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# A SEARCH FOR EXPERIMENTS TO EXPLOIT THE SPACE SHUTTLE ENVIRONMENT

## VOLUME ONE


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# A SEARCH FOR EXPERIMENTS TO EXPLOIT THE SPACE SHUTTLE ENVIRONMENT

by

John B. Fenn

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RELAY DEVELOPMENT CORPORATION

226 Pleasant Point Road

Branford, Connecticut
06405

203-488-5428

First of Two Volumes

## Abstract

This study extends an earlier search for worthwhile experiments in pure and applied physics and chemistry which might take advantage of conditions achievable aboard the Space Shuttle. Of particular interest were the very large pumping speeds at high or ultra high vacuum, the highly non-equilibrium composition of the ambient atmosphere, and the relative absence of gravitational effects. Ideas and suggestions were solicited in the course of visits to 31 research establishments in Western Europe, India and Japan, conversations with over 90 scientists, and presentations at three international meetings. Intriguing possibilities emerged in five arenas: (1) Spectroscopy of the transition state in chemical reactions; (2) Flame structure and analysis; (3) Solid propellant combustion; (4) Analysis of atmospheric composition; (5) Turbulence Effects on Aerosol Coagulation.

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## Summary

This report comprises a geographic and substantive extension of an earlier attempt in 1976 to identify worthwhile experiments which might advantageously be carried out aboard a Space Shuttle in orbit. The earlier investigation focussed on experiments with free jets which would take advantage of the very high pumping speed available in