(122)	C(123)	121.3(4)
C(231)	C(232)	C(233)	120.3(4)	C(234)	C(233)	C(232)	120.4(4)
C(29)	C(210)	C(211)	119.3(3)	C(233)	C(234)	C(235)	119.8(4)
C(29)	C(210)	C(218)	121.0(3)	C(234)	C(235)	C(236)	120.8(4)
C(211)	C(210)	C(218)	119.6(3)	C(231)	C(236)	C(235)	120.1(4)
N(212)	C(211)	C(210)	122.5(3)	C(302)	O(301)	C(305)	102.5(9)
N(212)	C(211)	C(231)	116.2(3)	C(303)	C(304)	C(305)	104.4(10)
C(210)	C(211)	C(231)	121.3(3)	O(301)	C(302)	C(303)	117.8(11)
N(212)	C(213)	C(28)	122.2(3)	C(304)	C(305)	O(301)	106.4(9)
N(212)	C(213)	C(214)	116.8(3)	C(302)	C(303)	C(304)	106.3(13)

Absorbance

Tables 3.13-3.15 contain all of the solid state absorbance data as well as dihedral angle values for all of the compounds used in this study. The data has been roughly divided into three categories. The first is the parent group. This group contains compounds with ligands that contain only hydrogen atoms in the 2 and 9 positions of the phenanthroline (or 6 and 6' of bipyridine) ligand. There may be substitution at other places on the ligand, but only the 2,9 positions are being considered. The second group is referred to as the alkyl group. This group contains ligands with alkyl groups in the 2 and 9 positions of the phenanthroline (or 6 and 6' of bipyridine) ligand. Again, this group may have other substituents on the ligands, but only the positions directly adjacent to the chelating nitrogens are being considered. The third and final group is the aryl group. This group contains molecules with aryl functionalities in the positions adjacent to the nitrogen atoms.

Table 3.13. Absorbance and dihedral angle data for the parent group.

Compound	CH_2Cl_2 Abs (nm)	Solid Abs (nm)	Θ_Z (deg)	Θ_Z Ref.
$[Cu(phen)_2]ClO_4$	435	620	49.9	8
$[Cu(phen)_2]BPh_4$	435	480, 550		
$[Cu(tmp)_2]PF_6$	430	575		
$[Cu(tmp)_2]BPh_4$	430	450, 485	81.9	this work
$[Cu(bipy)_2]ClO_4$		460, 530	75.2	27
$[Cu(bipy)_2]BPh_4$		475, 550		

Table 3.14. Absorbance and dihedral angle data for the aryl group.

Compound	CH_2Cl_2 Abs (nm)	Solid Abs (nm)	Θ_Z (deg)	Θ_Z Ref.
$[Cu(dpp)_2]BF_4$	441, 560	475, 540	(71.8)[a]	20
$[Cu(dpp)_2]PF_6$	441, 560	475, 540	79.8	21
$[Cu(dpp)_2]TFPB$	441, 560	450, 550		
$[Cu(dpdmp)_2]PF_6$	440, 550	425, 530		
$[Cu(dptmp)_2]PF_6$	467	490	87.8	this work
$[Cu(dptmp)_2]TFPB$	467	480		

a Data extrapolated from the value for $[Cu(dpp)_2]CuCl_2$

Table 3.15. Absorbance and dihedral angle data for the alkyl group.

Compound	CH_2Cl_2 Abs (nm)	Solid Abs (nm)	Θ_Z (deg)	Θ_Z Ref.
$[Cu(dmp)_2]Br$	455	475, 550	79.9	3
$[Cu(dmp)_2]NO_3$	455	475, 550	72.4, 85.4[a]	6
$[Cu(dmp)_2]ClO_4$	455	460, 545	81.8	5
$[Cu(dmp)_2]TFPB$	455	460		
$[Cu(bcp)_2]BF_4$	479	480	88.1	20
$[Cu(bcp)_2]BPh_4$	479	480, 560		
$[Cu(dbp)_2]PF_6$	457	470	(87.4)[b]	9
$[Cu(dbdmp)_2]PF_6$	456	470		
$[Cu(dbtmp)_2]PF_6$	453	460		
$[Cu(dnpp)_2]PF_6$	449	425, 550	66.3	4
$[Cu(dipp)_2]Cl$	445	460		
$[Cu(dipp)_2]PF_6$	445	460		
$[Cu(dipp)_2]TFPB$	445	465	88.9	this work
$[Cu(dcyp)_2]PF_6$	457	470		
$[Cu(dsbp)_2]Cl$	455	460		
$[Cu(dsbp)_2]PF_6$	455	470, 515		
$[Cu(dmbp)_2]BF_4$		450, 550	80.8	28
$[Cu(dmbp)_2]BPh_4$		485		
$[Cu(tmbp)_2]BF_4$		440, 540		
$[Cu(tmbp)_2]ClO_4$		440, 540	75.0	29

a This nitrate salt was a dihydrate
b Data extrapolated from $[Cu(di\text{-}n\text{-}pentyl\text{-}phen)_2]CuCl_2$

An overlay of the solid state absorbance spectra for $[Cu(phen)_2]ClO_4$, $[Cu(phen)_2]BPh_4$, $[Cu(tmp)_2]PF_6$, and $[Cu(tmp)_2]BPh_4$ is shown in Figure 3.9. Based on the aforementioned spectra and the two known Θ_Z values for phen]ClO_4 and tmp]BPh_4, it seems reasonable to estimate a Θ_Z of ~80° for phen]BPh_4 and a Θ_Z of ~60° for tmp]PF_6. This suggests that large anions tend to open up the crystal lattice and allow the copper complex to "open up" and approach a Θ_Z of 90°. The dihedral angle can also be estimated by examining the color of the salt. For instance, phen]ClO_4 and tmp]PF_6 are both purple, while phen]BPh_4 and tmp]BPh_4 are red-orange in color.

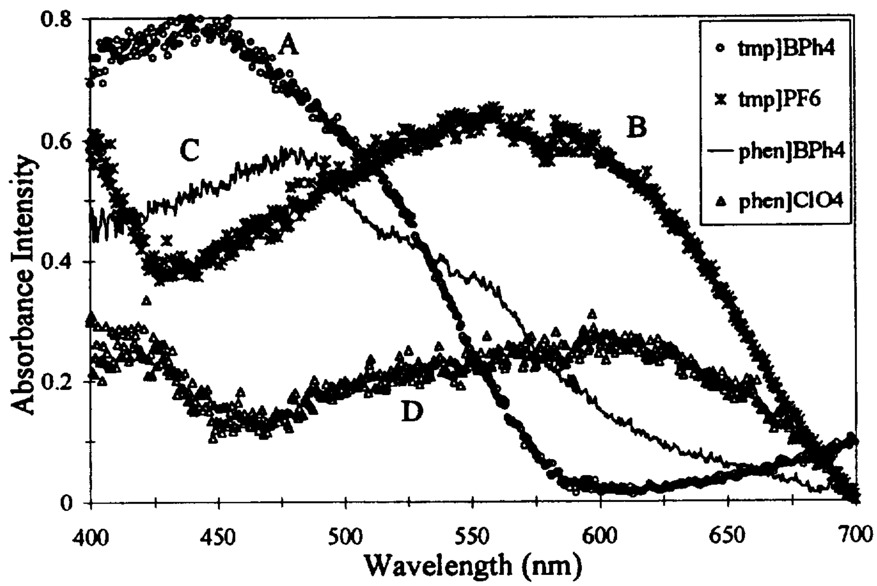


Figure 3.9. Solid state absorbance spectra for selected compounds of the parent group. A = $[Cu(tmp)_2]BPh_4$, B = $[Cu(tmp)_2]PF_6$, C = $[Cu(phen)_2]BPh_4$, D = $[Cu(phen)_2]ClO_4$. NB V-51.

For the aryl group, simple examination of the color of the salt is not sufficient. All of the aryl group compounds are a wine-red colored solid. The difference in these compounds can only be observed in their spectra. All of the dpp and dpdmp salts have similar absorption spectra, indicating similar structures in the solid state, see Figure 3.10. The stand outs are the salts of dptmp. These compounds exhibit only one peak, like the compounds in the parent and alkyl groups. This phenomena has been discussed previously.[11] Interestingly, for the aryl group, the anion seems to have only a limited effect on the absorption spectrum. This could be indicating that the structure of the molecule is determined by the ligands and not the lattice forces.

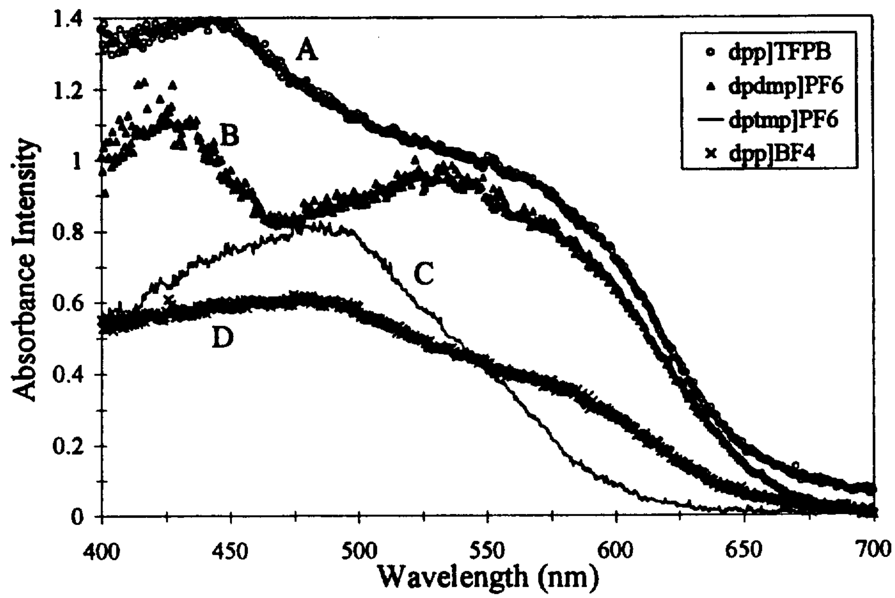


Figure 3.10. Solid state absorbance spectra for selected compounds of the aryl group. A = $[Cu(dpp)_2]TFPB$, B = $[Cu(dpdmp)_2]PF_6$, C = $[Cu(dptmp)_2]PF_6$, D = $[Cu(dpp)_2]BF_4$. NB V-52

For the alkyl group, there are three apparent trends. The first is that ligands with small substituents in positions 2 and 9 are anion dependent, especially dmp. The absorption maxima for dmp complexes vary, as does Θ_Z, with dmp]TFPB having the highest energy absorbance maximum.

The second trend is that bulky substituents in the 2,9 positions override any influence the anion has. For example, for dipp, the absorbance maxima does not change as the anion goes from Cl^- to PF_6^- to TFPB. Considering the vast size difference between Cl^- and TFPB, that is quite a feat to be that consistent. Based on earlier evidence, the *iso*-propyl groups must be keeping the phenanthroline ligands from flattening and therefore keeping a similar Θ_Z throughout the series of dipp compounds.

The third trend is based on the fact that as Θ_Z maximizes, so does the absorbance energy. For instance, the compounds dmp]TFPB, bcp]BF_4, dbp]PF_6, and dipp]TFPB all have absorbance maxima around 460 nm, except bcp]BF_4 which is red-shifted due to the 4,7-diphenyl substitution it has. Most of these compounds have a reported Θ_Z, or at least one that can be estimated easily, that is 85° or greater. These compounds do not exhibit the pronounced shoulders in their absorbance spectra that are indicative of a flattening distortion, consistent with the idea of a large Θ_Z. On the other hand, for compounds like dmp]Br and dnpp]PF_6, their spectra show low energy shoulders and their measured Θ_Z's are quite low compared to the first group. Figure 3.11 contains a sampling of the absorption spectra discussed above.

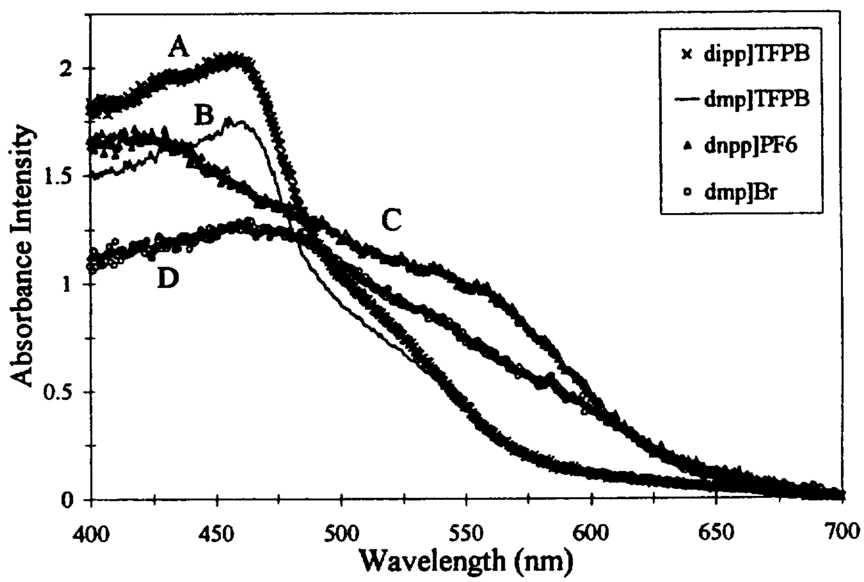


Figure 3.11. Solid state absorbance spectra for select compounds of the alkyl group. A = $[Cu(dipp)_2]$TFPB, B = $[Cu(dmp)_2]$TFPB, C = $[Cu(dnpp)_2]PF_6$, D = $[Cu(dmp)_2]$Br. NB V-52, 53, 54

Luminescence

One of the most interesting aspects of this project is the solid state luminescence measurements that were made. The data taken on the parent group, shown in Table 3.16, shows that for the first time, a non-2,9-substituted phenanthroline complex emits!

There have been many reports over the years that $[Cu(phen)_2]^+$ does not emit in any state,[1] but by using a large anion to increase lattice spacing, and consequently the dihedral angle, $[Cu(phen)_2]BPh_4$ and $[Cu(tmp)_2]BPh_4$ can be made to emit. Further, even $[Cu(bipy)_2]^+$ salts give a measurable emission signal at room temperature. The signal is weaker than the phen and tmp complexes, but it is nonetheless measurable. Figure 3.12 contains the uncorrected emission spectra for the parent group complexes that show room temperature emission. These signals were checked against, and found to be different than free ligand, free anion, and the empty sample holder.

Table 3.16. Luminescence and dihedral angle data for the parent group.

Compound	CH_2Cl_2 Em (nm)	CH_2Cl_2 τ (ns)	Solid Em (nm)	Solid τ (ns)	Θ_Z (deg)	Θ_Z Ref.
$[Cu(phen)_2]ClO_4$	---	---	---	---	49.9	8
$[Cu(phen)_2]BPh_4$	---	---	695	20		
$[Cu(tmp)_2]PF_6$	---	---	---	---		
$[Cu(tmp)_2]BPh_4$	---	---	700	15	81.9	this work
$[Cu(bipy)_2]ClO_4$	---	---	660	<10	75.2	27
$[Cu(bipy)_2]BPh_4$	---	---	660	~10		

Luminescence data for the aryl group is shown in Table 3.17. Analysis of this data shows that the emission energy of the dptmp complexes is sharply shifted to higher energy relative to the dpp and dpdmp complexes. This shift to higher energy is also followed by dramatic increases in the excited state lifetimes of the dptmp complexes. With lifetimes of 1.5 μs and 4.7 μs in the solid at room temperature, the $[Cu(dptmp)_2]^+$ cation has become the longest lived copper phenanthroline in both the solid and solution states. This increase in emission energy and lifetime are most likely consequences of the increased dihedral angle, based on the data reported for $dpp]PF_6$ and that extrapolated for dpp]BF_4. A comparison of the uncorrected emission spectra for dpp]PF_6, dpdmp]PF_6, and dptmp]PF_6 is shown in Figure 3.13.

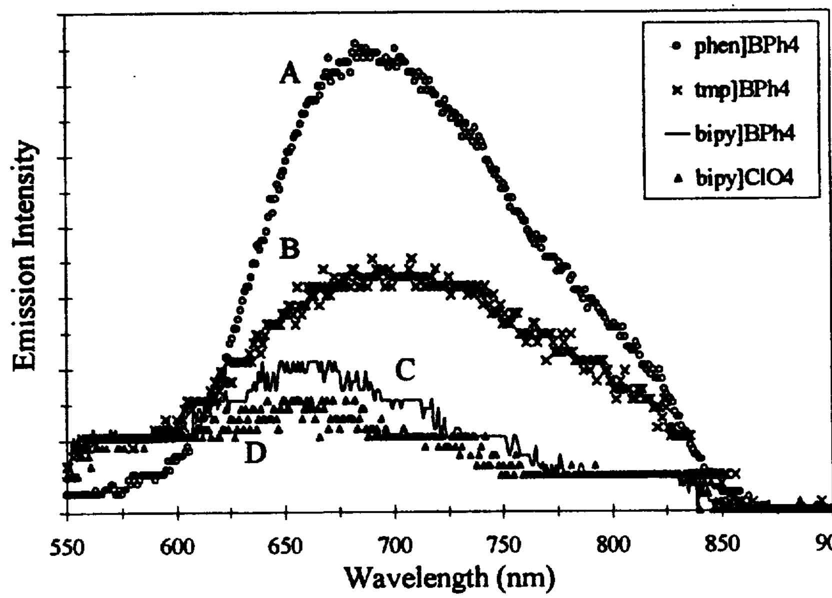


Figure 3.12. Room temperature solid state emission spectra from the parent group. A = $[Cu(phen)_2]BPh_4$, B = $[Cu(tmp)_2]BPh_4$, C = $[Cu(bipy)_2]BPh_4$, D = $[Cu(bipy)_2]ClO_4$. NB V-70, 71

Table 3.17. Luminescence and dihedral angle data for the aryl group.

Compound	CH_2Cl_2 Em (nm)	CH_2Cl_2 τ (ns)	Solid Em (nm)	Solid τ (ns)	Θ_Z (deg)	Θ_Z Ref.
$[Cu(dpp)_2]BF_4$	675[b]	310[b]	695	280	(71.8)[a]	21
$[Cu(dpp)_2]PF_6$	685[c]	270[c]	670	780	79.8	22
$[Cu(dpp)_2]$TFPB	680[d]	280[d]	700	310		
$[Cu(dpdmp)_2]PF_6$	685[c]	310[c]	690	325		
$[Cu(dptmp)_2]PF_6$	670[c]	480[c]	655	1570	87.8	this work
$[Cu(dptmp)_2]$TFPB	671[d]	495[d]	625	4710		

a Data extrapolated from the value for $[Cu(dpp)_2]CuCl_2$
b Data taken from ref. r19
c Data taken from ref. r11
d Data taken from ref. r23

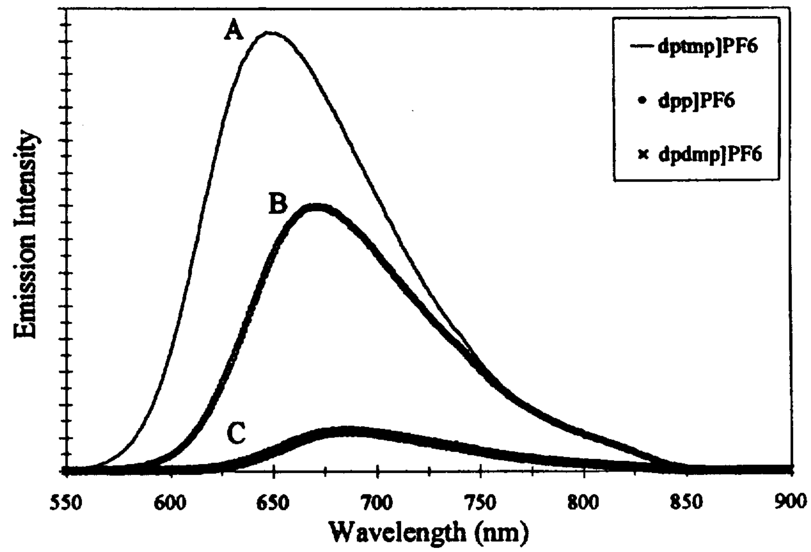


Figure 3.13. Room temperature solid state emission spectra for selected compounds of the aryl group. A = $[Cu(dptmp)_2]PF_6$, B = $[Cu(dpp)_2]PF_6$, C = $[Cu(dpdmp)_2]PF_6$. NB V-68, 69

For the alkyl group, the data is much more difficult to categorize, see Table 3.18. The main reason is the lack of dihedral angle data for a majority of the compounds presented in the table; however, two general trends can be theorized. The first is that with an increasing Θ_Z, the emission maxima shifts to higher energy. The dnpp complex is an exception to the rule. Figure 3.14 shows an overlay of some emission spectra that illustrate this idea. The second is that with an increasing Θ_Z, the excited state lifetime also increases.

These two trends are not surprising, if Θ_Z is examined more closely. Θ_Z refers to the angle between the two phenanthroline ligands, which also refers to the symmetry of the cation. The closer the symmetry of the cation is to D_{2d} (or tetrahedral coordination geometry), the larger Θ_Z. A more tetrahedral structure tends to offer a more stable ground state and a more destabilized excited state. This in turn causes a larger energy difference between the ground and excited states and therefore a higher energy emission. A consequence of the large energy difference between the ground and excited states is an excited state that takes longer to decay, or span the gap to return to the ground state.

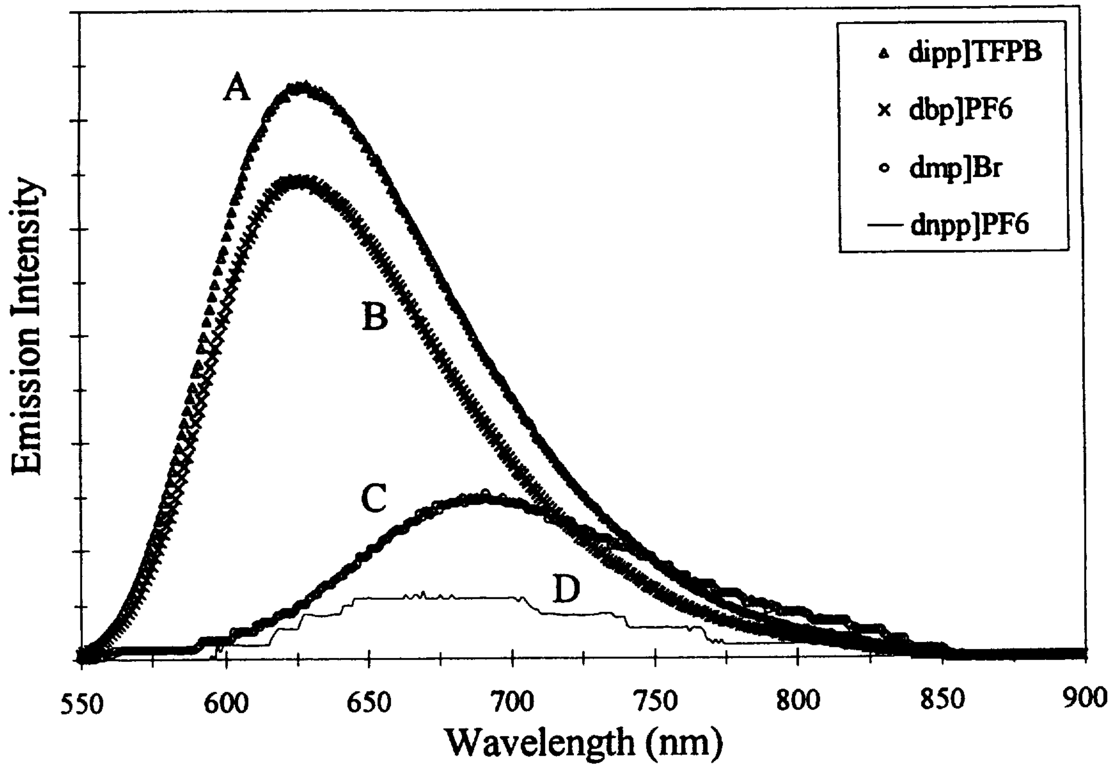


Figure 3.14. Room temperature solid state emission spectra for selected compounds of the alkyl group. A = [Cu(dipp)$_2$]TFPB, B = [Cu(dbp)$_2$]PF$_6$, C = [Cu(dmp)$_2$]Br, D = [Cu(dnpp)$_2$]PF$_6$. NB V-66, 67

Table 3.18. Luminescence and dihedral angle data for the alkyl group.

Compound	CH_2Cl_2 Em (nm)	CH_2Cl_2 τ (ns)	Solid Em (nm)	Solid τ (ns)	Θ_Z (deg)	Θ_Z Ref.
$[Cu(dmp)_2]Br$			690	250	79.9	3
$[Cu(dmp)_2]NO_3$			680	300	72.4, 85.4[a]	6
$[Cu(dmp)_2]ClO_4$			670	235	81.8	5
$[Cu(dmp)_2]TFPB$			650	690		
$[Cu(bcp)_2]BF_4$	685	80	690	135	88.1	20
$[Cu(dbp)_2]PF_6$	670[e]	150[e]	625	1240	(87.4)[b]	9
$[Cu(dbdmp)_2]PF_6$	670[e]	145[e]	630	740		
$[Cu(dbtmp)_2]PF_6$	635[e]	330[e]	635	1710		
$[Cu(dnpp)_2]PF_6$	665[c]	260[c]	670	595	66.3	4
$[Cu(dipp)_2]Cl$			625	1420		
$[Cu(dipp)_2]PF_6$			630	1290		
$[Cu(dipp)_2]TFPB$	650[f]	365[f]	625	1330	88.9	this work
$[Cu(dcyp)_2]PF_6$	649[f]	360[f]	630	765		
$[Cu(dsbp)_2]Cl$			625	1020		
$[Cu(dsbp)_2]PF_6$	650[c]	400[c]	625	1240		
$[Cu(dmbp)_2]BF_4$			685		80.8	28
$[Cu(dmbp)_2]BPh_4$			670			
$[Cu(tmbp)_2]BF_4$	725[d]	18[d]	695	65		
$[Cu(tmbp)_2]ClO_4$			695	230	75.0	29

a This nitrate salt was a dihydrate
b Data extrapolated from $[Cu(di\text{-}n\text{-}pentyl\text{-}phen)_2]CuCl_2$
c Data taken from ref. 31
d Data taken from ref. 14
e Data taken from ref. 11
f Data taken from ref. 30

Discussion

Controlling the Dihedral Angle

Table 3.19 lists dihedral angles based on reported crystal structures in the literature. This table contains both spectrally characterized and spectrally uncharacterized compounds (those not examined in this report). Examination of this data reveals two controlling factors as to the dihedral angle: ligand-ligand repulsions and anions. Thus, for the same cation, a different anion can induce a drastic change in the dihedral angle. The most obvious reason is packing forces overcome ligand-ligand repulsions and force the copper complex into a flattened geometry.[4] Or, the anion can be large and bulky and reduce the packing forces and allow the geometry to open up. By the same token, a complex with little to no steric bulk in the 2 and 9 positions of the ligand is one that can flatten.[8] On the other hand, a complex with bulky groups in the 2 and 9 positions is one that is rigid and keeps a tetrahedral-like coordination geometry around the copper center.

What the data above signifies is that the dihedral angle can be systematically varied to give a copper complex with a specific angle. For example, $[Cu(phen)_2]^+$ cations all show smallish dihedral angles.[8, 23] It is presumed that this is due to the lack of steric blocks in positions 2 and 9 to keep a more rigid structure.[8] However, by switching to a larger anion such as BPh_4^-, crystals of $[Cu(tmp)_2]^+$ were able to be grown which show a much larger dihedral angle. The result of this finding is the room temperature solid state emission from $[Cu(tmp)_2]BPh_4$ and $[Cu(phen)_2]BPh_4$, which is assumed to have a much similar dihedral angle even though no crystal data exists.

Table 3.19. Dihedral angle data for copper bis-phenanthroline complexes.

Compound	Θ_Z[a]	Ref.	Compound	Θ_Z[a]	Ref.
$[Cu(phen)_2]CuBr_2$	77.8	8	$[Cu(phen)_2]ClO_4$	49.9	8
$[Cu(phen)_2]_2[Cu(OAc)_2]$ $[OAc]$•HOAc[b]	68.5	23	$[Cu(bipy)_2]ClO_4$	75.2	27
$[Cu(tmp)_2]BPh_4$	81.9	c	$[Cu(dmp)_2]Br$•H_2O	79.9	3
$[Cu(dmp)_2]NO_3$	72.4	6	$[Cu(dmp)_2]NO_3$•$3H_2O$	85.4	3
$[Cu(dmp)_2]ClO_4$	81.8	5	$[Cu(dmp)_2]_2[TCNQ]_2$	88.8	7
$[Cu(dmbp)_2]BF_4$	80.8	28	$[Cu(tmbp)_2]ClO_4$	75.0	29
$[Cu(bcp)_2]BF_4$•CH_3OH	88.1	20	$[Cu(tmbp)_2]Cl$•$2H_2O$	79.0	3
$[Cu(n\text{-pentylphen})_2]CuCl_2$	87.4	9	$[Cu(dnpp)_2]PF_6$	66.3	4[d]
$[Cu(dipp)_2]TFPB$	88.9	c	$[Cu(dptmp)_2]PF_6$•THF	87.8	c
$[Cu(bfp)_2]PF_6$[e]	87	24	$[Cu(ocp)_2]BF_4$•CH_2Cl_2[d]	89.4	25
$[Cu(dap)_2]BF_4$[e]	~71	26	$[Cu(dpp)_2]CuCl_2$•⅔CH_3CN	71.8	21
$[Cu(dpp)_2]PF_6$	79.8	22			

a in degrees
b OAc = acetate
c this work
d the previously reported value of 75° is erroneous
e bfp = 2,9-bis(trifluromethyl)-1,10-phenanthroline
f ocp = 2,3,4,5,6,7,8,9-octachloro-1,10-phenanthroline
g dap = 2,9-bis(*p*-anisolyl)-1,10-phenanthroline

The other facet of the crystal data from above is that the dihedral angle can be controlled by modifying the steric size of the 2,9 substituents. For instance, *iso*-propyl, Cl,[25] CF_3,[19] and *n*-pentyl[9] groups are all rather large and all of their structures show very nearly 90° dihedral angles, even though their anions range from BF_4^- to PF_6^- to $CuCl_2^-$ to $TFPB^-$. What this steric control offers is the ability to create a very nearly D_{2d} copper phenanthroline cation, which has a very long lifetime in the solid state. One exception is the substituent *neo*-pentyl.[4] When this molecule crystallized, it distorted the *neo*-pentyl groups in a way as to flatten its structure. The fact that the *tert*-butyl part was out away from the phenanthroline core one methylene unit was probably the reason for the unusual packing which lead to the small dihedral angle.[4] This molecule also showed very long Cu-N bonds which indicate excessive strain in the cation. This molecule does not lessen ones ability to induce a change in the dihedral angle by altering the sterics.

The dihedral angle can also be forced to increase by placing steric locks on remote positions of the phenanthroline as well.[20] In the case of $[Cu(dptmp)_2]^+$, the 3 and 8 methyls act as locks on the 2,9 phenyls, keeping them in a very twisted orientation, with respect to the phenanthroline core. This lack of mobility of the phenyl groups does not allow for the flattening distortion seen in other 2,9-bis(aryl)-phenanthroline complexes.[21, 22, 26] The dptmp crystal structure does, however; still show the rocking distortion so common to 2,9-bis(aryl)-phenanthroline complexes.[21, 22, 26] This rocking distortion is no doubt caused by the intramolecular π-stacking that occurs after the distortion.[21, 22]

Electronic Structure

The dihedral angle obviously effects the electronic structure of the copper complex, see Tables 3.13 through 3.18. Based on the changes seen in the absorption spectra, the energy of the orbitals involved in the MLCT absorbance are obviously being altered. Kaizu et al[1] have performed DV-Xα computations on the model complex $[Cu(ethane\text{-}diimine)_2]^+$ in order to better understand the changes.

Figure 3.15 shows the highest occupied and lowest unoccupied molecular orbitals, as calculated in ref. 1, and how they change with the dihedral angle. Analysis of the calculated orbitals for percent composition revealed that all of the highest occupied orbitals shown were predominately Cu 3d in character and all of the lowest unoccupied orbitals shown were predominately N 2p and C 2p in character. From these calculations, it is obvious that the lowest allowed transition is MLCT in nature and that the energy decreases in the order: 90° > 60° > 40°. The solid state absorption-dihedral angle correlation presented above is supported by the orbital energy data.[1] As the dihedral angle is maximizing, so is ΔE_{MLCT}.

The emission data correlate with the calculated energy level data. For example, in the aryl group, the dptmp complex has a larger Θ_Z, higher energy emission, longer lifetime, and based on the Θ_Z a larger ΔE_{MLCT} than dpp]PF_6, see Table 3.17. Similarly, Table 3.18 shows that in the alkyl group, Θ_Z, emission energy, and lifetime all increase in the order:

dmp]Br ~ dmp]ClO_4 < dbp]PF_6 ~ dipp]TFPB

Based on the reported dihedral angles for these molecules, the calculated ΔE_{MLCT} also increases the that order. And most importantly, in the parent group, the large dihedral angles of tmp]BPh_4 and, presumably, phen]BPh_4, lead to emissive compounds with measurable lifetimes. These molecules would be calculated to have larger ΔE_{MLCT} values than their non-emissive counterparts tmp]PF_6 and phen]ClO_4.

The one limit to this data is that it does not predict boundaries. For example, the one exception to many of the trends is dnpp]PF_6. This molecule has an extremely small Θ_Z (66.3°)[4] yet it has a moderate energy emission maximum and a considerable lifetime, while tmp]BPh_4 has a large Θ_Z (81.9°) a low energy emission and a very short lifetime. The electronic differences in the ligands may be responsible for the photophysical differences,[11] however it does not explain why the dnpp]PF_6 complex does not fit the trends of other alkyl group molecules. Regardless, the data presented here along with that of Kaizu et al[1] gives a pretty clear picture of the flattening distortion and its effects on the photochemistry of copper phenanthrolines.[6]

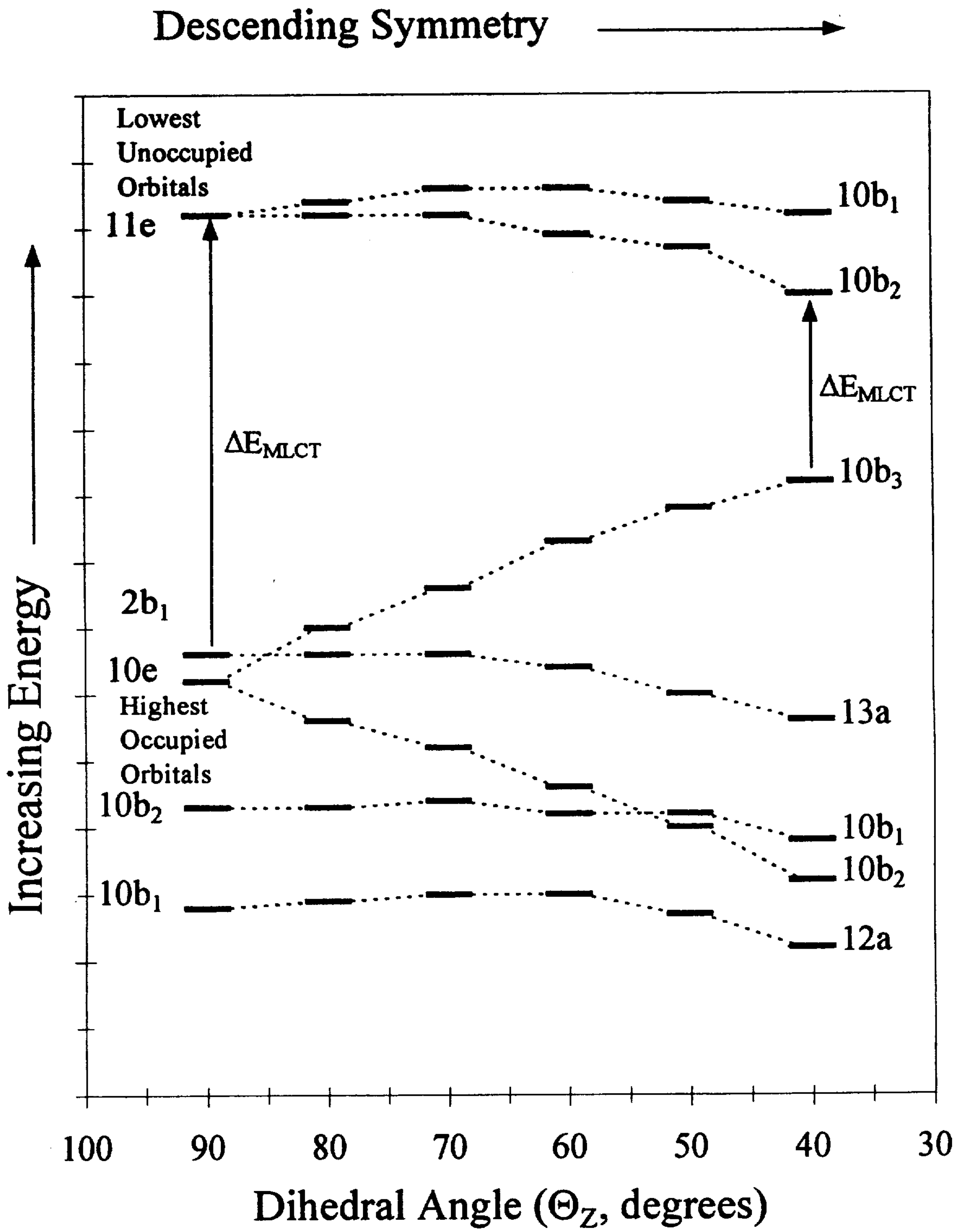


Figure 3.19. Energies of the highest occupied and lowest unoccupied molecular orbitals of $[Cu(ethane\text{-}diimine)_2]^+$, as predicted by DV-X$\alpha$ calculations in ref 1.

Conclusion

The correlation between the computational, structural and photophysical data presented above indicates that the solid state is a good media in which to study the flattening distortion that copper phenanthrolines undergo in solution.[10] In the solid state, the molecules are predisposed to a specific amount of flattening, which can be changed by altering the anion or the steric bulk of the 2,9 positions. The amount of flattening will then dictate the photochemistry the copper complex is able to perform. It is a very good example of the impact the flattening distortion, proposed by McMillin et al, has on the photochemistry of copper phenanthrolines.[10]

APPENDICES

Appendix A: Crystal Data for $[Cu(dptmp)_2]PF_6$•THF

Table A.1. Anisotropic temperature factor coefficients - U's[a] for $[Cu(dptmp)_2]PF_6$•THF.

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Cu	0.0415(3)	0.0599(3)	0.0473(3)	0.00107(19)	-0.00415(17)	-0.00195(19)
P(1)	0.0894(11)	0.0920(10)	0.1125(12)	-0.0125(8)	0.0008(9)	0.0246(9)
F(1)	0.191(6)	0.125(4)	0.466(13)	0.000(4)	0.087(7)	-0.053(6)
F(2)	0.193(7)	0.399(12)	0.340(11)	0.107(8)	-0.160(8)	-0.028(10)
F(3)	0.187(6)	0.595(17)	0.166(5)	-0.036(8)	0.057(5)	0.154(8)
F(4)	0.258(8)	0.291(8)	0.147(5)	0.119(6)	-0.046(5)	0.022(5)
F(5)	0.468(16)	0.213(7)	0.397(14)	-0.043(9)	0.323(14)	0.016(8)
F(6)	0.218(6)	0.115(3)	0.224(6)	0.008(4)	-0.016(5)	0.002(4)
O(301)	0.144(6)	0.243(9)	0.224(8)	-0.024(6)	-0.016(5)	0.074(7)
N(11)	0.0424(15)	0.0528(16)	0.0449(15)	0.0079(12)	0.0012(12)	0.0010(12)
N(21)	0.0376(15)	0.0618(17)	0.0447(15)	0.0036(12)	0.0001(11)	0.0024(13)
N(112)	0.0419(15)	0.0535(16)	0.0428(14)	0.0054(12)	-0.0011(11)	0.0033(12)
N(212)	0.0353(14)	0.0544(16)	0.0460(15)	0.0037(12)	0.0014(11)	0.0054(12)
C(12)	0.047(2)	0.063(2)	0.054(2)	0.0122(16)	0.0056(16)	0.0097(17)
C(13)	0.055(2)	0.077(3)	0.059(2)	0.018(2)	0.0045(18)	0.018(2)
C(14)	0.050(2)	0.086(3)	0.051(2)	0.021(2)	-0.0011(16)	0.0095(19)
C(15)	0.0403(18)	0.071(2)	0.0470(18)	0.0101(16)	-0.0014(14)	-0.0012(17)
C(16)	0.047(2)	0.079(3)	0.055(2)	0.0030(19)	-0.0103(17)	-0.011(2)
C(17)	0.051(2)	0.063(2)	0.072(3)	-0.0045(18)	-0.0031(19)	-0.014(2)
C(18)	0.048(2)	0.060(2)	0.060(2)	0.0042(16)	0.0054(16)	-0.0042(17)
C(19)	0.061(2)	0.056(2)	0.081(3)	-0.0009(19)	0.011(2)	0.003(2)
C(22)	0.0384(18)	0.079(3)	0.051(2)	0.0046(17)	0.0011(15)	0.0017(18)
C(23)	0.038(2)	0.106(3)	0.060(2)	0.007(2)	0.0012(17)	-0.001(2)
C(24)	0.0378(19)	0.090(3)	0.059(2)	0.0028(19)	-0.0047(16)	0.000(2)
C(25)	0.0385(18)	0.072(2)	0.054(2)	-0.0017(16)	-0.0020(15)	0.0027(17)
C(26)	0.050(2)	0.094(3)	0.052(2)	-0.003(2)	-0.0075(17)	-0.012(2)
C(27)	0.051(2)	0.083(3)	0.053(2)	0.001(2)	0.0007(17)	-0.0133(19)
C(28)	0.0455(19)	0.056(2)	0.0446(17)	0.0028(15)	0.0031(14)	0.0002(15)
C(29)	0.052(2)	0.0508(19)	0.0491(18)	0.0069(15)	0.0083(15)	0.0051(15)
C(110)	0.075(3)	0.067(3)	0.074(3)	0.006(2)	0.011(2)	0.022(2)
C(111)	0.057(2)	0.063(2)	0.054(2)	0.0077(18)	0.0069(17)	0.0096(18)
C(113)	0.0405(17)	0.0537(19)	0.0460(18)	0.0039(14)	0.0015(14)	-0.0038(15)
C(114)	0.0363(17)	0.059(2)	0.0441(17)	0.0054(14)	-0.0022(13)	0.0000(15)
C(115)	0.096(4)	0.103(4)	0.098(4)	0.026(3)	-0.006(3)	0.046(3)
C(116)	0.070(3)	0.131(5)	0.068(3)	0.021(3)	-0.020(2)	0.021(3)
C(117)	0.088(4)	0.068(3)	0.133(5)	-0.014(3)	0.008(3)	0.011(3)
C(118)	0.112(5)	0.084(4)	0.114(5)	-0.004(3)	0.000(4)	0.043(3)
C(121)	0.057(2)	0.061(2)	0.061(2)	0.0080(18)	0.0111(18)	0.0158(18)
C(122)	0.069(3)	0.062(2)	0.075(3)	0.003(2)	0.017(2)	0.006(2)
C(123)	0.084(4)	0.076(3)	0.093(4)	-0.011(3)	0.021(3)	-0.006(3)
C(124)	0.093(4)	0.081(3)	0.108(4)	-0.022(3)	0.017(3)	0.005(3)
C(125)	0.090(4)	0.091(4)	0.115(5)	-0.013(3)	0.031(3)	0.033(3)
C(126)	0.081(3)	0.087(3)	0.071(3)	0.001(3)	0.016(2)	0.020(2)
C(131)	0.059(2)	0.083(3)	0.061(2)	0.009(2)	0.0018(19)	0.026(2)
C(132)	0.096(4)	0.076(3)	0.064(3)	0.019(3)	-0.007(2)	0.015(2)
C(133)	0.108(5)	0.110(4)	0.070(3)	0.009(4)	-0.016(3)	0.019(3)
C(134)	0.084(4)	0.209(8)	0.085(4)	0.008(5)	-0.025(3)	0.045(5)
C(135)	0.088(5)	0.305(12)	0.086(5)	0.068(6)	0.000(4)	0.037(6)
C(136)	0.078(4)	0.210(8)	0.065(3)	0.053(4)	0.001(3)	0.018(4)
C(210)	0.0387(17)	0.058(2)	0.0534(19)	0.0082(15)	0.0079(14)	0.0072(16)
C(211)	0.0402(17)	0.0531(19)	0.0490(18)	0.0054(14)	0.0039(14)	0.0108(15)
C(213)	0.0349(16)	0.0511(18)	0.0465(17)	0.0025(13)	-0.0012(13)	0.0045(14)
C(214)	0.0376(17)	0.060(2)	0.0458(18)	0.0008(15)	-0.0010(14)	0.0022(15)
C(215)	0.039(2)	0.171(6)	0.097(4)	0.012(3)	0.004(2)	-0.027(4)
C(216)	0.043(2)	0.138(5)	0.072(3)	0.005(3)	-0.013(2)	-0.004(3)
C(217)	0.067(3)	0.073(3)	0.059(2)	0.010(2)	0.014(2)	-0.009(2)
C(218)	0.048(2)	0.087(3)	0.070(3)	0.016(2)	0.0110(19)	0.000(2)
C(221)	0.0321(17)	0.081(3)	0.059(2)	0.0072(17)	0.0025(15)	-0.0025(19)
C(222)	0.064(3)	0.095(3)	0.059(2)	0.004(2)	0.007(2)	0.002(2)
C(223)	0.083(4)	0.114(4)	0.065(3)	-0.009(3)	0.009(2)	0.011(3)

Table A.1, continued

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
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C(224)	0.061(3)	0.133(5)	0.064(3)	0.001(3)	0.009(2)	-0.017(3)
C(225)	0.067(3)	0.109(4)	0.098(4)	0.026(3)	0.012(3)	-0.021(3)
C(226)	0.070(3)	0.098(4)	0.073(3)	0.022(3)	0.005(2)	0.001(3)
C(231)	0.0382(18)	0.058(2)	0.055(2)	0.0063(15)	0.0078(15)	0.0035(16)
C(232)	0.058(2)	0.070(3)	0.072(3)	-0.003(2)	0.001(2)	0.006(2)
C(233)	0.059(3)	0.074(3)	0.093(3)	-0.015(2)	0.006(2)	0.002(2)
C(234)	0.046(2)	0.092(3)	0.080(3)	-0.004(2)	0.002(2)	-0.017(3)
C(235)	0.051(2)	0.113(4)	0.060(2)	0.016(2)	-0.0049(19)	-0.002(2)
C(236)	0.048(2)	0.077(3)	0.059(2)	0.0094(18)	0.0018(17)	0.0100(19)
C(302)	0.131(10)	0.141(9)	0.63(4)	0.003(7)	-0.036(14)	0.167(15)
C(303)	0.131(10)	0.164(11)	0.74(4)	-0.021(9)	-0.068(17)	0.179(18)
C(304)	0.103(7)	0.143(9)	0.49(3)	0.017(7)	0.031(11)	0.111(12)
C(305)	0.157(10)	0.191(11)	0.216(11)	0.053(9)	0.033(8)	0.050(9)

a The form of the anisotropic temperature factor is:
$\exp[-2\pi \{h^2a^{*2}U(1,1) + k^2b^{*2}U(2,2) + l^2c^{*2}U(3,3) + 2hka^*b^*U(1,2) + 2hla^*c^*U(1,3) + 2klb^*c^*U(2,3)\}]$ where a^*, b^*, and c^* are reciprocal lattice constants.

Table A.2. Torsion angles in degrees for [Cu(dptmp)$_2$]PF$_6$•THF.

Atom 1	Atom 2	Atom 3	Atom 4	Angle	
N(21)	Cu	N(11)	C(12)	-35.62	(0.39)
N(21)	Cu	N(11)	C(114)	152.63	(0.23)
N(112)	Cu	N(11)	C(12)	179.61	(0.33)
N(112)	Cu	N(11)	C(114)	7.86	(0.23)
N(212)	Cu	N(11)	C(12)	73.26	(0.33)
N(212)	Cu	N(11)	C(114)	-98.49	(0.24)
N(11)	Cu	N(21)	C(22)	-62.66	(0.36)
N(11)	Cu	N(21)	C(214)	123.35	(0.26)
N(112)	Cu	N(21)	C(22)	70.18	(0.34)
N(112)	Cu	N(21)	C(214)	-103.81	(0.26)
N(212)	Cu	N(21)	C(22)	176.56	(0.32)
N(212)	Cu	N(21)	C(214)	2.57	(0.25)
N(11)	Cu	N(112)	C(111)	-177.66	(0.32)
N(11)	Cu	N(112)	C(113)	-8.93	(0.23)
N(21)	Cu	N(112)	C(111)	30.68	(0.36)
N(21)	Cu	N(112)	C(113)	-160.59	(0.22)
N(212)	Cu	N(112)	C(111)	-62.70	(0.32)
N(212)	Cu	N(112)	C(113)	106.03	(0.23)
N(11)	Cu	N(212)	C(211)	38.61	(0.35)
N(11)	Cu	N(212)	C(213)	-142.17	(0.20)
N(21)	Cu	N(212)	C(211)	-179.24	(0.33)
N(21)	Cu	N(212)	C(213)	-0.02	(0.28)
N(112)	Cu	N(212)	C(211)	-51.13	(0.34)
N(112)	Cu	N(212)	C(213)	128.09	(0.20)
C(305)	O(301)	C(302)	C(303)	-8.90	(2.21)
C(302)	O(301)	C(305)	C(304)	-1.82	(1.60)
Cu	N(11)	C(12)	C(13)	-168.40	(0.29)
Cu	N(11)	C(12)	C(121)	9.77	(0.50)
C(114)	N(11)	C(12)	C(13)	2.90	(0.55)
C(114)	N(11)	C(12)	C(121)	-178.93	(0.33)
Cu	N(11)	C(114)	C(15)	173.36	(0.29)
Cu	N(11)	C(114)	C(113)	-5.63	(0.39)
C(12)	N(11)	C(114)	C(15)	0.50	(0.53)
C(12)	N(11)	C(114)	C(113)	-178.49	(0.33)
Cu	N(21)	C(22)	C(23)	-172.47	(0.34)
Cu	N(21)	C(22)	C(221)	11.51	(0.50)
C(214)	N(21)	C(22)	C(23)	1.33	(0.58)
C(214)	N(21)	C(22)	C(221)	-174.70	(0.34)
Cu	N(21)	C(214)	C(25)	173.94	(0.31)
Cu	N(21)	C(214)	C(213)	-4.76	(0.42)
C(22)	N(21)	C(214)	C(25)	-0.65	(0.55)
C(22)	N(21)	C(214)	C(213)	-179.35	(0.32)
Cu	N(112)	C(111)	C(110)	165.16	(0.32)
Cu	N(112)	C(111)	C(131)	-15.61	(0.49)
C(113)	N(112)	C(111)	C(110)	-2.93	(0.57)
C(113)	N(112)	C(111)	C(131)	176.31	(0.33)
Cu	N(112)	C(113)	C(18)	-169.85	(0.30)
Cu	N(112)	C(113)	C(114)	8.59	(0.39)
C(111)	N(112)	C(113)	C(18)	0.12	(0.52)
C(111)	N(112)	C(113)	C(114)	178.57	(0.33)
Cu	N(212)	C(211)	C(210)	-176.55	(0.27)
Cu	N(212)	C(211)	C(231)	5.14	(0.51)
C(213)	N(212)	C(211)	C(210)	4.28	(0.52)
C(213)	N(212)	C(211)	C(231)	-174.02	(0.30)
Cu	N(212)	C(213)	C(28)	179.97	(0.32)
Cu	N(212)	C(213)	C(214)	-2.43	(0.34)
C(211)	N(212)	C(213)	C(28)	-0.69	(0.47)
C(211)	N(212)	C(213)	C(214)	176.92	(0.32)
N(11)	C(12)	C(13)	C(14)	-4.23	(0.62)
N(11)	C(12)	C(13)	C(115)	172.75	(0.41)
C(121)	C(12)	C(13)	C(14)	177.74	(0.39)
C(121)	C(12)	C(13)	C(115)	-5.28	(0.63)
N(11)	C(12)	C(121)	C(122)	-52.30	(0.54)
N(11)	C(12)	C(121)	C(126)	125.78	(0.45)

Table A.2, continued

Atom 1	Atom 2	Atom 3	Atom 4	Angle
C(13)	C(12)	C(121)	C(122)	125.86 (0.48)
C(13)	C(12)	C(121)	C(126)	-56.07 (0.59)
C(12)	C(13)	C(14)	C(15)	2.03 (0.60)
C(12)	C(13)	C(14)	C(116)	-179.86 (0.40)
C(115)	C(13)	C(14)	C(15)	-174.85 (0.42)
C(115)	C(13)	C(14)	C(116)	3.26 (0.66)
C(13)	C(14)	C(15)	C(16)	177.81 (0.38)
C(13)	C(14)	C(15)	C(114)	1.13 (0.56)
C(116)	C(14)	C(15)	C(16)	-0.34 (0.60)
C(116)	C(14)	C(15)	C(114)	-177.02 (0.37)
C(14)	C(15)	C(16)	C(17)	-173.84 (0.40)
C(114)	C(15)	C(16)	C(17)	2.83 (0.59)
C(14)	C(15)	C(114)	N(11)	-2.53 (0.55)
C(14)	C(15)	C(114)	C(113)	176.44 (0.34)
C(16)	C(15)	C(114)	N(11)	-179.41 (0.34)
C(16)	C(15)	C(114)	C(113)	-0.44 (0.53)
C(15)	C(16)	C(17)	C(18)	-2.21 (0.64)
C(16)	C(17)	C(18)	C(19)	177.88 (0.41)
C(16)	C(17)	C(18)	C(113)	-0.84 (0.61)
C(17)	C(18)	C(19)	C(110)	178.48 (0.41)
C(17)	C(18)	C(19)	C(117)	-1.39 (0.67)
C(113)	C(18)	C(19)	C(110)	-2.81 (0.60)
C(113)	C(18)	C(19)	C(117)	177.32 (0.43)
C(17)	C(18)	C(113)	N(112)	-178.45 (0.35)
C(17)	C(18)	C(113)	C(114)	3.16 (0.55)
C(19)	C(18)	C(113)	N(112)	2.75 (0.58)
C(19)	C(18)	C(113)	C(114)	-175.65 (0.35)
C(18)	C(19)	C(110)	C(111)	0.25 (0.64)
C(18)	C(19)	C(110)	C(118)	179.46 (0.45)
C(117)	C(19)	C(110)	C(111)	-179.89 (0.47)
C(117)	C(19)	C(110)	C(118)	-0.68 (0.73)
N(21)	C(22)	C(23)	C(24)	-0.45 (0.70)
N(21)	C(22)	C(23)	C(215)	178.83 (0.45)
C(221)	C(22)	C(23)	C(24)	175.44 (0.41)
C(221)	C(22)	C(23)	C(215)	-5.28 (0.70)
N(21)	C(22)	C(221)	C(222)	73.38 (0.52)
N(21)	C(22)	C(221)	C(226)	-110.26 (0.47)
C(23)	C(22)	C(221)	C(222)	-102.76 (0.52)
C(23)	C(22)	C(221)	C(226)	73.61 (0.59)
C(22)	C(23)	C(24)	C(25)	-1.11 (0.68)
C(22)	C(23)	C(24)	C(216)	178.47 (0.46)
C(215)	C(23)	C(24)	C(25)	179.62 (0.47)
C(215)	C(23)	C(24)	C(216)	-0.79 (0.77)
C(23)	C(24)	C(25)	C(26)	-177.88 (0.46)
C(23)	C(24)	C(25)	C(214)	1.72 (0.63)
C(216)	C(24)	C(25)	C(26)	2.54 (0.69)
C(216)	C(24)	C(25)	C(214)	-177.86 (0.44)
C(24)	C(25)	C(26)	C(27)	178.96 (0.45)
C(214)	C(25)	C(26)	C(27)	-0.64 (0.72)
C(24)	C(25)	C(214)	N(21)	-0.87 (0.61)
C(24)	C(25)	C(214)	C(213)	177.80 (0.35)
C(26)	C(25)	C(214)	N(21)	178.75 (0.40)
C(26)	C(25)	C(214)	C(213)	-2.57 (0.59)
C(25)	C(26)	C(27)	C(28)	2.76 (0.74)
C(26)	C(27)	C(28)	C(29)	178.14 (0.44)
C(26)	C(27)	C(28)	C(213)	-1.53 (0.61)
C(27)	C(28)	C(29)	C(210)	-174.86 (0.38)
C(27)	C(28)	C(29)	C(217)	4.90 (0.61)
C(213)	C(28)	C(29)	C(210)	4.80 (0.56)
C(213)	C(28)	C(29)	C(217)	-175.44 (0.34)
C(27)	C(28)	C(213)	N(212)	175.79 (0.32)
C(27)	C(28)	C(213)	C(214)	-1.71 (0.51)
C(29)	C(28)	C(213)	N(212)	-3.89 (0.52)
C(29)	C(28)	C(213)	C(214)	178.60 (0.35)

Table A.2, continued

Atom 1	Atom 2	Atom 3	Atom 4	Angle
C(28)	C(29)	C(210)	C(211)	-1.44 (0.57)
C(28)	C(29)	C(210)	C(218)	178.92 (0.39)
C(217)	C(29)	C(210)	C(211)	178.81 (0.36)
C(217)	C(29)	C(210)	C(218)	-0.83 (0.60)
C(19)	C(110)	C(111)	N(112)	2.76 (0.66)
C(19)	C(110)	C(111)	C(131)	-176.42 (0.40)
C(118)	C(110)	C(111)	N(112)	-176.47 (0.43)
C(118)	C(110)	C(111)	C(131)	4.35 (0.67)
N(112)	C(111)	C(131)	C(132)	81.48 (0.53)
N(112)	C(111)	C(131)	C(136)	-98.87 (0.56)
C(110)	C(111)	C(131)	C(132)	-99.28 (0.55)
C(110)	C(111)	C(131)	C(136)	80.37 (0.64)
N(112)	C(113)	C(114)	N(11)	-1.99 (0.49)
N(112)	C(113)	C(114)	C(15)	178.98 (0.32)
C(18)	C(113)	C(114)	N(11)	176.50 (0.34)
C(18)	C(113)	C(114)	C(15)	-2.53 (0.54)
C(12)	C(121)	C(122)	C(123)	177.65 (0.43)
C(126)	C(121)	C(122)	C(123)	-0.51 (0.69)
C(12)	C(121)	C(126)	C(125)	-177.66 (0.46)
C(122)	C(121)	C(126)	C(125)	0.48 (0.72)
C(121)	C(122)	C(123)	C(124)	0.74 (0.80)
C(122)	C(123)	C(124)	C(125)	-0.91 (0.87)
C(123)	C(124)	C(125)	C(126)	0.90 (0.92)
C(124)	C(125)	C(126)	C(121)	-0.69 (0.87)
C(111)	C(131)	C(132)	C(133)	-178.01 (0.49)
C(136)	C(131)	C(132)	C(133)	2.33 (0.82)
C(111)	C(131)	C(136)	C(135)	179.88 (0.71)
C(132)	C(131)	C(136)	C(135)	-0.46 (1.04)
C(131)	C(132)	C(133)	C(134)	-0.95 (0.97)
C(132)	C(133)	C(134)	C(135)	-2.27 (1.23)
C(133)	C(134)	C(135)	C(136)	4.06 (1.39)
C(134)	C(135)	C(136)	C(131)	-2.67 (1.32)
C(29)	C(210)	C(211)	N(212)	-3.24 (0.59)
C(29)	C(210)	C(211)	C(231)	174.99 (0.36)
C(218)	C(210)	C(211)	N(212)	176.41 (0.38)
C(218)	C(210)	C(211)	C(231)	-5.37 (0.58)
N(212)	C(211)	C(231)	C(232)	99.53 (0.42)
N(212)	C(211)	C(231)	C(236)	-82.10 (0.48)
C(210)	C(211)	C(231)	C(232)	-78.80 (0.51)
C(210)	C(211)	C(231)	C(236)	99.57 (0.46)
N(212)	C(213)	C(214)	N(21)	4.88 (0.47)
N(212)	C(213)	C(214)	C(25)	-173.87 (0.33)
C(28)	C(213)	C(214)	N(21)	-177.49 (0.32)
C(28)	C(213)	C(214)	C(25)	3.77 (0.53)
C(22)	C(221)	C(222)	C(223)	174.25 (0.44)
C(226)	C(221)	C(222)	C(223)	-2.26 (0.73)
C(22)	C(221)	C(226)	C(225)	-174.87 (0.44)
C(222)	C(221)	C(226)	C(225)	1.49 (0.72)
C(221)	C(222)	C(223)	C(224)	1.17 (0.80)
C(222)	C(223)	C(224)	C(225)	0.72 (0.84)
C(223)	C(224)	C(225)	C(226)	-1.47 (0.84)
C(224)	C(225)	C(226)	C(221)	0.34 (0.80)
C(211)	C(231)	C(232)	C(233)	179.19 (0.40)
C(236)	C(231)	C(232)	C(233)	0.78 (0.61)
C(211)	C(231)	C(236)	C(235)	-178.37 (0.37)
C(232)	C(231)	C(236)	C(235)	0.02 (0.84)
C(231)	C(232)	C(233)	C(234)	-0.84 (0.71)
C(232)	C(233)	C(234)	C(235)	0.10 (0.71)
C(233)	C(234)	C(235)	C(236)	0.70 (0.68)
C(234)	C(235)	C(236)	C(231)	-0.75 (0.64)
O(301)	C(302)	C(303)	C(304)	16.60 (2.70)
C(302)	C(303)	C(304)	C(305)	-15.48 (2.20)
C(303)	C(304)	C(305)	O(301)	10.85 (1.80)

Table A.3. Structure factors (F^2_{obs} & F^2_{calc})[a] for $[Cu(dptmp)_2]PF_6{\bullet}THF$.

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
3	0	0	3879	3799	11	2	0	337	356	11	4	0	-1	1	9	6	0	904	708	9	8	0	227	237
4	0	0	2968	2626	12	2	0	836	723	12	4	0	288	265	10	6	0	12	27	10	8	0	77	74
5	0	0	996	817	13	2	0	0	3	13	4	0	12	3	11	6	0	9	15	11	8	0	87	71
6	0	0	22	65	14	2	0	11	4	14	4	0	10	3	12	6	0	149	125	12	8	0	53	58
7	0	0	1845	1814	15	2	0	14	3	15	4	0	17	8	13	6	0	67	69	13	8	0	34	30
8	0	0	1722	1465	16	2	0	-8	0	-18	5	0	26	2	14	6	0	-7	1	14	8	0	-11	0
9	0	0	1365	1173	-16	3	0	18	26	-17	5	0	61	28	15	6	0	76	36	-17	9	0	31	7
10	0	0	955	977	-15	3	0	11	15	-16	5	0	11	5	-18	7	0	-19	3	-16	9	0	32	31
11	0	0	57	68	-14	3	0	68	72	-15	5	0	-2	1	-17	7	0	81	54	-15	9	0	15	16
12	0	0	120	129	-13	3	0	1	0	-14	5	0	102	89	-16	7	0	24	27	-14	9	0	-8	0
13	0	0	282	261	-12	3	0	68	68	-13	5	0	37	36	-15	7	0	15	10	-13	9	0	15	10
14	0	0	544	429	-11	3	0	137	134	-12	5	0	22	26	-14	7	0	36	24	-12	9	0	82	74
15	0	0	60	38	-10	3	0	272	237	-11	5	0	397	354	-13	7	0	69	63	-11	9	0	17	41
16	0	0	18	40	-9	3	0	154	153	-10	5	0	809	759	-12	7	0	7	0	-10	9	0	45	52
-16	1	0	27	12	-8	3	0	889	749	-9	5	0	153	152	-11	7	0	71	84	-9	9	0	466	417
-15	1	0	68	48	-7	3	0	7	3	-8	5	0	265	293	-10	7	0	168	199	-8	9	0	79	88
-14	1	0	-2	14	-6	3	0	1635	1373	-7	5	0	199	227	-9	7	0	471	424	-7	9	0	-3	5
-13	1	0	17	1	-5	3	0	20	6	-6	5	0	1786	2025	-8	7	0	7	3	-6	9	0	897	819
-12	1	0	127	98	-4	3	0	25	32	-5	5	0	2	0	-7	7	0	23	16	-5	9	0	396	324
-11	1	0	65	76	-3	3	0	2362	2630	-4	5	0	4398	4103	-6	7	0	341	360	-4	9	0	152	173
-10	1	0	758	659	-2	3	0	1372	1354	-3	5	0	168	178	-5	7	0	169	194	-3	9	0	537	627
-9	1	0	477	428	-1	3	0	19	9	-2	5	0	1	4	-4	7	0	790	730	-2	9	0	264	198
-8	1	0	285	273	1	3	0	671	588	-1	5	0	2651	2871	-3	7	0	1482	1715	-1	9	0	1151	1282
-7	1	0	94	96	2	3	0	2	11	0	5	0	2304	2576	-2	7	0	482	409	0	9	0	86	111
-6	1	0	492	464	3	3	0	48	57	1	5	0	55	77	-1	7	0	7	4	1	9	0	100	84
-5	1	0	3044	3267	4	3	0	502	427	2	5	0	592	428	0	7	0	3686	4249	2	9	0	878	838
-4	1	0	2902	3009	5	3	0	465	490	3	5	0	4498	4128	1	7	0	7	25	3	9	0	-1	0
-3	1	0	859	867	6	3	0	10	5	4	5	0	8554	7165	2	7	0	290	473	4	9	0	378	424
3	1	0	9400	9017	7	3	0	525	582	5	5	0	32	17	3	7	0	816	853	5	9	0	360	297
4	1	0	537	565	8	3	0	95	76	6	5	0	456	413	4	7	0	958	885	6	9	0	42	33
5	1	0	2592	2466	9	3	0	452	361	7	5	0	2	3	5	7	0	525	489	7	9	0	271	268
6	1	0	193	215	10	3	0	435	402	8	5	0	283	218	6	7	0	11	24	8	9	0	616	569
7	1	0	106	112	11	3	0	711	707	9	5	0	173	129	7	7	0	73	102	9	9	0	102	65
8	1	0	248	298	12	3	0	35	27	10	5	0	138	133	8	7	0	629	557	10	9	0	4	7
9	1	0	951	872	13	3	0	102	80	11	5	0	277	287	9	7	0	11	31	11	9	0	33	38
10	1	0	1293	1152	14	3	0	8	3	12	5	0	2	2	10	7	0	95	86	12	9	0	51	65
11	1	0	97	73	15	3	0	9	2	13	5	0	62	50	11	7	0	297	261	13	9	0	17	8
12	1	0	2063	1949	-18	4	0	8	7	14	5	0	5	15	12	7	0	61	67	-17	10	0	85	2
13	1	0	852	761	-17	4	0	22	24	15	5	0	-10	0	13	7	0	38	19	-16	10	0	-15	6
14	1	0	143	212	-16	4	0	103	102	-18	6	0	12	1	14	7	0	51	39	-15	10	0	-12	3
15	1	0	1	8	-15	4	0	17	5	-17	6	0	-13	15	-17	8	0	-10	1	-14	10	0	0	16
16	1	0	14	5	-14	4	0	14	9	-16	6	0	-1	19	-16	8	0	7	1	-13	10	0	32	51
-16	2	0	62	58	-13	4	0	130	129	-15	6	0	4	12	-15	8	0	-1	4	-12	10	0	76	65
-15	2	0	22	10	-12	4	0	178	156	-14	6	0	-1	0	-14	8	0	14	6	-11	10	0	19	6
-14	2	0	31	24	-11	4	0	13	2	-13	6	0	44	33	-13	8	0	-5	12	-10	10	0	14	12
-13	2	0	228	203	-10	4	0	90	87	-12	6	0	334	364	-12	8	0	-3	4	-9	10	0	51	49
-12	2	0	-5	3	-9	4	0	2706	2565	-11	6	0	128	88	-11	8	0	81	62	-8	10	0	49	39
-11	2	0	19	9	-8	4	0	460	400	-10	6	0	22	27	-10	8	0	23	34	-7	10	0	80	73
-10	2	0	95	144	-7	4	0	37	70	-9	6	0	426	394	-9	8	0	25	27	-6	10	0	297	278
-9	2	0	716	617	-6	4	0	249	152	-8	6	0	754	657	-8	8	0	176	135	-5	10	0	-2	2
-8	2	0	-2	2	-5	4	0	802	895	-7	6	0	158	129	-7	8	0	11	10	-4	10	0	128	113
-7	2	0	293	358	-4	4	0	119	82	-6	6	0	132	112	-6	8	0	3	5	-3	10	0	1517	1366
-6	2	0	1047	1312	-3	4	0	25	12	-5	6	0	2897	2839	-5	8	0	904	870	-2	10	0	355	323
-5	2	0	3	12	-2	4	0	2205	2135	-4	6	0	486	528	-4	8	0	801	745	-1	10	0	6	7
-4	2	0	714	788	-1	4	0	862	1090	-3	6	0	7	13	-3	8	0	648	618	0	10	0	1101	1037
-3	2	0	19034	14924	0	4	0	1435	1368	-2	6	0	1153	1258	-2	8	0	69	51	1	10	0	60	63
-2	2	0	37913	29271	1	4	0	8	18	-1	6	0	1935	2298	-1	8	0	55	55	2	10	0	136	115
2	2	0	5110	5120	2	4	0	207	251	0	6	0	413	454	0	8	0	339	433	3	10	0	278	286
3	2	0	493	564	3	4	0	47	36	1	6	0	573	406	1	8	0	10	18	4	10	0	0	10
4	2	0	8224	8178	4	4	0	2	26	2	6	0	2405	2375	2	8	0	23	22	5	10	0	70	80
5	2	0	80	117	5	4	0	2061	1955	3	6	0	3158	3065	3	8	0	980	1093	6	10	0	37	36
6	2	0	352	327	6	4	0	5	4	4	6	0	210	258	4	8	0	382	387	7	10	0	69	58
7	2	0	353	390	7	4	0	-1	3	5	6	0	1919	1803	5	8	0	11	17	8	10	0	86	99
8	2	0	3033	2660	8	4	0	1110	1041	6	6	0	1108	1247	6	8	0	196	169	9	10	0	3	11
9	2	0	433	458	9	4	0	599	542	7	6	0	23	21	7	8	0	-3	1	10	10	0	40	14
10	2	0	38	55	10	4	0	542	571	8	6	0	616	638	8	8	0	2	3	11	10	0	62	46
12	10	0	14	1	-6	13	0	-2	3	-7	16	0	75	25	0	-17	1	24	23	3	-14	1	3	8
13	10	0	15	0	-5	13	0	20	2	-6	16	0	34	0	1	-17	1	22	14	4	-14	1	53	44
-16	11	0	12	1	-4	13	0	8	21	-5	16	0	14	8	2	-17	1	-7	1	5	-14	1	9	3
-15	11	0	-14	0	-3	13	0	176	167	-4	16	0	41	25	3	-17	1	4	7	6	-14	1	-2	22
-14	11	0	-9	2	-2	13	0	460	407	-3	16	0	-5	3	4	-17	1	9	9	7	-14	1	78	54
-13	11	0	-4	4	-1	13	0	273	229	-2	16	0	-4	1	5	-17	1	-10	1	8	-14	1	40	44
-12	11	0	98	95	0	13	0	326	301	-1	16	0	30	30	6	-17	1	16	3	9	-14	1	5	6
-11	11	0	21	36	1	13	0	33	38	0	16	0	17	17	7	-17	1	2	9	10	-14	1	-7	0
-10	11	0	-4	5	2	13	0	14	17	1	16	0	1	2	8	-17	1	14	0	11	-14	1	4	7
-9	11	0	94	77	3	13	0	87	96	2	16	0	46	55	9	-17	1	4	3	12	-14	1	-8	0
-8	11	0	212	192	4	13	0	18	21	3	16	0	23	44	10	-17	1	2	7	13	-14	1	4	8
-7	11	0	153	164	5	13	0	-4	1	4	16	0	-5	4	-7	-16	1	-13	4	14	-14	1	28	3
-6	11	0	-1	3	6	13	0	31	31	5	16	0	9	5	-6	-16	1	-13	2	-11	-13	1	-7	4
-5	11	0	83	52	7	13	0	1	2	6	16	0	-9	4	-5	-16	1	15	5	-10	-13	1	6	7
-4	11	0	117	128	8	13	0	1	8	7	16	0	2	0	-4	-16	1	28	26	-9	-13	1	47	26
-3	11	0	38	42	9	13	0	-7	1	-9	17	0	47	18	-3	-16	1	1	0	-8	-13	1	-1	3
-2	11	0	628	528	10	13	0	9	0	-8	17	0	-6	16	-2	-16	1	20	6	-7	-13	1	4	1
-1	11	0	403	334	-14	14	0	16	0	-7	17	0	12	1	-1	-16	1	37	35	-6	-13	1	17	15
0	11	0	165	147	-13	14	0	14	10	-6	17	0	23	9	0	-16	1	5	6	-5	-13	1	41	35
1	11	0	5	0	-12	14	0	64	21	-5	17	0	-7	5	1	-16	1	-1	0	-4	-13	1	-3	7
2	11	0	80	59	-11	14	0	23	7	-4	17	0	-1	2	2	-16	1	5	2	-3	-13	1	42	39
3	11	0	7	13	-10	14	0	16	8	-3	17	0	-6	2	3	-16	1	10	1	-2	-13	1	123	123
4	11	0	27	21	-9	14	0	0	3	-2	17	0	5	3	4	-16	1	0	1	-1	-13	1	190	184
5	11	0	21	31	-8	14	0	4	4	-1	17	0	14	7	5	-16	1	1	9	0	-13	1	8	9
6	11	0	44	39	-7	14	0	5	1	0	17	0	-5	9	6	-16	1	48	12	1	-13	1	-1	12
7	11	0	19	5	-6	14	0	11	13	1	17	0	15	23	7	-16	1	-6	2	2	-13	1	41	37
8	11	0	7	19	-5	14	0	5	1	2	17	0	36	13	8	-16	1	4	0	3	-13	1	7	13
9	11	0	86	66	-4	14	0	31	33	3	17	0	-5	2	9	-16	1	3	0	4	-13	1	22	10
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-14	12	0	75	33	1	14	0	61	66	-4	18	0	-1	9	-7	-15	1	-11	8	9	-13	1	45	48
-13	12	0	35	42	2	14	0	41	34	-3	18	0	13	6	-6	-15	1	24	26	10	-13	1	6	19
-12	12	0	33	42	3	14	0	-3	0	-2	18	0	-1	2	-5	-15	1	17	16	11	-13	1	-7	0
-11	12	0	31	21	4	14	0	7	5	-1	18	0	5	0	-4	-15	1	4	1	12	-13	1	34	41
-10	12	0	18	7	5	14	0	20	20	0	18	0	-1	0	-3	-15	1	19	15	13	-13	1	20	16

Table A.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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-8	12	0	3	2	7	14	0	22	14	2	18	0	4	18	-1	-15	1	13	5	15	-13	1	11	1
-7	12	0	28	41	8	14	0	14	0	3	18	0	11	4	0	-15	1	19	20	-12	-12	1	-4	5
-6	12	0	97	92	9	14	0	-7	1	-1	19	0	8	1	1	-15	1	21	10	-11	-12	1	-6	0
-5	12	0	17	17	-12	15	0	-11	1	-2	-19	1	-2	7	2	-15	1	5	3	-10	-12	1	53	49
-4	12	0	4	2	-11	15	0	5	7	-1	-19	1	-9	1	3	-15	1	-4	0	-9	-12	1	24	31
-3	12	0	20	18	-10	15	0	15	10	0	-19	1	6	4	4	-15	1	19	26	-8	-12	1	17	22
-2	12	0	175	157	-9	15	0	31	10	1	-19	1	39	3	5	-15	1	42	36	-7	-12	1	74	76
-1	12	0	67	49	-8	15	0	16	12	2	-19	1	-1	0	6	-15	1	0	4	-6	-12	1	79	64
0	12	0	116	100	-7	15	0	-5	1	3	-19	1	-13	2	7	-15	1	1	1	-5	-12	1	6	1
1	12	0	73	81	-6	15	0	5	5	4	-19	1	-1	7	8	-15	1	39	11	-4	-12	1	72	86
2	12	0	110	142	-5	15	0	22	10	-4	-18	1	-4	2	9	-15	1	36	4	-3	-12	1	87	63
3	12	0	-3	5	-4	15	0	82	84	-3	-18	1	6	7	10	-15	1	-1	0	-2	-12	1	35	30
4	12	0	79	80	-3	15	0	68	86	-2	-18	1	14	34	11	-15	1	-10	2	-1	-12	1	81	91
5	12	0	126	130	-2	15	0	-3	3	-1	-18	1	26	57	12	-15	1	41	4	0	-12	1	103	101
6	12	0	6	1	-1	15	0	27	13	0	-18	1	1	13	13	-15	1	8	0	1	-12	1	110	133
7	12	0	2	0	0	15	0	119	144	1	-18	1	10	0	-10	-14	1	-11	4	2	-12	1	4	2
8	12	0	4	4	1	15	0	46	46	2	-18	1	21	4	-9	-14	1	34	4	3	-12	1	121	97
9	12	0	-5	1	2	15	0	13	13	3	-18	1	-5	0	-8	-14	1	17	0	4	-12	1	206	193
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-9	-11	1	2	17	-5	-9	1	46	37	-4	-7	1	1219	1206	-6	-5	1	404	410	-9	-3	1	136	118
-8	-11	1	63	63	-4	-9	1	363	312	-3	-7	1	945	987	-5	-5	1	241	302	-8	-3	1	669	680
-7	-11	1	168	171	-3	-9	1	373	292	-2	-7	1	121	185	-4	-5	1	-1	5	-7	-3	1	6	2
-6	-11	1	-2	6	-2	-9	1	98	125	-1	-7	1	23	44	-3	-5	1	419	397	-6	-3	1	1029	934
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8	-11	1	23	18	12	-9	1	46	34	13	-7	1	10	1	11	-5	1	246	241	9	-3	1	520	544
9	-11	1	46	51	13	-9	1	0	1	14	-7	1	4	12	12	-5	1	112	100	10	-3	1	998	834
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12	-11	1	39	31	16	-9	1	0	18	17	-7	1	24	3	15	-5	1	-3	14	13	-3	1	283	283
13	-11	1	56	21	17	-9	1	33	16	18	-7	1	-5	0	16	-5	1	110	121	14	-3	1	12	0
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-12	-10	1	47	53	-10	-8	1	21	21	-11	-6	1	351	351	-13	-4	1	99	120	-14	-2	1	113	109
-11	-10	1	-5	4	-9	-8	1	52	51	-10	-6	1	-3	4	-12	-4	1	0	7	-13	-2	1	375	384
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-9	-10	1	64	66	-7	-8	1	58	41	-8	-6	1	373	418	-10	-4	1	1059	1020	-11	-2	1	16	27
-8	-10	1	146	171	-6	-8	1	532	527	-7	-6	1	456	329	-9	-4	1	0	3	-10	-2	1	16	24
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-4	-10	1	200	191	-2	-8	1	248	220	-3	-6	1	225	210	-5	-4	1	584	427	-6	-2	1	134	176
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-2	-10	1	174	159	0	-8	1	83	134	-1	-6	1	3956	4282	-3	-4	1	1136	1169	-4	-2	1	874	1029
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1	-10	1	173	157	3	-8	1	662	546	2	-6	1	2955	3088	0	-4	1	900	923	-1	-2	1	372	474
2	-10	1	284	272	4	-8	1	611	488	3	-6	1	239	214	1	-4	1	7314	7251	2	-2	1	7969	7810
3	-10	1	-2	3	5	-8	1	145	133	4	-6	1	146	154	2	-4	1	1337	1327	3	-2	1	764	918
4	-10	1	266	217	6	-8	1	59	75	5	-6	1	310	265	3	-4	1	3535	4019	4	-2	1	34	17
5	-10	1	434	434	7	-8	1	100	72	6	-6	1	2	3	4	-4	1	137	161	5	-2	1	30	14
6	-10	1	152	126	8	-8	1	716	582	7	-6	1	5	5	5	-4	1	368	264	6	-2	1	5	4
7	-10	1	-1	2	9	-8	1	135	141	8	-6	1	-2	6	6	-4	1	52	46	7	-2	1	2534	2391
8	-10	1	199	197	10	-8	1	45	46	9	-6	1	159	146	7	-4	1	401	529	8	-2	1	1426	1492
9	-10	1	126	105	11	-8	1	68	61	10	-6	1	288	256	8	-4	1	4	9	9	-2	1	1092	1139
10	-10	1	46	27	12	-8	1	119	119	11	-6	1	-3	1	9	-4	1	16	22	10	-2	1	511	453
11	-10	1	68	77	13	-8	1	94	83	12	-6	1	10	17	10	-4	1	1383	1147	11	-2	1	104	106
12	-10	1	59	57	14	-8	1	-5	13	13	-6	1	143	134	11	-4	1	42	25	12	-2	1	208	182
13	-10	1	40	51	15	-8	1	16	7	14	-6	1	46	36	12	-4	1	9	14	13	-2	1	10	5
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15	-10	1	-8	2	17	-8	1	42	28	16	-6	1	-8	0	14	-4	1	57	71	15	-2	1	28	15
16	-10	1	-13	7	18	-8	1	-4	0	17	-6	1	13	7	15	-4	1	7	29	16	-2	1	16	11
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-13	-9	1	8	15	-12	-7	1	34	14	-14	-5	1	-6	6	18	-4	1	11	4	-14	-1	1	367	323
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-11	-1	1	234	222	3	1	1	7903	6942	5	3	1	2513	2508	5	5	1	898	1040	4	7	1	581	436
-10	-1	1	1172	1195	4	1	1	6733	6191	6	3	1	755	824	6	5	1	531	486	5	7	1	446	489
-9	-1	1	15	21	5	1	1	436	385	7	3	1	141	127	7	5	1	10	1	6	7	1	121	111
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-6	-1	1	72	72	8	1	1	2193	2350	10	3	1	-2	3	10	5	1	9	1	9	7	1	27	28
-5	-1	1	138	142	9	1	1	63	92	11	3	1	379	352	11	5	1	115	104	10	7	1	164	131
-4	-1	1	5512	5671	10	1	1	36	50	12	3	1	246	284	12	5	1	74	79	11	7	1	13	1
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Table A.3, continued

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4	-1	1	15827	14418	13	1	1	1	28	15	3	1	2	6	15	5	1	-11	3	14	7	1	-12	13
5	-1	1	276	314	14	1	1	19	13	-18	4	1	-16	7	-18	6	1	48	3	-17	8	1	-19	7
6	-1	1	389	368	15	1	1	-1	10	-16	4	1	40	12	-17	6	1	48	29	-16	8	1	22	36
7	-1	1	1991	1951	16	1	1	-6	5	-15	4	1	3	9	-16	6	1	32	24	-15	8	1	-9	4
8	-1	1	40	71	-16	2	1	85	94	-14	4	1	83	70	-15	6	1	17	0	-14	8	1	7	3
9	-1	1	239	355	-15	2	1	5	1	-13	4	1	24	20	-14	6	1	25	31	-13	8	1	-1	9
10	-1	1	25	11	-14	2	1	61	31	-12	4	1	344	395	-13	6	1	34	40	-12	8	1	70	63
11	-1	1	20	6	-13	2	1	43	53	-11	4	1	1250	1148	-12	6	1	84	100	-11	8	1	14	22
12	-1	1	41	42	-12	2	1	120	99	-10	4	1	2008	1771	-11	6	1	61	41	-10	8	1	184	181
13	-1	1	120	103	-11	2	1	340	264	-9	4	1	13	26	-10	6	1	311	241	-9	8	1	240	225
14	-1	1	104	89	-10	2	1	200	191	-8	4	1	815	878	-9	6	1	74	105	-8	8	1	180	135
15	-1	1	-1	2	-9	2	1	223	200	-7	4	1	89	107	-8	6	1	17	7	-7	8	1	131	106
16	-1	1	46	27	-8	2	1	289	391	-6	4	1	1331	1263	-7	6	1	318	327	-6	8	1	445	401
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Table A.3, continued

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-4	-11	2	117	94	0	-9	2	186	130	0	-7	2	225	334	-2	-5	2	19	23	-6	-3	2	1544	1737
-3	-11	2	260	239	1	-9	2	248	260	1	-7	2	22	41	-1	-5	2	1968	2248	-5	-3	2	2409	1910
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-10	-2	2	606	489	-4	0	2	14	27	3	2	2	1343	1510	4	4	2	3134	3076	2	6	2	758	873
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-8	-2	2	579	590	2	0	2	30	4	5	2	2	1555	1466	6	4	2	90	131	4	6	2	1056	1022
-7	-2	2	705	775	3	0	2	840	798	6	2	2	3140	2952	7	4	2	142	142	5	6	2	262	252
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-4	-2	2	591	663	6	0	2	348	386	9	2	2	520	477	10	4	2	0	3	8	6	2	410	396
-3	-2	2	2	6	7	0	2	46	91	10	2	2	2165	2133	11	4	2	53	65	9	6	2	212	163
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2	-2	2	104	70	10	0	2	402	395	13	2	2	5	11	14	4	2	48	53	12	6	2	93	105
3	-2	2	156	127	11	0	2	458	444	14	2	2	68	95	15	4	2	22	1	13	6	2	13	22
4	-2	2	272	283	12	0	2	6	0	15	2	2	2	1	-18	5	2	1	1	14	6	2	35	27
5	-2	2	144	130	13	0	2	92	99	16	2	2	43	0	-17	5	2	6	9	-17	7	2	-3	1

Table A.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
6	-2	2	5325	5407	14	0	2	69	55	-16	3	2	-9	2	-16	5	2	11	4	-15	7	2	-4	2
7	-2	2	215	182	15	0	2	-1	3	-15	3	2	-7	12	-15	5	2	-1	14	-14	7	2	41	24
8	-2	2	988	827	16	0	2	-13	5	-14	3	2	21	26	-14	5	2	1	12	-13	7	2	28	20
9	-2	2	302	292	-16	1	2	297	326	-13	3	2	23	12	-13	5	2	7	11	-12	7	2	63	59
10	-2	2	594	563	-15	1	2	80	99	-12	3	2	661	712	-12	5	2	28	14	-11	7	2	26	17
11	-2	2	132	130	-14	1	2	44	31	-11	3	2	446	428	-11	5	2	167	138	-10	7	2	52	30
12	-2	2	215	197	-13	1	2	13	24	-10	3	2	347	286	-10	5	2	200	221	-9	7	2	108	70
13	-2	2	81	132	-12	1	2	283	260	-9	3	2	116	129	-9	5	2	64	76	-8	7	2	70	42
14	-2	2	41	38	-11	1	2	68	90	-8	3	2	610	568	-8	5	2	523	559	-7	7	2	95	105
15	-2	2	-1	9	-10	1	2	260	250	-7	3	2	30	39	-7	5	2	685	664	-6	7	2	640	690
16	-2	2	46	23	-9	1	2	891	870	-6	3	2	4979	4385	-6	5	2	364	394	-5	7	2	69	46
-16	-1	2	65	81	-8	1	2	1065	1102	-5	3	2	233	252	-5	5	2	15	24	-4	7	2	294	241
-15	-1	2	-6	8	-7	1	2	16	4	-4	3	2	4157	4135	-4	5	2	1678	1695	-3	7	2	3409	3466
-14	-1	2	10	7	-6	1	2	543	750	-3	3	2	5711	5825	-3	5	2	1208	1223	-2	7	2	1165	980
-13	-1	2	203	201	-5	1	2	83	86	-2	3	2	255	237	-2	5	2	246	287	-1	7	2	467	540
-12	-1	2	335	348	-4	1	2	8411	7267	-1	3	2	4169	3801	-1	5	2	32	30	0	7	2	2726	2761
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-9	-1	2	666	518	1	1	2	107	217	2	3	2	437	689	2	5	2	1411	1552	3	7	2	493	645
-8	-1	2	56	65	2	1	2	2319	2091	3	3	2	2	9	3	5	2	560	857	4	7	2	34	42
-7	-1	2	834	667	3	1	2	130	88	4	3	2	345	347	4	5	2	0	2	5	7	2	87	123
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12	-1	2	102	99	-15	2	2	-9	2	-13	4	2	70	58	-15	6	2	62	51	-10	8	2	5	2
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8	8	2	22	39	-12	11	2	63	48	2	13	2	132	88	6	16	2	11	1	4	-16	3	0	3
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12	9	2	45	41	-5	12	2	0	8	-8	15	2	8	12	6	-18	3	-1	4	-9	-14	3	5	3
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-8	10	2	625	486	3	12	2	3	9	0	15	2	16	15	-1	-17	3	-2	2	-1	-14	3	34	40
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-6	10	2	226	195	5	12	2	132	150	2	15	2	83	94	1	-17	3	4	10	1	-14	3	14	3
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-3	10	2	356	347	8	12	2	95	123	5	15	2	9	4	4	-17	3	18	11	4	-14	3	74	78
-2	10	2	170	159	9	12	2	-7	2	6	15	2	26	4	5	-17	3	5	1	5	-14	3	2	1
-1	10	2	3	15	10	12	2	-8	3	7	15	2	3	0	6	-17	3	-5	5	6	-14	3	15	24
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Table A.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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2	10	2	26	25	-12	13	2	4	14	-8	16	2	23	7	9	-17	3	4	10	9	-14	3	0	0
3	10	2	66	63	-11	13	2	23	34	-7	16	2	13	14	10	-17	3	-13	2	10	-14	3	7	14
4	10	2	15	12	-10	13	2	21	28	-6	16	2	5	15	-8	-16	3	-9	2	11	-14	3	13	2
5	10	2	45	43	-9	13	2	28	22	-5	16	2	2	10	-7	-16	3	18	2	12	-14	3	1	3
6	10	2	177	233	-8	13	2	-2	2	-4	16	2	8	5	-6	-16	3	25	5	13	-14	3	18	7
7	10	2	27	41	-7	13	2	94	105	-3	16	2	0	3	-5	-16	3	21	18	14	-14	3	-10	2
8	10	2	63	53	-6	13	2	-2	2	-2	16	2	3	12	-4	-16	3	36	19	-12	-13	3	-5	0
9	10	2	24	24	-5	13	2	-4	4	-1	16	2	18	17	-3	-16	3	20	2	-11	-13	3	-10	0
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-9	-13	3	20	19	-1	-11	3	14	13	1	-9	3	440	379	1	-7	3	1769	1969	-1	-5	3	758	613
-8	-13	3	10	8	0	-11	3	261	264	2	-9	3	480	488	2	-7	3	456	365	0	-5	3	1112	959
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-3	-13	3	-3	1	5	-11	3	414	336	7	-9	3	146	131	7	-7	3	-2	4	5	-5	3	333	245
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8	-12	3	72	112	12	-10	3	4	4	13	-8	3	73	92	13	-6	3	389	386	9	-4	3	465	454
9	-12	3	-4	1	13	-10	3	27	12	14	-8	3	-4	2	14	-6	3	47	55	10	-4	3	423	454
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-9	-11	3	23	34	-7	-9	3	430	364	-7	-7	3	112	58	-9	-5	3	493	525	-13	-3	3	60	58
-8	-11	3	52	48	-6	-9	3	8	4	-6	-7	3	7	15	-8	-5	3	731	655	-12	-3	3	226	192
-7	-11	3	38	37	-5	-9	3	117	184	-5	-7	3	208	195	-7	-5	3	594	561	-11	-3	3	208	148
-6	-11	3	13	20	-4	-9	3	1636	1378	-4	-7	3	505	411	-6	-5	3	926	992	-10	-3	3	107	91
-5	-11	3	63	53	-3	-9	3	7	28	-3	-7	3	17	27	-5	-5	3	514	657	-9	-3	3	173	172
-4	-11	3	795	728	-2	-9	3	82	85	-2	-7	3	11	1	-4	-5	3	127	140	-8	-3	3	84	66
-3	-11	3	112	77	-1	-9	3	757	762	-1	-7	3	161	249	-3	-5	3	723	826	-7	-3	3	62	19
-6	-3	3	1477	1402	-6	-1	3	1074	940	-3	1	3	53114	35287	-2	3	3	168	189	-1	5	3	147	131
-5	-3	3	557	647	-5	-1	3	24	17	-1	1	3	4718	4982	-1	3	3	831	894	0	5	3	166	115
-4	-3	3	295	292	-4	-1	3	1957	2385	0	1	3	552	655	0	3	3	409	370	1	5	3	2972	3492
-3	-3	3	935	1044	-3	-1	3	359	383	1	1	3	1298	1305	1	3	3	2484	2471	2	5	3	9	3
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-1	-3	3	4395	4840	-1	-1	3	377	326	3	1	3	42	89	3	3	3	1282	1271	4	5	3	352	380
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5	-3	3	2907	3077	7	-1	3	816	805	9	1	3	111	130	9	3	3	731	676	10	5	3	10	21
6	-3	3	473	535	8	-1	3	374	356	10	1	3	2157	1966	10	3	3	27	6	11	5	3	274	231
7	-3	3	372	469	9	-1	3	66	67	11	1	3	456	399	11	3	3	21	3	12	5	3	83	72
8	-3	3	431	421	10	-1	3	338	376	12	1	3	77	100	12	3	3	22	20	13	5	3	6	1
9	-3	3	407	366	11	-1	3	449	411	13	1	3	163	140	13	3	3	57	46	14	5	3	29	4
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11	-3	3	8	5	13	-1	3	127	159	15	1	3	6	1	15	3	3	32	1	-17	6	3	10	5
12	-3	3	157	154	14	-1	3	2	0	16	1	3	-4	6	-16	4	3	6	3	-16	6	3	14	0
13	-3	3	155	163	15	-1	3	-6	0	-16	2	3	4	1	-15	4	3	33	29	-15	6	3	88	57
14	-3	3	21	0	16	-1	3	10	32	-15	2	3	7	3	-14	4	3	3	24	-14	6	3	167	149
15	-3	3	36	18	-16	0	3	270	258	-14	2	3	6	2	-13	4	3	-7	1	-13	6	3	208	198
17	-3	3	-5	0	-15	0	3	95	121	-13	2	3	3	6	-12	4	3	-5	4	-12	6	3	105	121
18	-3	3	-11	8	-14	0	3	102	87	-12	2	3	96	99	-11	4	3	165	173	-11	6	3	144	127
-16	-2	3	79	58	-13	0	3	61	71	-11	2	3	73	62	-10	4	3	10	1	-10	6	3	114	118
-15	-2	3	16	21	-12	0	3	182	198	-10	2	3	23	13	-9	4	3	4	6	-9	6	3	1	2
-14	-2	3	10	2	-11	0	3	132	108	-9	2	3	35	58	-8	4	3	517	509	-8	6	3	62	89
-13	-2	3	-6	12	-10	0	3	155	142	-8	2	3	1177	1075	-7	4	3	154	169	-7	6	3	883	808
-12	-2	3	18	10	-9	0	3	195	284	-7	2	3	2	7	-6	4	3	1227	1115	-6	6	3	186	128

Table A.3, continued

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-10	-2	3	189	187	-7	0	3	831	804	-5	2	3	5216	5171	-4	4	3	1996	2220	-4	6	3	1369	1651
-9	-2	3	2	2	-6	0	3	160	125	-4	2	3	2783	2963	-3	4	3	868	840	-3	6	3	983	864
-8	-2	3	66	73	-5	0	3	841	1099	-3	2	3	15861	12896	-2	4	3	48	27	-2	6	3	334	433
-7	-2	3	2011	1820	-4	0	3	1107	1201	-2	2	3	8863	8364	-1	4	3	2989	3337	-1	6	3	3911	3773
-6	-2	3	6	7	-3	0	3	1516	1457	-1	2	3	1158	849	0	4	3	16	36	0	6	3	1863	1865
-5	-2	3	84	35	-2	0	3	1740	1580	0	2	3	36	79	1	4	3	0	1	1	6	3	4480	4234
-4	-2	3	12	20	-1	0	3	5784	5105	1	2	3	2400	2577	2	4	3	4	11	2	6	3	27	5
-3	-2	3	34	35	1	0	3	9338	8246	2	2	3	1160	1237	3	4	3	65	78	3	6	3	34	23
-2	-2	3	5739	5887	2	0	3	2123	2656	3	2	3	1402	1468	4	4	3	760	575	4	6	3	675	765
-1	-2	3	603	691	3	0	3	239	249	4	2	3	1844	1711	5	4	3	14	25	5	6	3	55	66
0	-2	3	2312	2318	4	0	3	180	130	5	2	3	6001	5468	6	4	3	530	592	6	6	3	45	51
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3	-2	3	116	141	7	0	3	28	23	8	2	3	1015	932	9	4	3	24	17	9	6	3	16	37
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Table A.3, continued

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3	-14	4	13	2	13	-12	4	18	14	-13	-9	4	20	23	-13	-7	4	-2	1	-14	-5	4	57	66
4	-14	4	30	50	14	-12	4	14	0	-12	-9	4	83	99	-12	-7	4	48	40	-13	-5	4	10	7
5	-14	4	191	167	15	-12	4	-6	4	-11	-9	4	30	26	-11	-7	4	-4	3	-12	-5	4	228	163
6	-14	4	78	76	16	-12	4	2	0	-10	-9	4	13	4	-10	-7	4	96	81	-11	-5	4	196	183
7	-14	4	0	1	-13	-11	4	22	5	-9	-9	4	11	23	-9	-7	4	65	71	-10	-5	4	453	419
8	-14	4	8	6	-12	-11	4	7	24	-8	-9	4	107	78	-8	-7	4	77	93	-9	-5	4	32	27
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-15	-2	4	56	37	-13	0	4	62	72	-11	2	4	317	220	-9	4	4	272	229	-7	6	4	118	114
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Table A.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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-11	-2	4	36	33	-9	0	4	3	3	-7	2	4	784	855	-5	4	4	331	400	-3	6	4	1642	1401
-10	-2	4	6	0	-8	0	4	943	852	-6	2	4	775	698	-4	4	4	683	683	-2	6	4	2519	2330
-9	-2	4	1144	1082	-7	0	4	179	187	-5	2	4	99	126	-3	4	4	5370	5139	-1	6	4	1321	1255
-8	-2	4	2644	2320	-6	0	4	3706	3171	-4	2	4	1817	1906	-2	4	4	4725	4004	0	6	4	18	12
-7	-2	4	1199	1278	-5	0	4	43	57	-3	2	4	2614	2529	-1	4	4	50	60	1	6	4	160	194
-6	-2	4	110	77	-4	0	4	1838	1709	-2	2	4	257	291	0	4	4	47	114	2	6	4	1082	1106
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3	-2	4	1154	1334	5	0	4	551	451	7	2	4	622	703	9	4	4	83	69	11	6	4	20	19
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-11	-13	5	-11	2	-1	-11	5	85	72	3	-9	5	7	15	5	-7	5	31	30	5	-5	5	430	391
-10	-13	5	8	56	0	-11	5	8	9	4	-9	5	139	131	6	-7	5	341	335	6	-5	5	340	354
-9	-13	5	33	45	1	-11	5	8	11	5	-9	5	136	143	7	-7	5	1063	1034	7	-5	5	244	306
-8	-13	5	27	30	2	-11	5	243	190	6	-9	5	200	187	8	-7	5	549	477	8	-5	5	292	269
-7	-13	5	14	17	3	-11	5	29	32	7	-9	5	558	563	9	-7	5	47	61	9	-5	5	29	24
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Table A.3, continued

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-4	-13	5	21	10	6	-11	5	4	1	10	-9	5	-1	12	12	-7	5	10	2	12	-5	5	9	8
-3	-13	5	184	163	7	-11	5	21	30	11	-9	5	148	167	13	-7	5	136	98	13	-5	5	-4	1
-2	-13	5	171	146	8	-11	5	11	21	12	-9	5	47	41	14	-7	5	101	110	14	-5	5	34	28
-1	-13	5	0	4	9	-11	5	74	63	13	-9	5	122	142	15	-7	5	8	0	15	-5	5	12	13
0	-13	5	11	14	10	-11	5	43	22	14	-9	5	6	11	16	-7	5	0	9	16	-5	5	14	8
1	-13	5	127	121	11	-11	5	20	12	15	-9	5	13	1	-16	-6	5	21	18	-16	-4	5	23	10
2	-13	5	47	68	12	-11	5	18	11	16	-9	5	22	31	-15	-6	5	68	50	-15	-4	5	101	85
3	-13	5	9	0	13	-11	5	17	22	-15	-8	5	10	8	-14	-6	5	35	50	-14	-4	5	97	76
4	-13	5	67	80	14	-11	5	58	0	-14	-8	5	-9	0	-13	-6	5	22	7	-13	-4	5	-5	0
5	-13	5	187	204	15	-11	5	25	2	-13	-8	5	28	34	-12	-6	5	56	58	-12	-4	5	86	91
6	-13	5	7	5	-14	-10	5	15	0	-12	-8	5	18	28	-11	-6	5	65	68	-11	-4	5	295	236
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8	-13	5	74	92	-12	-10	5	15	16	-10	-8	5	118	134	-9	-6	5	47	50	-9	-4	5	6	9
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-10	-12	5	3	14	-3	-10	5	200	180	-1	-8	5	1252	1026	0	-6	5	14	22	0	-4	5	9	3
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-11	-11	5	6	0	-7	-9	5	428	357	-5	-7	5	19	20	-5	-5	5	175	238	-5	-3	5	774	1010
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-7	-11	5	11	9	-3	-9	5	38	22	-1	-7	5	512	509	-1	-5	5	2308	2181	-1	-3	5	2007	2091
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5	-3	5	1814	1726	6	-1	5	49	59	8	1	5	21	4	11	3	5	41	61	-17	6	5	76	6
6	-3	5	21	49	7	-1	5	816	797	9	1	5	87	59	12	3	5	15	15	-16	6	5	6	6
7	-3	5	254	245	8	-1	5	186	172	10	1	5	445	453	13	3	5	39	46	-15	6	5	49	51
8	-3	5	699	675	9	-1	5	565	470	11	1	5	97	73	14	3	5	21	43	-14	6	5	23	16
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13	-3	5	41	23	14	-1	5	11	0	-16	2	5	14	6	-12	4	5	188	195	-9	6	5	61	70
14	-3	5	43	21	15	-1	5	-6	1	-15	2	5	47	26	-11	4	5	232	238	-8	6	5	307	355
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-16	-2	5	-5	6	-14	0	5	0	3	-12	2	5	-4	2	-8	4	5	716	586	-5	6	5	284	221
-15	-2	5	13	28	-13	0	5	23	32	-11	2	5	292	357	-7	4	5	1161	1118	-4	6	5	1111	1083
-14	-2	5	14	25	-12	0	5	1	9	-10	2	5	459	395	-6	4	5	3138	2822	-3	6	5	-1	3
-13	-2	5	12	3	-11	0	5	21	9	-9	2	5	520	481	-5	4	5	379	395	-2	6	5	0	2
-12	-2	5	0	22	-10	0	5	925	783	-8	2	5	488	402	-4	4	5	19	46	-1	6	5	74	102
-11	-2	5	214	177	-9	0	5	54	38	-7	2	5	1817	1594	-3	4	5	314	306	0	6	5	121	141
-10	-2	5	755	661	-8	0	5	185	177	-6	2	5	8384	8033	-2	4	5	3405	3139	1	6	5	544	583
-9	-2	5	163	173	-7	0	5	721	831	-5	2	5	3822	3790	-1	4	5	767	781	2	6	5	778	814
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-7	-2	5	1442	1570	-5	0	5	2853	3017	-3	2	5	74	46	1	4	5	17	20	4	6	5	555	562
-6	-2	5	37	21	-4	0	5	73	44	-2	2	5	1546	1751	2	4	5	1257	1224	5	6	5	5	6
-5	-2	5	576	714	-3	0	5	3588	3615	-1	2	5	492	474	3	4	5	409	467	6	6	5	38	44
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-2	-2	5	342	390	0	0	5	376	380	2	2	5	135	139	6	4	5	2217	2165	9	6	5	12	2
-1	-2	5	1818	2277	1	0	5	2218	2525	3	2	5	24	10	7	4	5	2399	2181	10	6	5	294	311
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5	-2	5	94	52	7	0	5	273	358	9	2	5	185	162	13	4	5	140	139	-14	7	5	-4	9
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7	-2	5	2071	2385	9	0	5	3	5	11	2	5	211	250	-17	5	5	-16	27	-12	7	5	107	117
8	-2	5	178	144	10	0	5	63	86	12	2	5	178	164	-16	5	5	56	23	-11	7	5	31	13
9	-2	5	359	348	11	0	5	267	244	13	2	5	8	3	-15	5	5	5	1	-10	7	5	-3	2
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12	-2	5	33	15	14	0	5	56	54	-15	3	5	9	11	-12	5	5	48	35	-7	7	5	166	164
13	-2	5	86	71	15	0	5	34	18	-14	3	5	41	40	-11	5	5	22	49	-6	7	5	148	187
14	-2	5	92	99	-16	1	5	11	8	-13	3	5	27	39	-10	5	5	163	106	-5	7	5	604	532
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Table A.3, continued

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-15	-1	5	31	49	-13	1	5	7	4	-10	3	5	442	367	-7	5	5	894	818	-2	7	5	587	590
-14	-1	5	-7	6	-12	1	5	8	10	-9	3	5	8	2	-6	5	5	646	698	-1	7	5	218	240
-13	-1	5	13	14	-11	1	5	124	139	-8	3	5	338	357	-5	5	5	99	70	0	7	5	-2	1
-12	-1	5	130	134	-10	1	5	50	43	-7	3	5	4683	4249	-4	5	5	302	377	1	7	5	849	800
-11	-1	5	148	151	-9	1	5	110	74	-6	3	5	10518	9088	-3	5	5	1005	1180	2	7	5	175	134
-10	-1	5	4	3	-8	1	5	512	545	-5	3	5	3232	3057	-2	5	5	518	514	3	7	5	144	111
-9	-1	5	0	10	-7	1	5	1037	1005	-4	3	5	421	199	-1	5	5	1365	1139	4	7	5	202	162
-8	-1	5	513	532	-6	1	5	472	480	-3	3	5	1010	936	0	5	5	18	35	5	7	5	316	321
-7	-1	5	241	181	-5	1	5	96	132	-2	3	5	1261	1405	1	5	5	3627	3643	6	7	5	214	179
-6	-1	5	344	358	-4	1	5	697	757	-1	3	5	21	12	2	5	5	717	679	7	7	5	11	5
-5	-1	5	506	568	-3	1	5	2481	2501	0	3	5	157	237	3	5	5	9	6	8	7	5	22	13
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-2	-1	5	3	5	0	1	5	431	400	3	3	5	875	948	6	5	5	709	708	11	7	5	28	28
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Table A.3, continued

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13	-12	6	34	25	-10	-9	6	5	0	-7	-7	6	97	91	-5	-5	6	22	5	-4	-3	6	1429	1276
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-13	-11	6	-11	3	-8	-9	6	-1	1	-5	-7	6	331	293	-3	-5	6	361	338	-2	-3	6	1502	1649
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-11	-11	6	-7	9	-6	-9	6	580	553	-3	-7	6	59	59	-1	-5	6	553	334	0	-3	6	1805	2462
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-10	-1	6	777	781	-7	1	6	50	50	-3	3	6	9	11	2	5	6	215	230	9	7	6	127	117
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Table A.3, continued

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4	0	6	5	18	8	2	6	32	24	13	4	6	-5	10	-11	7	6	237	181	-1	9	6	309	253
5	0	6	182	177	9	2	6	117	130	-17	5	6	41	1	-10	7	6	34	55	0	9	6	24	25
6	0	6	1954	1873	10	2	6	362	319	-16	5	6	8	2	-9	7	6	348	291	1	9	6	188	138
7	0	6	4	5	11	2	6	44	66	-15	5	6	37	50	-8	7	6	48	54	2	9	6	107	91
8	0	6	52	49	12	2	6	26	12	-14	5	6	-1	1	-7	7	6	1215	1236	3	9	6	206	223
4	9	6	228	222	-5	12	6	14	3	6	15	6	2	25	-1	-15	7	15	12	-5	-12	7	-3	4
5	9	6	239	257	-4	12	6	13	14	-7	16	6	23	1	0	-15	7	1	1	-4	-12	7	170	160
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7	9	6	71	68	-2	12	6	27	25	-5	16	6	34	22	2	-15	7	14	2	-2	-12	7	5	0
8	9	6	178	163	-1	12	6	18	24	-4	16	6	-3	5	3	-15	7	-3	0	-1	-12	7	90	77
9	9	6	8	10	0	12	6	19	9	-3	16	6	44	17	4	-15	7	2	9	0	-12	7	94	85
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-9	-9	7	9	7	-5	-7	7	8	14	-3	-5	7	4	3	-1	-3	7	1057	1068	-1	-1	7	4221	3822
-8	-9	7	83	83	-4	-7	7	807	706	-2	-5	7	5	3	0	-3	7	0	1	0	-1	7	678	780
-7	-9	7	422	332	-3	-7	7	195	245	-1	-5	7	360	343	1	-3	7	833	766	1	-1	7	1171	1282
-6	-9	7	121	137	-2	-7	7	32	16	0	-5	7	239	337	2	-3	7	34	34	2	-1	7	2454	2276
-5	-9	7	174	150	-1	-7	7	472	386	1	-5	7	623	471	3	-3	7	285	318	3	-1	7	1002	869
-4	-9	7	6	1	0	-7	7	123	159	2	-5	7	75	30	4	-3	7	2218	2137	4	-1	7	39	37
-3	-9	7	160	128	1	-7	7	48	21	3	-5	7	423	299	5	-3	7	408	397	5	-1	7	200	257
-2	-9	7	46	71	2	-7	7	690	553	4	-5	7	3801	3546	6	-3	7	18	37	6	-1	7	137	153
-1	-9	7	365	322	3	-7	7	142	161	5	-5	7	652	662	7	-3	7	49	77	7	-1	7	216	212
0	-9	7	48	36	4	-7	7	594	449	6	-5	7	121	118	8	-3	7	56	40	8	-1	7	127	100
1	-9	7	252	269	5	-7	7	30	37	7	-5	7	449	398	9	-3	7	64	59	9	-1	7	277	279
2	-9	7	589	483	6	-7	7	53	51	8	-5	7	284	284	10	-3	7	1	2	10	-1	7	164	143
3	-9	7	176	179	7	-7	7	-1	7	9	-5	7	5	0	11	-3	7	65	54	11	-1	7	90	101
4	-9	7	229	213	8	-7	7	394	362	10	-5	7	498	443	12	-3	7	170	144	12	-1	7	160	159
5	-9	7	2	1	9	-7	7	142	144	11	-5	7	235	221	13	-3	7	17	27	13	-1	7	57	39
6	-9	7	90	96	10	-7	7	27	32	12	-5	7	35	19	14	-3	7	27	37	14	-1	7	19	9
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Table A.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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9	-9	7	22	21	13	-7	7	8	24	15	-5	7	8	5	-16	-2	7	-8	2	-14	0	7	38	54
10	-9	7	7	6	14	-7	7	18	37	-16	-4	7	11	1	-15	-2	7	16	20	-13	0	7	143	107
11	-9	7	1	19	15	-7	7	1	2	-15	-4	7	30	25	-14	-2	7	17	19	-12	0	7	212	220
12	-9	7	2	4	-16	-6	7	30	12	-14	-4	7	110	68	-13	-2	7	1	14	-11	0	7	30	20
13	-9	7	35	51	-15	-6	7	15	1	-13	-4	7	7	0	-12	-2	7	-8	2	-10	0	7	325	259
14	-9	7	15	14	-14	-6	7	-3	1	-12	-4	7	104	120	-11	-2	7	47	55	-9	0	7	156	113
-15	-8	7	-10	11	-13	-6	7	14	11	-11	-4	7	239	199	-10	-2	7	724	657	-8	0	7	8	11
-14	-8	7	-8	0	-12	-6	7	43	39	-10	-4	7	45	57	-9	-2	7	35	35	-7	0	7	139	203
-13	-8	7	64	52	-11	-6	7	115	95	-9	-4	7	10	11	-8	-2	7	119	104	-6	0	7	213	160
-12	-8	7	38	26	-10	-6	7	4	2	-8	-4	7	218	186	-7	-2	7	1726	1660	-5	0	7	18	43
-11	-8	7	2	6	-9	-6	7	113	83	-7	-4	7	521	518	-6	-2	7	275	267	-4	0	7	461	692
-10	-8	7	92	58	-8	-6	7	434	412	-6	-4	7	478	460	-5	-2	7	12	1	-3	0	7	681	511
-9	-8	7	98	84	-7	-6	7	4	0	-5	-4	7	49	47	-4	-2	7	1537	1652	-2	0	7	2969	3208
-8	-8	7	421	387	-6	-6	7	141	111	-4	-4	7	741	815	-3	-2	7	365	305	-1	0	7	-2	1
-7	-8	7	13	11	-5	-6	7	34	27	-3	-4	7	679	817	-2	-2	7	372	431	0	0	7	407	390
-6	-8	7	17	6	-4	-6	7	393	369	-2	-4	7	32	37	-1	-2	7	937	1266	1	0	7	4779	4600
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-4	1	7	750	911	1	3	7	782	654	7	5	7	467	482	-12	8	7	24	13	2	10	7	0	2
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8	1	7	131	156	13	3	7	33	34	-10	6	7	21	14	0	8	7	78	69	-9	11	7	0	0
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10	1	7	286	307	-15	4	7	37	13	-8	6	7	26	21	2	8	7	1972	1808	-7	11	7	7	21
11	1	7	32	33	-14	4	7	-6	3	-7	6	7	976	947	3	8	7	19	22	-6	11	7	16	20
12	1	7	21	15	-13	4	7	24	4	-6	6	7	29	33	4	8	7	227	212	-5	11	7	5	8
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-11	2	7	-4	1	-5	4	7	230	177	2	6	7	1940	1967	-15	9	7	21	7	3	11	7	80	65
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-2	2	7	2109	2032	4	4	7	74	93	11	6	7	31	14	-6	9	7	19	21	-11	12	7	-7	1
-1	2	7	809	742	5	4	7	181	152	12	6	7	16	21	-5	9	7	39	34	-10	12	7	6	5
0	2	7	24	14	6	4	7	723	626	-16	7	7	26	6	-4	9	7	22	2	-9	12	7	58	60
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2	2	7	1664	1592	8	4	7	5	3	-14	7	7	6	1	-2	9	7	274	267	-7	12	7	42	30
3	2	7	37	30	9	4	7	235	243	-13	7	7	5	15	-1	9	7	42	33	-6	12	7	61	70
4	2	7	881	876	10	4	7	68	64	-12	7	7	5	23	0	9	7	251	232	-5	12	7	138	120
5	2	7	209	238	11	4	7	41	68	-11	7	7	14	7	1	9	7	115	97	-4	12	7	43	63
6	2	7	93	125	12	4	7	21	21	-10	7	7	242	260	2	9	7	22	26	-3	12	7	9	2
7	2	7	545	568	13	4	7	41	14	-9	7	7	39	48	3	9	7	8	9	-2	12	7	121	103
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9	2	7	97	103	-15	5	7	-5	5	-7	7	7	290	251	5	9	7	206	186	0	12	7	3	0
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-10	3	7	37	26	-4	5	7	164	191	4	7	7	15	16	-9	10	7	94	62	-10	13	7	-5	5
-9	3	7	8	8	-3	5	7	433	395	5	7	7	23	13	-8	10	7	8	2	-9	13	7	24	7
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-7	3	7	533	485	-1	5	7	5	12	7	7	7	22	36	-6	10	7	175	161	-7	13	7	23	6
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Table A.3, continued

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0	13	7	94	80	4	-17	8	26	10	-3	-13	8	52	42	-12	-10	8	15	22	-3	-8	8	59	30
1	13	7	61	62	5	-17	8	-1	7	-2	-13	8	15	15	-11	-10	8	26	9	-2	-8	8	148	97
2	13	7	8	1	6	-17	8	3	0	-1	-13	8	57	35	-10	-10	8	-4	2	-1	-8	8	5	8
3	13	7	4	12	7	-17	8	29	1	0	-13	8	320	340	-9	-10	8	18	18	0	-8	8	50	20
4	13	7	17	16	8	-17	8	16	1	1	-13	8	8	16	-8	-10	8	72	47	1	-8	8	35	22
5	13	7	24	1	9	-17	8	-1	1	2	-13	8	13	19	-7	-10	8	-1	7	2	-8	8	47	66
6	13	7	45	48	10	-17	8	-2	0	3	-13	8	14	20	-6	-10	8	68	55	3	-8	8	268	242
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-9	14	7	26	7	-2	-16	8	-3	8	5	-13	8	5	7	-4	-10	8	-1	1	5	-8	8	223	214
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-7	14	7	1	0	0	-16	8	17	23	7	-13	8	32	12	-2	-10	8	59	41	7	-8	8	183	195
-6	14	7	-3	1	1	-16	8	5	7	8	-13	8	1	3	-1	-10	8	101	108	8	-8	8	188	170
-5	14	7	14	38	2	-16	8	-3	1	9	-13	8	21	20	0	-10	8	178	209	9	-8	8	105	103
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6	-18	8	1	2	12	-14	8	12	1	7	-11	8	116	91	-10	-8	8	13	33	-5	-6	8	27	42
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Table A.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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7	-5	8	186	165	11	-3	8	10	11	13	-1	8	27	19	-12	2	8	26	26	-5	4	8	3	3
8	-5	8	3	1	12	-3	8	83	72	14	-1	8	107	131	-11	2	8	255	257	-4	4	8	110	117
9	-5	8	204	187	13	-3	8	95	102	-16	0	8	0	0	-10	2	8	122	154	-3	4	8	256	229
10	-5	8	68	58	14	-3	8	20	21	-15	0	8	29	49	-9	2	8	29	31	-2	4	8	55	72
11	-5	8	5	1	-17	-2	8	49	2	-14	0	8	3	3	-8	2	8	14	2	-1	4	8	9	24
12	-5	8	124	95	-16	-2	8	7	0	-13	0	8	-2	0	-7	2	8	68	73	0	4	8	1431	1384
13	-5	8	122	121	-15	-2	8	62	29	-12	0	8	95	108	-6	2	8	58	51	1	4	8	1003	984
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-6	-12	9	-2	3	9	-10	9	0	0	-11	-7	9	85	83	-6	-5	9	164	145	-3	-3	9	1190	1098
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Table A.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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-3	-12	9	34	24	12	-10	9	2	13	-8	-7	9	10	2	-3	-5	9	44	58	0	-3	9	36	22
-2	-12	9	14	7	13	-10	9	30	1	-7	-7	9	81	71	-2	-5	9	1164	1033	1	-3	9	342	311
-1	-12	9	130	132	-13	-9	9	40	4	-6	-7	9	51	60	-1	-5	9	14	12	2	-3	9	613	679
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1	-12	9	6	6	-11	-9	9	21	34	-4	-7	9	256	232	1	-5	9	842	655	4	-3	9	497	522
2	-12	9	86	65	-10	-9	9	27	10	-3	-7	9	105	128	2	-5	9	243	200	5	-3	9	156	139
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4	-12	9	22	8	-8	-9	9	23	25	-1	-7	9	208	154	4	-5	9	83	84	7	-3	9	97	132
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-5	0	9	100	122	1	2	9	188	177	9	4	9	121	107	-6	7	9	213	209	-12	10	9	24	14
-4	0	9	488	528	2	2	9	576	646	10	4	9	20	16	-5	7	9	92	77	-11	10	9	19	6
-3	0	9	144	122	3	2	9	11	22	11	4	9	20	5	-4	7	9	10	20	-10	10	9	30	36
-2	0	9	17	55	4	2	9	336	310	-16	5	9	-16	1	-3	7	9	121	119	-9	10	9	37	41
-1	0	9	72	93	5	2	9	376	365	-15	5	9	28	2	-2	7	9	1102	1038	-8	10	9	4	13
0	0	9	332	405	6	2	9	124	127	-14	5	9	115	98	-1	7	9	8	5	-7	10	9	2	4
1	0	9	676	660	7	2	9	305	306	-13	5	9	39	27	0	7	9	88	55	-6	10	9	3	4
2	0	9	47	54	8	2	9	698	599	-12	5	9	29	27	1	7	9	1048	950	-5	10	9	8	5
3	0	9	312	285	9	2	9	402	413	-11	5	9	6	1	2	7	9	113	110	-4	10	9	4	9
4	0	9	1127	1140	10	2	9	97	69	-10	5	9	238	205	3	7	9	182	169	-3	10	9	152	151
5	0	9	12	16	11	2	9	151	129	-9	5	9	105	141	4	7	9	214	213	-2	10	9	63	50
6	0	9	28	13	12	2	9	147	137	-8	5	9	63	42	5	7	9	164	163	-1	10	9	30	22
7	0	9	170	178	-16	3	9	-10	7	-7	5	9	1203	1031	6	7	9	9	0	0	10	9	67	73
8	0	9	114	68	-15	3	9	13	5	-6	5	9	21	27	7	7	9	145	148	1	10	9	178	164
9	0	9	102	139	-14	3	9	52	37	-5	5	9	11	12	8	7	9	189	156	2	10	9	27	32
10	0	9	143	144	-13	3	9	11	1	-4	5	9	242	214	9	7	9	74	64	3	10	9	37	31

Table A.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
11	0	9	133	125	-12	3	9	8	18	-3	5	9	351	301	10	7	9	24	13	4	10	9	65	38
12	0	9	12	10	-11	3	9	315	314	-2	5	9	356	356	-15	8	9	-13	5	5	10	9	27	40
13	0	9	-9	15	-10	3	9	239	197	-1	5	9	11	1	-14	8	9	13	1	6	10	9	-4	2
-16	1	9	14	4	-9	3	9	74	79	0	5	9	96	104	-13	8	9	15	0	7	10	9	0	41
-15	1	9	70	73	-8	3	9	190	147	1	5	9	633	568	-12	8	9	-6	1	-13	11	9	-4	10
-14	1	9	43	58	-7	3	9	629	587	2	5	9	490	480	-11	8	9	2	10	-12	11	9	-15	2
-13	1	9	-5	12	-6	3	9	21	4	3	5	9	14	32	-10	8	9	53	76	-11	11	9	23	11
-12	1	9	27	4	-5	3	9	34	38	4	5	9	197	155	-9	8	9	9	7	-10	11	9	21	1
-11	1	9	125	124	-4	3	9	692	561	5	5	9	8	1	-8	8	9	24	54	-9	11	9	17	6
-10	1	9	49	36	-3	3	9	60	63	6	5	9	6	1	-7	8	9	161	130	-8	11	9	23	31
-9	1	9	7	0	-2	3	9	-2	1	7	5	9	458	429	-6	8	9	84	82	-7	11	9	2	0
-8	1	9	91	115	-1	3	9	170	176	8	5	9	54	46	-5	8	9	27	17	-6	11	9	4	5
-7	1	9	20	18	0	3	9	212	284	9	5	9	-1	7	-4	8	9	19	21	-5	11	9	108	80
-6	1	9	7	17	1	3	9	17	15	10	5	9	30	39	-3	8	9	230	210	-4	11	9	188	179
-5	1	9	1813	1559	2	3	9	799	741	11	5	9	38	26	-2	8	9	13	3	-3	11	9	4	11
-2	11	9	89	82	-1	15	9	-14	2	10	-14	10	18	20	13	-11	10	-19	2	2	-8	10	1	1
-1	11	9	222	201	0	15	9	120	12	11	-14	10	-16	2	-11	-10	10	3	6	3	-8	10	139	124
0	11	9	35	36	1	15	9	57	8	-6	-13	10	-11	17	-10	-10	10	-3	0	4	-8	10	6	4
1	11	9	-1	1	2	15	9	-19	0	-5	-13	10	68	24	-9	-10	10	35	27	5	-8	10	136	148
2	11	9	29	40	3	15	9	-14	3	-4	-13	10	-8	2	-8	-10	10	8	11	6	-8	10	392	357
3	11	9	69	70	4	15	9	51	12	-3	-13	10	-3	1	-7	-10	10	-2	2	7	-8	10	80	70
4	11	9	25	26	-3	16	9	-18	5	-2	-13	10	1	1	-6	-10	10	-10	3	8	-8	10	14	9
5	11	9	25	1	-2	16	9	33	0	-1	-13	10	8	2	-5	-10	10	2	13	9	-8	10	177	139
6	11	9	10	30	-1	16	9	42	1	0	-13	10	-1	1	-4	-10	10	10	30	10	-8	10	46	51
7	11	9	40	10	0	16	9	-19	1	1	-13	10	62	62	-3	-10	10	7	29	11	-8	10	0	4
-11	12	9	1	3	-1	-18	10	-11	0	2	-13	10	31	35	-2	-10	10	295	264	12	-8	10	25	17
-10	12	9	-5	1	0	-18	10	3	0	3	-13	10	14	12	-1	-10	10	351	320	13	-8	10	13	32
-9	12	9	-6	2	1	-18	10	-7	0	4	-13	10	1	1	0	-10	10	19	11	-14	-7	10	6	1
-8	12	9	8	2	2	-18	10	-8	0	5	-13	10	8	0	1	-10	10	231	175	-13	-7	10	-6	10
-7	12	9	32	23	3	-18	10	21	1	6	-13	10	11	12	2	-10	10	251	284	-12	-7	10	25	21
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1	12	9	49	40	2	-17	10	54	16	-7	-12	10	23	22	10	-10	10	40	50	-4	-7	10	130	137
2	12	9	31	33	3	-17	10	12	1	-6	-12	10	39	76	11	-10	10	-4	0	-3	-7	10	203	197
3	12	9	2	6	4	-17	10	3	0	-5	-12	10	-8	0	12	-10	10	18	10	-2	-7	10	244	257
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5	12	9	-5	3	6	-17	10	112	0	-3	-12	10	54	52	-12	-9	10	22	2	0	-7	10	48	23
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-9	13	9	40	1	0	-16	10	44	70	0	-12	10	9	2	-9	-9	10	47	55	3	-7	10	106	113
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-1	13	9	2	15	8	-16	10	3	3	8	-12	10	5	12	0	-9	10	137	152	11	-7	10	114	97
0	13	9	42	50	9	-16	10	15	4	9	-12	10	4	8	1	-9	10	62	59	12	-7	10	94	85
1	13	9	20	26	-2	-15	10	5	21	10	-12	10	18	16	2	-9	10	79	84	13	-7	10	-5	8
2	13	9	13	5	-1	-15	10	28	28	11	-12	10	13	5	3	-9	10	58	50	-14	-6	10	2	11
3	13	9	79	52	0	-15	10	0	0	12	-12	10	42	2	4	-9	10	209	158	-13	-6	10	1	1
4	13	9	27	15	1	-15	10	56	58	13	-12	10	-7	1	5	-9	10	121	124	-12	-6	10	-4	10
5	13	9	23	5	2	-15	10	37	29	-10	-11	10	2	21	6	-9	10	8	9	-11	-6	10	7	1
6	13	9	33	7	3	-15	10	3	5	-9	-11	10	2	0	7	-9	10	77	72	-10	-6	10	-3	4
-9	14	9	5	4	4	-15	10	5	1	-8	-11	10	33	28	8	-9	10	24	26	-9	-6	10	46	48
-8	14	9	7	6	5	-15	10	9	11	-7	-11	10	14	15	9	-9	10	4	9	-8	-6	10	198	198
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-6	14	9	-15	0	7	-15	10	-3	0	-5	-11	10	-1	18	11	-9	10	125	132	-6	-6	10	34	46
-5	14	9	46	6	8	-15	10	12	7	-4	-11	10	22	32	12	-9	10	27	35	-5	-6	10	31	28
-4	14	9	0	3	9	-15	10	2	14	-3	-11	10	32	70	13	-9	10	48	0	-4	-6	10	67	46
-3	14	9	-8	8	10	-15	10	-2	2	-2	-11	10	-1	4	-13	-8	10	-7	0	-3	-6	10	378	305
-2	14	9	38	57	-4	-14	10	-14	0	-1	-11	10	21	3	-12	-8	10	5	14	-2	-6	10	40	33
-1	14	9	12	33	-3	-14	10	26	22	0	-11	10	2	2	-11	-8	10	-4	17	-1	-6	10	83	101
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1	14	9	62	15	-1	-14	10	-7	1	2	-11	10	89	91	-9	-8	10	18	16	1	-6	10	30	69
2	14	9	29	11	0	-14	10	106	99	3	-11	10	110	117	-8	-8	10	-2	3	2	-6	10	375	329
3	14	9	22	6	1	-14	10	15	17	4	-11	10	5	10	-7	-8	10	18	9	3	-6	10	93	115
4	14	9	14	1	2	-14	10	9	0	5	-11	10	6	4	-6	-8	10	28	38	4	-6	10	1335	1275
5	14	9	-2	4	3	-14	10	12	13	6	-11	10	156	156	-5	-8	10	344	274	5	-6	10	623	618
-7	15	9	-14	1	4	-14	10	1	7	7	-11	10	25	19	-4	-8	10	187	164	6	-6	10	994	932
-6	15	9	-1	2	5	-14	10	14	8	8	-11	10	2	0	-3	-8	10	-6	0	7	-6	10	202	206
-5	15	9	-11	0	6	-14	10	5	2	9	-11	10	8	6	-2	-8	10	260	274	8	-6	10	39	29
-4	15	9	7	6	7	-14	10	-3	2	10	-11	10	5	7	-1	-8	10	274	228	9	-6	10	18	13
-3	15	9	16	19	8	-14	10	-4	6	11	-11	10	31	27	0	-8	10	60	59	10	-6	10	46	53
-2	15	9	24	8	9	-14	10	13	10	12	-11	10	28	7	1	-8	10	26	43	11	-6	10	16	26
12	-6	10	-3	0	-11	-3	10	213	162	-5	-1	10	239	211	1	1	10	317	413	9	3	10	41	42
13	-6	10	-12	1	-10	-3	10	-4	2	-4	-1	10	346	313	2	1	10	1436	1285	10	3	10	8	4
-15	-5	10	25	11	-9	-3	10	37	36	-3	-1	10	492	574	3	1	10	1026	1014	11	3	10	37	21
-14	-5	10	8	1	-8	-3	10	305	291	-2	-1	10	302	281	4	1	10	138	151	-15	4	10	4	19
-13	-5	10	16	0	-7	-3	10	274	247	-1	-1	10	-2	1	5	1	10	296	265	-14	4	10	165	146
-12	-5	10	13	15	-6	-3	10	8	3	0	-1	10	528	468	6	1	10	114	141	-13	4	10	14	10
-11	-5	10	32	37	-5	-3	10	161	167	1	-1	10	119	162	7	1	10	97	82	-12	4	10	-5	0
-10	-5	10	23	14	-4	-3	10	313	307	2	-1	10	26	47	8	1	10	769	707	-11	4	10	47	27
-9	-5	10	107	88	-3	-3	10	0	1	3	-1	10	836	808	9	1	10	83	91	-10	4	10	54	39
-8	-5	10	174	177	-2	-3	10	2252	2376	4	-1	10	444	359	10	1	10	149	131	-9	4	10	0	0
-7	-5	10	54	59	-1	-3	10	746	688	5	-1	10	199	257	11	1	10	130	107	-8	4	10	269	250
-6	-5	10	238	216	0	-3	10	1018	1041	6	-1	10	570	594	12	1	10	19	35	-7	4	10	281	326
-5	-5	10	161	192	1	-3	10	1	0	7	-1	10	112	73	-16	2	10	25	1	-6	4	10	-4	1
-4	-5	10	480	478	2	-3	10	545	600	8	-1	10	7	14	-15	2	10	10	17	-5	4	10	92	107
-3	-5	10	61	57	3	-3	10	1069	977	9	-1	10	44	48	-14	2	10	62	32	-4	4	10	245	264
-2	-5	10	831	790	4	-3	10	165	144	10	-1	10	190	153	-13	2	10	1	1	-3	4	10	113	100
-1	-5	10	957	816	5	-3	10	29	14	11	-1	10	43	38	-12	2	10	41	47	-2	4	10	11	3
0	-5	10	4	1	6	-3	10	200	177	12	-1	10	0	0	-11	2	10	82	81	-1	4	10	91	115
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2	-5	10	273	240	8	-3	10	0	1	-16	0	10	19	8	-9	2	10	48	34	1	4	10	7	1
3	-5	10	27	27	9	-3	10	52	47	-15	0	10	56	37	-8	2	10	349	318	2	4	10	1504	1437
4	-5	10	250	271	10	-3	10	259	284	-14	0	10	18	24	-7	2	10	1395	1358	3	4	10	72	67
5	-5	10	378	403	11	-3	10	53	43	-13	0	10	14	4	-6	2	10	119	49	4	4	10	8	5

Table A.3, continued

H K L	Obs	Calc	H K L	Obs	Calc	H K L	Obs	Calc	H K L	Obs	Calc	H K L	Obs	Calc
6 -5 10	436	372	12 -3 10	72	63	-12 0 10	43	22	-5 2 10	359	343	5 4 10	-1	1
7 -5 10	19	12	13 -3 10	91	49	-11 0 10	66	29	-4 2 10	598	635	6 4 10	226	178
8 -5 10	133	125	-16 -2 10	24	3	-10 0 10	56	35	-3 2 10	91	69	7 4 10	113	108
9 -5 10	78	67	-15 -2 10	-9	9	-9 0 10	8	1	-2 2 10	-2	1	8 4 10	44	44
10 -5 10	19	31	-14 -2 10	24	8	-8 0 10	123	132	-1 2 10	27	49	9 4 10	60	66
11 -5 10	35	38	-13 -2 10	29	26	-7 0 10	357	385	0 2 10	5	2	10 4 10	75	65
12 -5 10	50	45	-12 -2 10	36	22	-6 0 10	117	125	1 2 10	-1	0	-15 5 10	28	12
13 -5 10	-1	2	-11 -2 10	17	28	-5 0 10	161	140	2 2 10	1153	1232	-14 5 10	23	4
-16 -4 10	25	0	-10 -2 10	73	65	-4 0 10	1043	1099	3 2 10	1079	971	-13 5 10	75	90
-15 -4 10	8	5	-9 -2 10	84	84	-3 0 10	1	0	4 2 10	372	439	-12 5 10	91	92
-14 -4 10	27	33	-8 -2 10	45	81	-2 0 10	563	525	5 2 10	8	18	-11 5 10	131	118
-13 -4 10	-3	17	-7 -2 10	12	11	-1 0 10	548	553	6 2 10	453	415	-10 5 10	55	72
-12 -4 10	98	94	-6 -2 10	519	523	0 0 10	170	167	7 2 10	243	224	-9 5 10	-4	1
-11 -4 10	41	30	-5 -2 10	18	34	1 0 10	40	49	8 2 10	1	0	-8 5 10	98	57
-10 -4 10	133	126	-4 -2 10	29	27	2 0 10	725	742	9 2 10	338	314	-7 5 10	47	25
-9 -4 10	70	71	-3 -2 10	1452	1386	3 0 10	217	210	10 2 10	165	164	-6 5 10	127	106
-8 -4 10	5	5	-2 -2 10	18	12	4 0 10	11	15	11 2 10	79	89	-5 5 10	177	153
-7 -4 10	171	153	-1 -2 10	10	10	5 0 10	158	122	12 2 10	83	7	-4 5 10	15	19
-6 -4 10	192	179	0 -2 10	3	1	6 0 10	67	52	-16 3 10	12	6	-3 5 10	129	131
-5 -4 10	79	72	1 -2 10	997	1031	7 0 10	35	19	-15 3 10	-7	3	-2 5 10	559	585
-4 -4 10	9	6	2 -2 10	369	395	8 0 10	30	48	-14 3 10	26	15	-1 5 10	894	780
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Table A.3, continued

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3	3	11	7	6	-9	6	11	62	46	-10	9	11	40	1	4	12	11	-13	4	2	-14	12	9	2
4	3	11	501	465	-8	6	11	133	119	-9	9	11	17	7	5	12	11	52	8	3	-14	12	23	21
5	3	11	147	102	-7	6	11	-5	2	-8	9	11	4	17	-9	13	11	3	11	4	-14	12	9	13
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-1	4	11	14	21	-10	7	11	130	104	-6	10	11	18	8	0	14	11	9	0	-5	-12	12	16	16
0	4	11	-1	0	-9	7	11	34	34	-5	10	11	5	3	1	14	11	-3	0	-4	-12	12	-5	0
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Table A.3, continued

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4	4	11	126	125	-5	7	11	221	208	-1	10	11	37	22	-3	15	11	41	7	0	-12	12	8	16
5	4	11	286	262	-4	7	11	20	20	0	10	11	164	138	-2	15	11	97	4	1	-12	12	8	0
6	4	11	47	41	-3	7	11	305	289	1	10	11	145	148	-1	15	11	-10	1	2	-12	12	-4	1
7	4	11	66	59	-2	7	11	365	359	2	10	11	0	6	0	15	11	49	1	3	-12	12	10	11
8	4	11	169	156	-1	7	11	110	96	3	10	11	114	104	1	15	11	61	4	4	-12	12	32	29
9	4	11	125	129	0	7	11	-3	1	4	10	11	112	106	2	-18	12	-5	1	5	-12	12	26	32
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12	-10	12	-7	10	4	-7	12	62	46	-12	-4	12	20	9	-3	-2	12	539	570	5	0	12	114	115
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-8	-9	12	1	3	7	-7	12	53	67	-9	-4	12	3	0	0	-2	12	37	27	8	0	12	40	46
-7	-9	12	36	5	8	-7	12	64	58	-8	-4	12	-2	0	1	-2	12	43	53	9	0	12	49	75
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9	-9	12	3	0	-3	-6	12	55	65	8	-4	12	90	78	-12	-1	12	0	10	-3	1	12	323	292
10	-9	12	10	1	-2	-6	12	415	416	9	-4	12	32	20	-11	-1	12	96	76	-2	1	12	46	60
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12	-9	12	16	13	0	-6	12	83	71	11	-4	12	30	25	-9	-1	12	12	1	0	1	12	464	361
13	-9	12	32	6	1	-6	12	10	19	12	-4	12	9	8	-8	-1	12	43	38	1	1	12	269	322
-11	-8	12	-1	4	2	-6	12	20	32	-15	-3	12	33	14	-7	-1	12	841	866	2	1	12	832	888
-10	-8	12	15	5	3	-6	12	435	385	-14	-3	12	0	0	-6	-1	12	7	0	3	1	12	779	717
-9	-8	12	46	37	4	-6	12	35	30	-13	-3	12	-6	3	-5	-1	12	345	302	4	1	12	18	9
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-7	-8	12	42	18	6	-6	12	226	193	-11	-3	12	37	58	-3	-1	12	37	48	6	1	12	100	110
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2	-8	12	156	166	-13	-5	12	-5	0	-2	-3	12	302	309	6	-1	12	539	581	-12	2	12	54	14
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4	-8	12	1	0	-11	-5	12	0	1	0	-3	12	51	72	8	-1	12	-5	4	-10	2	12	0	6
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8	-8	12	40	52	-7	-5	12	9	7	4	-3	12	-3	7	12	-1	12	31	10	-6	2	12	13	18
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Table A.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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2	2	12	33	24	-9	5	12	74	58	-11	8	12	-7	2	2	11	12	1	3	0	-13	13	34	28
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Table A.3, continued

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Table A.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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7	-5	14	4	0	-3	-2	14	55	77	10	0	14	-10	0	0	3	14	324	275	0	6	14	163	159
8	-5	14	95	80	-2	-2	14	102	97	-15	1	14	-6	0	1	3	14	204	200	1	6	14	136	133
9	-5	14	65	94	-1	-2	14	18	18	-14	1	14	15	2	2	3	14	-1	4	2	6	14	8	4
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0	-13	15	5	7	6	-8	15	-2	3	9	-5	15	32	29	6	-2	15	68	68	2	1	15	1	19

Table A.3, continued

H K L	Obs	Calc	H K L	Obs	Calc	H K L	Obs	Calc	H K L	Obs	Calc	H K L	Obs	Calc
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-4-12 15	-11	2	9 -8 15	-7	0	-10 -4 15	-4	5	9 -2 15	-4	3	5 1 15	78	60
-3-12 15	-3	0	10 -8 15	15	12	-9 -4 15	38	31	10 -2 15	-3	2	6 1 15	61	85
-2-12 15	14	29	-9 -7 15	-2	4	-8 -4 15	127	128	-12 -1 15	18	0	7 1 15	21	32
-1-12 15	38	35	-8 -7 15	-7	2	-7 -4 15	-1	1	-11 -1 16	6	5	8 1 15	68	41
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1-12 15	19	0	-6 -7 15	1	0	-5 -4 15	113	106	-9 -1 15	37	33	-13 2 15	-15	5
2-12 15	8	5	-5 -7 15	111	92	-4 -4 15	0	0	-8 -1 15	19	13	-12 2 15	-5	0
-6-11 15	41	4	-4 -7 15	64	60	-3 -4 15	3	8	-7 -1 15	41	41	-11 2 15	-1	6
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9 -2 16	13	12	-11 2 16	16	20	-5 5 16	25	22	-2 10 16	0	15	-7 -5 17	2	13
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-5 -1 16	35	41	-3 2 16	50	47	3 5 16	-13	0	-2-11 17	-12	9	1 -5 17	11	8
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-1 -1 16	67	49	1 2 16	59	70	-10 6 16	20	21	-3-10 17	4	1	5 -5 17	4	30
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2 -1 16	110	103	4 2 16	16	4	-7 6 16	33	13	-7 -9 17	-13	7	8 -5 17	-9	0
3 -1 16	77	95	5 2 16	39	32	-6 6 16	-7	6	-6 -9 17	7	3	-9 -4 17	70	5
4 -1 16	20	19	6 2 16	9	0	-5 6 16	4	7	-5 -9 17	22	0	-8 -4 17	55	8
5 -1 16	34	24	7 2 16	-1	0	-4 6 16	83	66	-4 -9 17	-10	8	-7 -4 17	4	0
6 -1 16	118	120	8 2 16	74	12	-3 6 16	67	47	-3 -9 17	25	19	-6 -4 17	8	3

Table A.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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8	-1	16	17	4	-11	3	16	-6	0	-1	6	16	38	32	-1	-9	17	11	1	-4	-4	17	7	9
9	-1	16	6	22	-10	3	16	29	19	0	6	16	-1	5	0	-9	17	5	4	-3	-4	17	14	13
-11	0	16	-2	3	-9	3	16	60	39	1	6	16	0	2	-7	-8	17	8	35	-2	-4	17	55	53
-10	0	16	1	19	-8	3	16	-3	2	2	6	16	2	1	-6	-8	17	8	2	-1	-4	17	3	0
-9	0	16	28	18	-7	3	16	11	12	3	6	16	74	51	-5	-8	17	-9	5	0	-4	17	-1	0
-8	0	16	-6	0	-6	3	16	20	15	4	6	16	5	27	-4	-8	17	22	14	1	-4	17	63	57
-7	0	16	18	1	-5	3	16	5	1	-11	7	16	12	15	-3	-8	17	15	18	2	-4	17	69	67
-6	0	16	13	19	-4	3	16	67	56	-10	7	16	-13	1	-2	-8	17	-6	0	3	-4	17	72	44
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-4	0	16	21	35	-2	3	16	29	30	-8	7	16	12	5	0	-8	17	5	9	5	-4	17	13	21
-3	0	16	69	66	-1	3	16	33	39	-7	7	16	4	2	1	-8	17	9	5	6	-4	17	70	34
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1	0	16	64	110	3	3	16	67	59	-3	7	16	19	7	-5	-7	17	23	43	-8	-3	17	3	7
2	0	16	82	48	4	3	16	69	60	-2	7	16	39	35	-4	-7	17	32	12	-7	-3	17	7	9
3	0	16	8	0	5	3	16	14	26	-1	7	16	38	44	-3	-7	17	0	0	-6	-3	17	-1	1
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9	0	16	33	3	-9	4	16	-5	2	-8	8	16	3	0	3	-7	17	26	31	0	-3	17	77	68
-12	1	16	-9	20	-8	4	16	18	4	-7	8	16	31	5	4	-7	17	11	9	1	-3	17	21	27
-11	1	16	-1	20	-7	4	16	0	0	-6	8	16	4	9	5	-7	17	25	13	2	-3	17	7	0
-10	1	16	14	15	-6	4	16	9	0	-5	8	16	8	15	6	-7	17	26	9	3	-3	17	0	16
-9	1	16	16	0	-5	4	16	-5	3	-4	8	16	-6	10	-8	-6	17	26	8	4	-3	17	5	11
-8	1	16	13	24	-4	4	16	-4	12	-3	8	16	19	20	-7	-6	17	74	63	5	-3	17	12	0
-7	1	16	29	20	-3	4	16	0	1	-2	8	16	8	19	-6	-6	17	27	40	6	-3	17	8	3
-6	1	16	8	14	-2	4	16	9	4	-1	8	16	24	0	-5	-6	17	16	4	7	-3	17	23	14
-5	1	16	19	12	-1	4	16	80	87	0	8	16	12	11	-4	-6	17	9	13	8	-3	17	-1	9
-4	1	16	87	81	0	4	16	64	50	-9	9	16	15	3	-3	-6	17	19	21	9	-3	17	4	12
-3	1	16	47	46	1	4	16	-3	0	-8	9	16	-12	14	-2	-6	17	46	52	-9	-2	17	14	12
-2	1	16	-3	0	2	4	16	29	25	-7	9	16	18	30	-1	-6	17	17	3	-8	-2	17	36	33
-1	1	16	85	87	3	4	16	26	51	-6	9	16	59	69	0	-6	17	3	8	-7	-2	17	5	2
0	1	16	37	39	4	4	16	27	2	-5	9	16	-1	18	1	-6	17	49	55	-6	-2	17	0	0
1	1	16	-4	1	5	4	16	11	5	-4	9	16	2	0	2	-6	17	27	40	-5	-2	17	4	5
2	1	16	26	46	6	4	16	-9	9	-2	9	16	31	12	3	-6	17	27	3	-4	-2	17	-3	1
3	1	16	133	127	-12	5	16	59	0	-1	9	16	11	19	4	-6	17	-4	0	-3	-2	17	9	9
4	1	16	49	59	-11	5	16	9	0	-8	10	16	10	1	5	-6	17	22	0	-2	-2	17	164	144
-1	-2	17	105	95	6	1	17	-9	5	-3	5	17	28	18	-2	-6	18	-5	6	-4	-1	18	79	78
0	-2	17	3	7	7	1	17	9	2	-2	5	17	22	0	-8	-5	18	9	0	-3	-1	18	0	0
1	-2	17	19	18	-12	2	17	27	0	-1	5	17	18	10	-7	-5	18	10	3	-2	-1	18	2	1
2	-2	17	42	30	-11	2	17	-4	5	0	5	17	17	0	-6	-5	18	30	16	-1	-1	18	56	51
3	-2	17	41	35	-10	2	17	54	44	1	5	17	-4	0	-5	-5	18	0	1	0	-1	18	21	9
4	-2	17	9	1	-9	2	17	34	20	2	5	17	45	6	-4	-5	18	-8	1	1	-1	18	-4	2
5	-2	17	30	16	-8	2	17	26	10	3	5	17	55	40	-3	-5	18	14	3	2	-1	18	40	21
6	-2	17	40	49	-7	2	17	12	14	4	5	17	47	1	-2	-5	18	24	22	3	-1	18	39	36
7	-2	17	8	9	-6	2	17	7	9	-11	6	17	0	10	-1	-5	18	2	2	4	-1	18	18	6
8	-2	17	4	15	-5	2	17	12	0	-10	6	17	-2	1	0	-5	18	26	25	5	-1	18	-4	21
9	-2	17	20	28	-4	2	17	38	30	-9	6	17	-1	0	1	-5	18	38	50	6	-1	18	10	4
-10	-1	17	-8	2	-3	2	17	34	34	-8	6	17	6	0	2	-5	18	33	50	7	-1	18	-11	23
-9	-1	17	3	2	-2	2	17	7	6	-7	6	17	10	0	3	-5	18	19	5	-8	0	18	9	0
-8	-1	17	3	4	-1	2	17	67	80	-6	6	17	5	2	4	-5	18	-2	3	-7	0	18	9	9
-7	-1	17	4	3	0	2	17	260	234	-5	6	17	-1	1	5	-5	18	35	29	-6	0	18	12	17
-6	-1	17	-2	2	1	2	17	58	38	-4	6	17	0	6	-8	-4	18	11	13	-5	0	18	8	15
-5	-1	17	16	21	2	2	17	-1	0	-3	6	17	-1	8	-7	-4	18	-1	0	-4	0	18	3	3
-4	-1	17	144	148	3	2	17	27	40	-2	6	17	45	32	-6	-4	18	16	6	-3	0	18	0	5
-3	-1	17	179	189	4	2	17	5	23	-1	6	17	-4	4	-5	-4	18	30	21	-2	0	18	12	4
-2	-1	17	50	49	5	2	17	18	10	0	6	17	18	3	-4	-4	18	45	38	-1	0	18	3	3
-1	-1	17	5	3	6	2	17	8	3	1	6	17	-11	7	-3	-4	18	67	63	0	0	18	36	33
0	-1	17	33	39	7	2	17	6	32	2	6	17	22	48	-2	-4	18	12	4	1	0	18	19	24
1	-1	17	43	31	-12	3	17	20	3	-10	7	17	19	3	-1	-4	18	13	17	2	0	18	6	21
2	-1	17	10	0	-11	3	17	11	16	-9	7	17	26	1	0	-4	18	43	35	3	0	18	-11	6
3	-1	17	6	1	-10	3	17	-6	1	-8	7	17	20	8	1	-4	18	6	7	4	0	18	72	57
4	-1	17	15	23	-9	3	17	11	26	-7	7	17	16	21	2	-4	18	55	19	5	0	18	27	19
5	-1	17	12	8	-8	3	17	24	12	-6	7	17	11	33	3	-4	18	45	24	6	0	18	23	2
6	-1	17	5	14	-7	3	17	14	1	-5	7	17	30	9	4	-4	18	11	4	7	0	18	28	22
7	-1	17	9	5	-6	3	17	14	5	-4	7	17	7	23	5	-4	18	-6	1	-12	1	18	-15	8
8	-1	17	15	2	-5	3	17	27	18	-3	7	17	26	34	6	-4	18	64	46	-11	1	18	-7	13
-10	0	17	-7	2	-4	3	17	-3	0	-2	7	17	-3	5	7	-4	18	-8	7	-10	1	18	23	28
-9	0	17	-7	1	-3	3	17	-3	4	-1	7	17	0	12	-7	-3	18	4	0	-9	1	18	8	0
-8	0	17	20	19	-2	3	17	28	15	0	7	17	-13	22	-6	-3	18	-10	0	-8	1	18	11	7
-7	0	17	11	5	-1	3	17	36	35	-9	8	17	1	11	-5	-3	18	6	0	-7	1	18	24	6
-6	0	17	9	3	0	3	17	2	0	-8	8	17	-7	12	-4	-3	18	0	0	-6	1	18	24	16
-5	0	17	56	46	1	3	17	62	35	-7	8	17	13	14	-3	-3	18	39	45	-5	1	18	7	4
-4	0	17	108	102	2	3	17	33	34	-6	8	17	34	8	-2	-3	18	49	42	-4	1	18	16	7
-3	0	17	15	14	3	3	17	17	26	-5	8	17	61	25	-1	-3	18	42	29	-3	1	18	-4	0
-2	0	17	-2	2	4	3	17	9	7	-4	8	17	9	5	0	-3	18	1	2	-2	1	18	7	6
-1	0	17	60	52	5	3	17	18	23	-3	8	17	-5	0	1	-3	18	13	16	-1	1	18	55	62
0	0	17	45	37	6	3	17	25	29	-8	9	17	-12	0	2	-3	18	46	45	0	1	18	23	53
1	0	17	0	0	-11	4	17	3	3	-7	9	17	14	8	3	-3	18	-9	8	1	1	18	10	1
2	0	17	31	28	-10	4	17	23	26	-6	9	17	43	37	4	-3	18	-4	0	2	1	18	4	3
3	0	17	84	104	-9	4	17	17	0	-5	9	17	-7	2	5	-3	18	14	20	3	1	18	27	33
4	0	17	21	9	-8	4	17	11	3	-4	9	17	53	29	6	-3	18	0	8	4	1	18	1	14
5	0	17	13	28	-7	4	17	0	6	-6	10	17	0	2	7	-3	18	32	28	5	1	18	0	2
6	0	17	9	22	-6	4	17	19	37	-6	-9	18	9	0	8	-3	18	28	15	6	1	18	47	7
7	0	17	11	20	-5	4	17	5	4	-5	-9	18	-10	2	-7	-2	18	2	0	-11	2	18	-10	6
8	0	17	33	32	-4	4	17	9	16	-4	-9	18	38	1	-6	-2	18	14	6	-10	2	18	8	7
-11	1	17	-12	7	-3	4	17	34	42	-7	-8	18	25	10	-5	-2	18	93	88	-9	2	18	46	28
-10	1	17	4	2	-2	4	17	7	8	-6	-8	18	16	26	-4	-2	18	270	270	-8	2	18	8	4
-9	1	17	8	6	-1	4	17	33	12	-5	-8	18	9	2	-3	-2	18	149	152	-7	2	18	20	8
-8	1	17	-5	0	0	4	17	37	38	-4	-8	18	10	3	-2	-2	18	10	14	-6	2	18	16	2
-7	1	17	12	2	1	4	17	-3	3	-3	-8	18	28	11	-1	-2	18	25	30	-5	2	18	5	10
-6	1	17	11	5	2	4	17	-1	8	-7	-7	18	-14	21	0	-2	18	38	39	-4	2	18	-5	0
-5	1	17	28	17	3	4	17	13	4	-6	-7	18	30	12	1	-2	18	15	2	-3	2	18	19	27
-4	1	17	6	3	4	4	17	30	60	-5	-7	18	-9	1	2	-2	18	-5	1	-2	2	18	29	25
-3	1	17	29	26	5	4	17	14	12	-4	-7	18	2	7	3	-2	18	33	10	-1	2	18	21	12
-2	1	17	39	45	-11	5	17	27	16	-3	-7	18	21	18	4	-2	18	2	4	0	2	18	32	50
-1	1	17	6	1	-10	5	17	2	5	-2	-7	18	-7	5	5	-2	18	24	0	1	2	18	37	25
0	1	17	51	57	-9	5	17	8	2	-8	-6	18	2	7	6	-2	18	28	12	2	2	18	50	20
1	1	17	150	115	-8	5	17	-7	0	-7	-6	18	-4	8	7	-2	18	-8	0	3	2	18	15	14
2	1	17	54	56	-7	5	17	5	5	-6	-6	18	40	4	8	-2	18	1	1	4	2	18	47	16

Table A.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
3	1	17	18	11	-6	5	17	-5	0	-5	-6	18	0	19	-7	-1	18	-5	0	5	2	18	54	46
4	1	17	56	37	-5	5	17	17	6	-4	-6	18	-8	7	-6	-1	18	48	29	6	2	18	-13	20
5	1	17	50	47	-4	5	17	5	20	-3	-6	18	9	16	-5	-1	18	96	107	-11	3	18	-17	1
-10	3	18	-1	16	-7	-4	19	34	5	4	1	19	19	26	-7	0	20	45	34					
-9	3	18	16	3	-7	-3	19	11	2	5	1	19	23	4	-6	0	20	19	29					
-8	3	18	14	5	-6	-3	19	-5	4	-11	2	19	-18	2	-10	1	20	-15	1					
-7	3	18	22	11	-3	-3	19	16	13	-10	2	19	-14	5	-9	1	20	-11	6					
-6	3	18	6	12	-2	-3	19	5	0	-9	2	19	-6	4	-8	1	20	-23	10					
-5	3	18	24	3	-1	-3	19	0	29	-8	2	19	36	3	-7	1	20	0	14					
-4	3	18	13	18	0	-3	19	54	40	-7	2	19	27	3	-1	1	20	15	7					
-3	3	18	16	19	1	-3	19	-6	1	-6	2	19	3	1	0	1	20	-3	0					
-2	3	18	-1	3	2	-3	19	8	6	-5	2	19	23	5	1	1	20	-3	0					
-1	3	18	63	38	3	-3	19	42	40	-4	2	19	18	16	-8	2	20	31	0					
0	3	18	22	38	-5	-2	19	81	36	-3	2	19	-8	4	-3	2	20	-9	10					
1	3	18	-4	0	-4	-2	19	27	9	-2	2	19	13	0	-2	2	20	35	15					
2	3	18	-13	1	-3	-2	19	17	5	-1	2	19	29	20	-1	2	20	-14	6					
3	3	18	0	16	-2	-2	19	30	21	0	2	19	-4	2	0	2	20	8	3					
4	3	18	18	30	-1	-2	19	43	34	1	2	19	14	0	1	2	20	53	2					
5	3	18	0	2	0	-2	19	10	2	2	2	19	-6	0	2	2	20	41	17					
-11	4	18	-4	8	1	-2	19	38	22	3	2	19	-10	25	-4	3	20	52	21					
-10	4	18	22	1	2	-2	19	26	13	4	2	19	32	4	-3	3	20	-13	9					
-9	4	18	-8	8	3	-2	19	25	14	-10	3	19	6	0	-2	3	20	-11	6					
-8	4	18	5	1	4	-2	19	-8	3	-9	3	19	-12	8	-1	3	20	-16	6					
-7	4	18	13	8	5	-2	19	11	3	-8	3	19	-7	1	0	3	20	15	14					
-6	4	18	13	3	-7	-1	19	46	8	-7	3	19	-7	1	-4	4	20	78	3					
-5	4	18	2	2	-6	-1	19	18	4	-6	3	19	1	1	-3	4	20	17	0					
-4	4	18	5	0	-5	-1	19	-5	1	-5	3	19	-6	2	-2	4	20	43	4					
-3	4	18	-5	3	-4	-1	19	9	22	-4	3	19	2	4	-1	4	20	0	0					
-2	4	18	17	24	-3	-1	19	22	18	-3	3	19	39	15										
-1	4	18	45	51	-2	-1	19	18	9	-2	3	19	33	64										
0	4	18	8	6	-1	-1	19	11	0	-1	3	19	22	42										
1	4	18	35	2	0	-1	19	45	43	0	3	19	16	10										
2	4	18	10	20	1	-1	19	15	5	1	3	19	4	0										
3	4	18	9	10	2	-1	19	-2	1	2	3	19	56	23										
4	4	18	-15	14	3	-1	19	-11	12	3	3	19	-10	4										
-10	5	18	-1	2	4	-1	19	-12	11	-9	4	19	29	1										
-9	5	18	8	0	5	-1	19	19	1	-8	4	19	20	3										
-8	5	18	-5	0	6	-1	19	25	3	-7	4	19	5	3										
-7	5	18	5	0	-10	0	19	25	7	-6	4	19	31	27										
-6	5	18	-7	4	-9	0	19	21	4	-5	4	19	-7	11										
-5	5	18	-6	1	-8	0	19	-6	4	-4	4	19	12	27										
-4	5	18	12	16	-7	0	19	-3	0	-3	4	19	4	38										
-3	5	18	32	27	-6	0	19	2	0	-2	4	19	39	42										
-2	5	18	31	40	-5	0	19	-5	10	-1	4	19	-1	2										
-1	5	18	-13	0	-4	0	19	20	8	0	4	19	19	9										
0	5	18	0	1	-3	0	19	5	1	1	4	19	-11	21										
1	5	18	0	14	-2	0	19	-5	2	2	4	19	-11	3										
2	5	18	60	28	-1	0	19	21	15	-9	5	19	-9	9										
-10	6	18	31	1	0	0	19	14	4	-8	5	19	7	3										
-9	6	18	-17	7	1	0	19	30	25	-7	5	19	5	5										
-8	6	18	41	6	2	0	19	11	11	-6	5	19	10	27										
-7	6	18	14	11	3	0	19	42	21	-5	5	19	50	19										
-6	6	18	30	43	4	0	19	20	0	-4	5	19	-1	8										
-5	6	18	13	2	5	0	19	46	15	-3	5	19	-11	5										
-4	6	18	0	9	-11	1	19	-14	0	-2	5	19	-2	1										
-3	6	18	1	15	-10	1	19	-2	10	-1	5	19	17	11										
-2	6	18	-10	1	-9	1	19	4	4	0	5	19	14	2										
-1	6	18	51	13	-8	1	19	-9	2	-8	6	19	34	2										
0	6	18	21	13	-7	1	19	17	0	-5	6	19	85	42										
-9	7	18	-12	7	-6	1	19	11	6	-4	6	19	0	8										
-8	7	18	30	0	-5	1	19	16	4	-3	6	19	39	0										
-7	7	18	-16	0	-4	1	19	15	3	-6	-2	20	-11	2										
-6	7	18	-6	19	-3	1	19	9	15	-9	-1	20	-8	7										
-5	7	18	63	67	-2	1	19	-6	3	-8	-1	20	-8	0										
-4	7	18	15	0	-1	1	19	12	0	-7	-1	20	-4	5										
-3	7	18	2	0	0	1	19	33	12	-6	-1	20	15	12										
-8	8	18	-9	0	1	1	19	13	0	-10	0	20	-15	1										
-7	8	18	55	19	2	1	19	-13	2	-9	0	20	-5	2										
-6	8	18	0	48	3	1	19	-1	3	-8	0	20	10	22										

a Reflections flagged with an asterisk were considered unobserved.

Table A.4. Atomic Multiplicities for $[Cu(dptmp)_2]PF_6 \cdot THF$.

Name	Multiplicity	Name	Multiplicity	Name	Multiplicity
Cu	1.000	P(1)	1.000	F(1)	1.000
F(2)	1.000	F(3)	1.000	F(4)	1.000
F(5)	1.000	F(6)	1.000	O(301)	1.000
N(11)	1.000	N(21)	1.000	N(112)	1.000
N(212)	1.000	C(12)	1.000	C(13)	1.000
C(14)	1.000	C(15)	1.000	C(16)	1.000
C(17)	1.000	C(18)	1.000	C(19)	1.000
C(22)	1.000	C(23)	1.000	C(24)	1.000
C(25)	1.000	C(26)	1.000	C(27)	1.000
C(28)	1.000	C(29)	1.000	C(110)	1.000
C(111)	1.000	C(113)	1.000	C(114)	1.000
C(115)	1.000	C(116)	1.000	C(117)	1.000
C(118)	1.000	C(121)	1.000	C(122)	1.000
C(123)	1.000	C(124)	1.000	C(125)	1.000
C(126)	1.000	C(131)	1.000	C(132)	1.000
C(133)	1.000	C(134)	1.000	C(135)	1.000
C(136)	1.000	C(210)	1.000	C(211)	1.000
C(213)	1.000	C(214)	1.000	C(215)	1.000
C(216)	1.000	C(217)	1.000	C(218)	1.000
C(221)	1.000	C(222)	1.000	C(223)	1.000
C(224)	1.000	C(225)	1.000	C(226)	1.000
C(231)	1.000	C(232)	1.000	C(233)	1.000
C(234)	1.000	C(235)	1.000	C(236)	1.000
C(302)	1.000	C(303)	1.000	C(304)	1.000
C(305)	1.000	H(16)	1.000	H(17)	1.000
H(26)	1.000	H(27)	1.000	H(11A)	1.000
H(11B)	1.000	H(11C)	1.000	H(11D)	1.000
H(11E)	1.000	H(11F)	1.000	H(11G)	1.000
H(11H)	1.000	H(11I)	1.000	H(11J)	1.000
H(11K)	1.000	H(11L)	1.000	H(122)	1.000
H(123)	1.000	H(124)	1.000	H(125)	1.000
H(126)	1.000	H(132)	1.000	H(133)	1.000
H(134)	1.000	H(135)	1.000	H(136)	1.000
H(21A)	1.000	H(21B)	1.000	H(21C)	1.000
H(21D)	1.000	H(21E)	1.000	H(21F)	1.000
H(21G)	1.000	H(21H)	1.000	H(21I)	1.000
H(21J)	1.000	H(21K)	1.000	H(21L)	1.000
H(222)	1.000	H(223)	1.000	H(224)	1.000
H(225)	1.000	H(226)	1.000	H(232)	1.000
H(233)	1.000	H(234)	1.000	H(235)	1.000
H(236)	1.000	H(30A)	1.000	H(30B)	1.000
H(30C)	1.000	H(30D)	1.000	H(30E)	1.000
H(30F)	1.000	H(30G)	1.000	H(30H)	1.000

Appendix B: Crystal Data for $[Cu(tmp)_2]BPh_4$

Table B.1. Anisotropic temperature factor coefficients - U's[a] for $[Cu(tmp)_2]BPh_4$.

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Cu	0.02901(19)	0.0909(3)	0.0675(3)	0.01038(16)	0.00946(16)	0.0006(2)
N(11)	0.0327(12)	0.0647(14)	0.0473(14)	0.0005(9)	0.0090(10)	0.0047(11)
N(21)	0.0378(12)	0.0650(14)	0.0529(15)	0.0091(10)	0.0086(11)	0.0044(12)
N(112)	0.0377(12)	0.0616(13)	0.0518(14)	0.0054(10)	0.0081(10)	-0.0022(11)
N(212)	0.0381(12)	0.0650(14)	0.0492(14)	0.0019(10)	0.0066(10)	-0.0013(11)
C(12)	0.0502(17)	0.0686(18)	0.0476(17)	-0.0100(13)	0.0074(13)	-0.0007(14)
C(13)	0.070(2)	0.0618(17)	0.0490(18)	-0.0033(15)	0.0199(16)	0.0032(14)
C(14)	0.0612(19)	0.0535(16)	0.0579(19)	0.0089(13)	0.0276(15)	0.0089(14)
C(15)	0.0399(15)	0.0534(15)	0.0586(18)	0.0079(11)	0.0190(13)	0.0093(13)
C(16)	0.0380(16)	0.080(2)	0.088(3)	0.0153(14)	0.0222(16)	0.0069(19)
C(17)	0.0271(14)	0.083(2)	0.093(3)	0.0052(14)	0.0093(15)	0.014(2)
C(18)	0.0342(14)	0.0596(16)	0.0593(18)	0.0000(11)	0.0019(12)	0.0116(14)
C(19)	0.0478(17)	0.0600(17)	0.064(2)	-0.0070(13)	-0.0060(15)	0.0115(15)
C(22)	0.0573(19)	0.076(2)	0.0578(19)	0.0091(15)	0.0116(15)	0.0090(16)
C(23)	0.088(3)	0.0579(18)	0.060(2)	-0.0052(16)	0.0306(19)	-0.0046(15)
C(24)	0.064(2)	0.0625(18)	0.081(2)	-0.0143(15)	0.0338(18)	-0.0193(17)
C(25)	0.0420(16)	0.0576(16)	0.078(2)	-0.0068(12)	0.0208(15)	-0.0144(16)
C(26)	0.0279(15)	0.086(2)	0.119(3)	-0.0035(14)	0.0147(17)	-0.017(2)
C(27)	0.0361(16)	0.077(2)	0.108(3)	0.0112(14)	-0.0007(18)	-0.008(2)
C(28)	0.0382(15)	0.0555(16)	0.073(2)	0.0094(12)	-0.0055(14)	-0.0166(15)
C(29)	0.069(2)	0.0510(17)	0.063(2)	0.0140(14)	-0.0163(16)	-0.0106(15)
C(31)	0.0415(14)	0.0465(14)	0.0498(16)	0.0057(11)	0.0009(12)	0.0002(12)
C(32)	0.0504(16)	0.0555(16)	0.0490(16)	0.0103(12)	0.0041(13)	0.0009(13)
C(33)	0.0587(19)	0.070(2)	0.064(2)	0.0249(15)	0.0033(16)	-0.0058(16)
C(34)	0.069(2)	0.0470(16)	0.090(3)	0.0162(15)	-0.0046(19)	-0.0011(16)
C(35)	0.062(2)	0.0493(16)	0.098(3)	0.0016(14)	0.0073(19)	0.0108(17)
C(36)	0.0505(17)	0.0531(16)	0.085(2)	0.0049(13)	0.0180(16)	0.0067(15)
C(41)	0.0343(13)	0.0532(15)	0.0461(16)	0.0069(11)	0.0042(11)	0.0044(12)
C(42)	0.0438(15)	0.0602(16)	0.0520(17)	0.0083(12)	0.0088(13)	0.0111(13)
C(43)	0.0477(17)	0.092(2)	0.0428(18)	0.0129(15)	0.0057(13)	0.0158(16)
C(44)	0.0420(16)	0.090(2)	0.0495(19)	0.0049(14)	0.0045(13)	-0.0137(16)
C(45)	0.0514(17)	0.0643(17)	0.0539(19)	0.0033(13)	0.0046(14)	-0.0121(15)
C(46)	0.0591(18)	0.0557(16)	0.0433(16)	0.0018(13)	0.0048(13)	0.0016(13)
C(51)	0.0499(15)	0.0416(13)	0.0424(15)	0.0068(11)	0.0058(12)	0.0058(11)
C(52)	0.0545(17)	0.0502(15)	0.0582(19)	0.0098(13)	-0.0009(14)	-0.0077(13)
C(53)	0.0507(18)	0.0682(19)	0.080(2)	0.0182(15)	-0.0010(16)	-0.0105(17)
C(54)	0.0505(18)	0.0695(19)	0.071(2)	0.0091(14)	-0.0051(16)	-0.0021(17)
C(55)	0.065(2)	0.076(2)	0.061(2)	0.0039(16)	-0.0084(16)	-0.0120(16)
C(56)	0.0549(18)	0.0663(18)	0.0540(18)	0.0116(14)	0.0025(14)	-0.0137(14)
C(61)	0.0618(18)	0.0427(14)	0.0472(17)	0.0054(12)	0.0138(14)	-0.0009(12)
C(62)	0.090(3)	0.0607(18)	0.055(2)	0.0082(16)	0.0154(18)	0.0117(15)
C(63)	0.158(5)	0.074(2)	0.074(3)	0.007(3)	0.043(3)	0.023(2)
C(64)	0.148(5)	0.073(2)	0.096(3)	-0.026(3)	0.065(3)	0.002(2)
C(65)	0.096(3)	0.077(2)	0.098(3)	-0.030(2)	0.047(3)	-0.020(2)
C(66)	0.064(2)	0.0681(19)	0.066(2)	-0.0071(15)	0.0177(17)	-0.0033(16)
C(110)	0.070(2)	0.0616(17)	0.0553(19)	-0.0051(15)	-0.0007(16)	0.0021(15)
C(111)	0.0535(18)	0.0713(19)	0.0574(19)	0.0074(14)	0.0072(15)	-0.0068(16)
C(113)	0.0303(12)	0.0526(14)	0.0510(16)	0.0042(10)	0.0071(11)	0.0088(12)
C(114)	0.0316(13)	0.0533(15)	0.0497(16)	0.0030(10)	0.0118(11)	0.0092(12)
C(115)	0.110(3)	0.092(3)	0.069(2)	-0.009(2)	0.021(2)	-0.020(2)
C(116)	0.092(3)	0.073(2)	0.082(3)	0.0240(18)	0.042(2)	0.0073(18)
C(117)	0.062(2)	0.093(3)	0.092(3)	-0.0192(18)	-0.013(2)	0.006(2)
C(118)	0.105(3)	0.088(3)	0.076(3)	-0.011(2)	-0.009(2)	-0.019(2)
C(210)	0.081(2)	0.0588(18)	0.0521(19)	0.0028(16)	-0.0041(16)	-0.0036(14)
C(211)	0.0590(19)	0.0693(18)	0.0505(18)	-0.0042(15)	0.0081(15)	0.0004(15)
C(213)	0.0305(13)	0.0501(14)	0.0533(17)	0.0014(10)	0.0023(11)	-0.0089(12)
C(214)	0.0321(13)	0.0521(15)	0.0573(17)	0.0011(11)	0.0091(12)	-0.0105(13)
C(215)	0.136(4)	0.093(3)	0.077(3)	-0.003(3)	0.045(3)	0.011(2)
C(216)	0.088(3)	0.102(3)	0.122(4)	-0.037(2)	0.057(3)	-0.014(3)
C(217)	0.095(3)	0.084(3)	0.106(3)	0.037(2)	-0.036(2)	-0.007(2)

Table B.1, continued

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C(218)	0.142(4)	0.079(2)	0.069(3)	0.009(2)	0.007(3)	0.017(2)
B	0.0465(17)	0.0462(16)	0.0428(17)	0.0062(13)	0.0051(13)	0.0031(13)

a The form of the anisotropic temperature factor is:
$\exp[-2\pi \{h^2a^{*2}U(1,1) + k^2b^{*2}U(2,2) + l^2c^{*2}U(3,3) + 2hka^*b^*U(1,2) + 2hla^*c^*U(1,3) + 2klb^*c^*U(2,3)\}]$ where a^*, b^*, and c^* are reciprocal lattice constants.

Table B.2. Torsion angles in degrees for $[Cu(tmp)_2]BPh_4$

Atom 1	Atom 2	Atom 3	Atom 4	Angle	
N(21)	Cu	N(11)	C(12)	-56.41	(0.27)
N(21)	Cu	N(11)	C(114)	125.00	(0.18)
N(112)	Cu	N(11)	C(12)	178.85	(0.25)
N(112)	Cu	N(11)	C(114)	0.26	(0.18)
N(212)	Cu	N(11)	C(12)	44.79	(0.26)
N(212)	Cu	N(11)	C(114)	-133.80	(0.18)
N(11)	Cu	N(21)	C(22)	-59.84	(0.28)
N(11)	Cu	N(21)	C(214)	116.44	(0.19)
N(112)	Cu	N(21)	C(22)	44.79	(0.27)
N(112)	Cu	N(21)	C(214)	-138.94	(0.18)
N(212)	Cu	N(21)	C(22)	-179.56	(0.26)
N(212)	Cu	N(21)	C(214)	-3.29	(0.19)
N(11)	Cu	N(112)	C(111)	-179.71	(0.26)
N(11)	Cu	N(112)	C(113)	-1.32	(0.18)
N(21)	Cu	N(112)	C(111)	52.20	(0.27)
N(21)	Cu	N(112)	C(113)	-129.41	(0.18)
N(212)	Cu	N(112)	C(111)	-58.22	(0.29)
N(212)	Cu	N(112)	C(113)	120.17	(0.19)
N(11)	Cu	N(212)	C(211)	51.78	(0.27)
N(11)	Cu	N(212)	C(213)	-124.34	(0.18)
N(21)	Cu	N(212)	C(211)	178.87	(0.26)
N(21)	Cu	N(212)	C(213)	2.74	(0.19)
N(112)	Cu	N(212)	C(211)	-53.85	(0.29)
N(112)	Cu	N(212)	C(213)	130.02	(0.19)
Cu	N(11)	C(12)	C(13)	178.93	(0.21)
C(114)	N(11)	C(12)	C(13)	-2.53	(0.41)
Cu	N(11)	C(114)	C(15)	178.68	(0.22)
Cu	N(11)	C(114)	C(113)	0.82	(0.30)
C(12)	N(11)	C(114)	C(15)	-0.12	(0.40)
C(12)	N(11)	C(114)	C(113)	-177.99	(0.25)
Cu	N(21)	C(22)	C(23)	175.73	(0.23)
C(214)	N(21)	C(22)	C(23)	-0.42	(0.43)
Cu	N(21)	C(214)	C(25)	-175.07	(0.23)
Cu	N(21)	C(214)	C(213)	3.33	(0.32)
C(22)	N(21)	C(214)	C(25)	1.75	(0.41)
C(22)	N(21)	C(214)	C(213)	-179.84	(0.28)
Cu	N(112)	C(111)	C(110)	177.14	(0.23)
C(113)	N(112)	C(111)	C(110)	-1.21	(0.43)
Cu	N(112)	C(113)	C(18)	-176.09	(0.23)
Cu	N(112)	C(113)	C(114)	2.16	(0.31)
C(111)	N(112)	C(113)	C(18)	2.56	(0.40)
C(111)	N(112)	C(113)	C(114)	-179.19	(0.25)
Cu	N(212)	C(211)	C(210)	-179.73	(0.22)
C(213)	N(212)	C(211)	C(210)	-3.74	(0.43)
Cu	N(212)	C(213)	C(28)	177.07	(0.23)
Cu	N(212)	C(213)	C(214)	-1.81	(0.31)
C(211)	N(212)	C(213)	C(28)	0.33	(0.40)
C(211)	N(212)	C(213)	C(214)	-178.55	(0.26)
N(11)	C(12)	C(13)	C(14)	2.25	(0.45)
N(11)	C(12)	C(13)	C(115)	-179.04	(0.29)
C(12)	C(13)	C(14)	C(15)	0.72	(0.43)
C(12)	C(13)	C(14)	C(116)	-179.84	(0.29)
C(115)	C(13)	C(14)	C(15)	-177.91	(0.30)
C(115)	C(13)	C(14)	C(116)	1.53	(0.48)
C(13)	C(14)	C(15)	C(16)	175.59	(0.29)
C(13)	C(14)	C(15)	C(114)	-3.09	(0.43)
C(116)	C(14)	C(15)	C(16)	-3.84	(0.47)
C(116)	C(14)	C(15)	C(114)	177.48	(0.28)
C(14)	C(15)	C(16)	C(17)	-179.14	(0.33)
C(114)	C(15)	C(16)	C(17)	-0.44	(0.47)
C(14)	C(15)	C(114)	N(11)	2.89	(0.43)
C(14)	C(15)	C(114)	C(113)	-179.32	(0.27)
C(16)	C(15)	C(114)	N(11)	-175.89	(0.27)
C(16)	C(15)	C(114)	C(113)	1.90	(0.42)

Table B.2, continued

Atom 1	Atom 2	Atom 3	Atom 4	Angle	
C(15)	C(16)	C(17)	C(18)	-1.33	(0.55)
C(16)	C(17)	C(18)	C(19)	-179.24	(0.33)
C(16)	C(17)	C(18)	C(113)	1.57	(0.50)
C(17)	C(18)	C(19)	C(110)	179.10	(0.31)
C(17)	C(18)	C(19)	C(117)	-1.53	(0.50)
C(113)	C(18)	C(19)	C(110)	-1.73	(0.45)
C(113)	C(18)	C(19)	C(117)	177.65	(0.30)
C(17)	C(18)	C(113)	N(112)	178.09	(0.29)
C(17)	C(18)	C(113)	C(114)	-0.08	(0.42)
C(19)	C(18)	C(113)	N(112)	-1.14	(0.45)
C(19)	C(18)	C(113)	C(114)	-179.31	(0.28)
C(18)	C(19)	C(110)	C(111)	2.97	(0.45)
C(18)	C(19)	C(110)	C(118)	-178.17	(0.30)
C(117)	C(19)	C(110)	C(111)	-176.41	(0.30)
C(117)	C(19)	C(110)	C(118)	2.45	(0.50)
N(21)	C(22)	C(23)	C(24)	-1.42	(0.48)
N(21)	C(22)	C(23)	C(215)	179.46	(0.30)
C(22)	C(23)	C(24)	C(25)	1.89	(0.46)
C(22)	C(23)	C(24)	C(216)	-178.60	(0.31)
C(215)	C(23)	C(24)	C(25)	-179.04	(0.31)
C(215)	C(23)	C(24)	C(216)	0.47	(0.51)
C(23)	C(24)	C(25)	C(26)	-179.46	(0.34)
C(23)	C(24)	C(25)	C(214)	-0.68	(0.46)
C(216)	C(24)	C(25)	C(26)	1.03	(0.53)
C(216)	C(24)	C(25)	C(214)	179.82	(0.32)
C(24)	C(25)	C(26)	C(27)	-179.27	(0.36)
C(214)	C(25)	C(26)	C(27)	1.92	(0.55)
C(24)	C(25)	C(214)	N(21)	-1.23	(0.46)
C(24)	C(25)	C(214)	C(213)	-179.59	(0.29)
C(26)	C(25)	C(214)	N(21)	177.65	(0.30)
C(26)	C(25)	C(214)	C(213)	-0.70	(0.45)
C(25)	C(26)	C(27)	C(28)	-0.96	(0.62)
C(26)	C(27)	C(28)	C(29)	179.54	(0.37)
C(26)	C(27)	C(28)	C(213)	-1.24	(0.55)
C(27)	C(28)	C(29)	C(210)	176.37	(0.33)
C(27)	C(28)	C(29)	C(217)	-2.68	(0.51)
C(213)	C(28)	C(29)	C(210)	-2.84	(0.46)
C(213)	C(28)	C(29)	C(217)	178.11	(0.30)
C(27)	C(28)	C(213)	N(212)	-176.39	(0.29)
C(27)	C(28)	C(213)	C(214)	2.43	(0.46)
C(29)	C(28)	C(213)	N(212)	2.87	(0.45)
C(29)	C(28)	C(213)	C(214)	-178.31	(0.28)
C(28)	C(29)	C(210)	C(211)	-0.19	(0.46)
C(28)	C(29)	C(210)	C(218)	-178.55	(0.30)
C(217)	C(29)	C(210)	C(211)	178.84	(0.30)
C(217)	C(29)	C(210)	C(218)	0.49	(0.50)
C(36)	C(31)	C(32)	C(33)	-0.24	(0.43)
B	C(31)	C(32)	C(33)	175.17	(0.28)
C(32)	C(31)	C(36)	C(35)	-0.06	(0.44)
B	C(31)	C(36)	C(35)	-175.64	(0.30)
C(32)	C(31)	B	C(41)	115.35	(0.30)
C(32)	C(31)	B	C(51)	-124.63	(0.28)
C(32)	C(31)	B	C(61)	-2.95	(0.38)
C(36)	C(31)	B	C(41)	-69.53	(0.34)
C(36)	C(31)	B	C(51)	50.50	(0.35)
C(36)	C(31)	B	C(61)	172.18	(0.27)
C(31)	C(32)	C(33)	C(34)	0.33	(0.49)
C(32)	C(33)	C(34)	C(35)	-0.09	(0.56)
C(33)	C(34)	C(35)	C(36)	-0.20	(0.54)
C(34)	C(35)	C(36)	C(31)	0.28	(0.54)
C(46)	C(41)	C(42)	C(43)	-0.31	(0.39)
B	C(41)	C(42)	C(43)	176.99	(0.26)
C(42)	C(41)	C(46)	C(45)	0.37	(0.42)
B	C(41)	C(46)	C(45)	-177.09	(0.27)

Table B.2, continued

Atom 1	Atom 2	Atom 3	Atom 4	Angle
C(42)	C(41)	B	C(31)	21.25 (0.37)
C(42)	C(41)	B	C(51)	-98.03 (0.29)
C(42)	C(41)	B	C(61)	142.27 (0.26)
C(46)	C(41)	B	C(31)	-161.58 (0.24)
C(46)	C(41)	B	C(51)	79.14 (0.29)
C(46)	C(41)	B	C(61)	-40.56 (0.32)
C(41)	C(42)	C(43)	C(44)	-0.26 (0.42)
C(42)	C(43)	C(44)	C(45)	0.77 (0.43)
C(43)	C(44)	C(45)	C(46)	-0.71 (0.44)
C(44)	C(45)	C(46)	C(41)	0.13 (0.46)
C(56)	C(51)	C(52)	C(53)	0.41 (0.41)
B	C(51)	C(52)	C(53)	-179.32 (0.27)
C(52)	C(51)	C(56)	C(55)	0.04 (0.45)
B	C(51)	C(56)	C(55)	179.79 (0.28)
C(52)	C(51)	B	C(31)	-143.45 (0.26)
C(52)	C(51)	B	C(41)	-21.30 (0.34)
C(52)	C(51)	B	C(61)	95.16 (0.31)
C(56)	C(51)	B	C(31)	36.84 (0.33)
C(56)	C(51)	B	C(41)	158.98 (0.24)
C(56)	C(51)	B	C(61)	-84.55 (0.29)
C(51)	C(52)	C(53)	C(54)	-0.40 (0.49)
C(52)	C(53)	C(54)	C(55)	-0.08 (0.49)
C(53)	C(54)	C(55)	C(56)	0.52 (0.48)
C(54)	C(55)	C(56)	C(51)	-0.52 (0.47)
C(66)	C(61)	C(62)	C(63)	-0.82 (0.46)
B	C(61)	C(62)	C(63)	-177.70 (0.31)
C(62)	C(61)	C(66)	C(65)	1.47 (0.47)
B	C(61)	C(66)	C(65)	178.46 (0.31)
C(62)	C(61)	B	C(31)	-115.84 (0.31)
C(62)	C(61)	B	C(41)	122.06 (0.30)
C(62)	C(61)	B	C(51)	3.79 (0.38)
C(66)	C(61)	B	C(31)	67.46 (0.34)
C(66)	C(61)	B	C(41)	-54.64 (0.34)
C(66)	C(61)	B	C(51)	-172.91 (0.25)
C(61)	C(62)	C(63)	C(64)	-0.04 (0.56)
C(62)	C(63)	C(64)	C(65)	0.32 (0.66)
C(63)	C(64)	C(65)	C(66)	0.31 (0.65)
C(64)	C(65)	C(66)	C(61)	-1.27 (0.59)
C(19)	C(110)	C(111)	N(112)	-1.59 (0.48)
C(118)	C(110)	C(111)	N(112)	179.50 (0.30)
N(112)	C(113)	C(114)	N(11)	-2.02 (0.38)
N(112)	C(113)	C(114)	C(15)	-179.94 (0.29)
C(18)	C(113)	C(114)	N(11)	176.25 (0.26)
C(18)	C(113)	C(114)	C(15)	-1.66 (0.43)
C(29)	C(210)	C(211)	N(212)	3.73 (0.48)
C(218)	C(210)	C(211)	N(212)	-177.82 (0.29)
N(212)	C(213)	C(214)	N(21)	-1.02 (0.39)
N(212)	C(213)	C(214)	C(25)	177.42 (0.26)
C(28)	C(213)	C(214)	N(21)	-179.91 (0.29)
C(28)	C(213)	C(214)	C(25)	-1.47 (0.45)

Table B.3. Structure factors (F^2_{obs} & F^2_{calc})^a for $[Cu(tmp)_2]BPh_4$.

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
4	0	0	51182	54965	12	3	0	1082	1142	11	6	0	905	869	14	9	0	-11	8	-12	1	1	29	18
6	0	0	21571	21824	13	3	0	2324	2369	12	6	0	253	293	15	9	0	12	2	-11	1	1	97	100
8	0	0	8741	8758	14	3	0	996	1042	13	6	0	5	6	16	9	0	-3	1	-10	1	1	942	834
10	0	0	8792	8962	15	3	0	99	100	14	6	0	104	91	17	9	0	1	3	-9	1	1	236	288
12	0	0	7350	7772	16	3	0	674	766	15	6	0	98	98	18	9	0	78	7	-8	1	1	585	425
14	0	0	2354	2169	17	3	0	105	102	16	6	0	88	113	0	10	0	4	47	-7	1	1	1607	1557
16	0	0	297	339	18	3	0	136	78	17	6	0	71	60	1	10	0	258	275	-6	1	1	875	792
18	0	0	561	586	19	3	0	-14	6	18	6	0	131	148	2	10	0	118	150	-5	1	1	5302	5719
20	0	0	1385	1268	20	3	0	266	254	19	6	0	53	103	3	10	0	16	15	-4	1	1	561	557
22	0	0	-2	112	21	3	0	20	9	20	6	0	144	75	4	10	0	70	75	-3	1	1	1078	1137
1	1	0	513	1158	22	3	0	10	86	21	6	0	63	39	5	10	0	31	87	-2	1	1	113	154
2	1	0	143	173	0	4	0	117	117	1	7	0	32	32	6	10	0	38	45	-1	1	1	87	147
3	1	0	2075	2176	1	4	0	7595	7953	2	7	0	688	676	7	10	0	371	461	1	1	1	6594	12989
4	1	0	734	838	2	4	0	250	243	3	7	0	682	620	8	10	0	5	3	2	1	1	3579	3846
5	1	0	374	418	3	4	0	7275	7622	4	7	0	538	535	9	10	0	118	123	3	1	1	20	7
6	1	0	1257	1236	4	4	0	235	185	5	7	0	28	16	10	10	0	135	147	4	1	1	2583	2812
7	1	0	1675	1567	5	4	0	14325	14689	6	7	0	101	106	11	10	0	49	20	5	1	1	454	404
8	1	0	775	540	6	4	0	41	42	7	7	0	6	16	12	10	0	14	18	6	1	1	9990	10214
9	1	0	2091	1988	7	4	0	8171	8404	8	7	0	43	44	13	10	0	-14	27	7	1	1	9216	8542
10	1	0	2012	1970	8	4	0	130	163	9	7	0	-4	1	14	10	0	-4	1	8	1	1	4078	4000
11	1	0	35	38	9	4	0	2036	2173	10	7	0	7	5	1	11	0	87	5	9	1	1	-1	2
12	1	0	1844	1659	10	4	0	115	108	11	7	0	-4	1	2	11	0	-17	3	10	1	1	3846	3765
13	1	0	127	103	11	4	0	1353	1193	12	7	0	32	54	3	11	0	170	163	11	1	1	41	39
14	1	0	771	701	12	4	0	578	487	13	7	0	166	158	4	11	0	45	48	12	1	1	595	573
15	1	0	476	453	13	4	0	1085	1109	14	7	0	56	63	5	11	0	2	25	13	1	1	229	229
16	1	0	22	35	14	4	0	22	0	15	7	0	24	54	6	11	0	42	40	14	1	1	5388	5034
17	1	0	19	9	15	4	0	96	60	16	7	0	16	7	7	11	0	-27	2	15	1	1	10	8
18	1	0	132	156	16	4	0	-10	7	17	7	0	83	31	8	11	0	-32	33	16	1	1	23	24
19	1	0	-9	6	17	4	0	493	511	18	7	0	0	6	9	11	0	141	58	17	1	1	28	0
20	1	0	93	105	18	4	0	-18	2	19	7	0	29	1	2	12	0	53	2	18	1	1	86	54
21	1	0	8	1	19	4	0	485	524	20	7	0	-12	0	3	12	0	56	3	19	1	1	18	49
22	1	0	28	5	20	4	0	127	36	21	7	0	-5	7	4	12	0	-40	1	20	1	1	20	77
0	2	0	4526	4921	21	4	0	124	141	0	8	0	921	735	5	12	0	12	26	21	1	1	41	6
1	2	0	2280	2399	22	4	0	1	12	1	8	0	108	62	6	12	0	-56	29	22	1	1	99	27
2	2	0	26126	32171	1	5	0	94	83	2	8	0	49	28	7	12	0	83	20	-22	2	1	-5	21
3	2	0	2396	2397	2	5	0	105	97	3	8	0	-6	8	8	12	0	-3	13	-21	2	1	28	34
4	2	0	2821	3057	3	5	0	898	826	4	8	0	145	176	-21	0	1	584	664	-20	2	1	226	250
5	2	0	101	150	4	5	0	635	556	5	8	0	177	178	-19	0	1	543	552	-19	2	1	107	61
6	2	0	173	219	5	5	0	1496	1590	6	8	0	106	94	-17	0	1	1167	1082	-18	2	1	116	127
7	2	0	6195	6450	6	5	0	145	120	7	8	0	216	188	-15	0	1	35	52	-17	2	1	485	401
8	2	0	5589	5380	7	5	0	196	167	8	8	0	383	367	-13	0	1	5043	5029	-16	2	1	80	96
9	2	0	656	695	8	5	0	67	42	9	8	0	11	1	-11	0	1	2528	2557	-15	2	1	118	114
10	2	0	1876	1953	9	5	0	416	407	10	8	0	55	34	-9	0	1	327	457	-14	2	1	526	479
11	2	0	412	403	10	5	0	31	26	11	8	0	278	282	-7	0	1	3216	2667	-13	2	1	1895	1890
12	2	0	3896	4013	11	5	0	1094	1090	12	8	0	176	160	-5	0	1	29437	28703	-12	2	1	2942	2962
13	2	0	3388	3336	12	5	0	74	34	13	8	0	66	89	-3	0	1	7184	9050	-11	2	1	1380	1352
14	2	0	334	265	13	5	0	93	86	14	8	0	291	333	3	0	1	29773	33969	-10	2	1	839	1102
15	2	0	130	101	14	5	0	6	3	15	8	0	66	23	5	0	1	1462	1360	-9	2	1	4096	4052
16	2	0	480	466	15	5	0	968	1049	16	8	0	154	115	7	0	1	4120	4505	-8	2	1	13350	13198
17	2	0	1006	973	16	5	0	32	0	17	8	0	-2	0	9	0	1	7599	7576	-7	2	1	2998	3123
18	2	0	470	419	17	5	0	149	186	18	8	0	124	89	11	0	1	2242	2332	-6	2	1	3084	3251
19	2	0	429	441	18	5	0	44	39	19	8	0	4	2	13	0	1	9914	10102	-5	2	1	206	207
20	2	0	381	380	19	5	0	98	95	20	8	0	47	13	15	0	1	260	324	-4	2	1	10233	10809
21	2	0	213	240	20	5	0	88	82	1	9	0	7	16	17	0	1	1845	1872	-3	2	1	7562	7693
22	2	0	-4	22	21	5	0	-13	2	2	9	0	4	2	19	0	1	645	636	-2	2	1	11427	12947
1	3	0	1398	1491	0	6	0	3374	3188	3	9	0	162	166	21	0	1	630	600	-1	2	1	16566	17745
2	3	0	419	430	1	6	0	1365	1370	4	9	0	-32	1	-22	1	1	58	0	0	2	1	5	12550
3	3	0	12	17	2	6	0	43	38	5	9	0	307	195	-21	1	1	-25	0	1	2	1	4419	4597
4	3	0	41	36	3	6	0	128	113	6	9	0	89	77	-20	1	1	81	120	2	2	1	7864	8523
5	3	0	1795	1822	4	6	0	1765	1770	7	9	0	4	0	-19	1	1	23	33	3	2	1	684	757
6	3	0	32	69	5	6	0	899	812	8	9	0	8	10	-18	1	1	290	326	4	2	1	6875	7280
7	3	0	4325	3883	6	6	0	443	486	9	9	0	372	335	-17	1	1	58	23	5	2	1	1673	1766
8	3	0	374	346	7	6	0	36	16	10	9	0	20	1	-16	1	1	224	189	6	2	1	4590	4947
9	3	0	115	132	8	6	0	17	18	11	9	0	31	29	-15	1	1	777	708	7	2	1	2713	2857
10	3	0	49	15	9	6	0	156	152	12	9	0	41	50	-14	1	1	1583	1513	8	2	1	669	702
11	3	0	108	81	10	6	0	48	63	13	9	0	62	47	-13	1	1	1815	1815	9	2	1	3625	3522
10	2	1	1813	1976	-14	4	1	866	829	9	5	1	806	724	-11	7	1	188	156	13	8	1	314	277
11	2	1	2442	2383	-13	4	1	80	76	10	5	1	35	40	-10	7	1	8	5	14	8	1	45	20
12	2	1	817	767	-12	4	1	1784	1758	11	5	1	927	887	-9	7	1	2	7	15	8	1	211	173
13	2	1	1658	1532	-11	4	1	12	7	12	5	1	771	724	-8	7	1	30	9	16	8	1	10	10
14	2	1	1952	2067	-10	4	1	2157	2216	13	5	1	112	111	-7	7	1	36	28	17	8	1	151	151
15	2	1	45	27	-9	4	1	184	188	14	5	1	74	63	-6	7	1	7	10	18	8	1	18	12
16	2	1	805	794	-8	4	1	610	781	15	5	1	273	283	-5	7	1	19	14	19	8	1	51	7
17	2	1	541	489	-7	4	1	79	61	16	5	1	101	99	-4	7	1	159	161	20	8	1	-34	0
18	2	1	390	379	-6	4	1	14432	14367	17	5	1	244	226	-3	7	1	1287	1267	-18	9	1	102	1
19	2	1	302	306	-5	4	1	2070	2112	18	5	1	94	69	-2	7	1	164	150	-17	9	1	44	1
20	2	1	487	518	-4	4	1	644	804	19	5	1	81	93	-1	7	1	873	868	-16	9	1	-24	8
21	2	1	10	27	-3	4	1	406	390	20	5	1	9	8	0	7	1	10	39	-15	9	1	11	5
22	2	1	37	99	-2	4	1	1307	1667	21	5	1	-44	20	1	7	1	138	100	-14	9	1	5	2
-22	3	1	-44	4	-1	4	1	19	1	-21	6	1	-6	29	2	7	1	64	61	-13	9	1	22	20
-21	3	1	112	65	0	4	1	4	18	-20	6	1	15	1	3	7	1	278	223	-12	9	1	44	53
-20	3	1	41	8	1	4	1	690	728	-19	6	1	135	96	4	7	1	147	139	-11	9	1	15	28
-19	3	1	60	63	2	4	1	983	1011	-18	6	1	210	203	5	7	1	23	5	-10	9	1	75	36
-18	3	1	38	29	3	4	1	722	634	-17	6	1	128	200	6	7	1	206	186	-9	9	1	8	22
-17	3	1	19	13	4	4	1	3601	3634	-16	6	1	233	273	7	7	1	-9	3	-8	9	1	9	16
-16	3	1	64	74	5	4	1	36	25	-15	6	1	98	93	8	7	1	88	79	-7	9	1	30	21
-15	3	1	61	75	6	4	1	3026	3128	-14	6	1	475	481	9	7	1	53	33	-6	9	1	9	0
-14	3	1	190	231	7	4	1	353	318	-13	6	1	301	274	10	7	1	399	384	-5	9	1	181	0
-13	3	1	114	100	8	4	1	742	824	-12	6	1	519	522	11	7	1	490	408	-4	9	1	-27	0
-12	3	1	1203	1201	9	4	1	650	585	-11	6	1	178	170	12	7	1	150	162	-3	9	1	-10	6
-11	3	1	1475	1435	10	4	1	1244	1327	-10	6	1	1365	1292	13	7	1	35	1	-2	9	1	11	21
-10	3	1	1274	977	11	4	1	-5	0	-9	6	1	392	379	14	7	1	296	251	-1	9	1	-9	0
-9	3	1	521	499	12	4	1	1765	1651	-8	6	1	904	954	15	7	1	-22	5	0	9	1	44	48
-8	3	1	1338	985	13	4	1	411	399	-7	6	1	1411	1459	16	7	1	31	9	1	9	1	38	49
-7	3	1	220	221	14	4	1	125	108	-6	6	1	438	425	17	7	1	-9	2	2	9	1	-7	0
-6	3	1	2954	2683	15	4	1	-3	8	-5	6	1	3209	2835	18	7	1	46	10	3	9	1	130	147
-5	3	1	660	586	16	4	1	465	446	-4	6	1	2318	2305	19	7	1	-24	6	4	9	1	96	82
-4	3	1	6	0	17	4	1	59	75	-3	6	1	3396	3424	20	7	1	8	17	5	9	1	95	53
-3	3	1	663	573	18	4	1	577	636	-2	6	1	669	712	21	7	1	26	1	6	9	1	10	1
-2	3	1	2581	2819	19	4	1	117	52	-1	6	1	1711	1733	-20	8	1	82	1	7	9	1	86	112
-1	3	1	13	3	20	4	1	252	228	0	6	1	283	283	-19	8	1	23	6	8	9	1	50	49
0	3	1	673	792	21	4	1	-19	4	1	6	1	1274	1269	-18	8	1	39	15	9	9	1	7	13
1	3	1	19	21	-21	5	1	36	41	2	6	1	1134	1161	-17	8	1	87	102	10	9	1	42	26

Table B.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
2	3	1	4	4	-20	5	1	-4	7	3	6	1	1076	1162	-16	8	1	4	14	11	9	1	249	279
3	3	1	994	1122	-19	5	1	8	9	4	6	1	96	88	-15	8	1	58	76	12	9	1	102	70
4	3	1	339	326	-18	5	1	32	1	5	6	1	2298	2274	-14	8	1	32	33	13	9	1	119	111
5	3	1	689	629	-17	5	1	103	115	6	6	1	356	328	-13	8	1	272	235	14	9	1	46	16
6	3	1	33	28	-16	5	1	-10	1	7	6	1	663	692	-12	8	1	9	15	15	9	1	66	78
7	3	1	3866	3796	-15	5	1	224	254	8	6	1	425	459	-11	8	1	21	28	16	9	1	-15	1
8	3	1	5892	5910	-14	5	1	26	5	9	6	1	1488	1444	-10	8	1	4	0	17	9	1	28	18
9	3	1	1094	1177	-13	5	1	17	22	10	6	1	6	2	-9	8	1	396	343	18	9	1	52	6
10	3	1	45	31	-12	5	1	669	667	11	6	1	448	434	-8	8	1	194	177	-14	10	1	95	108
11	3	1	221	265	-11	5	1	108	121	12	6	1	153	133	-7	8	1	621	630	-13	10	1	15	0
12	3	1	125	125	-10	5	1	375	392	13	6	1	529	548	-6	8	1	13	23	-12	10	1	77	103
13	3	1	60	70	-9	5	1	28	40	14	6	1	40	36	-5	8	1	888	938	-11	10	1	18	7
14	3	1	131	138	-8	5	1	265	212	15	6	1	125	117	-4	8	1	81	85	-10	10	1	40	59
15	3	1	32	32	-7	5	1	901	758	16	6	1	114	107	-3	8	1	298	350	-9	10	1	19	18
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8	10	1	29	6	-17	1	2	107	100	4	2	2	25	8	-19	4	2	626	693	4	5	2	172	184
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22	0	2	44	105	-2	2	2	274	267	19	3	2	49	20	-2	5	2	2512	2445	21	6	2	-59	64
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Table B.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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-4	7	2	190	162	20	8	2	-26	13	13	10	2	36	29	-10	1	3	132	194	12	2	3	1261	1202
-3	7	2	186	195	-18	9	2	99	0	14	10	2	24	7	-9	1	3	2564	2250	13	2	3	354	389
-2	7	2	1489	1315	-17	9	2	34	0	-9	11	2	4	26	-8	1	3	393	331	14	2	3	508	453
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0	7	2	-12	0	-15	9	2	23	4	-7	11	2	45	0	-6	1	3	4042	4256	16	2	3	125	154
1	7	2	20	2	-14	9	2	26	0	-6	11	2	34	60	-5	1	3	77	101	17	2	3	467	481
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6	7	2	57	48	-9	9	2	100	79	-1	11	2	27	47	0	1	3	1730	1876	22	2	3	501	12
7	7	2	554	509	-8	9	2	17	12	0	11	2	-21	0	1	1	3	-2	22475	-22	3	3	18	83
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Table B.3, continued

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6	8	4	66	40	0	10	4	-3	5	21	0	5	34	6	1	2	5	32777	33607	-21	4	5	70	18
7	8	4	6	9	1	10	4	58	41	-22	1	5	81	63	2	2	5	800	984	-20	4	5	174	198
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9	8	4	317	308	3	10	4	31	6	-20	1	5	106	120	4	2	5	2343	2367	-18	4	5	335	327
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11	8	4	62	2	5	10	4	126	141	-18	1	5	256	305	6	2	5	714	719	-16	4	5	326	284
12	8	4	0	4	6	10	4	17	37	-17	1	5	32	2	7	2	5	2130	2262	-15	4	5	1	9
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Table B.3, continued

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15	8	4	14	27	9	10	4	30	7	-14	1	5	6406	6074	10	2	5	1009	1069	-12	4	5	3748	3600
16	8	4	94	67	10	10	4	35	4	-13	1	5	770	762	11	2	5	427	428	-11	4	5	96	72
17	8	4	-24	1	11	10	4	-11	4	-12	1	5	1132	1087	12	2	5	1625	1636	-10	4	5	1004	992
18	8	4	-16	3	12	10	4	9	2	-11	1	5	10	16	13	2	5	527	500	-9	4	5	455	330
19	8	4	51	86	13	10	4	26	0	-10	1	5	5321	5241	14	2	5	112	97	-8	4	5	2695	2800
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-19	6	5	173	181	5	7	5	232	250	-8	9	5	11	10	2	11	5	72	61	5	1	6	10365	11387
-18	6	5	14	32	6	7	5	245	246	-7	9	5	170	158	3	11	5	43	2	6	1	6	14100	13461
-17	6	5	388	431	7	7	5	225	224	-6	9	5	75	30	4	11	5	-35	2	7	1	6	8815	8456
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2	6	5	557	486	-15	8	5	65	57	13	9	5	26	37	-14	0	6	1451	1298	-18	2	6	444	441
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Table B.3, continued

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7	6	5	1375	1444	-10	8	5	307	310	-15	10	5	54	17	-4	0	6	9	16	-13	2	6	3858	3652
8	6	5	350	324	-9	8	5	96	79	-14	10	5	129	92	-2	0	6	10266	10745	-12	2	6	1366	1317
9	6	5	19	12	-8	8	5	163	138	-13	10	5	-13	1	0	0	6	83	65	-11	2	6	3239	3116
10	6	5	53	64	-7	8	5	216	232	-12	10	5	216	201	2	0	6	14543	15249	-10	2	6	541	547
11	6	5	801	722	-6	8	5	104	80	-11	10	5	32	49	4	0	6	9819	10287	-9	2	6	2874	2756
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13	6	5	766	883	-4	8	5	3	7	-9	10	5	23	6	8	0	6	1788	1610	-7	2	6	7118	6792
14	6	5	142	141	-3	8	5	7	5	-8	10	5	145	126	10	0	6	843	815	-6	2	6	41	18
15	6	5	22	6	-2	8	5	99	81	-7	10	5	69	66	12	0	6	24	2	-5	2	6	688	691
16	6	5	120	136	-1	8	5	476	451	-6	10	5	264	245	14	0	6	56	12	-4	2	6	3213	3579
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12	2	6	578	620	-10	4	6	13	3	12	5	6	54	52	-6	7	6	165	137	19	8	6	75	1
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14	2	6	220	239	-8	4	6	141	161	14	5	6	28	3	-4	7	6	178	182	-17	9	6	26	9
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Table B.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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4	11	6	10	8	10	1	7	4140	4212	-12	3	7	276	257	10	4	7	271	280	-9	6	7	2	8
5	11	6	12	23	11	1	7	92	97	-11	3	7	510	505	11	4	7	168	169	-8	6	7	341	374
6	11	6	21	0	12	1	7	3600	3455	-10	3	7	311	258	12	4	7	266	280	-7	6	7	159	197
7	11	6	-35	16	13	1	7	285	267	-9	3	7	3325	3360	13	4	7	315	307	-6	6	7	143	131
8	11	6	-15	0	14	1	7	1091	1040	-8	3	7	-5	1	14	4	7	19	20	-5	6	7	775	819
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-5	12	6	4	1	17	1	7	145	99	-5	3	7	3266	3162	17	4	7	11	2	-2	6	7	355	404
-4	12	6	77	13	18	1	7	720	722	-4	3	7	4811	4575	18	4	7	68	5	-1	6	7	744	735
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-21	0	7	797	833	-22	2	7	36	4	0	3	7	41	28	-21	5	7	23	1	3	6	7	925	1124
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16	7	7	36	20	3	9	7	-5	8	-2	12	7	13	1	21	1	8	73	30	0	3	8	9027	9465
17	7	7	64	0	4	9	7	13	1	-22	0	8	6	66	-22	2	8	161	145	1	3	8	4642	4036
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-5	8	7	1248	1234	-10	10	7	7	4	16	0	8	-13	0	-3	2	8	2908	2624	20	3	8	242	93
-4	8	7	96	88	-9	10	7	36	37	18	0	8	-26	10	-2	2	8	7859	8042	-22	4	8	55	1
-3	8	7	95	68	-8	10	7	34	37	20	0	8	105	30	-1	2	8	7	13	-21	4	8	91	75
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0	8	7	22	23	-5	10	7	77	77	-20	1	8	49	34	2	2	8	321	261	-18	4	8	53	77
1	8	7	-6	1	-4	10	7	72	58	-19	1	8	202	195	3	2	8	803	850	-17	4	8	84	69
2	8	7	239	250	-3	10	7	84	100	-18	1	8	90	105	4	2	8	16	5	-16	4	8	-9	2
3	8	7	2	1	-2	10	7	15	1	-17	1	8	139	177	5	2	8	802	681	-15	4	8	8	12
4	8	7	11	10	-1	10	7	4	37	-16	1	8	42	8	6	2	8	1892	1591	-14	4	8	45	76
5	8	7	416	413	0	10	7	130	148	-15	1	8	3293	3160	7	2	8	233	200	-13	4	8	1585	1464
6	8	7	0	3	1	10	7	33	34	-14	1	8	1052	1055	8	2	8	167	144	-12	4	8	840	775

Table B.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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8	8	7	628	599	3	10	7	57	79	-12	1	8	689	718	10	2	8	-6	1	-10	4	8	160	180
9	8	7	18	11	4	10	7	11	2	-11	1	8	2736	2704	11	2	8	450	425	-9	4	8	92	95
10	8	7	55	60	5	10	7	-8	1	-10	1	8	1386	1441	12	2	8	19	26	-8	4	8	46	52
11	8	7	73	79	6	10	7	27	50	-9	1	8	14	10	13	2	8	67	57	-7	4	8	164	223
-6	4	8	123	111	18	5	8	270	285	0	7	8	420	412	-12	9	8	41	7	2	11	8	1	50
-5	4	8	297	293	19	5	8	16	20	1	7	8	511	488	-11	9	8	17	17	3	11	8	96	53
-4	4	8	311	324	20	5	8	48	65	2	7	8	514	473	-10	9	8	208	188	4	11	8	28	3
-3	4	8	2538	2096	-21	6	8	-32	0	3	7	8	1001	903	-9	9	8	122	87	5	11	8	47	12
-2	4	8	753	645	-20	6	8	5	30	4	7	8	1014	1086	-8	9	8	61	55	6	11	8	60	56
-1	4	8	6593	6585	-19	6	8	3	0	5	7	8	195	152	-7	9	8	86	66	7	11	8	154	20
0	4	8	2189	2038	-18	6	8	148	82	6	7	8	1	1	-6	9	8	130	111	8	11	8	0	93
1	4	8	266	273	-17	6	8	13	18	7	7	8	2233	2073	-5	9	8	42	40	-6	12	8	42	2
2	4	8	618	527	-16	6	8	56	63	8	7	8	596	648	-4	9	8	11	0	-5	12	8	39	1
3	4	8	265	217	-15	6	8	54	28	9	7	8	1082	1009	-3	9	8	60	68	-4	12	8	10	14
4	4	8	185	138	-14	6	8	352	319	10	7	8	21	0	-2	9	8	66	95	-3	12	8	122	3
5	4	8	1182	1070	-13	6	8	81	65	11	7	8	474	481	-1	9	8	12	5	-21	0	9	634	610
6	4	8	631	560	-12	6	8	294	263	12	7	8	12	7	0	9	8	147	117	-19	0	9	363	335
7	4	8	771	669	-11	6	8	199	218	13	7	8	160	129	1	9	8	86	98	-17	0	9	1125	1204
8	4	8	388	396	-10	6	8	119	104	14	7	8	129	165	2	9	8	41	50	-15	0	9	1127	1236
9	4	8	6	31	-9	6	8	5	8	15	7	8	156	167	3	9	8	15	4	-13	0	9	44	46
10	4	8	169	195	-8	6	8	896	892	16	7	8	7	30	4	9	8	225	234	-11	0	9	988	922
11	4	8	122	105	-7	6	8	406	403	17	7	8	-3	62	5	9	8	19	1	-9	0	9	1360	1209
12	4	8	88	54	-6	6	8	194	205	18	7	8	35	15	6	9	8	18	27	-7	0	9	407	351
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15	4	8	15	14	-3	6	8	21	29	-19	8	8	29	4	9	9	8	48	41	-1	0	9	73	77
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-8	5	8	331	323	16	6	8	44	35	0	8	8	104	102	-3	10	8	11	22	-14	1	9	5377	4859
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2	5	8	1306	1282	-16	7	8	21	31	10	8	8	7	1	7	10	8	-4	3	-4	1	9	1028	1179
3	5	8	306	327	-15	7	8	164	152	11	8	8	37	45	8	10	8	-2	0	-3	1	9	34	46
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8	5	8	411	395	-10	7	8	232	251	16	8	8	-7	0	-8	11	8	70	60	2	1	9	17496	18801
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10	5	8	315	273	-8	7	8	539	547	18	8	8	-5	3	-6	11	8	87	9	4	1	9	11862	11979
11	5	8	1407	1442	-7	7	8	97	78	19	8	8	39	37	-5	11	8	-11	17	5	1	9	443	522
12	5	8	1360	1244	-6	7	8	143	124	-18	9	8	138	0	-4	11	8	110	4	6	1	9	29413	28642
13	5	8	410	410	-5	7	8	318	333	-17	9	8	20	14	-3	11	8	0	15	7	1	9	1093	792
14	5	8	580	568	-4	7	8	69	60	-16	9	8	58	1	-2	11	8	53	22	8	1	9	1617	1743
15	5	8	3	3	-3	7	8	173	166	-15	9	8	21	0	-1	11	8	22	2	9	1	9	310	284
16	5	8	462	509	-2	7	8	211	220	-14	9	8	-1	14	0	11	8	182	251	10	1	9	2508	2446
17	5	8	1	1	-1	7	8	55	40	-13	9	8	40	34	1	11	8	-10	0	11	1	9	216	169
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16	1	9	847	867	-4	3	9	143	154	19	4	9	143	113	1	6	9	8	0	-14	8	9	16	2
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18	1	9	439	308	-2	3	9	4596	4344	-21	5	9	57	48	3	6	9	30	39	-12	8	9	28	2
19	1	9	82	64	-1	3	9	1093	1295	-20	5	9	45	55	4	6	9	622	561	-11	8	9	70	88
20	1	9	243	301	0	3	9	529	620	-19	5	9	227	226	5	6	9	51	67	-10	8	9	0	12
-22	2	9	123	5	1	3	9	2350	2647	-18	5	9	236	182	6	6	9	0	14	-9	8	9	39	25
-21	2	9	152	136	2	3	9	3989	3598	-17	5	9	371	382	7	6	9	23	28	-8	8	9	70	80
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-19	2	9	75	73	4	3	9	78	45	-15	5	9	20	3	9	6	9	589	556	-6	8	9	123	130
-18	2	9	391	432	5	3	9	302	300	-14	5	9	67	62	10	6	9	35	38	-5	8	9	565	624
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-8	2	9	771	779	15	3	9	202	223	-4	5	9	447	407	-21	7	9	7	15	5	8	9	773	854
-7	2	9	453	370	16	3	9	109	101	-3	5	9	842	782	-20	7	9	38	71	6	8	9	39	22
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Table B.3, continued

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2	2	9	266	254	-18	4	9	427	464	6	5	9	671	635	-11	7	9	-1	8	15	8	9	5	0
3	2	9	558	527	-17	4	9	61	25	7	5	9	1889	1964	-10	7	9	642	662	16	8	9	15	2
4	2	9	426	417	-16	4	9	34	26	8	5	9	93	96	-9	7	9	-5	6	17	8	9	20	17
5	2	9	97	86	-15	4	9	260	281	9	5	9	70	26	-8	7	9	157	145	18	8	9	-1	0
6	2	9	943	872	-14	4	9	1415	1343	10	5	9	88	113	-7	7	9	226	296	-18	9	9	73	9
7	2	9	2927	2512	-13	4	9	471	432	11	5	9	625	525	-6	7	9	1110	1097	-17	9	9	11	0
8	2	9	1494	1291	-12	4	9	474	495	12	5	9	482	444	-5	7	9	37	42	-16	9	9	65	26
9	2	9	17	28	-11	4	9	23	7	13	5	9	254	242	-4	7	9	101	100	-15	9	9	17	3
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Table B.3, continued

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-9	7	10	524	442	17	8	10	8	0	-6	11	10	21	19	7	1	11	1475	1284	-12	3	11	77	51
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Table B.3, continued

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7	10	12	14	40	4	1	13	2092	2019	-12	3	13	9	3	13	4	13	17	1	-5	6	13	438	371
8	10	12	-1	11	5	1	13	520	494	-11	3	13	713	650	14	4	13	734	749	-4	6	13	187	205
9	10	12	11	3	6	1	13	887	894	-10	3	13	24	11	15	4	13	26	31	-3	6	13	6131	6039
10	10	12	2	1	7	1	13	1674	1533	-9	3	13	51	40	16	4	13	78	73	-2	6	13	11	15
-7	11	12	213	32	8	1	13	67	37	-8	3	13	1146	1138	17	4	13	2	1	-1	6	13	16	14
-6	11	12	34	25	9	1	13	757	749	-7	3	13	1172	1350	18	4	13	105	129	0	6	13	834	790
-5	11	12	-9	2	10	1	13	518	398	-6	3	13	197	159	19	4	13	54	4	1	6	13	360	363
-4	11	12	58	1	11	1	13	13	4	-5	3	13	916	851	20	4	13	6	67	2	6	13	1600	1536
-3	11	12	17	21	12	1	13	17	5	-4	3	13	313	307	21	4	13	114	11	3	6	13	146	140
-2	11	12	22	15	13	1	13	274	298	-3	3	13	3260	3308	-21	5	13	84	96	4	6	13	1020	983
-1	11	12	9	2	14	1	13	419	433	-2	3	13	4	8	-20	5	13	-9	26	5	6	13	45	41

Table B.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
0	11	12	29	17	15	1	13	30	1	-1	3	13	389	465	-19	5	13	152	169	6	6	13	39	17
1	11	12	45	1	16	1	13	431	491	0	3	13	860	749	-18	5	13	73	98	7	6	13	550	495
2	11	12	7	6	17	1	13	26	10	1	3	13	1915	1832	-17	5	13	218	201	8	6	13	44	50
3	11	12	37	3	18	1	13	131	173	2	3	13	922	849	-16	5	13	270	280	9	6	13	252	225
4	11	12	-1	2	19	1	13	-46	13	3	3	13	2041	2153	-15	5	13	93	108	10	6	13	47	30
5	11	12	120	2	-21	2	13	32	6	4	3	13	572	523	-14	5	13	-4	6	11	6	13	86	85
6	11	12	58	0	-20	2	13	64	65	5	3	13	1980	1872	-13	5	13	1555	1538	12	6	13	18	12
7	11	12	-1	1	-19	2	13	54	34	6	3	13	1466	1253	-12	5	13	331	270	13	6	13	32	24
-21	0	13	-33	10	-18	2	13	167	203	7	3	13	2313	2153	-11	5	13	845	780	14	6	13	120	225
-19	0	13	-16	12	-17	2	13	142	178	8	3	13	322	303	-10	5	13	275	319	15	6	13	82	111
-17	0	13	5	0	-16	2	13	29	26	9	3	13	3	10	-9	5	13	24	4	16	6	13	15	4
-15	0	13	122	161	-15	2	13	406	417	10	3	13	172	160	-8	5	13	131	131	17	6	13	49	24
-13	0	13	28	31	-14	2	13	36	38	11	3	13	1357	1357	-7	5	13	332	266	18	6	13	11	2
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-7	0	13	6638	6558	-11	2	13	180	200	14	3	13	104	74	-4	5	13	170	179	-18	7	13	93	55
-5	0	13	1734	1536	-10	2	13	377	375	15	3	13	198	175	-3	5	13	379	423	-17	7	13	26	13
-3	0	13	583	592	-9	2	13	216	192	16	3	13	121	139	-2	5	13	116	121	-16	7	13	53	13
-1	0	13	735	771	-8	2	13	22	2	17	3	13	200	154	-1	5	13	1833	1674	-15	7	13	93	124
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3	0	13	759	702	-6	2	13	378	392	19	3	13	150	132	1	5	13	57	100	-13	7	13	58	12
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7	0	13	86	94	-4	2	13	1390	1276	-20	4	13	12	3	3	5	13	42	55	-11	7	13	70	55
9	0	13	223	226	-3	2	13	3101	2982	-19	4	13	16	3	4	5	13	72	75	-10	7	13	233	242
11	0	13	83	45	-2	2	13	26	43	-18	4	13	-13	8	5	5	13	134	181	-9	7	13	52	60
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17	0	13	287	230	1	2	13	775	516	-15	4	13	-4	0	8	5	13	8	19	-6	7	13	346	343
19	0	13	228	325	2	2	13	3356	3215	-14	4	13	91	93	9	5	13	234	218	-5	7	13	252	259
-22	1	13	222	116	3	2	13	331	289	-13	4	13	21	8	10	5	13	6	10	-4	7	13	422	411
-21	1	13	109	128	4	2	13	1353	1471	-12	4	13	22	5	11	5	13	27	20	-3	7	13	170	163
-20	1	13	486	509	5	2	13	8	26	-11	4	13	156	160	12	5	13	3	6	-2	7	13	923	874
-19	1	13	143	98	6	2	13	1295	1251	-10	4	13	871	862	13	5	13	245	218	-1	7	13	28	46
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-13	1	13	50	53	12	2	13	23	7	-4	4	13	866	889	19	5	13	67	41	5	7	13	6	0
-12	1	13	1106	1013	13	2	13	79	82	-3	4	13	0	2	-21	6	13	34	29	6	7	13	348	349
-11	1	13	23	28	14	2	13	120	126	-2	4	13	114	82	-20	6	13	-19	2	7	7	13	15	0
-10	1	13	1746	1775	15	2	13	159	158	-1	4	13	48	35	-19	6	13	10	7	8	7	13	158	169
-9	1	13	709	565	16	2	13	69	109	0	4	13	758	790	-18	6	13	31	11	9	7	13	233	162
-8	1	13	5915	5756	17	2	13	37	12	1	4	13	68	106	-17	6	13	-9	16	10	7	13	106	133
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1	1	13	1264	1140	-15	3	13	496	459	10	4	13	728	682	-8	6	13	357	339	-19	8	13	-6	10
2	1	13	177	228	-14	3	13	113	117	11	4	13	113	136	-7	6	13	60	50	-18	8	13	38	13
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-14	8	13	9	0	-14	10	13	29	9	-14	1	14	724	646	11	2	14	70	46	-4	4	14	41	49
-13	8	13	-1	0	-13	10	13	26	1	-13	1	14	91	69	12	2	14	-13	3	-3	4	14	648	667
-12	8	13	19	38	-12	10	13	-21	11	-12	1	14	717	727	13	2	14	26	25	-2	4	14	8	2
-11	8	13	32	45	-11	10	13	33	0	-11	1	14	335	347	14	2	14	125	118	-1	4	14	54	54
-10	8	13	2	10	-10	10	13	63	46	-10	1	14	732	786	15	2	14	334	329	0	4	14	10	16
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-8	8	13	14	15	-8	10	13	94	82	-8	1	14	9	11	17	2	14	98	51	2	4	14	265	197
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-6	8	13	203	226	-6	10	13	83	49	-6	1	14	6193	5951	19	2	14	41	41	4	4	14	189	169
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-4	8	13	721	750	-4	10	13	19	40	-4	1	14	498	499	-20	3	14	405	468	6	4	14	412	388
-3	8	13	-1	3	-3	10	13	11	3	-3	1	14	3282	3399	-19	3	14	4	6	7	4	14	350	323
-2	8	13	214	235	-2	10	13	18	27	-2	1	14	80	126	-18	3	14	543	576	8	4	14	100	75
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0	8	13	7	3	0	10	13	45	12	0	1	14	28	10	-16	3	14	638	659	10	4	14	195	234
1	8	13	6	1	1	10	13	-9	7	1	1	14	902	1029	-15	3	14	427	457	11	4	14	331	341
2	8	13	154	178	2	10	13	106	119	2	1	14	845	837	-14	3	14	3928	3756	12	4	14	36	21
3	8	13	2	1	3	10	13	31	40	3	1	14	1806	1788	-13	3	14	7	22	13	4	14	418	469
4	8	13	23	11	4	10	13	27	12	4	1	14	42	52	-12	3	14	708	639	14	4	14	35	15
5	8	13	122	94	5	10	13	0	0	5	1	14	899	976	-11	3	14	6	4	15	4	14	46	58
6	8	13	5	1	6	10	13	11	0	6	1	14	1478	1360	-10	3	14	2062	1950	16	4	14	33	29
7	8	13	54	95	7	10	13	22	28	7	1	14	271	232	-9	3	14	142	105	17	4	14	195	176
8	8	13	4	8	8	10	13	52	49	8	1	14	113	168	-8	3	14	1883	1996	18	4	14	23	36
9	8	13	176	136	9	10	13	22	4	9	1	14	184	180	-7	3	14	282	262	19	4	14	65	5
10	8	13	75	69	10	10	13	41	10	10	1	14	320	292	-6	3	14	3122	2799	20	4	14	-49	5
11	8	13	26	32	-6	11	13	55	11	11	1	14	670	634	-5	3	14	50	24	21	4	14	116	119
12	8	13	30	1	-5	11	13	34	15	12	1	14	36	70	-4	3	14	523	551	-21	5	14	207	30
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14	8	13	-18	4	-3	11	13	18	21	14	1	14	32	1	-2	3	14	1193	1216	-19	5	14	11	22
15	8	13	100	37	-2	11	13	5	1	15	1	14	268	295	-1	3	14	35	10	-18	5	14	41	31
16	8	13	0	0	-1	11	13	41	49	16	1	14	87	26	0	3	14	87	102	-17	5	14	108	92
17	8	13	25	14	0	11	13	18	1	17	1	14	26	40	1	3	14	391	345	-16	5	14	22	15
-18	9	13	80	84	1	11	13	40	10	18	1	14	28	11	2	3	14	399	457	-15	5	14	97	129
-17	9	13	175	4	2	11	13	2	1	19	1	14	213	18	3	3	14	538	508	-14	5	14	527	540
-16	9	13	-2	17	3	11	13	-13	60	-21	2	14	9	3	4	3	14	142	175	-13	5	14	169	139
-15	9	13	46	55	4	11	13	11	2	-20	2	14	39	48	5	3	14	1428	1284	-12	5	14	576	579
-14	9	13	103	92	5	11	13	13	11	-19	2	14	-13	9	6	3	14	2430	2323	-11	5	14	627	656
-13	9	13	57	59	6	11	13	-20	0	-18	2	14	25	1	7	3	14	194	187	-10	5	14	774	775
-12	9	13	86	52	-20	0	14	-17	4	-17	2	14	96	70	8	3	14	173	219	-9	5	14	97	91
-11	9	13	116	102	-18	0	14	12	46	-16	2	14	883	904	9	3	14	-13	3	-8	5	14	49	50
-10	9	13	14	52	-16	0	14	577	582	-15	2	14	494	497	10	3	14	0	13	-7	5	14	1955	1886
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-8	9	13	24	53	-12	0	14	114	127	-13	2	14	197	185	12	3	14	101	91	-5	5	14	32	19
-7	9	13	-4	0	-10	0	14	296	324	-12	2	14	171	172	13	3	14	59	149	-4	5	14	97	37
-6	9	13	148	150	-8	0	14	3940	3639	-11	2	14	67	82	14	3	14	115	113	-3	5	14	98	103
-5	9	13	81	73	-6	0	14	1917	1909	-10	2	14	216	264	15	3	14	216	183	-2	5	14	2047	1961

Table B.3, continued

H	K	L	Obs	Calc
-4	9	13	41	29
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2	9	13	245	295
3	9	13	4	8
4	9	13	47	33
5	9	13	28	16
6	9	13	10	15
7	9	13	-2	6
8	9	13	134	131
9	9	13	24	37
10	9	13	51	5
11	9	13	19	30
12	9	13	11	1
13	9	13	30	29
17	5	14	28	3
18	5	14	47	87
19	5	14	0	54
-20	6	14	11	5
-19	6	14	11	2
-18	6	14	4	0
-17	6	14	209	138
-16	6	14	62	2
-15	6	14	-5	57
-14	6	14	114	84
-13	6	14	160	150
-12	6	14	30	29
-11	6	14	16	19
-10	6	14	14	0
-9	6	14	17	4
-8	6	14	6	18
-7	6	14	152	121
-6	6	14	482	539
-5	6	14	299	304
-4	6	14	228	184
-3	6	14	2382	2494
-2	6	14	1177	1100
-1	6	14	1923	1932
0	6	14	1452	1414
1	6	14	1838	1675
2	6	14	644	595
3	6	14	-1	5
4	6	14	88	48
5	6	14	80	97
6	6	14	52	48
7	6	14	0	2
8	6	14	172	153
9	6	14	-9	8
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11	6	14	51	17
12	6	14	34	11
13	6	14	74	90
14	6	14	82	81
15	6	14	8	0
16	6	14	77	67
17	6	14	49	0
18	6	14	36	8
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-19	7	14	152	134
-18	7	14	33	10
-17	7	14	106	182
-16	7	14	64	11
-15	7	14	16	9
-14	7	14	138	126
-13	7	14	372	432
-12	7	14	-20	2
-11	7	14	43	56
-10	7	14	45	28
-9	7	14	1062	1068
-8	7	14	18	1
-7	7	14	656	733
-6	7	14	16	11
-5	7	14	377	347
-4	7	14	119	122
-3	7	14	50	62
-2	7	14	1	2
-1	7	14	496	543
0	7	14	159	166
1	7	14	217	246
2	7	14	45	2
3	7	14	45	64
-18	4	15	65	54
-17	4	15	316	315
-16	4	15	625	686
-15	4	15	6	26
-14	4	15	24	6
-13	4	15	25	12
-12	4	15	14	3
-11	4	15	240	257
-10	4	15	600	628
-9	4	15	437	435
-8	4	15	18	2
-7	4	15	305	291
-6	4	15	1097	1089
-5	4	15	402	330
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-1	4	15	53	47
0	4	15	1340	1305

H	K	L	Obs	Calc
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2	0	14	1876	1856
4	0	14	2976	3360
6	0	14	2337	2438
8	0	14	256	247
10	0	14	247	286
12	0	14	99	86
14	0	14	137	199
16	0	14	55	85
18	0	14	137	185
-22	1	14	32	27
-21	1	14	127	153
-20	1	14	181	217
-19	1	14	479	387
-18	1	14	400	465
-17	1	14	492	483
4	7	14	20	36
5	7	14	117	117
6	7	14	-16	3
7	7	14	27	44
8	7	14	1	14
9	7	14	58	78
10	7	14	29	46
11	7	14	152	135
12	7	14	20	7
13	7	14	1	30
14	7	14	15	6
15	7	14	-4	7
16	7	14	-26	1
17	7	14	-13	4
-19	8	14	-5	35
-18	8	14	110	34
-17	8	14	16	2
-16	8	14	58	20
-15	8	14	7	1
-14	8	14	-5	14
-13	8	14	33	4
-12	8	14	44	13
-11	8	14	46	43
-10	8	14	219	227
-9	8	14	142	108
-8	8	14	35	10
-7	8	14	49	39
-6	8	14	54	51
-5	8	14	329	341
-4	8	14	105	101
-3	8	14	6	10
-2	8	14	29	33
-1	8	14	367	401
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1	8	14	56	39
2	8	14	83	93
3	8	14	22	24
4	8	14	85	105
5	8	14	14	15
6	8	14	33	23
7	8	14	37	50
8	8	14	268	221
9	8	14	92	110
10	8	14	129	105
11	8	14	79	91
12	8	14	13	2
13	8	14	19	1
14	8	14	114	115
15	8	14	-1	9
16	8	14	1	3
17	8	14	13	1
-18	9	14	-54	3
-17	9	14	26	9
-16	9	14	164	58
-15	9	14	79	9
-14	9	14	11	12
-13	9	14	-22	11
-12	9	14	86	14
-11	9	14	84	64
-10	9	14	67	49
-9	9	14	60	24
-8	9	14	4	8
-7	9	14	152	162
-6	9	14	29	24
-5	9	14	73	87
-4	9	14	88	62
6	5	15	725	772
7	5	15	690	598
8	5	15	27	38
9	5	15	304	382
10	5	15	14	6
11	5	15	83	86
12	5	15	-11	3
13	5	15	173	152
14	5	15	69	55
15	5	15	-22	1
16	5	15	143	128
17	5	15	17	4
18	5	15	50	17
19	5	15	15	105
-20	6	15	-45	44
-19	6	15	-31	21
-18	6	15	-29	2
-17	6	15	118	117
-16	6	15	6	7

H	K	L	Obs	Calc
-9	2	14	117	151
-8	2	14	1021	876
-7	2	14	70	50
-6	2	14	370	384
-5	2	14	168	222
-4	2	14	646	716
-3	2	14	236	247
-2	2	14	1041	977
-1	2	14	1433	1295
0	2	14	1607	1574
1	2	14	604	606
2	2	14	350	332
3	2	14	347	362
4	2	14	-11	8
5	2	14	45	69
6	2	14	2142	2106
7	2	14	893	876
8	2	14	11	2
-3	9	14	14	18
-2	9	14	25	28
-1	9	14	14	20
0	9	14	8	8
1	9	14	0	13
2	9	14	7	7
3	9	14	62	89
4	9	14	22	6
5	9	14	7	0
6	9	14	21	0
7	9	14	43	40
8	9	14	28	4
9	9	14	59	54
10	9	14	59	56
11	9	14	30	53
12	9	14	20	71
13	9	14	-20	4
14	9	14	-7	29
-13	10	14	-44	8
-12	10	14	44	7
-11	10	14	107	34
-10	10	14	28	15
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-7	10	14	67	71
-6	10	14	23	5
-5	10	14	-1	2
-4	10	14	6	21
-3	10	14	4	1
-2	10	14	-14	0
-1	10	14	24	10
0	10	14	2	11
1	10	14	4	5
2	10	14	-10	10
3	10	14	24	20
4	10	14	50	58
5	10	14	19	0
6	10	14	36	1
7	10	14	10	9
8	10	14	8	5
9	10	14	35	6
-6	11	14	210	5
-5	11	14	55	10
-4	11	14	36	16
-3	11	14	-8	1
-2	11	14	8	5
-1	11	14	30	0
0	11	14	24	13
1	11	14	49	6
2	11	14	-1	23
3	11	14	89	1
4	11	14	-33	17
5	11	14	29	2
6	11	14	-5	4
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-19	0	15	4	7
-17	0	15	32	2
-15	0	15	485	489
-13	0	15	406	388
-11	0	15	235	220
-9	0	15	369	346
-7	0	15	49	51
-5	0	15	90	102
-3	0	15	1991	1949
-1	0	15	724	481
1	0	15	8825	8697
-6	7	15	305	306
-5	7	15	1	5
-4	7	15	39	44
-3	7	15	467	470
-2	7	15	18	20
-1	7	15	37	24
0	7	15	668	705
1	7	15	0	2
2	7	15	6	12
3	7	15	-4	1
4	7	15	108	79
5	7	15	-7	2
6	7	15	55	22
7	7	15	69	70
8	7	15	79	151
9	7	15	37	67
10	7	15	99	89
11	7	15	-19	20
12	7	15	33	64

H	K	L	Obs	Calc
16	3	14	77	89
17	3	14	36	38
18	3	14	35	18
-21	4	14	-32	37
-20	4	14	20	4
-19	4	14	70	30
-18	4	14	46	70
-17	4	14	65	47
-16	4	14	17	0
-15	4	14	181	240
-14	4	14	19	1
-13	4	14	51	69
-12	4	14	110	140
-11	4	14	61	56
-10	4	14	21	40
-9	4	14	231	268
-8	4	14	209	262
-7	4	14	144	115
3	0	15	4459	4518
5	0	15	2832	2541
7	0	15	2913	3097
9	0	15	566	635
11	0	15	261	274
13	0	15	179	114
15	0	15	399	347
17	0	15	-1	3
-21	1	15	29	71
-20	1	15	293	340
-19	1	15	59	24
-18	1	15	546	530
-17	1	15	362	357
-16	1	15	906	912
-15	1	15	-1	1
-14	1	15	732	684
-13	1	15	126	105
-12	1	15	1621	1527
-11	1	15	134	132
-10	1	15	410	418
-9	1	15	395	400
-8	1	15	2027	1972
-7	1	15	28	2
-6	1	15	1370	1453
-5	1	15	1483	1450
-4	1	15	2301	2342
-3	1	15	-7	3
-2	1	15	319	368
-1	1	15	288	250
0	1	15	492	474
1	1	15	0	19
2	1	15	2577	2487
3	1	15	207	179
4	1	15	2441	2387
5	1	15	23	32
6	1	15	1809	1827
7	1	15	143	116
8	1	15	2921	2967
9	1	15	153	133
10	1	15	1470	1517
11	1	15	-8	1
12	1	15	323	325
13	1	15	28	58
14	1	15	362	343
15	1	15	35	71
16	1	15	233	190
17	1	15	36	4
18	1	15	-11	30
-21	2	15	-9	22
-20	2	15	11	28
-19	2	15	36	67
-18	2	15	-9	14
-17	2	15	12	1
-16	2	15	57	47
-15	2	15	8	23
-14	2	15	107	136
-13	2	15	22	27
-12	2	15	92	74
-11	2	15	104	111
-10	2	15	290	244
-9	2	15	6	6
-8	2	15	1081	1101
-7	2	15	28	53
-6	2	15	1234	1162
-5	2	15	138	179
-4	2	15	1091	994
-10	9	15	47	47
-9	9	15	75	110
-8	9	15	13	1
-7	9	15	2	1
-6	9	15	27	9
-5	9	15	42	47
-4	9	15	2	16
-3	9	15	13	12
-2	9	15	-10	11
-1	9	15	9	15
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1	9	15	-10	11
2	9	15	6	11
3	9	15	13	5
4	9	15	32	21
5	9	15	19	8
6	9	15	19	43
7	9	15	4	28
8	9	15	29	5

H	K	L	Obs	Calc
-1	5	14	375	405
0	5	14	1767	1800
1	5	14	705	699
2	5	14	527	610
3	5	14	76	37
4	5	14	-1	3
5	5	14	-2	3
6	5	14	628	611
7	5	14	2	9
8	5	14	62	64
9	5	14	25	11
10	5	14	204	197
11	5	14	5	17
12	5	14	200	191
13	5	14	215	199
14	5	14	0	10
15	5	14	52	12
16	5	14	83	23
-3	2	15	244	259
-2	2	15	233	258
-1	2	15	334	323
0	2	15	245	257
1	2	15	22	18
2	2	15	529	479
3	2	15	1458	1374
4	2	15	744	808
5	2	15	755	770
6	2	15	408	457
7	2	15	320	292
8	2	15	1887	1870
9	2	15	133	107
10	2	15	819	782
11	2	15	597	675
12	2	15	11	2
13	2	15	215	230
14	2	15	296	298
15	2	15	220	219
16	2	15	323	256
17	2	15	51	99
18	2	15	-16	43
-21	3	15	36	25
-20	3	15	9	2
-19	3	15	103	170
-18	3	15	70	92
-17	3	15	0	25
-16	3	15	70	99
-15	3	15	1008	993
-14	3	15	94	137
-13	3	15	609	563
-12	3	15	10	10
-11	3	15	1807	1710
-10	3	15	134	131
-9	3	15	114	107
-8	3	15	64	62
-7	3	15	4839	4593
-6	3	15	377	355
-5	3	15	1860	1765
-4	3	15	35	25
-3	3	15	1291	1326
-2	3	15	35	12
-1	3	15	1258	1256
0	3	15	7	3
1	3	15	636	545
2	3	15	77	54
3	3	15	1525	1550
4	3	15	412	388
5	3	15	1706	1595
6	3	15	342	315
7	3	15	542	487
8	3	15	83	73
9	3	15	28	1
10	3	15	23	79
11	3	15	302	349
12	3	15	82	105
13	3	15	66	63
14	3	15	123	121
15	3	15	180	195
16	3	15	-23	0
17	3	15	79	81
18	3	15	130	19
22	3	15	-45	30
-21	4	15	2	89
-20	4	15	2	0
-19	4	15	99	31
-6	0	16	947	856
-4	0	16	2259	2405
-2	0	16	5805	6007
0	0	16	3280	2611
2	0	16	7975	7215
4	0	16	941	1234
6	0	16	198	160
8	0	16	1208	1141
10	0	16	927	791
12	0	16	408	362
14	0	16	619	598
16	0	16	872	872
18	0	16	489	520
-21	1	16	190	62
-20	1	16	191	165
-19	1	16	176	190
-18	1	16	49	8
-17	1	16	1009	1011
-16	1	16	314	246

Table B.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
1	4	15	88	96	-15	6	15	180	187	13	7	15	-1	26	9	9	15	-11	8	-15	1	16	313	323
2	4	15	781	749	-14	6	15	65	29	14	7	15	13	6	10	9	15	11	47	-14	1	16	0	6
3	4	15	73	28	-13	6	15	58	33	15	7	15	53	11	11	9	15	109	146	-13	1	16	446	372
4	4	15	1502	1318	-12	6	15	107	105	16	7	15	58	1	12	9	15	44	7	-12	1	16	81	51
5	4	15	154	156	-11	6	15	308	288	17	7	15	24	4	13	9	15	19	2	-11	1	16	533	524
6	4	15	4	6	-10	6	15	326	373	-18	8	15	-7	11	14	9	15	104	4	-10	1	16	63	61
7	4	15	540	509	-9	6	15	169	175	-17	8	15	54	57	-13	10	15	34	15	-9	1	16	312	298
8	4	15	616	666	-8	6	15	731	671	-16	8	15	20	16	-12	10	15	109	1	-8	1	16	10	1
9	4	15	12	5	-7	6	15	7	7	-15	8	15	22	12	-11	10	15	-2	9	-7	1	16	3956	3742
10	4	15	378	363	-6	6	15	11	21	-14	8	15	15	20	-10	10	15	-34	0	-6	1	16	17	4
11	4	15	42	46	-5	6	15	146	138	-13	8	15	60	15	-9	10	15	32	2	-5	1	16	1457	1258
12	4	15	266	236	-4	6	15	548	543	-12	8	15	97	110	-8	10	15	-1	3	-4	1	16	135	98
13	4	15	53	24	-3	6	15	2489	2382	-11	8	15	221	210	-7	10	15	-2	4	-3	1	16	1444	1418
14	4	15	200	175	-2	6	15	1669	1803	-10	8	15	32	0	-6	10	15	43	43	-2	1	16	72	57
15	4	15	59	52	-1	6	15	78	55	-9	8	15	84	75	-5	10	15	95	120	-1	1	16	406	427
16	4	15	3	3	0	6	15	1269	1282	-8	8	15	83	108	-4	10	15	31	24	0	1	16	370	429
17	4	15	45	26	1	6	15	1364	1284	-7	8	15	126	131	-3	10	15	19	27	1	1	16	127	122
18	4	15	-40	19	2	6	15	84	79	-6	8	15	0	0	-2	10	15	6	0	2	1	16	420	353
19	4	15	28	41	3	6	15	388	338	-5	8	15	38	45	-1	10	15	27	34	3	1	16	399	330
20	4	15	183	12	4	6	15	0	6	-4	8	15	79	101	0	10	15	24	14	4	1	16	163	155
21	4	15	19	1	5	6	15	162	155	-3	8	15	165	153	1	10	15	48	36	5	1	16	209	172
-20	5	15	133	20	6	6	15	49	61	-2	8	15	8	6	2	10	15	21	24	6	1	16	189	203
-19	5	15	139	74	7	6	15	167	164	-1	8	15	79	55	3	10	15	39	32	7	1	16	33	18
-18	5	15	133	56	8	6	15	89	78	0	8	15	15	17	4	10	15	26	11	8	1	16	1147	1244
-17	5	15	156	147	9	6	15	14	30	1	8	15	321	330	5	10	15	-4	10	9	1	16	50	31
-16	5	15	133	97	10	6	15	75	75	2	8	15	0	3	6	10	15	2	1	10	1	16	53	61
-15	5	15	238	252	11	6	15	32	24	3	8	15	221	160	7	10	15	6	4	11	1	16	45	72
-14	5	15	297	301	12	6	15	223	178	4	8	15	65	50	8	10	15	42	29	12	1	16	465	471
-13	5	15	445	464	13	6	15	-5	3	5	8	15	231	166	9	10	15	39	4	13	1	16	89	36
-12	5	15	69	46	14	6	15	75	99	6	8	15	-11	0	-5	11	15	-64	23	14	1	16	28	4
-11	5	15	471	571	15	6	15	135	144	7	8	15	36	42	-4	11	15	-43	1	15	1	16	79	58
-10	5	15	104	92	16	6	15	37	9	8	8	15	9	0	-3	11	15	40	9	16	1	16	72	1
-9	5	15	-1	2	17	6	15	31	3	9	8	15	113	112	-2	11	15	66	6	17	1	16	20	16
-8	5	15	695	683	-20	7	15	77	56	10	8	15	-16	3	-1	11	15	17	8	18	1	16	81	4
-7	5	15	41	47	-19	7	15	10	1	11	8	15	79	105	0	11	15	-10	22	-21	2	16	34	12
-6	5	15	22	14	-18	7	15	3	16	12	8	15	43	10	1	11	15	43	0	-20	2	16	65	76
-5	5	15	12	2	-17	7	15	-23	6	13	8	15	32	0	2	11	15	-30	23	-19	2	16	4	6
-4	5	15	105	108	-16	7	15	3	4	14	8	15	60	6	3	11	15	35	22	-18	2	16	89	38
-3	5	15	441	374	-15	7	15	6	2	15	8	15	108	10	4	11	15	51	1	-17	2	16	21	13
-2	5	15	871	905	-14	7	15	21	11	16	8	15	5	7	5	11	15	11	30	-16	2	16	350	339
-1	5	15	1490	1485	-13	7	15	52	57	-17	9	15	74	12	-20	0	16	105	160	-15	2	16	-14	3
0	5	15	467	453	-12	7	15	431	420	-16	9	15	-39	4	-18	0	16	97	117	-14	2	16	69	44
1	5	15	147	176	-11	7	15	10	10	-15	9	15	83	0	-16	0	16	320	376	-13	2	16	26	39
2	5	15	39	23	-10	7	15	112	114	-14	9	15	44	35	-14	0	16	677	694	-12	2	16	13	2
3	5	15	515	534	-9	7	15	16	13	-13	9	15	22	23	-12	0	16	123	102	-11	2	16	18	21
4	5	15	255	295	-8	7	15	284	299	-12	9	15	51	3	-10	0	16	31	17	-10	2	16	286	272
5	5	15	317	367	-7	7	15	23	20	-11	9	15	-21	1	-8	0	16	699	702	-9	2	16	308	274
-8	2	16	34	25	19	3	16	124	2	1	5	16	-10	4	-11	7	16	36	29	-14	9	16	-12	1
-7	2	16	843	777	20	3	16	75	24	2	5	16	73	59	-10	7	16	32	6	-13	9	16	33	34
-6	2	16	349	396	21	3	16	53	0	3	5	16	16	0	-9	7	16	24	4	-12	9	16	11	9
-5	2	16	33	9	22	3	16	-2	0	4	5	16	17	30	-8	7	16	19	0	-11	9	16	94	82
-4	2	16	627	524	-20	4	16	76	41	5	5	16	959	921	-7	7	16	37	39	-10	9	16	54	17
-3	2	16	127	101	-19	4	16	7	4	6	5	16	569	577	-6	7	16	54	85	-9	9	16	47	5
-2	2	16	940	971	-18	4	16	-1	6	7	5	16	194	202	-5	7	16	62	57	-8	9	16	66	70
-1	2	16	500	539	-17	4	16	115	118	8	5	16	62	51	-4	7	16	358	365	-7	9	16	2	2
0	2	16	2873	2701	-16	4	16	20	0	9	5	16	-7	0	-3	7	16	18	24	-6	9	16	18	10
1	2	16	120	109	-15	4	16	316	327	10	5	16	22	29	-2	7	16	80	122	-5	9	16	15	18
2	2	16	503	451	-14	4	16	156	126	11	5	16	20	3	-1	7	16	277	331	-4	9	16	14	1
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4	2	16	143	143	-12	4	16	79	68	13	5	16	0	2	1	7	16	389	459	-2	9	16	15	14
5	2	16	615	592	-11	4	16	538	503	14	5	16	24	32	2	7	16	126	86	-1	9	16	14	33
6	2	16	1048	1037	-10	4	16	137	136	15	5	16	38	10	3	7	16	13	4	0	9	16	71	80
7	2	16	43	35	-9	4	16	220	249	16	5	16	43	15	4	7	16	-14	2	1	9	16	61	68
8	2	16	354	358	-8	4	16	452	468	17	5	16	-4	18	5	7	16	-29	0	2	9	16	4	0
9	2	16	406	418	-7	4	16	2	9	18	5	16	16	1	6	7	16	17	0	3	9	16	23	11
10	2	16	266	265	-6	4	16	36	57	19	5	16	-11	9	7	7	16	-3	5	4	9	16	39	0
11	2	16	69	51	-5	4	16	1013	875	-20	6	16	24	24	8	7	16	25	11	5	9	16	-4	1
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14	2	16	346	354	-2	4	16	106	97	-17	6	16	97	94	11	7	16	6	1	8	9	16	8	0
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5	3	16	100	124	-13	5	16	253	223	13	6	16	180	184	6	8	16	146	166	-2	11	16	4	16
6	3	16	2465	2406	-12	5	16	477	520	14	6	16	104	140	7	8	16	39	2	-1	11	16	24	1
7	3	16	495	568	-11	5	16	19	21	15	6	16	44	9	8	8	16	-4	5	0	11	16	42	1
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Table B.3, continued

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11	3	16	81	45	-7	5	16	495	444	-19	7	16	249	154	12	8	16	27	0	4	11	16	34	12
12	3	16	67	109	-6	5	16	2524	2527	-18	7	16	53	62	13	8	16	35	0	5	11	16	-17	15
13	3	16	-9	8	-5	5	16	282	338	-17	7	16	36	27	14	8	16	50	60	-19	0	17	45	20
14	3	16	6	1	-4	5	16	104	109	-16	7	16	53	22	15	8	16	6	22	-17	0	17	586	578
15	3	16	108	116	-3	5	16	114	85	-15	7	16	8	5	16	8	16	199	35	-15	0	17	476	495
16	3	16	32	42	-2	5	16	941	970	-14	7	16	161	144	-17	9	16	-39	12	-13	0	17	143	122
17	3	16	55	9	-1	5	16	-3	1	-13	7	16	134	157	-16	9	16	25	28	-11	0	17	1095	1098
18	3	16	116	42	0	5	16	37	46	-12	7	16	80	62	-15	9	16	82	20	-9	0	17	923	836
-7	0	17	2310	2325	-6	2	17	1327	1298	22	3	17	-10	14	4	5	17	97	102	-7	7	17	23	21
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7	0	17	587	714	1	2	17	1248	1198	-14	4	17	201	225	11	5	17	72	63	0	7	17	907	1066
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7	9	17	42	3	-10	1	18	412	420	21	2	18	-49	9	3	4	18	855	746	-10	6	18	143	136
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9	9	17	-7	0	-8	1	18	165	117	-19	3	18	-25	2	5	4	18	273	295	-8	6	18	110	83
10	9	17	50	67	-7	1	18	448	442	-18	3	18	141	125	6	4	18	114	112	-7	6	18	44	35
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12	9	17	13	17	-5	1	18	20	20	-16	3	18	284	274	8	4	18	91	62	-5	6	18	332	356
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-12	10	17	-17	1	-3	1	18	13	2	-14	3	18	489	506	10	4	18	-1	2	-3	6	18	12	4
-11	10	17	-40	7	-2	1	18	687	628	-13	3	18	48	49	11	4	18	259	279	-2	6	18	52	52
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Table B.3, continued

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-6	10	17	8	2	3	1	18	264	241	-8	3	18	400	386	16	4	18	26	53	3	6	18	-19	6
-5	10	17	34	3	4	1	18	20	18	-7	3	18	-6	12	17	4	18	32	41	4	6	18	545	548
-4	10	17	56	20	5	1	18	89	86	-6	3	18	993	995	18	4	18	156	29	5	6	18	93	87
-3	10	17	2	1	6	1	18	19	25	-5	3	18	-12	17	19	4	18	126	18	6	6	18	71	152
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Table B.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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Table B.3, continued

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Table B.3, continued

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Table B.3, continued

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6	1	25	18	28	1	3	25	19	1	-4	5	25	19	3	-3	7	25	2	4	-6	10	25	16	11
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Table B.3, continued

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12	1	25	18	18	7	3	25	-1	11	2	5	25	22	21	3	7	25	0	1	0	10	25	15	13
13	1	25	17	0	8	3	25	80	35	3	5	25	-10	6	4	7	25	135	151	1	10	25	40	0
14	1	25	184	4	9	3	25	81	83	4	5	25	43	13	5	7	25	16	1	2	10	25	18	4
15	1	25	63	44	10	3	25	53	21	5	5	25	58	17	6	7	25	53	46	3	10	25	50	8
16	1	25	71	34	11	3	25	31	10	6	5	25	21	1	7	7	25	7	40	4	10	25	-20	8
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-2	2	26	141	133	-6	4	26	17	8	-7	6	26	24	11	2	8	26	15	23	9	0	27	81	58
-1	2	26	161	178	-5	4	26	52	73	-6	6	26	73	63	3	8	26	10	6	11	0	27	148	14
0	2	26	164	124	-4	4	26	19	16	-5	6	26	-20	0	4	8	26	15	0	13	0	27	-13	0
1	2	26	0	3	-3	4	26	130	126	-4	6	26	37	69	5	8	26	-8	2	15	0	27	27	0
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4	2	26	145	152	0	4	26	8	64	-1	6	26	72	75	8	8	26	96	5	-17	1	27	135	14
5	2	26	146	130	1	4	26	121	135	0	6	26	4	35	9	8	26	15	0	-16	1	27	46	27
6	2	26	21	51	2	4	26	20	1	1	6	26	13	3	10	8	26	17	7	-15	1	27	-18	9
7	2	26	45	31	3	4	26	2	10	2	6	26	12	25	-11	9	26	-27	0	-14	1	27	37	37
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Table B.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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10	2	26	30	17	6	4	26	31	1	5	6	26	111	115	-8	9	26	-5	0	-11	1	27	6	27
11	2	26	22	14	7	4	26	8	0	6	6	26	-10	2	-7	9	26	2	0	-10	1	27	560	673
12	2	26	17	23	8	4	26	126	14	7	6	26	21	17	-6	9	26	-31	12	-9	1	27	60	75
13	2	26	13	0	9	4	26	37	17	8	6	26	-6	0	-5	9	26	44	20	-8	1	27	39	10
14	2	26	22	0	10	4	26	4	9	9	6	26	38	34	-4	9	26	126	12	-7	1	27	190	208
15	2	26	27	3	11	4	26	-18	1	10	6	26	-18	3	-3	9	26	108	14	-6	1	27	11	15
16	2	26	32	1	12	4	26	56	0	11	6	26	70	3	-2	9	26	52	3	-5	1	27	6	1
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4	1	27	24	37	0	3	27	33	0	-1	5	27	115	138	5	7	27	5	4	0	11	27	28	11
5	1	27	171	199	1	3	27	82	36	0	5	27	33	6	6	7	27	15	0	-18	0	28	-40	8
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-7	3	27	132	87	-8	5	27	40	18	-2	7	27	0	9	3	10	27	74	1	-12	2	28	6	11
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-3	3	27	12	7	-4	5	27	-20	4	2	7	27	16	0	-3	11	27	-2	2	-8	2	28	-15	3
-2	3	27	-5	3	-3	5	27	64	105	3	7	27	17	24	-2	11	27	4	0	-7	2	28	-10	3
-6	2	28	271	230	-6	4	28	66	3	-1	6	28	-25	7	-4	9	28	-3	22	8	1	29	85	92
-5	2	28	41	5	-5	4	28	27	0	0	6	28	40	31	-3	9	28	-2	2	9	1	29	35	0
-4	2	28	-8	16	-4	4	28	23	29	1	6	28	29	8	-2	9	28	35	0	10	1	29	49	47
-3	2	28	38	1	-3	4	28	31	0	2	6	28	5	14	-1	9	28	-2	1	11	1	29	23	4
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8	2	28	58	22	8	4	28	11	14	13	6	28	35	0	-3	10	28	133	1	-11	2	29	9	14
9	2	28	-36	34	9	4	28	-65	7	-13	7	28	230	0	-2	10	28	-74	0	-10	2	29	128	176
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12	2	28	0	0	12	4	28	-7	34	-10	7	28	-14	2	1	10	28	63	3	-7	2	29	0	8
13	2	28	-47	10	13	4	28	-42	7	-9	7	28	-26	2	2	10	28	8	1	-6	2	29	51	43
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Table B.3, continued

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-16	3	28	-9	16	-13	5	28	2	4	-4	7	28	59	39	-15	0	29	-34	60	-1	2	29	17	11
-15	3	28	-25	8	-12	5	28	-34	4	-3	7	28	62	20	-13	0	29	-6	57	0	2	29	9	16
-14	3	28	24	1	-11	5	28	34	1	-2	7	28	24	4	-11	0	29	70	42	1	2	29	54	26
-13	3	28	10	10	-10	5	28	45	7	-1	7	28	65	8	-9	0	29	250	278	2	2	29	41	25
-12	3	28	20	23	-9	5	28	102	52	0	7	28	41	15	-7	0	29	62	5	3	2	29	10	18
-11	3	28	-24	3	-8	5	28	93	58	1	7	28	10	30	-5	0	29	295	306	4	2	29	0	1
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-9	3	28	-22	1	-6	5	28	52	33	3	7	28	88	56	-1	0	29	-1	0	6	2	29	30	0
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-7	3	28	40	13	-4	5	28	28	19	5	7	28	94	77	3	0	29	27	24	8	2	29	32	7
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Table B.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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3	8	30	-34	0	-17	2	31	-10	3	-8	4	31	8	1	-9	7	31	63	3	-2	1	32	70	11
4	8	30	-16	0	-16	2	31	85	0	-7	4	31	31	7	-8	7	31	64	0	-1	1	32	31	42
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Table B.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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0	3	34	138	16	1	7	34	49	1	-3	3	35	140	13	-9	1	36	52	12	-5	5	36	69	1
1	3	34	19	6	2	7	34	-14	2	-2	3	35	79	4	-8	1	36	247	4	-4	5	36	11	8
2	3	34	57	32	-13	0	35	60	2	-1	3	35	72	26	-7	1	36	-31	39	-3	5	36	113	3
3	3	34	11	27	-11	0	35	117	7	0	3	35	12	0	-6	1	36	70	10	-2	5	36	-83	9
4	3	34	111	0	-9	0	35	-47	21	1	3	35	21	13	-5	1	36	61	24	-1	5	36	62	1
5	3	34	-10	3	-7	0	35	12	3	2	3	35	-89	3	-4	1	36	22	14	0	5	36	12	0
6	3	34	107	3	-5	0	35	97	18	3	3	35	50	22	-3	1	36	-21	23	-7	6	36	0	0
-14	4	34	33	2	-3	0	35	32	23	4	3	35	67	5	-2	1	36	41	0	-6	6	36	42	1
-5	6	36	-28	0	-6	1	38	97	0															

Table B.3, continued

H	K	L	Obs	Calc
-4	6	36	-61	1
-3	6	36	34	0
-2	6	36	32	0
-1	6	36	-69	0
-9	0	37	-11	11
-7	0	37	-21	10
-5	0	37	368	7
-3	0	37	96	0
-1	0	37	29	0
1	0	37	-21	1
-11	1	37	36	14
-10	1	37	-55	0
-9	1	37	-28	14
-8	1	37	74	1
-7	1	37	63	0
-6	1	37	-11	4
-5	1	37	38	2
-4	1	37	-51	0
-3	1	37	14	1
-2	1	37	200	0
-1	1	37	19	1
0	1	37	21	0
1	1	37	85	2
-11	2	37	88	0
-10	2	37	139	12
-9	2	37	59	7
-8	2	37	-36	4
-7	2	37	148	4
-6	2	37	325	0
-5	2	37	49	5
-4	2	37	96	10
-3	2	37	-3	0
-2	2	37	-14	10
-1	2	37	30	0
0	2	37	107	1
-12	3	37	-57	6
-11	3	37	150	9
-10	3	37	-33	5
-9	3	37	49	38
-8	3	37	48	1
-7	3	37	253	1
-6	3	37	-100	0
-5	3	37	49	10
-4	3	37	-36	3
-3	3	37	199	0
-2	3	37	56	1
-1	3	37	-65	1
0	3	37	10	1
-10	4	37	118	2
-9	4	37	48	0
-8	4	37	67	0
-7	4	37	21	0
-6	4	37	-27	34
-5	4	37	-28	2
-4	4	37	375	4
-3	4	37	85	6
-2	4	37	100	7
-1	4	37	-15	1
-8	5	37	111	2
-7	5	37	-52	2
-6	5	37	17	2
-5	5	37	-39	5
-4	5	37	-39	2
-3	5	37	80	4
-4	6	37	-57	0
-5	1	38	-13	3
-4	1	38	19	0
-3	1	38	-103	1
-7	2	38	67	22
-6	2	38	-43	8
-5	2	38	46	0
-4	2	38	-30	1
-7	3	38	98	1
-6	3	38	283	1
-5	3	38	-100	0
-6	4	38	0	0

a Reflections flagged with an asterisk were considered unobserved.

Table B.4. Atomic multiplicities for $[Cu(tmp)_2]BPh_4$.

Name	Multiplicity	Name	Multiplicity	Name	Multiplicity
Cu	1.000	N(11)	1.000	N(21)	1.000
N(112)	1.000	N(212)	1.000	C(12)	1.000
C(13)	1.000	C(14)	1.000	C(15)	1.000
C(16)	1.000	C(17)	1.000	C(18)	1.000
C(19)	1.000	C(22)	1.000	C(23)	1.000
C(24)	1.000	C(25)	1.000	C(26)	1.000
C(27)	1.000	C(28)	1.000	C(29)	1.000
C(31)	1.000	C(32)	1.000	C(33)	1.000
C(34)	1.000	C(35)	1.000	C(36)	1.000
C(41)	1.000	C(42)	1.000	C(43)	1.000
C(44)	1.000	C(45)	1.000	C(46)	1.000
C(51)	1.000	C(52)	1.000	C(53)	1.000
C(54)	1.000	C(55)	1.000	C(56)	1.000
C(61)	1.000	C(62)	1.000	C(63)	1.000
C(64)	1.000	C(65)	1.000	C(66)	1.000
C(110)	1.000	C(111)	1.000	C(113)	1.000
C(114)	1.000	C(115)	1.000	C(116)	1.000
C(117)	1.000	C(118)	1.000	C(210)	1.000
C(211)	1.000	C(213)	1.000	C(214)	1.000
C(215)	1.000	C(216)	1.000	C(217)	1.000
C(218)	1.000	B	1.000	H(12)	1.000
H(16)	1.000	H(17)	1.000	H(22)	1.000
H(26)	1.000	H(27)	1.000	H(32)	1.000
H(33)	1.000	H(34)	1.000	H(35)	1.000
H(36)	1.000	H(42)	1.000	H(43)	1.000
H(44)	1.000	H(45)	1.000	H(46)	1.000
H(52)	1.000	H(53)	1.000	H(54)	1.000
H(55)	1.000	H(56)	1.000	H(62)	1.000
H(63)	1.000	H(64)	1.000	H(65)	1.000
H(66)	1.000	H(111)	1.000	H(11A)	1.000
H(11B)	1.000	H(11C)	1.000	H(11D)	1.000
H(11E)	1.000	H(11F)	1.000	H(11G)	1.000
H(11H)	1.000	H(11I)	1.000	H(11J)	1.000
H(11K)	1.000	H(11L)	1.000	H(211)	1.000
H(21A)	1.000	H(21B)	1.000	H(21C)	1.000
H(21D)	1.000	H(21E)	1.000	H(21F)	1.000
H(21G)	1.000	H(21H)	1.000	H(21I)	1.000
H(21J)	1.000	H(21K)	1.000	H(21L)	1.000

Appendix C: Crystal Data for [Cu(dipp)$_2$]TFPB

Table C.1. Anisotropic temperature factor coefficients - U's[a] for [Cu(dipp)$_2$]TFPB.

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
Cu	0.0759(5)	0.0646(5)	0.0557(5)	0.0267(4)	0.0361(4)	0.0232(4)
N(11)	0.063(3)	0.069(3)	0.059(3)	0.029(2)	0.028(2)	0.023(2)
N(21)	0.073(3)	0.060(3)	0.065(3)	0.022(2)	0.034(3)	0.029(2)
N(112)	0.107(4)	0.070(3)	0.069(3)	0.041(3)	0.053(3)	0.037(3)
N(212)	0.072(3)	0.053(3)	0.061(3)	0.022(2)	0.032(2)	0.022(2)
C(12)	0.081(4)	0.059(4)	0.084(5)	0.017(3)	0.033(4)	0.018(3)
C(13)	0.123(7)	0.064(5)	0.104(6)	0.020(4)	0.044(5)	0.010(4)
C(14)	0.127(7)	0.073(5)	0.079(5)	0.031(5)	0.029(5)	0.006(4)
C(15)	0.106(5)	0.101(6)	0.051(4)	0.054(5)	0.024(4)	0.014(4)
C(16)	0.196(11)	0.127(8)	0.070(5)	0.080(8)	0.068(6)	0.028(5)
C(17)	0.261(15)	0.159(10)	0.080(6)	0.103(11)	0.110(8)	0.052(7)
C(18)	0.223(11)	0.134(8)	0.103(6)	0.093(8)	0.115(8)	0.076(6)
C(19)	0.38(2)	0.166(12)	0.165(12)	0.113(14)	0.209(15)	0.098(10)
C(22)	0.075(4)	0.092(5)	0.073(4)	0.033(4)	0.028(3)	0.040(4)
C(23)	0.099(6)	0.138(7)	0.087(5)	0.052(5)	0.027(5)	0.057(5)
C(24)	0.115(7)	0.114(7)	0.072(5)	0.037(5)	0.017(5)	0.043(5)
C(25)	0.124(6)	0.067(4)	0.056(4)	0.027(4)	0.038(4)	0.028(3)
C(26)	0.156(8)	0.074(5)	0.059(4)	0.026(5)	0.049(5)	0.026(4)
C(27)	0.148(8)	0.070(5)	0.070(5)	0.027(5)	0.067(5)	0.023(4)
C(28)	0.104(5)	0.053(4)	0.076(4)	0.021(3)	0.055(4)	0.023(3)
C(29)	0.112(6)	0.084(5)	0.111(7)	0.038(4)	0.077(5)	0.031(5)
C(110)	0.38(2)	0.139(10)	0.204(14)	0.101(13)	0.216(16)	0.119(10)
C(111)	0.183(9)	0.097(6)	0.119(7)	0.056(6)	0.105(7)	0.068(5)
C(113)	0.106(5)	0.101(5)	0.065(4)	0.055(4)	0.049(4)	0.046(4)
C(114)	0.073(4)	0.078(4)	0.053(3)	0.039(3)	0.018(3)	0.023(3)
C(115)	0.125(6)	0.065(4)	0.108(6)	0.019(4)	0.075(5)	0.033(4)
C(116)	0.149(11)	0.257(18)	0.183(13)	-0.014(11)	0.106(11)	0.027(12)
C(117)	0.269(19)	0.39(3)	0.189(14)	0.19(2)	0.154(14)	0.211(18)
C(118)	0.256(14)	0.079(6)	0.163(10)	0.063(8)	0.149(11)	0.070(6)
C(119)	0.34(2)	0.162(12)	0.255(18)	0.169(15)	0.201(18)	0.120(13)
C(120)	0.24(2)	0.147(13)	0.222(18)	0.004(13)	0.089(15)	0.022(12)
C(210)	0.089(5)	0.091(5)	0.109(6)	0.040(4)	0.055(5)	0.029(5)
C(211)	0.076(4)	0.068(4)	0.084(4)	0.032(3)	0.044(4)	0.029(3)
C(213)	0.083(4)	0.043(3)	0.066(4)	0.019(3)	0.044(3)	0.022(3)
C(214)	0.084(4)	0.048(3)	0.055(3)	0.017(3)	0.033(3)	0.020(3)
C(215)	0.079(5)	0.148(8)	0.085(5)	0.052(5)	0.036(4)	0.054(5)
C(216)	0.148(10)	0.133(10)	0.183(12)	0.043(8)	0.092(9)	0.003(8)
C(217)	0.106(7)	0.194(12)	0.185(12)	0.022(8)	0.083(8)	0.077(10)
C(218)	0.085(5)	0.117(6)	0.098(6)	0.055(5)	0.037(4)	0.048(5)
C(219)	0.146(10)	0.198(13)	0.107(8)	-0.024(9)	0.019(7)	0.045(8)
C(220)	0.232(15)	0.207(13)	0.143(10)	0.150(12)	0.078(10)	0.098(10)
F(331)	0.310(11)	0.128(5)	0.125(5)	0.090(6)	0.010(6)	0.072(4)
F(332)	0.145(5)	0.223(8)	0.388(14)	0.122(6)	0.128(7)	0.229(9)
F(333)	0.166(5)	0.080(3)	0.224(7)	0.006(3)	-0.004(5)	0.090(4)
F(351)	0.193(8)	0.156(7)	0.357(15)	-0.101(7)	-0.162(10)	0.138(9)
F(352)	0.051(3)	0.59(3)	0.140(6)	0.015(7)	0.003(4)	-0.068(10)
F(353)	0.105(4)	0.281(10)	0.167(6)	-0.056(5)	-0.045(4)	0.134(7)
F(431)	0.107(4)	0.205(6)	0.157(5)	0.092(4)	0.048(3)	0.119(5)
F(432)	0.122(5)	0.514(18)	0.199(7)	0.185(8)	0.111(5)	0.219(10)
F(433)	0.091(4)	0.138(6)	0.382(15)	0.002(4)	-0.102(7)	0.068(7)
F(451)	0.279(10)	0.344(13)	0.107(4)	0.180(10)	0.119(6)	0.121(6)
F(452)	0.415(14)	0.164(6)	0.097(4)	-0.064(8)	-0.006(6)	0.100(5)
F(453)	0.129(5)	0.342(11)	0.101(4)	0.011(6)	0.008(4)	0.144(6)
F(531)	0.124(4)	0.199(6)	0.080(3)	0.010(4)	0.055(3)	0.051(4)
F(532)	0.076(3)	0.227(6)	0.111(4)	0.011(3)	0.044(3)	0.081(4)
F(533)	0.286(9)	0.243(8)	0.354(12)	0.155(8)	0.247(10)	0.258(10)
F(551)	0.086(3)	0.147(5)	0.114(4)	-0.029(3)	0.028(3)	0.017(3)
F(552)	0.137(5)	0.219(7)	0.093(4)	-0.089(5)	-0.040(3)	0.080(4)
F(553)	0.144(5)	0.073(3)	0.192(6)	-0.015(3)	0.051(4)	0.024(3)
F(631)	0.486(16)	0.342(12)	0.537(18)	0.343(13)	0.454(16)	0.402(14)

Table C.1, continued

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
F(632)	0.306(11)	0.109(5)	0.168(6)	0.013(5)	0.086(7)	0.084(5)
F(633)	0.176(6)	0.269(10)	0.265(9)	0.045(6)	0.050(6)	0.235(9)
F(651)	0.175(6)	0.303(9)	0.269(8)	0.188(7)	0.172(6)	0.217(8)
F(652)	0.177(7)	0.64(3)	0.262(10)	0.205(13)	0.179(8)	0.321(16)
F(653)	0.187(8)	0.170(7)	0.62(3)	0.047(6)	0.298(14)	0.102(11)
C(31)	0.050(3)	0.047(3)	0.044(3)	0.012(2)	0.022(2)	0.016(2)
C(32)	0.055(3)	0.056(3)	0.060(3)	0.018(3)	0.025(3)	0.024(3)
C(33)	0.065(4)	0.048(3)	0.071(4)	0.013(3)	0.027(3)	0.021(3)
C(34)	0.077(4)	0.052(3)	0.087(4)	0.008(3)	0.035(4)	0.027(3)
C(35)	0.058(3)	0.066(4)	0.060(3)	0.002(3)	0.019(3)	0.014(3)
C(36)	0.055(3)	0.061(3)	0.046(3)	0.013(3)	0.020(2)	0.018(3)
C(41)	0.048(3)	0.051(3)	0.045(3)	0.010(2)	0.014(2)	0.023(2)
C(42)	0.049(3)	0.073(4)	0.046(3)	0.014(3)	0.016(2)	0.029(3)
C(43)	0.048(3)	0.089(4)	0.070(4)	0.018(3)	0.022(3)	0.041(3)
C(44)	0.066(4)	0.093(5)	0.078(4)	0.025(3)	0.043(3)	0.044(4)
C(45)	0.064(4)	0.074(4)	0.058(3)	0.022(3)	0.031(3)	0.034(3)
C(46)	0.054(3)	0.064(3)	0.050(3)	0.018(3)	0.019(2)	0.027(3)
C(51)	0.054(3)	0.043(3)	0.048(3)	0.014(2)	0.019(2)	0.020(2)
C(52)	0.054(3)	0.062(3)	0.050(3)	0.010(3)	0.018(2)	0.028(3)
C(53)	0.067(4)	0.080(4)	0.047(3)	0.012(3)	0.024(3)	0.029(3)
C(54)	0.078(4)	0.078(4)	0.042(3)	0.007(3)	0.016(3)	0.021(3)
C(55)	0.064(3)	0.060(3)	0.051(3)	0.001(3)	0.014(3)	0.019(3)
C(56)	0.063(3)	0.052(3)	0.054(3)	0.007(3)	0.021(3)	0.025(3)
C(61)	0.053(3)	0.052(3)	0.041(3)	0.012(2)	0.015(2)	0.019(2)
C(62)	0.061(3)	0.055(3)	0.058(3)	0.019(3)	0.026(3)	0.026(3)
C(63)	0.078(4)	0.064(4)	0.068(4)	0.028(3)	0.034(3)	0.034(3)
C(64)	0.083(4)	0.089(5)	0.087(4)	0.050(4)	0.043(4)	0.052(4)
C(65)	0.065(4)	0.091(5)	0.086(4)	0.039(3)	0.043(3)	0.053(4)
C(66)	0.059(3)	0.073(4)	0.071(4)	0.024(3)	0.032(3)	0.045(3)
C(331)	0.090(5)	0.063(5)	0.119(7)	0.022(4)	0.022(5)	0.042(4)
C(351)	0.062(5)	0.107(6)	0.087(5)	-0.021(4)	0.018(4)	0.030(5)
C(431)	0.053(4)	0.177(9)	0.114(7)	0.032(5)	0.037(5)	0.079(7)
C(451)	0.093(5)	0.133(7)	0.074(5)	0.040(5)	0.048(4)	0.065(5)
C(531)	0.083(5)	0.143(8)	0.053(4)	0.003(5)	0.018(3)	0.045(5)
C(551)	0.091(5)	0.079(5)	0.059(4)	-0.012(4)	0.018(4)	0.018(4)
C(631)	0.126(6)	0.088(6)	0.121(6)	0.070(5)	0.076(6)	0.072(5)
C(651)	0.106(7)	0.175(10)	0.165(9)	0.076(7)	0.094(7)	0.130(8)
B	0.047(3)	0.054(3)	0.047(3)	0.014(3)	0.018(3)	0.025(3)

a The form of the anisotropic temperature factor is:
$\exp[-2\pi\ (h^2a^{*2}U(1,1) + k^2b^{*2}U(2,2) + l^2c^{*2}U(3,3) + 2hka^*b^*U(1,2) + 2hla^*c^*U(1,3) + 2klb^*c^*U(2,3))]$ where a^*, b^*, and c^* are reciprocal lattice constants.

Table C.2. Torsion angles in degrees for [Cu(dipp)$_2$]TFPB.

Atom 1	Atom 2	Atom 3	Atom 4	Angle
N(21)	Cu	N(11)	C(12)	57.04 (0.70)
N(21)	Cu	N(11)	C(114)	-120.21 (0.47)
N(112)	Cu	N(11)	C(12)	-179.95 (0.82)
N(112)	Cu	N(11)	C(114)	2.81 (0.48)
N(212)	Cu	N(11)	C(12)	-42.79 (0.72)
N(212)	Cu	N(11)	C(114)	139.97 (0.45)
N(11)	Cu	N(21)	C(22)	59.68 (0.71)
N(11)	Cu	N(21)	C(214)	-116.65 (0.45)
N(112)	Cu	N(21)	C(22)	-39.61 (0.73)
N(112)	Cu	N(21)	C(214)	144.06 (0.44)
N(212)	Cu	N(21)	C(22)	-176.64 (0.68)
N(212)	Cu	N(21)	C(214)	7.03 (0.44)
N(11)	Cu	N(112)	C(111)	-179.40 (0.84)
N(11)	Cu	N(112)	C(113)	-2.80 (0.51)
N(21)	Cu	N(112)	C(111)	-61.28 (0.89)
N(21)	Cu	N(112)	C(113)	115.32 (0.50)
N(212)	Cu	N(112)	C(111)	51.55 (0.90)
N(212)	Cu	N(112)	C(113)	-131.85 (0.51)
N(11)	Cu	N(212)	C(211)	-63.57 (0.71)
N(11)	Cu	N(212)	C(213)	110.93 (0.46)
N(21)	Cu	N(212)	C(211)	178.11 (0.68)
N(21)	Cu	N(212)	C(213)	-7.39 (0.45)
N(112)	Cu	N(212)	C(211)	49.63 (0.75)
N(112)	Cu	N(212)	C(213)	-135.87 (0.44)
Cu	N(11)	C(12)	C(13)	-179.32 (0.63)
Cu	N(11)	C(12)	C(115)	-0.77 (1.06)
C(114)	N(11)	C(12)	C(13)	-2.28 (1.11)
C(114)	N(11)	C(12)	C(115)	176.27 (0.71)
Cu	N(11)	C(114)	C(15)	178.09 (0.61)
Cu	N(11)	C(114)	C(113)	-2.33 (0.82)
C(12)	N(11)	C(114)	C(15)	0.49 (1.07)
C(12)	N(11)	C(114)	C(113)	-179.93 (0.74)
Cu	N(21)	C(22)	C(23)	-175.67 (0.70)
Cu	N(21)	C(22)	C(215)	4.10 (1.11)
C(214)	N(21)	C(22)	C(23)	0.41 (1.17)
C(214)	N(21)	C(22)	C(215)	-179.83 (0.73)
Cu	N(21)	C(214)	C(25)	175.99 (0.59)
Cu	N(21)	C(214)	C(213)	-5.63 (0.74)
C(22)	N(21)	C(214)	C(25)	-0.87 (1.03)
C(22)	N(21)	C(214)	C(213)	177.51 (0.66)
Cu	N(112)	C(111)	C(110)	173.02 (1.10)
Cu	N(112)	C(111)	C(118)	-3.38 (1.52)
C(113)	N(112)	C(111)	C(110)	-3.32 (1.68)
C(113)	N(112)	C(111)	C(118)	-179.72 (0.99)
Cu	N(112)	C(113)	C(18)	-176.15 (0.81)
Cu	N(112)	C(113)	C(114)	2.43 (0.89)
C(111)	N(112)	C(113)	C(18)	0.79 (1.33)
C(111)	N(112)	C(113)	C(114)	179.37 (0.84)
Cu	N(212)	C(211)	C(210)	173.81 (0.64)
Cu	N(212)	C(211)	C(218)	-7.24 (1.11)
C(213)	N(212)	C(211)	C(210)	-0.37 (1.15)
C(213)	N(212)	C(211)	C(218)	178.58 (0.71)
Cu	N(212)	C(213)	C(28)	-174.92 (0.55)
Cu	N(212)	C(213)	C(214)	6.58 (0.77)
C(211)	N(212)	C(213)	C(28)	0.32 (1.03)
C(211)	N(212)	C(213)	C(214)	-178.19 (0.67)
N(11)	C(12)	C(13)	C(14)	2.57 (1.36)
C(115)	C(12)	C(13)	C(14)	-175.94 (0.90)
C(12)	C(13)	C(14)	C(15)	-0.98 (1.51)
C(13)	C(14)	C(15)	C(16)	179.56 (1.05)
C(13)	C(14)	C(15)	C(114)	-0.72 (1.38)
C(14)	C(15)	C(16)	C(17)	179.93 (1.09)
C(114)	C(15)	C(16)	C(17)	0.22 (1.77)
C(14)	C(15)	C(114)	N(11)	1.02 (1.20)

Table C.2, continued

Atom 1	Atom 2	Atom 3	Atom 4	Angle	
C(14)	C(15)	C(114)	C(113)	-178.55 (	0.81)
C(16)	C(15)	C(114)	N(11)	-179.25 (	0.89)
C(16)	C(15)	C(114)	C(113)	1.19 (	1.29)
C(15)	C(16)	C(17)	C(18)	-0.99 (	2.21)
C(16)	C(17)	C(18)	C(19)	177.34 (	1.63)
C(16)	C(17)	C(18)	C(113)	0.35 (	2.10)
C(17)	C(18)	C(19)	C(110)	179.90 (	1.64)
C(113)	C(18)	C(19)	C(110)	-3.11 (	2.57)
C(17)	C(18)	C(113)	N(112)	179.63 (	1.04)
C(17)	C(18)	C(113)	C(114)	1.08 (	1.63)
C(19)	C(18)	C(113)	N(112)	2.37 (	1.78)
C(19)	C(18)	C(113)	C(114)	-176.18 (	1.25)
C(18)	C(19)	C(110)	C(111)	0.77 (	2.88)
N(21)	C(22)	C(23)	C(24)	0.75 (	1.53)
C(215)	C(22)	C(23)	C(24)	-179.00 (	0.98)
N(21)	C(22)	C(215)	C(216)	-97.82 (	0.97)
C(23)	C(22)	C(215)	C(216)	81.95 (	1.14)
C(22)	C(23)	C(24)	C(25)	-1.46 (	1.61)
C(23)	C(24)	C(25)	C(26)	-178.46 (	0.97)
C(23)	C(24)	C(25)	C(214)	0.99 (	1.39)
C(24)	C(25)	C(26)	C(27)	179.14 (	0.92)
C(214)	C(25)	C(26)	C(27)	-0.30 (	1.29)
C(24)	C(25)	C(214)	N(21)	0.18 (	1.17)
C(24)	C(25)	C(214)	C(213)	-178.14 (	0.76)
C(26)	C(25)	C(214)	N(21)	179.67 (	0.70)
C(26)	C(25)	C(214)	C(213)	1.35 (	1.13)
C(25)	C(26)	C(27)	C(28)	-1.39 (	1.35)
C(26)	C(27)	C(28)	C(29)	-176.96 (	0.85)
C(26)	C(27)	C(28)	C(213)	2.02 (	1.22)
C(27)	C(28)	C(29)	C(210)	179.51 (	0.88)
C(213)	C(28)	C(29)	C(210)	0.50 (	1.23)
C(27)	C(28)	C(213)	N(212)	-179.43 (	0.69)
C(27)	C(28)	C(213)	C(214)	-0.93 (	1.05)
C(29)	C(28)	C(213)	N(212)	-0.38 (	1.07)
C(29)	C(28)	C(213)	C(214)	178.12 (	0.70)
C(28)	C(29)	C(210)	C(211)	-0.58 (	1.45)
C(36)	C(31)	C(32)	C(33)	0.19 (	0.87)
B	C(31)	C(32)	C(33)	179.91 (	0.55)
C(32)	C(31)	C(36)	C(35)	-0.79 (	0.81)
B	C(31)	C(36)	C(35)	179.52 (	0.54)
C(32)	C(31)	B	C(41)	-77.03 (	0.59)
C(32)	C(31)	B	C(51)	45.16 (	0.67)
C(32)	C(31)	B	C(61)	159.99 (	0.49)
C(36)	C(31)	B	C(41)	102.65 (	0.60)
C(36)	C(31)	B	C(51)	-135.15 (	0.54)
C(36)	C(31)	B	C(61)	-20.32 (	0.73)
C(31)	C(32)	C(33)	C(34)	0.79 (	1.01)
C(32)	C(33)	C(34)	C(35)	-1.17 (	1.04)
C(33)	C(34)	C(35)	C(36)	0.60 (	1.04)
C(33)	C(34)	C(35)	C(351)	179.81 (	0.70)
C(34)	C(35)	C(36)	C(31)	0.41 (	0.96)
C(351)	C(35)	C(36)	C(31)	-178.80 (	0.62)
C(34)	C(35)	C(351)	F(351)	11.52 (	1.34)
C(34)	C(35)	C(351)	F(353)	134.69 (	0.98)
C(36)	C(35)	C(351)	F(351)	-169.26 (	0.96)
C(36)	C(35)	C(351)	F(353)	-46.09 (	1.19)
C(46)	C(41)	C(42)	C(43)	-1.35 (	0.98)
B	C(41)	C(42)	C(43)	-175.93 (	0.65)
C(42)	C(41)	C(46)	C(45)	3.28 (	0.96)
B	C(41)	C(46)	C(45)	177.92 (	0.61)
C(42)	C(41)	B	C(31)	91.01 (	0.65)
C(42)	C(41)	B	C(51)	-27.41 (	0.85)
C(42)	C(41)	B	C(61)	-147.21 (	0.58)
C(46)	C(41)	B	C(31)	-83.17 (	0.70)

Table C.2, continued

Atom 1	Atom 2	Atom 3	Atom 4	Angle
C(46)	C(41)	B	C(51)	158.41 (0.57)
C(46)	C(41)	B	C(61)	38.61 (0.80)
C(41)	C(42)	C(43)	C(44)	-1.52 (1.14)
C(42)	C(43)	C(44)	C(45)	2.56 (1.17)
C(43)	C(44)	C(45)	C(46)	-0.70 (1.13)
C(43)	C(44)	C(45)	C(451)	-179.75 (0.80)
C(44)	C(45)	C(46)	C(41)	-2.37 (1.07)
C(451)	C(45)	C(46)	C(41)	176.66 (0.75)
C(44)	C(45)	C(451)	F(451)	-39.29 (1.22)
C(44)	C(45)	C(451)	F(452)	78.05 (1.23)
C(44)	C(45)	C(451)	F(453)	-147.56 (0.93)
C(46)	C(45)	C(451)	F(451)	141.65 (0.87)
C(46)	C(45)	C(451)	F(452)	-101.00 (1.12)
C(46)	C(45)	C(451)	F(453)	33.38 (1.31)
C(56)	C(51)	C(52)	C(53)	-0.19 (0.93)
B	C(51)	C(52)	C(53)	174.09 (0.62)
C(52)	C(51)	C(56)	C(55)	-3.15 (0.90)
B	C(51)	C(56)	C(55)	-177.13 (0.58)
C(52)	C(51)	B	C(31)	35.36 (0.71)
C(52)	C(51)	B	C(41)	151.65 (0.57)
C(52)	C(51)	B	C(61)	-83.82 (0.64)
C(56)	C(51)	B	C(31)	-150.93 (0.56)
C(56)	C(51)	B	C(41)	-34.64 (0.82)
C(56)	C(51)	B	C(61)	89.89 (0.66)
C(51)	C(52)	C(53)	C(54)	2.29 (1.13)
C(51)	C(52)	C(53)	C(531)	-177.98 (0.71)
C(52)	C(53)	C(54)	C(55)	-1.00 (1.17)
C(531)	C(53)	C(54)	C(55)	179.28 (0.77)
C(52)	C(53)	C(531)	F(531)	157.42 (0.73)
C(52)	C(53)	C(531)	F(532)	46.04 (1.13)
C(52)	C(53)	C(531)	F(533)	-79.90 (1.03)
C(54)	C(53)	C(531)	F(531)	-22.85 (1.18)
C(54)	C(53)	C(531)	F(532)	-134.23 (0.84)
C(54)	C(53)	C(531)	F(533)	99.83 (1.04)
C(53)	C(54)	C(55)	C(56)	-2.33 (1.12)
C(53)	C(54)	C(55)	C(551)	179.67 (0.74)
C(54)	C(55)	C(56)	C(51)	4.56 (1.05)
C(551)	C(55)	C(56)	C(51)	-177.46 (0.67)
C(54)	C(55)	C(551)	F(551)	-151.46 (0.77)
C(54)	C(55)	C(551)	F(552)	-28.07 (1.10)
C(54)	C(55)	C(551)	F(553)	92.36 (0.90)
C(56)	C(55)	C(551)	F(551)	30.51 (1.11)
C(56)	C(55)	C(551)	F(552)	153.90 (0.73)
C(56)	C(55)	C(551)	F(553)	-85.66 (0.87)
C(66)	C(61)	C(62)	C(63)	3.22 (0.84)
B	C(61)	C(62)	C(63)	178.50 (0.54)
C(62)	C(61)	C(66)	C(65)	-0.40 (0.85)
B	C(61)	C(66)	C(65)	-175.98 (0.56)
C(62)	C(61)	B	C(31)	135.86 (0.55)
C(62)	C(61)	B	C(41)	17.95 (0.76)
C(62)	C(61)	B	C(51)	-107.05 (0.58)
C(66)	C(61)	B	C(31)	-49.06 (0.64)
C(66)	C(61)	B	C(41)	-166.97 (0.49)
C(66)	C(61)	B	C(51)	68.03 (0.63)
C(61)	C(62)	C(63)	C(64)	-3.66 (0.97)
C(61)	C(62)	C(63)	C(631)	176.88 (0.64)
C(62)	C(63)	C(64)	C(65)	1.05 (1.02)
C(631)	C(63)	C(64)	C(65)	-179.50 (0.70)
C(62)	C(63)	C(631)	F(631)	-18.83 (1.34)
C(62)	C(63)	C(631)	F(632)	109.39 (1.01)
C(62)	C(63)	C(631)	F(633)	-141.63 (0.86)
C(64)	C(63)	C(631)	F(631)	161.72 (1.03)
C(64)	C(63)	C(631)	F(632)	-70.06 (1.16)
C(64)	C(63)	C(631)	F(633)	38.92 (1.16)

Table C.2, continued

Atom 1	Atom 2	Atom 3	Atom 4	Angle	
C(63)	C(64)	C(65)	C(66)	1.69	(1.05)
C(64)	C(65)	C(66)	C(61)	-2.07	(1.00)
C(19)	C(110)	C(111)	N(112)	2.57	(2.44)
C(19)	C(110)	C(111)	C(118)	178.92	(1.60)
N(112)	C(113)	C(114)	N(11)	-0.02	(1.20)
N(112)	C(113)	C(114)	C(15)	179.58	(0.71)
C(18)	C(113)	C(114)	N(11)	178.58	(0.87)
C(18)	C(113)	C(114)	C(15)	-1.83	(1.29)
C(29)	C(210)	C(211)	N(212)	0.52	(1.43)
C(29)	C(210)	C(211)	C(218)	-178.41	(0.90)
N(212)	C(213)	C(214)	N(21)	-0.55	(0.95)
N(212)	C(213)	C(214)	C(25)	177.86	(0.67)
C(28)	C(213)	C(214)	N(21)	-179.13	(0.61)
C(28)	C(213)	C(214)	C(25)	-0.72	(1.05)

Table C.3. Structure factors (F^2_{obs} & F^2_{calc})[a] for [Cu(dipp)$_2$]TFPB.

H	K	L	Obs	Calc
4	0	0	276	402
5	0	0	547	374
6	0	0	704	542
7	0	0	18	31
8	0	0	161	106
9	0	0	665	628
10	0	0	46	33
11	0	0	297	269
12	0	0	12	6
13	0	0	35	23
14	0	0	0	0
-14	1	0	85	103
-13	1	0	230	228
-12	1	0	9	1
-11	1	0	39	56
-10	1	0	19	16
-9	1	0	1017	972
-8	1	0	200	187
-7	1	0	1085	1117
-6	1	0	530	439
-5	1	0	1853	1548
-4	1	0	13875	15538
-3	1	0	2	732
3	1	0	2	559
4	1	0	677	807
5	1	0	9711	9290
6	1	0	111	74
7	1	0	54	42
8	1	0	507	564
9	1	0	408	432
10	1	0	4	9
11	1	0	16	10
12	1	0	11	1
13	1	0	12	2
-14	2	0	0	2
-13	2	0	17	4
-12	2	0	6	11
-11	2	0	337	329
-10	2	0	50	93
-9	2	0	250	263
-8	2	0	1288	1428
-7	2	0	13	1
-6	2	0	156	94
-5	2	0	2629	2155
-4	2	0	103	124
3	2	0	861	838
4	2	0	2732	2150
5	2	0	418	604
6	2	0	4525	4358
7	2	0	96	83
8	2	0	178	97
9	2	0	392	392
10	2	0	50	64
11	2	0	116	141
12	2	0	29	29
13	2	0	27	12
-14	3	0	6	2
-13	3	0	92	60
-12	3	0	0	1
-11	3	0	26	47
-10	3	0	255	273
-9	3	0	207	289
-8	3	0	65	4
-7	3	0	4869	5068
-6	3	0	246	286
-5	3	0	61	57
3	-16	1	9	22
4	-16	1	18	11
5	-16	1	8	1
6	-16	1	55	31
-1	-15	1	17	7
0	-15	1	6	0
1	-15	1	26	16
2	-15	1	181	142
3	-15	1	221	231
4	-15	1	163	145
5	-15	1	370	318
6	-15	1	33	22
7	-15	1	42	59
8	-15	1	2	11
9	-15	1	11	7
-3	-14	1	151	139
-2	-14	1	18	12
-1	-14	1	15	9
0	-14	1	255	273
1	-14	1	132	129
2	-14	1	116	103
3	-14	1	144	132
4	-14	1	33	31
5	-14	1	426	373
6	-14	1	34	25
7	-14	1	0	4
8	-14	1	79	75
9	-14	1	7	1
10	-14	1	12	34
-5	-13	1	21	31
-4	-13	1	38	21
-3	-13	1	151	170
-2	-13	1	1	1
-1	-13	1	-3	9
0	-13	1	193	213
1	-13	1	153	128
2	-13	1	8	7
-4	3	0	1373	1314
-3	3	0	1958	1354
2	3	0	906	898
3	3	0	244	272
4	3	0	367	306
5	3	0	7517	6735
6	3	0	80	62
7	3	0	426	409
8	3	0	339	238
9	3	0	3	2
10	3	0	18	6
11	3	0	14	1
12	3	0	13	25
-14	4	0	2	3
-13	4	0	50	45
-12	4	0	100	92
-11	4	0	-1	1
-10	4	0	615	501
-9	4	0	246	227
-8	4	0	1308	992
-7	4	0	79	33
-6	4	0	24	39
-5	4	0	4855	4113
-4	4	0	913	1172
-3	4	0	201	419
0	4	0	7112	7906
1	4	0	25	10
2	4	0	289	290
3	4	0	6	7
4	4	0	1214	996
5	4	0	495	835
6	4	0	23	16
7	4	0	8	2
8	4	0	3	19
9	4	0	1387	1277
10	4	0	12	4
11	4	0	80	84
12	4	0	17	25
-14	5	0	0	0
-13	5	0	27	6
-12	5	0	299	267
-11	5	0	266	250
-10	5	0	73	49
-9	5	0	138	134
-8	5	0	531	633
-7	5	0	767	475
-6	5	0	1448	1661
-5	5	0	2446	2204
-4	5	0	1697	1667
-3	5	0	204	310
-2	5	0	171	162
-1	5	0	195	155
0	5	0	1147	893
1	5	0	441	380
2	5	0	1980	2349
3	5	0	2213	1987
4	5	0	1373	1218
5	5	0	1290	1158
6	5	0	-3	0
7	5	0	2211	1738
8	5	0	38	42
9	5	0	-3	6
10	5	0	88	112
11	5	0	3	1
-14	6	0	1	0
-13	6	0	118	90
-6	-11	1	27	7
-5	-11	1	110	105
-4	-11	1	-2	12
-3	-11	1	57	33
-2	-11	1	-5	1
-1	-11	1	147	192
0	-11	1	203	122
1	-11	1	99	115
2	-11	1	822	974
3	-11	1	51	96
4	-11	1	806	833
5	-11	1	83	82
6	-11	1	189	180
7	-11	1	7	6
8	-11	1	27	26
9	-11	1	14	28
10	-11	1	35	39
11	-11	1	20	27
12	-11	1	39	41
13	-11	1	115	98
-8	-10	1	32	19
-7	-10	1	99	129
-6	-10	1	4	1
-5	-10	1	7	6
-4	-10	1	-4	7
-3	-10	1	194	167
-2	-10	1	257	288
-1	-10	1	596	417
0	-10	1	59	82
1	-10	1	218	296
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4	6	0	247	139
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5	-8	1	274	355
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6	8	0	92	122
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3	9	0	157	135
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7	9	0	84	94
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-8	10	0	585	631
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-5	10	0	0	11
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6	10	0	6	12
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3	-5	1	167	107
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-2	14	0	77	99
-1	14	0	31	19
0	14	0	236	202
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-8	15	0	-12	0
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14	-3	1	39	30
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-8	-2	1	41	24
-7	-2	1	312	279
-6	-2	1	2725	3276
-5	-2	1	4032	4243
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4	-2	1	593	682
5	-2	1	2855	2943
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7	-2	1	198	171
8	-2	1	295	189
9	-2	1	13	57
10	-2	1	61	70

Table C.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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5	-13	1	97	79	11	-10	1	81	79	3	-7	1	1832	1861	-11	-4	1	366	326	13	-2	1	20	33
6	-13	1	328	365	12	-10	1	92	129	4	-7	1	742	581	-10	-4	1	7	8	14	-2	1	2	7
7	-13	1	185	151	13	-10	1	65	68	5	-7	1	402	296	-9	-4	1	134	149	-14	-1	1	31	29
8	-13	1	79	50	-9	-9	1	12	17	6	-7	1	150	38	-8	-4	1	321	215	-13	-1	1	-5	4
9	-13	1	66	59	-8	-9	1	3	1	7	-7	1	132	87	-7	-4	1	893	875	-12	-1	1	-5	0
10	-13	1	0	1	-7	-9	1	197	153	8	-7	1	40	18	-6	-4	1	557	379	-11	-1	1	10	13
11	-13	1	11	3	-6	-9	1	4	1	9	-7	1	792	612	-5	-4	1	397	377	-10	-1	1	179	226
-6	-12	1	6	0	-5	-9	1	14	17	10	-7	1	45	66	-4	-4	1	3488	3238	-9	-1	1	65	62
-5	-12	1	182	210	-4	-9	1	463	584	11	-7	1	694	704	-3	-4	1	1479	1472	-8	-1	1	231	227
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-10	2	1	87	74	8	4	1	95	112	-4	7	1	2477	1986	-9	10	1	73	60	0	13	1	22	12
-9	2	1	207	146	9	4	1	3	3	-3	7	1	1690	1788	-8	10	1	234	283	1	13	1	41	22
-8	2	1	790	770	10	4	1	74	59	-2	7	1	96	128	-7	10	1	167	130	2	13	1	30	32
-7	2	1	601	468	11	4	1	15	5	-1	7	1	740	992	-6	10	1	18	69	3	13	1	45	35
-6	2	1	352	509	12	4	1	4	1	0	7	1	95	114	-5	10	1	32	46	-10	14	1	22	24
-5	2	1	2497	2177	-14	5	1	137	148	1	7	1	196	136	-4	10	1	1176	1164	-9	14	1	271	228
-4	2	1	1726	1585	-13	5	1	97	46	2	7	1	172	108	-3	10	1	749	680	-8	14	1	32	6
-3	2	1	9	6	-12	5	1	49	47	3	7	1	122	56	-2	10	1	428	418	-7	14	1	18	4
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5	2	1	1654	1416	-8	5	1	718	763	7	7	1	2	6	2	10	1	5	30	-3	14	1	84	83
6	2	1	141	281	-7	5	1	2684	2561	8	7	1	10	8	3	10	1	75	89	-2	14	1	219	237
7	2	1	47	52	-6	5	1	11	17	9	7	1	11	0	4	10	1	76	80	-1	14	1	2	3
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1	-16	2	75	10	8	-12	2	126	144	6	-9	2	881	920	-5	-6	2	261	173	8	-4	2	2577	2813
2	-16	2	94	62	9	-12	2	109	66	7	-9	2	45	108	-4	-6	2	875	761	9	-4	2	50	57
3	-16	2	61	79	10	-12	2	75	68	8	-9	2	3	5	-3	-6	2	708	815	10	-4	2	888	968
4	-16	2	96	141	11	-12	2	116	135	9	-9	2	176	170	-2	-6	2	3966	3550	11	-4	2	21	8

Table C.3, continued

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6	-16	2	168	209	-8	-11	2	61	50	11	-9	2	8	11	0	-6	2	5758	5150	13	-4	2	4	2
7	-16	2	-1	2	-7	-11	2	0	1	12	-9	2	188	191	1	-6	2	27	40	14	-4	2	21	16
-2	-15	2	72	63	-6	-11	2	33	50	13	-9	2	-6	1	2	-6	2	1538	1054	-13	-3	2	-2	0
-1	-15	2	60	21	-5	-11	2	36	24	-10	-8	2	25	16	3	-6	2	216	106	-12	-3	2	16	14
0	-15	2	225	206	-4	-11	2	1	2	-9	-8	2	90	45	4	-6	2	1328	1187	-11	-3	2	0	11
1	-15	2	19	27	-3	-11	2	135	115	-8	-8	2	221	208	5	-6	2	7170	5750	-10	-3	2	242	265
2	-15	2	193	192	-2	-11	2	353	395	-7	-8	2	39	28	6	-6	2	5	4	-9	-3	2	57	24
3	-15	2	122	118	-1	-11	2	6	18	-6	-8	2	291	236	7	-6	2	419	378	-8	-3	2	11	2
4	-15	2	4	28	0	-11	2	54	25	-5	-8	2	5	2	8	-6	2	300	336	-7	-3	2	2	6
5	-15	2	23	30	1	-11	2	113	98	-4	-8	2	51	22	9	-6	2	118	92	-6	-3	2	127	179
6	-15	2	154	173	2	-11	2	254	223	-3	-8	2	27	22	10	-6	2	515	565	-5	-3	2	1481	1346
7	-15	2	-8	9	3	-11	2	65	83	-2	-8	2	1800	1716	11	-6	2	8	16	-4	-3	2	809	860
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9	-15	2	18	12	5	-11	2	727	740	0	-8	2	5892	6308	13	-6	2	24	54	1	-3	2	1735	1774
-4	-14	2	7	18	6	-11	2	132	225	1	-8	2	5657	5034	14	-6	2	0	1	3	-3	2	7443	8400
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6	-13	2	5	2	9	-10	2	298	195	1	-7	2	966	868	13	-5	2	52	56	3	-2	2	17286	16116
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-5	-12	2	56	39	-7	-9	2	193	181	9	-7	2	247	212	-7	-4	2	36	25	11	-2	2	2	0
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-1	-12	2	235	242	-3	-9	2	344	333	13	-7	2	19	13	-3	-4	2	3021	3748	-13	-1	2	111	134
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-8	-1	2	705	820	-9	2	2	600	640	3	4	2	71	116	-9	7	2	72	77	-11	10	2	27	32
-7	-1	2	472	380	-8	2	2	885	831	4	4	2	320	213	-8	7	2	846	787	-10	10	2	42	15
-6	-1	2	2	13	-7	2	2	3658	3753	5	4	2	16	28	-7	7	2	1118	942	-9	10	2	66	82
-5	-1	2	53	41	-6	2	2	536	448	6	4	2	63	61	-6	7	2	498	337	-8	10	2	676	652
-4	-1	2	2294	1939	-5	2	2	638	743	7	4	2	432	364	-5	7	2	676	643	-7	10	2	8	21
-3	-1	2	1	87	-4	2	2	784	1039	8	4	2	13	18	-4	7	2	4216	4139	-6	10	2	441	323
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6	-1	2	675	542	1	2	2	5	44	-15	5	2	10	1	0	7	2	-2	7	-2	10	2	336	469
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9	-1	2	185	202	4	2	2	3622	3400	-12	5	2	1	0	3	7	2	21	44	1	10	2	540	551
10	-1	2	25	11	5	2	2	62	59	-11	5	2	156	110	4	7	2	44	75	2	10	2	10	0
11	-1	2	268	224	6	2	2	286	263	-10	5	2	23	49	5	7	2	0	2	3	10	2	211	214
12	-1	2	98	96	7	2	2	175	181	-9	5	2	347	284	6	7	2	83	84	4	10	2	137	107
13	-1	2	95	64	8	2	2	472	495	-8	5	2	171	235	7	7	2	258	200	5	10	2	159	146
-14	0	2	136	129	9	2	2	177	205	-7	5	2	383	340	8	7	2	6	2	6	10	2	1	4
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-12	0	2	117	155	11	2	2	118	151	-5	5	2	-6	3	-14	8	2	18	7	-12	11	2	133	158
-11	0	2	154	171	12	2	2	72	55	-4	5	2	434	297	-13	8	2	335	339	-11	11	2	66	58
-10	0	2	133	72	-15	3	2	13	10	-3	5	2	32	43	-12	8	2	92	86	-10	11	2	22	3
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-7	0	2	1772	1505	-12	3	2	88	88	0	5	2	444	546	-9	8	2	27	64	-7	11	2	269	193
-6	0	2	54	53	-11	3	2	895	936	1	5	2	74	104	-8	8	2	933	915	-6	11	2	284	255
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5	0	2	495	442	-6	3	2	828	597	6	5	2	600	612	-3	8	2	84	160	-1	11	2	376	314
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9	0	2	428	270	-1	3	2	3979	4104	10	5	2	17	19	1	8	2	321	495	3	11	2	53	58
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12	0	2	109	126	2	3	2	2076	1959	-14	6	2	4	5	4	8	2	348	353	-12	12	2	45	54
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-11	1	2	661	605	7	3	2	466	472	-9	6	2	7	1	-14	9	2	88	96	-7	12	2	0	6
-10	1	2	107	93	8	3	2	10	39	-8	6	2	567	632	-13	9	2	59	72	-6	12	2	54	76
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Table C.3, continued

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-7	1	2	1787	1430	11	3	2	17	35	-5	6	2	-3	3	-10	9	2	1	1	-3	12	2	414	407
-6	1	2	711	514	12	3	2	46	52	-4	6	2	4299	4000	-9	9	2	5	0	-2	12	2	41	80
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Table C.3, continued

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5	-1	3	688	909	-5	2	3	3724	2868	6	4	3	76	103	-5	7	3	1829	1531	-7	10	3	268	254
6	-1	3	11	31	-4	2	3	2637	2995	7	4	3	751	723	-4	7	3	432	424	-6	10	3	67	33
7	-1	3	565	476	-3	2	3	4817	5630	8	4	3	100	78	-3	7	3	4479	4043	-5	10	3	413	259
8	-1	3	64	40	-2	2	3	639	871	9	4	3	56	33	-2	7	3	331	174	-4	10	3	654	580
9	-1	3	173	157	-1	2	3	1123	872	10	4	3	96	113	-1	7	3	11	7	-3	10	3	235	198
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12	-1	3	72	87	2	2	3	767	724	-14	5	3	263	238	2	7	3	440	526	0	10	3	110	110
13	-1	3	28	9	3	2	3	641	685	-13	5	3	214	193	3	7	3	726	776	1	10	3	67	72
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2	-14	4	-6	4	10	-11	4	133	144	5	-8	4	232	128	-8	-5	4	2	1	9	-3	4	-3	4
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Table C.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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5	-14	4	526	492	-9	-10	4	-6	0	8	-8	4	24	9	-5	-5	4	3	8	12	-3	4	240	222
6	-14	4	46	33	-8	-10	4	123	126	9	-8	4	412	289	-4	-5	4	620	802	13	-3	4	3	5
7	-14	4	131	137	-7	-10	4	18	41	10	-8	4	-1	1	-3	-5	4	0	15	-14	-2	4	2	4
8	-14	4	25	51	-6	-10	4	49	47	11	-8	4	33	43	-2	-5	4	4905	4473	-13	-2	4	104	123
9	-14	4	99	84	-5	-10	4	21	8	12	-8	4	41	56	-1	-5	4	604	669	-12	-2	4	96	70
10	-14	4	32	29	-4	-10	4	544	454	13	-8	4	14	6	0	-5	4	495	464	-11	-2	4	23	13
-6	-13	4	-3	0	-3	-10	4	17	6	-12	-7	4	13	35	1	-5	4	2122	2093	-10	-2	4	652	556
-5	-13	4	163	175	-2	-10	4	1264	1149	-11	-7	4	22	3	2	-5	4	1546	1473	-9	-2	4	582	505
-4	-13	4	13	5	-1	-10	4	9	5	-10	-7	4	332	339	3	-5	4	147	64	-8	-2	4	646	621
-3	-13	4	12	4	0	-10	4	1513	1453	-9	-7	4	87	96	4	-5	4	1655	1452	-7	-2	4	304	272
-2	-13	4	82	113	1	-10	4	474	469	-8	-7	4	62	113	5	-5	4	5361	4704	-6	-2	4	2750	2698
-1	-13	4	140	70	2	-10	4	246	213	-7	-7	4	19	28	6	-5	4	157	134	-5	-2	4	4394	5084
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-3	-2	4	3818	4944	-14	1	4	209	219	-3	3	4	2024	2384	-15	6	4	11	7	4	8	4	67	86
-2	-2	4	6102	6787	-13	1	4	40	36	-2	3	4	148	123	-14	6	4	2	1	5	8	4	26	22
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-9	-1	4	13	23	6	1	4	447	347	-10	4	4	82	79	5	6	4	349	335	2	9	4	31	7
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-2	12	4	251	233	-7	-13	5	30	20	-5	-10	5	-4	1	13	-8	5	15	2	0	-5	5	276	292
-1	12	4	22	0	-6	-13	5	14	9	-4	-10	5	12	8	-12	-7	5	33	27	1	-5	5	399	369
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-4	14	4	74	81	-8	-12	5	21	11	-10	-9	5	39	21	6	-7	5	1042	887	-8	-4	5	74	106
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Table C.3, continued

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3	-17	5	51	53	-5	-12	5	105	111	-7	-9	5	30	66	9	-7	5	336	390	-5	-4	5	3950	3351
4	-17	5	48	58	-4	-12	5	178	232	-6	-9	5	8	24	10	-7	5	469	416	-4	-4	5	70	120
5	-17	5	38	21	-3	-12	5	279	269	-5	-9	5	548	609	11	-7	5	109	93	-3	-4	5	7905	7530
-2	-16	5	52	22	-2	-12	5	1161	1276	-4	-9	5	20	34	12	-7	5	333	488	-2	-4	5	2633	3004
-1	-16	5	9	0	-1	-12	5	299	230	-3	-9	5	3250	3228	13	-7	5	46	51	-1	-4	5	78	60
0	-16	5	62	84	0	-12	5	16	6	-2	-9	5	446	338	-12	-6	5	18	5	0	-4	5	218	277
1	-16	5	135	121	1	-12	5	197	154	-1	-9	5	617	914	-11	-6	5	246	217	1	-4	5	424	294
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3	-16	5	29	37	3	-12	5	20	32	1	-9	5	439	586	-9	-6	5	211	298	3	-4	5	1906	2152
4	-16	5	15	31	4	-12	5	178	182	2	-9	5	503	756	-8	-6	5	318	173	4	-4	5	136	267
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9	-3	5	16	7	-7	0	5	51	68	5	2	5	27	31	-7	5	5	45	13	-11	8	5	329	314
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4	-2	5	95	111	-12	1	5	385	379	0	3	5	3592	3950	-10	6	5	23	18	-9	9	5	146	146
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-10	-1	5	181	163	1	1	5	33	28	-13	4	5	10	21	3	6	5	375	403	4	9	5	61	67
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6	-1	5	745	725	-10	2	5	85	71	3	4	5	999	975	-4	7	5	8	15	1	10	5	19	7
7	-1	5	429	484	-9	2	5	2072	1921	4	4	5	184	204	-3	7	5	75	75	2	10	5	135	118
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Table C.3, continued

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3	-2	6	734	901	-12	1	6	32	34	2	3	6	679	693	-5	6	6	16	24	-1	9	6	10	16
4	-2	6	11	22	-11	1	6	477	535	3	3	6	1195	1228	-4	6	6	11	23	0	9	6	61	47
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6	-2	6	514	525	-9	1	6	117	64	5	3	6	570	430	-2	6	6	26	21	2	9	6	531	431
7	-2	6	109	115	-8	1	6	3360	3092	6	3	6	490	595	-1	6	6	195	154	3	9	6	45	38
8	-2	6	31	35	-7	1	6	650	467	7	3	6	0	0	0	6	6	394	393	4	9	6	22	21
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-10	-1	6	1586	1634	2	1	6	2538	2195	-9	4	6	346	176	-13	7	6	123	133	-4	10	6	-3	1
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Table C.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
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-7	-1	6	3155	1875	5	1	6	1323	1115	-6	4	6	36	55	-10	7	6	66	50	-1	10	6	42	16
-6	-1	6	10987	9874	6	1	6	982	1058	-5	4	6	1144	1071	-9	7	6	301	241	0	10	6	221	195
-5	-1	6	5006	4524	7	1	6	112	74	-4	4	6	1337	849	-8	7	6	63	50	1	10	6	25	18
-4	-1	6	82	82	8	1	6	29	28	-3	4	6	103	85	-7	7	6	1080	1253	2	10	6	67	39
-3	-1	6	5121	5324	9	1	6	185	139	-2	4	6	460	286	-6	7	6	18	42	3	10	6	26	21
-2	-1	6	4375	3972	10	1	6	5	2	-1	4	6	207	268	-5	7	6	163	167	-11	11	6	110	101
-1	-1	6	21	10	-15	2	6	20	23	0	4	6	8	2	-4	7	6	414	409	-10	11	6	1	7
0	-1	6	292	421	-14	2	6	320	304	1	4	6	-6	17	-3	7	6	277	220	-9	11	6	77	54
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2	-1	6	3318	3125	-12	2	6	21	8	3	4	6	666	510	-1	7	6	809	858	-7	11	6	0	2
3	-1	6	13	3	-11	2	6	441	448	4	4	6	28	15	0	7	6	218	219	-6	11	6	38	31
4	-1	6	758	782	-10	2	6	200	250	5	4	6	12	5	1	7	6	851	1019	-5	11	6	6	2
5	-1	6	43	69	-9	2	6	781	937	6	4	6	31	16	2	7	6	60	51	-4	11	6	70	128
6	-1	6	442	488	-8	2	6	33	29	7	4	6	7	0	3	7	6	423	470	-3	11	6	40	40
7	-1	6	223	253	-7	2	6	1270	1380	8	4	6	228	188	4	7	6	86	95	-2	11	6	10	19
8	-1	6	46	41	-6	2	6	44	33	9	4	6	15	21	5	7	6	16	12	-1	11	6	19	29
9	-1	6	72	52	-5	2	6	6034	6270	-15	5	6	56	47	6	7	6	33	27	0	11	6	238	204
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Table C.3, continued

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8	-1	7	473	435
9	-1	7	6	13
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-1	-3	8	92	44
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7	-14	8	13	19
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5	-1	8	315	378
6	-1	8	43	22
7	-1	8	149	116
8	-1	8	360	432
9	-1	8	41	51
10	-1	8	20	16
-15	0	8	47	26
-14	0	8	39	52
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-11	0	8	686	819
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Table C.3, continued

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2	-11	8	289	251	-1	-8	8	286	456	-9	-5	8	444	512	5	-3	8	122	77	-6	0	8	202	180
3	-11	8	29	65	0	-8	8	1804	1299	-8	-5	8	121	55	6	-3	8	161	144	-5	0	8	37	1
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5	-11	8	68	114	2	-8	8	405	373	-6	-5	8	1548	1467	8	-3	8	126	133	-3	0	8	769	586
6	-11	8	300	209	3	-8	8	296	265	-5	-5	8	1543	1495	9	-3	8	11	17	-2	0	8	2430	1606
7	-11	8	143	219	4	-8	8	76	111	-4	-5	8	7	8	10	-3	8	0	0	-1	0	8	888	996
8	-11	8	148	164	5	-8	8	104	154	-3	-5	8	741	587	11	-3	8	27	17	0	0	8	0	5
9	-11	8	9	11	6	-8	8	321	360	-2	-5	8	958	1002	-14	-2	8	33	29	1	0	8	1144	1025
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-9	-10	8	12	10	10	-8	8	1	0	2	-5	8	2343	2067	-10	-2	8	190	212	5	0	8	284	285
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2	-9	9	107	141	-4	-6	9	509	616	-12	-3	9	96	144	4	-1	9	40	44	-1	2	9	1224	1295
3	-9	9	802	665	-3	-6	9	1550	1395	-11	-3	9	16	26	5	-1	9	25	41	0	2	9	1405	1320
4	-9	9	192	112	-2	-6	9	2351	2436	-10	-3	9	37	51	6	-1	9	1722	1598	1	2	9	122	85
5	-9	9	575	453	-1	-6	9	1805	2081	-9	-3	9	214	170	7	-1	9	165	144	2	2	9	606	549
6	-9	9	90	69	0	-6	9	462	327	-8	-3	9	40	63	8	-1	9	218	241	3	2	9	26	10
7	-9	9	-6	32	1	-6	9	5181	5333	-7	-3	9	2514	2156	9	-1	9	6	4	4	2	9	-4	7
8	-9	9	-7	2	2	-6	9	171	298	-6	-3	9	107	183	-14	0	9	89	73	6	2	9	544	464

Table C.3, continued

H	K	L	Obs	Calc
9	-9	9	41	41
10	-9	9	59	29
-12	-8	9	14	5
-11	-8	9	10	14
-10	-8	9	291	278
-9	-8	9	-2	2
-8	-8	9	165	113
-7	-8	9	435	418
-6	-8	9	563	470
-5	-8	9	6	5
-4	-8	9	1566	1915
-3	-8	9	19	35
-2	-8	9	468	456
-1	-8	9	365	323
0	-8	9	34	18
1	-8	9	1609	1432
2	-8	9	71	42
3	-8	9	594	623
4	-8	9	11	5
5	-8	9	862	874
6	-8	9	135	173
7	-8	9	459	458
8	-8	9	95	76
9	-8	9	261	254
10	-8	9	12	9
11	-8	9	6	16
-12	-7	9	62	34
-11	-7	9	208	147
-10	-7	9	-1	6
-9	-7	9	295	287
-8	-7	9	77	121
-7	-7	9	40	31
-6	-7	9	2228	2799
-5	-7	9	376	443
-4	-7	9	95	165
-3	-7	9	4	11
-2	-7	9	123	85
-1	-7	9	108	68
0	-7	9	972	937
1	-7	9	2549	2945
2	-7	9	74	71
3	-7	9	4	6
4	-7	9	330	357
5	-7	9	283	231
6	-7	9	89	161
7	-7	9	15	9
8	-7	9	-4	2
9	-7	9	18	9
-9	5	9	1054	929
-8	5	9	75	77
-7	5	9	1244	1145
-6	5	9	20	42
-5	5	9	185	133
-4	5	9	446	394
-3	5	9	118	85
-2	5	9	358	392
-1	5	9	69	43
0	5	9	374	516
1	5	9	45	76
3	5	9	194	105
4	5	9	20	6
5	5	9	150	62
-13	6	9	274	276
-12	6	9	40	46
-11	6	9	469	410
-10	6	9	94	69
-9	6	9	727	598
-8	6	9	70	63
-7	6	9	352	437
-6	6	9	57	41
-5	6	9	25	21
-4	6	9	150	105
-3	6	9	189	153
-2	6	9	28	613
-1	6	9	29	24
0	6	9	13	8
1	6	9	76	90
2	6	9	95	138
3	6	9	106	127
4	6	9	159	15
-13	7	9	96	117
-12	7	9	25	28
-11	7	9	280	374
-10	7	9	0	2
-9	7	9	109	94
-8	7	9	5	5
-7	7	9	15	4
-6	7	9	532	456
-5	7	9	284	319
-4	7	9	285	273
-3	7	9	128	128
-2	7	9	521	600
-1	7	9	48	27
0	7	9	72	65
1	7	9	100	96
2	7	9	140	76
3	7	9	95	74
-12	8	9	17	6
-11	8	9	54	46
-10	8	9	27	17
-9	8	9	82	48
-8	8	9	47	55
-7	8	9	122	78

H	K	L	Obs	Calc
3	-6	9	1749	1549
4	-6	9	405	390
5	-6	9	977	860
6	-6	9	54	59
7	-6	9	34	48
8	-6	9	114	74
9	-6	9	54	44
10	-6	9	96	84
-13	-5	9	40	54
-12	-5	9	7	9
-11	-5	9	28	9
-10	-5	9	300	258
-9	-5	9	55	52
-8	-5	9	710	733
-7	-5	9	876	826
-6	-5	9	1543	1805
-5	-5	9	123	143
-4	-5	9	360	384
-3	-5	9	231	193
-2	-5	9	226	276
-1	-5	9	860	733
0	-5	9	412	492
1	-5	9	1834	1549
2	-5	9	535	565
3	-5	9	107	144
4	-5	9	131	96
5	-5	9	96	63
6	-5	9	35	17
7	-5	9	403	341
8	-5	9	250	224
9	-5	9	6	0
10	-5	9	2	2
-14	-4	9	2	4
-13	-4	9	38	22
-12	-4	9	30	37
-11	-4	9	11	26
-10	-4	9	251	313
-9	-4	9	146	109
-8	-4	9	430	480
-7	-4	9	607	528
-6	-4	9	7	9
-5	-4	9	1355	1358
-4	-4	9	10	6
-3	-4	9	53	38
-2	-4	9	10	3
-1	-4	9	3021	2889
0	-4	9	1565	1584
1	-4	9	4264	3936
-9	9	9	390	340
-8	9	9	13	2
-7	9	9	26	53
-6	9	9	171	130
-5	9	9	2	1
-4	9	9	208	189
-3	9	9	77	117
-2	9	9	345	362
-1	9	9	203	171
0	9	9	311	384
-10	10	9	22	19
-9	10	9	2	7
-8	10	9	105	97
-7	10	9	41	26
-6	10	9	168	103
-5	10	9	-2	0
-4	10	9	253	295
-3	10	9	108	99
-2	10	9	10	4
1	-17	10	0	12
2	-17	10	53	105
-3	-16	10	45	46
-2	-16	10	38	37
-1	-16	10	10	0
0	-16	10	11	9
1	-16	10	0	2
2	-16	10	113	52
3	-16	10	19	29
4	-16	10	75	53
5	-16	10	79	74
-5	-15	10	30	15
-4	-15	10	0	2
-3	-15	10	12	5
-2	-15	10	54	61
-1	-15	10	45	16
0	-15	10	80	88
1	-15	10	39	54
2	-15	10	16	7
3	-15	10	53	66
4	-15	10	10	5
5	-15	10	373	299
6	-15	10	76	53
7	-15	10	55	69
-6	-14	10	45	34
-5	-14	10	97	154
-4	-14	10	16	21
-3	-14	10	141	173
-2	-14	10	27	49
-1	-14	10	343	334
0	-14	10	169	127
1	-14	10	56	73
2	-14	10	45	50
3	-14	10	341	363
4	-14	10	28	40
5	-14	10	16	12

H	K	L	Obs	Calc
-5	-3	9	137	117
-4	-3	9	1460	1338
-3	-3	9	2681	2446
-2	-3	9	6877	6399
-1	-3	9	791	702
0	-3	9	398	264
1	-3	9	218	150
2	-3	9	138	73
3	-3	9	734	678
4	-3	9	1102	1056
5	-3	9	6	4
6	-3	9	827	685
7	-3	9	26	23
8	-3	9	28	21
9	-3	9	21	29
10	-3	9	50	36
-14	-2	9	65	67
-13	-2	9	24	34
-12	-2	9	105	68
-11	-2	9	72	52
-10	-2	9	654	601
-9	-2	9	11	15
-8	-2	9	227	261
-7	-2	9	50	38
-6	-2	9	29	12
-5	-2	9	122	121
-4	-2	9	1918	1399
-3	-2	9	1653	2159
-2	-2	9	198	170
-1	-2	9	7	22
0	-2	9	354	322
1	-2	9	49	49
2	-2	9	513	425
3	-2	9	49	86
4	-2	9	389	380
5	-2	9	139	176
6	-2	9	43	73
7	-2	9	1345	1276
8	-2	9	258	190
9	-2	9	97	112
10	-2	9	12	9
-14	-1	9	162	176
-13	-1	9	121	152
-12	-1	9	313	268
-11	-1	9	117	74
-10	-1	9	28	38
-9	-1	9	406	403
-8	-1	9	672	877
0	-13	10	137	102
1	-13	10	335	332
2	-13	10	80	73
3	-13	10	25	14
4	-13	10	30	30
5	-13	10	466	329
6	-13	10	58	82
7	-13	10	10	9
8	-13	10	33	15
-9	-12	10	10	1
-8	-12	10	111	138
-7	-12	10	22	27
-6	-12	10	88	112
-5	-12	10	179	193
-4	-12	10	241	271
-3	-12	10	68	89
-2	-12	10	146	153
-1	-12	10	195	252
0	-12	10	65	81
1	-12	10	434	377
2	-12	10	165	124
3	-12	10	694	617
4	-12	10	13	4
5	-12	10	74	77
6	-12	10	356	298
7	-12	10	142	115
8	-12	10	113	132
9	-12	10	7	2
-10	-11	10	77	61
-9	-11	10	25	10
-8	-11	10	34	57
-7	-11	10	-1	0
-6	-11	10	119	101
-5	-11	10	-5	1
-4	-11	10	4	1
-3	-11	10	244	210
-2	-11	10	3	5
-1	-11	10	11	7
0	-11	10	98	69
1	-11	10	291	418
2	-11	10	87	74
3	-11	10	46	46
4	-11	10	157	159
5	-11	10	66	67
6	-11	10	24	9
7	-11	10	12	9
8	-11	10	104	2
9	-11	10	36	57
-10	-10	10	94	105
-9	-10	10	41	24
-8	-10	10	78	90
-7	-10	10	303	232
-6	-10	10	349	347
-5	-10	10	299	222
-4	-10	10	415	369

H	K	L	Obs	Calc
-13	0	9	-1	1
-12	0	9	316	351
-11	0	9	262	336
-10	0	9	371	340
-9	0	9	39	3
-8	0	9	31	4
-7	0	9	358	267
-6	0	9	500	427
-5	0	9	932	999
-4	0	9	1842	1618
-3	0	9	1636	2040
-2	0	9	720	571
-1	0	9	2323	2101
0	0	9	1008	1004
1	0	9	24	33
2	0	9	126	159
3	0	9	255	317
4	0	9	116	53
5	0	9	9	15
6	0	9	28	32
7	0	9	23	22
8	0	9	11	2
9	0	9	5	1
-14	1	9	73	74
-13	1	9	134	118
-12	1	9	311	191
-11	1	9	66	73
-10	1	9	28	58
-9	1	9	781	710
-8	1	9	747	685
-7	1	9	14	28
-6	1	9	66	83
-5	1	9	80	122
-4	1	9	719	630
-3	1	9	3414	3424
-2	1	9	531	381
-1	1	9	2069	1979
0	1	9	48	26
1	1	9	1288	1297
2	1	9	23	2
3	1	9	35	33
4	1	9	292	264
5	1	9	82	96
6	1	9	33	32
7	1	9	2	11
8	1	9	117	131
-14	2	9	19	21
-13	2	9	110	141
8	-10	10	84	62
9	-10	10	27	15
10	-10	10	14	19
-11	-9	10	30	28
-10	-9	10	9	1
-9	-9	10	36	71
-8	-9	10	620	544
-7	-9	10	3	2
-6	-9	10	183	170
-5	-9	10	156	137
-4	-9	10	64	51
-3	-9	10	68	46
-2	-9	10	2372	2456
-1	-9	10	1832	1986
0	-9	10	1242	1087
1	-9	10	1140	1178
2	-9	10	52	75
3	-9	10	84	86
4	-9	10	68	75
5	-9	10	43	64
6	-9	10	133	133
7	-9	10	6	9
8	-9	10	5	1
9	-9	10	-3	2
10	-9	10	40	38
-12	-8	10	24	35
-11	-8	10	29	17
-10	-8	10	173	234
-9	-8	10	20	5
-8	-8	10	14	9
-7	-8	10	741	586
-6	-8	10	99	163
-5	-8	10	2	2
-4	-8	10	199	126
-3	-8	10	805	1078
-2	-8	10	87	17
-1	-8	10	53	118
0	-8	10	146	106
1	-8	10	319	315
2	-8	10	85	66
3	-8	10	381	318
4	-8	10	728	752
5	-8	10	180	171
6	-8	10	117	119
7	-8	10	1129	922
8	-8	10	41	39
9	-8	10	4	1
10	-8	10	0	10
-12	-7	10	22	1
-11	-7	10	62	40
-10	-7	10	133	121
-9	-7	10	113	105
-8	-7	10	184	170
-7	-7	10	434	378
-6	-7	10	424	246

H	K	L	Obs	Calc
7	2	9	-14	19
8	2	9	7	6
-14	3	9	92	106
-13	3	9	18	30
-12	3	9	4	1
-11	3	9	152	148
-10	3	9	5	1
-9	3	9	926	874
-8	3	9	309	355
-7	3	9	2038	2037
-6	3	9	171	307
-5	3	9	65	96
-4	3	9	917	865
-3	3	9	952	981
-2	3	9	106	65
-1	3	9	101	42
0	3	9	55	105
1	3	9	160	154
2	3	9	14	1
3	3	9	58	15
5	3	9	135	137
6	3	9	15	1
7	3	9	25	2
-14	4	9	42	52
-13	4	9	107	93
-12	4	9	13	6
-11	4	9	324	270
-10	4	9	0	0
-9	4	9	646	603
-8	4	9	275	362
-7	4	9	696	662
-6	4	9	614	480
-5	4	9	276	405
-4	4	9	52	16
-3	4	9	516	316
-2	4	9	129	151
-1	4	9	203	82
0	4	9	164	170
1	4	9	37	38
2	4	9	501	525
4	4	9	273	224
5	4	9	129	94
6	4	9	55	51
-14	5	9	49	34
-13	5	9	151	173
-12	5	9	24	31
-11	5	9	720	653
-10	5	9	52	38
6	-7	10	824	757
7	-7	10	56	11
8	-7	10	252	160
9	-7	10	96	61
10	-7	10	74	64
-13	-6	10	63	62
-12	-6	10	0	0
-11	-6	10	4	1
-10	-6	10	81	50
-9	-6	10	65	101
-8	-6	10	86	85
-7	-6	10	888	658
-6	-6	10	596	434
-5	-6	10	889	968
-4	-6	10	66	40
-3	-6	10	184	175
-2	-6	10	6	8
-1	-6	10	12	6
0	-6	10	3414	3242
1	-6	10	714	741
2	-6	10	1544	1535
3	-6	10	1058	982
4	-6	10	534	466
5	-6	10	7	0
6	-6	10	41	28
7	-6	10	114	112
8	-6	10	98	126
9	-6	10	-5	4
10	-6	10	20	4
-13	-5	10	21	23
-12	-5	10	27	24
-11	-5	10	131	113
-10	-5	10	1	0
-9	-5	10	739	883
-8	-5	10	92	105
-7	-5	10	526	678
-6	-5	10	9	0
-5	-5	10	394	414
-4	-5	10	82	140
-3	-5	10	432	479
-2	-5	10	149	128
-1	-5	10	17	23
0	-5	10	306	327
1	-5	10	30	18
2	-5	10	207	209
3	-5	10	493	498
4	-5	10	750	655
5	-5	10	175	173
6	-5	10	392	307
7	-5	10	25	25
8	-5	10	371	375
9	-5	10	274	264
10	-5	10	21	41
-13	-4	10	24	31
-12	-4	10	61	62

Table C.3, continued

H K L	Obs	Calc	H K L	Obs	Calc	H K L	Obs	Calc	H K L	Obs	Calc	H K L	Obs	Calc
-6 8 9	347	364	6-14 10	153	161	-3-10 10	187	176	-5 -7 10	1351	1169	-11 -4 10	709	713
-5 8 9	126	97	7-14 10	33	15	-2-10 10	1911	1630	-4 -7 10	66	69	-10 -4 10	3	4
-4 8 9	280	285	8-14 10	19	30	-1-10 10	1316	1339	-3 -7 10	449	532	-9 -4 10	275	227
-3 8 9	1	15	-8-13 10	82	47	0-10 10	11	19	-2 -7 10	80	74	-8 -4 10	7	15
-2 8 9	537	517	-7-13 10	30	21	1-10 10	1463	1274	-1 -7 10	1069	1001	-7 -4 10	34	23
-1 8 9	157	159	-6-13 10	-2	1	2-10 10	116	101	0 -7 10	212	167	-6 -4 10	756	550
0 8 9	5	7	-5-13 10	25	23	3-10 10	166	146	1 -7 10	3	6	-5 -4 10	496	548
1 8 9	-7	0	-4-13 10	5	1	4-10 10	19	43	2 -7 10	323	414	-4 -4 10	-2	8
2 8 9	9	4	-3-13 10	0	15	5-10 10	724	857	3 -7 10	41	86	-3 -4 10	2576	2157
-11 9 9	82	2	-2-13 10	13	1	6-10 10	98	91	4 -7 10	797	788	-2 -4 10	482	279
-10 9 9	119	129	-1-13 10	28	10	7-10 10	38	37	5 -7 10	-2	8	-1 -4 10	1083	1093
0 -4 10	770	705	-6 -1 10	366	409	-8 2 10	129	113	-4 5 10	913	920	-2-16 11	15	7
1 -4 10	3023	3149	-5 -1 10	66	46	-7 2 10	7	27	-3 5 10	429	417	-1-16 11	21	4
2 -4 10	480	463	-4 -1 10	1197	1256	-6 2 10	1631	1407	-2 5 10	128	125	0-16 11	2	1
3 -4 10	35	35	-3 -1 10	494	469	-5 2 10	472	335	-1 5 10	110	80	1-16 11	11	18
4 -4 10	30	21	-2 -1 10	841	543	-4 2 10	1261	1176	0 5 10	37	32	2-16 11	36	14
5 -4 10	139	214	-1 -1 10	89	49	-3 2 10	332	433	1 5 10	46	40	3-16 11	137	110
6 -4 10	88	86	0 -1 10	816	942	-2 2 10	800	868	2 5 10	0	7	4-16 11	17	34
7 -4 10	87	94	1 -1 10	10	3	-1 2 10	25	26	3 5 10	244	245	5-16 11	3	6
8 -4 10	14	11	2 -1 10	335	327	0 2 10	120	174	4 5 10	22	31	-5-15 11	14	24
9 -4 10	-3	0	3 -1 10	785	852	1 2 10	22	8	-13 6 10	59	111	-4-15 11	11	3
-14 -3 10	50	56	4 -1 10	5	1	2 2 10	146	106	-12 6 10	66	59	-3-15 11	-4	6
-13 -3 10	227	214	5 -1 10	22	42	3 2 10	69	72	-11 6 10	85	107	-2-15 11	7	3
-12 -3 10	92	60	6 -1 10	16	17	4 2 10	65	75	-10 6 10	203	205	-1-15 11	2	3
-11 -3 10	177	181	7 -1 10	35	8	5 2 10	123	85	-9 6 10	329	368	0-15 11	20	23
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Table C.3, continued

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-4	-10	11	31	14	-3	-7	11	4	1	-6	-4	11	576	589	-10	-1	11	166	189	-9	2	11	249	321
-3	-10	11	262	313	-2	-7	11	611	575	-5	-4	11	78	106	-9	-1	11	71	76	-8	2	11	665	560
-2	-10	11	745	797	-1	-7	11	157	136	-4	-4	11	656	685	-8	-1	11	226	361	-7	2	11	32	59
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-5	6	11	83	72	-3	-13	12	23	31	-9	-9	12	53	34	-5	-6	12	512	440	-5	-3	12	420	377
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-9	8	11	42	105	2	-12	12	74	45	-8	-8	12	133	90	-6	-5	12	47	42	-5	-2	12	254	307
-8	8	11	7	25	3	-12	12	441	404	-7	-8	12	497	521	-5	-5	12	202	167	-4	-2	12	62	44
-7	8	11	118	131	4	-12	12	439	460	-6	-8	12	31	19	-4	-5	12	57	64	-3	-2	12	2095	1999
-6	8	11	130	150	5	-12	12	22	44	-5	-8	12	190	105	-3	-5	12	586	816	-2	-2	12	67	33

Table C.3, continued

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-3	8	11	56	54	-9	-11	12	9	13	-2	-8	12	569	447	0	-5	12	127	159	1	-2	12	89	72
2	-2	12	700	571	5	1	12	20	7	-1	5	12	0	8	-5	-12	13	-3	1	7	-9	13	6	2
3	-2	12	0	0	-13	2	12	263	256	0	5	12	18	23	-4	-12	13	1	28	-11	-8	13	123	114
4	-2	12	3	2	-12	2	12	20	2	1	5	12	202	182	-3	-12	13	13	2	-10	-8	13	15	5
5	-2	12	32	22	-11	2	12	6	9	2	5	12	101	108	-2	-12	13	19	14	-9	-8	13	221	199
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7	-2	12	78	85	-9	2	12	250	232	-10	6	12	183	155	0	-12	13	34	26	-7	-8	13	162	97
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-9	-1	12	468	493	-3	2	12	847	781	-4	6	12	283	288	6	-12	13	44	36	-1	-8	13	105	62
-8	-1	12	62	62	-2	2	12	859	773	-3	6	12	77	83	7	-12	13	10	2	0	-8	13	36	32
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-7	-4	13	20	37	-2	-1	13	164	174	-8	3	13	166	174	-5	-13	14	102	63	-2	-9	14	64	55
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5	-4	13	62	95	-9	0	13	51	49	-11	4	13	-1	0	-7	-12	14	76	96	-8	-8	14	212	212
6	-4	13	12	8	-8	0	13	687	718	-10	4	13	218	237	-6	-12	14	42	19	-7	-8	14	271	156

Table C.3, continued

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-13	-3	13	117	130	-6	0	13	1109	1330	-8	4	13	14	3	-4	-12	14	260	216	-5	-8	14	-2	4
-12	-3	13	7	0	-5	0	13	1442	1334	-6	4	13	3	8	-3	-12	14	14	26	-4	-8	14	257	259
-11	-3	13	161	205	-4	0	13	1449	1264	-5	4	13	26	6	-2	-12	14	8	8	-3	-8	14	0	0
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-8	-3	13	53	21	-1	0	13	3	28	-2	4	13	95	103	1	-12	14	267	232	0	-8	14	6	2
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-1	-5	14	450	461	-10	-1	14	81	127	-7	3	14	2	2	2	-11	15	34	45	4	-7	15	242	215
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3	-5	14	35	331	-6	-1	14	91	86	-3	3	14	110	92	-9	-10	15	27	58	-9	-6	15	355	358
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-9	-4	15	340	287	-9	0	15	0	2	-3	-12	16	161	109	-3	-7	16	-6	0	2	-3	16	14	23
-8	-4	15	6	1	-8	0	15	93	72	-2	-12	16	20	8	-2	-7	16	399	413	-11	-2	16	28	31
-7	-4	15	83	56	-7	0	15	409	346	-1	-12	16	20	0	-1	-7	16	2	0	-10	-2	16	174	199

Table C.3, continued

H K L	Obs	Calc	H K L	Obs	Calc	H K L	Obs	Calc	H K L	Obs	Calc	H K L	Obs	Calc
-6 -4 15	278	278	-6 0 15	5	5	0-12 16	-4	0	0 -7 16	178	221	-9 -2 16	44	49
-5 -4 15	32	11	-5 0 15	126	85	1-12 16	19	7	1 -7 16	9	30	-8 -2 16	370	311
-4 -4 15	195	140	-4 0 15	1	1	2-12 16	60	39	2 -7 16	198	191	-7 -2 16	262	204
-3 -4 15	12	35	-3 0 15	78	57	3-12 16	2	1	3 -7 16	16	20	-6 -2 16	26	30
-2 -4 15	72	33	-2 0 15	38	52	-7-11 16	53	79	4 -7 16	9	5	-5 -2 16	111	121
-1 -4 15	374	268	-1 0 15	21	0	-6-11 16	15	3	-10 -6 16	0	1	-4 -2 16	22	28
0 -4 15	121	109	0 0 15	16	1	-5-11 16	332	316	-9 -6 16	39	49	-3 -2 16	28	33
1 -4 15	2	5	1 0 15	0	1	-4-11 16	102	115	-8 -6 16	-6	2	-2 -2 16	41	25
2 -4 15	8	9	2 0 15	14	16	-3-11 16	20	28	-7 -6 16	79	69	-1 -2 16	28	29
3 -4 15	6	6	-11 1 15	206	222	-2-11 16	513	489	-6 -6 16	415	501	0 -2 16	40	24
4 -4 15	18	15	-10 1 15	78	70	-1-11 16	93	73	-5 -6 16	126	125	1 -2 16	57	42
-12 -3 15	67	53	-9 1 15	242	245	0-11 16	298	335	-4 -6 16	161	146	2 -2 16	8	9
-11 -3 15	17	10	-8 1 15	423	350	1-11 16	72	91	-3 -6 16	9	0	-11 -1 16	14	10
-10 -3 15	5	3	-7 1 15	7	13	2-11 16	45	28	-2 -6 16	7	12	-10 -1 16	233	225
-9 -3 15	11	8	-6 1 15	367	309	3-11 16	14	32	-1 -6 16	90	138	-9 -1 16	5	1
-8 -3 15	27	36	-5 1 15	32	36	-8-10 16	44	67	0 -6 16	20	14	-8 -1 16	115	108
-7 -3 15	95	86	-4 1 15	3	15	-7-10 16	79	87	1 -6 16	193	201	-7 -1 16	0	1
-6 -3 15	141	122	-3 1 15	11	18	-6-10 16	62	43	2 -6 16	69	114	-6 -1 16	207	239
-5 -3 15	57	63	-2 1 15	165	145	-5-10 16	155	133	3 -6 16	102	81	-5 -1 16	224	217
-4 -3 15	699	629	-1 1 15	21	9	-4-10 16	189	179	4 -6 16	7	0	-4 -1 16	80	69
-3 -3 15	5	3	0 1 15	35	13	-3-10 16	67	46	-11 -5 16	36	53	-3 -1 16	270	246
-2 -3 15	279	314	1 1 15	109	96	-2-10 16	14	14	-10 -5 16	158	143	-2 -1 16	19	22
-1 -3 15	24	34	-11 2 15	13	14	-1-10 16	2	2	-9 -5 16	77	61	-1 -1 16	18	15
0 -3 15	131	142	-10 2 15	263	269	0-10 16	-1	1	-8 -5 16	303	339	0 -1 16	129	101
1 -3 15	34	40	-9 2 15	86	88	1-10 16	33	51	-7 -5 16	66	33	1 -1 16	21	12
2 -3 15	966	941	-8 2 15	44	79	2-10 16	16	9	-6 -5 16	22	24	-10 0 16	250	218
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-12 -2 15	24	9	-5 2 15	21	68	-9 -9 16	-5	1	-3 -5 16	51	72	-7 0 16	33	55
-11 -2 15	114	101	-4 2 15	27	21	-8 -9 16	51	20	-2 -5 16	185	164	-6 0 16	120	143
-10 -2 15	3	2	-3 2 15	71	51	-7 -9 16	221	222	-1 -5 16	30	39	-5 0 16	35	26
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-7 -2 15	674	584	0 2 15	4	8	-4 -9 16	264	271	2 -5 16	43	199	-2 0 16	4	4
-6 -2 15	13	13	-10 3 15	113	163	-3 -9 16	5	7	3 -5 16	27	39	-1 0 16	94	164
-5 -2 15	29	46	-9 3 15	3	1	-2 -9 16	666	612	-11 -4 16	179	159	0 0 16	158	148
-4 -2 15	76	69	-8 3 15	198	154	-1 -9 16	6	4	-10 -4 16	93	85	-10 1 16	48	50
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-1 -2 15	18	6	-5 3 15	-2	3	2 -9 16	25	37	-7 -4 16	275	287	-7 1 16	239	160
0 -2 15	174	184	-4 3 15	141	139	3 -9 16	2	0	-6 -4 16	78	45	-6 1 16	53	43
1 -2 15	0	1	-3 3 15	15	1	4 -9 16	44	34	-5 -4 16	27	7	-5 1 16	182	185
2 -2 15	70	104	-2 3 15	320	173	-10 -8 16	-1	2	-4 -4 16	52	27	-4 1 16	112	83
3 -2 15	11	14	-1 3 15	43	44	-9 -8 16	338	394	-3 -4 16	30	28	-3 1 16	37	36
-12 -1 15	-8	1	-8 4 15	83	96	-8 -8 16	50	58	-2 -4 16	72	101	-2 1 16	26	35
-11 -1 15	138	114	-7 4 15	37	36	-7 -8 16	80	69	-1 -4 16	47	51	-1 1 16	39	20
-10 -1 15	60	108	-6 4 15	59	70	-6 -8 16	636	644	0 -4 16	94	77	-9 2 16	122	106
-9 -1 15	204	239	-5 4 15	41	19	-5 -8 16	2	1	1 -4 16	116	195	-8 2 16	35	23
-8 -1 15	283	380	-4 4 15	58	48	-4 -8 16	363	422	2 -4 16	5	2	-7 2 16	19	19
-7 -1 15	8	9	-2-14 16	16	20	-3 -8 16	29	9	3 -4 16	169	196	-6 2 16	14	8
-6 -1 15	361	291	-1-14 16	120	129	-2 -8 16	9	14	-11 -3 16	7	3	-5 2 16	180	131
-5 -1 15	248	269	0-14 16	29	42	-1 -8 16	58	35	-10 -3 16	272	247	-4 2 16	0	0
-4 -1 15	33	19	-5-13 16	6	4	0 -8 16	2	1	-9 -3 16	7	5	-3 2 16	122	124
-3 -1 15	28	28	-4-13 16	8	3	1 -8 16	16	30	-8 -3 16	328	313	-5-12 17	7	8
-2 -1 15	3	10	-3-13 16	9	8	2 -8 16	0	1	-7 -3 16	278	234	-4-12 17	32	35
-1 -1 15	41	49	-2-13 16	196	215	4 -8 16	38	30	-6 -3 16	65	37	-3-12 17	14	30
0 -1 15	132	119	-1-13 16	16	9	-10 -7 16	74	72	-5 -3 16	461	497	-2-12 17	245	243
1 -1 15	12	47	0-13 16	254	261	-9 -7 16	2	1	-4 -3 16	130	135	-1-12 17	40	47
2 -1 15	185	166	1-13 16	207	233	-8 -7 16	107	106	-3 -3 16	47	61	0-12 17	7	3
3 -1 15	51	68	2-13 16	103	119	-7 -7 16	5	11	-2 -3 16	195	207	1-12 17	34	34
-12 0 15	51	57	-6-12 16	-4	0	-6 -7 16	218	173	-1 -3 16	264	235	-6-11 17	245	268
-5-11 17	18	31	-8 -5 17	2	1	-1-10 18	10	6						
-4-11 17	58	103	-7 -5 17	139	114	-6 -9 18	28	22						
-3-11 17	15	9	-6 -5 17	-4	4	-5 -9 18	40	36						
-2-11 17	21	18	-5 -5 17	12	18	-4 -9 18	14	10						
-1-11 17	69	59	-4 -5 17	12	11	-3 -9 18	20	13						
0-11 17	47	42	-3 -5 17	361	329	-2 -9 18	9	13						
1-11 17	18	10	-2 -5 17	9	2	-1 -9 18	128	97						
-7-10 17	19	6	-1 -5 17	272	256	0 -9 18	17	6						
-6-10 17	274	307	0 -5 17	0	3	-7 -8 18	3	7						
-5-10 17	124	79	2 -5 17	8	2	-6 -8 18	38	27						
-4-10 17	10	3	-10 -4 17	79	74	-5 -8 18	13	3						
-3-10 17	103	75	-9 -4 17	175	172	-4 -8 18	10	19						
-2-10 17	11	3	-8 -4 17	289	214	-3 -8 18	114	106						
-1-10 17	7	5	-7 -4 17	80	114	-2 -8 18	53	64						
0-10 17	7	7	-6 -4 17	40	36	-1 -8 18	0	2						
1-10 17	24	13	-5 -4 17	12	9	0 -8 18	151	176						
2-10 17	2	5	-4 -4 17	45	36	-8 -7 18	20	0						
-8 -9 17	33	25	-3 -4 17	221	203	-7 -7 18	45	74						
-7 -9 17	400	415	-2 -4 17	90	143	-6 -7 18	10	3						
-6 -9 17	71	76	-1 -4 17	95	82	-5 -7 18	30	23						
-5 -9 17	472	434	0 -4 17	154	179	-4 -7 18	7	19						
-4 -9 17	33	49	1 -4 17	78	105	-3 -7 18	22	13						
-3 -9 17	13	5	-10 -3 17	56	36	-2 -7 18	102	101						
-2 -9 17	316	269	-9 -3 17	149	112	-1 -7 18	28	45						
-1 -9 17	101	139	-8 -3 17	69	42	0 -7 18	20	7						
0 -9 17	28	0	-7 -3 17	375	315	-8 -6 18	21	26						
1 -9 17	7	4	-6 -3 17	142	113	-7 -6 18	139	157						
2 -9 17	6	3	-5 -3 17	360	362	-6 -6 18	41	14						
-9 -8 17	1	19	-4 -3 17	1	3	-5 -6 18	39	12						
-8 -8 17	79	64	-3 -3 17	65	120	-4 -6 18	169	133						
-7 -8 17	0	5	-2 -3 17	14	20	-3 -6 18	6	11						
-6 -8 17	4	1	-1 -3 17	2	1	-2 -6 18	61	66						
-5 -8 17	157	191	0 -3 17	2	33	-1 -6 18	5	1						
-4 -8 17	2	7	1 -3 17	6	2	0 -6 18	186	195						
-3 -8 17	26	22	-9 -2 17	323	277	-8 -5 18	75	61						
-2 -8 17	0	18	-8 -2 17	51	35	-7 -5 18	68	94						
-1 -8 17	53	26	-7 -2 17	151	144	-6 -5 18	7	76						
0 -8 17	94	99	-6 -2 17	6	8	-5 -5 18	43	10						
1 -8 17	49	50	-5 -2 17	51	55	-4 -5 18	129	149						
2 -8 17	59	80	-4 -2 17	48	46	-3 -5 18	11	18						
-9 -7 17	4	9	-3 -2 17	48	44	-2 -5 18	144	192						
-8 -7 17	22	29	-2 -2 17	82	94	-1 -5 18	13	3						

Table C.3, continued

H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc	H	K	L	Obs	Calc
-7	-7	17	129	127	0	-2	17	32	26	-8	-4	18	35	53										
-6	-7	17	-6	10	-9	-1	17	51	77	-7	-4	18	11	27										
-5	-7	17	19	2	-8	-1	17	-3	2	-6	-4	18	258	270										
-4	-7	17	25	22	-7	-1	17	123	98	-5	-4	18	28	112										
-3	-7	17	79	33	-6	-1	17	49	20	-4	-4	18	62	88										
-2	-7	17	81	54	-5	-1	17	263	262	-3	-4	18	4	6										
-1	-7	17	119	135	-4	-1	17	4	0	-2	-4	18	109	112										
0	-7	17	14	12	-3	-1	17	45	50	-1	-4	18	0	0										
1	-7	17	43	59	-2	-1	17	113	105	-8	-3	18	84	96										
2	-7	17	74	98	-1	-1	17	13	5	-7	-3	18	22	20										
-9	-6	17	-2	4	-8	0	17	16	7	-6	-3	18	70	55										
-8	-6	17	207	155	-7	0	17	52	46	-5	-3	18	12	5										
-7	-6	17	10	1	-6	0	17	-1	0	-4	-3	18	172	153										
-6	-6	17	178	221	-5	0	17	68	75	-3	-3	18	1	1										
-5	-6	17	180	168	-4	0	17	69	99	-2	-3	18	163	138										
-4	-6	17	80	75	-3	0	17	6	24	-7	-2	18	1	0										
-3	-6	17	0	5	-6	1	17	33	32	-6	-2	18	50	85										
-2	-6	17	16	30	-5	1	17	3	1	-5	-2	18	20	15										
-1	-6	17	24	18	-3	-11	18	33	26	-4	-2	18	26	26										
0	-6	17	1	0	-2	-11	18	-5	2	-3	-2	18	0	0										
1	-6	17	5	0	-5	-10	18	1	1															
2	-6	17	34	53	-4	-10	18	27	7															
-10	-5	17	61	52	-3	-10	18	66	97															
-9	-5	17	212	177	-2	-10	18	105	90															

a Reflections flagged with an asterisk were considered unobserved.

Table C.4. Atomic multiplicities for [Cu(dipp)$_2$]TFPB.

Name	Multiplicity	Name	Multiplicity	Name	Multiplicity
Cu	1.000	F(331)	1.000	F(332)	1.000
F(333)	1.000	F(351)	1.000	F(352)	1.000
F(353)	1.000	F(431)	1.000	F(432)	1.000
F(433)	1.000	F(451)	1.000	F(452)	1.000
F(453)	1.000	F(531)	1.000	F(532)	1.000
F(533)	1.000	F(551)	1.000	F(552)	1.000
F(553)	1.000	F(631)	1.000	F(632)	1.000
F(633)	1.000	F(651)	1.000	F(652)	1.000
F(653)	1.000	N(11)	1.000	N(21)	1.000
N(112)	1.000	N(212)	1.000	C(12)	1.000
C(13)	1.000	C(14)	1.000	C(15)	1.000
C(16)	1.000	C(17)	1.000	C(18)	1.000
C(19)	1.000	C(22)	1.000	C(23)	1.000
C(24)	1.000	C(25)	1.000	C(26)	1.000
C(27)	1.000	C(28)	1.000	C(29)	1.000
C(31)	1.000	C(32)	1.000	C(33)	1.000
C(34)	1.000	C(35)	1.000	C(36)	1.000
C(41)	1.000	C(42)	1.000	C(43)	1.000
C(44)	1.000	C(45)	1.000	C(46)	1.000
C(51)	1.000	C(52)	1.000	C(53)	1.000
C(54)	1.000	C(55)	1.000	C(56)	1.000
C(61)	1.000	C(62)	1.000	C(63)	1.000
C(64)	1.000	C(65)	1.000	C(66)	1.000
C(110)	1.000	C(111)	1.000	C(113)	1.000
C(114)	1.000	C(115)	1.000	C(116)	1.000
C(117)	1.000	C(118)	1.000	C(119)	1.000
C(120)	1.000	C(210)	1.000	C(211)	1.000
C(213)	1.000	C(214)	1.000	C(215)	1.000
C(216)	1.000	C(217)	1.000	C(218)	1.000
C(219)	1.000	C(220)	1.000	C(331)	1.000
C(351)	1.000	C(431)	1.000	C(451)	1.000
C(531)	1.000	C(551)	1.000	C(631)	1.000
C(651)	1.000	B	1.000	H(13)	1.000
H(14)	1.000	H(16)	1.000	H(17)	1.000
H(19)	1.000	H(23)	1.000	H(24)	1.000
H(26)	1.000	H(27)	1.000	H(29)	1.000
H(32)	1.000	H(34)	1.000	H(36)	1.000
H(42)	1.000	H(44)	1.000	H(46)	1.000
H(52)	1.000	H(54)	1.000	H(56)	1.000
H(62)	1.000	H(64)	1.000	H(66)	1.000
H(110)	1.000	H(115)	1.000	H(118)	1.000
H(11A)	1.000	H(11B)	1.000	H(11C)	1.000
H(11D)	1.000	H(11E)	1.000	H(11F)	1.000
H(11G)	1.000	H(11H)	1.000	H(11I)	1.000
H(12A)	1.000	H(12B)	1.000	H(12C)	1.000
H(210)	1.000	H(215)	1.000	H(218)	1.000
H(21A)	1.000	H(21B)	1.000	H(21C)	1.000
H(21D)	1.000	H(21E)	1.000	H(21F)	1.000
H(21G)	1.000	H(21H)	1.000	H(21I)	1.000
H(22A)	1.000	H(22B)	1.000	H(22C)	1.000

VITA

VITA

Corey Thomas Cunningham was born on April 4, 1973 in Danville, Indiana to Stephen and Brenda Cunningham. He spent his childhood in the nearby village of Pittsboro, Indiana. He graduated from Northwest Hendricks Junior Senior High School in Lizton, Indiana in June 1991. He then enrolled at Purdue University, in West Lafayette, Indiana where he stayed for the next 7 years. In May 1995 he completed the bachelors program and graduated with a B.S. in Chemistry. He spent the summer continuing his research under Dr. David R. McMillin and in early August of 1995 he married Dr. Kurstan Cunningham. In late August of 1995 he began his graduate career at Purdue University. While at Purdue, his research focused on the synthesis and photochemistry of transition metal coordination compounds. A little over three years later he defended his Doctor of Philosophy in Inorganic Chemistry under the supervision of Dr. David R. McMillin. He is currently (and forever more) remodeling a 90 year old house in Terre Haute, Indiana with his wife and their two dogs.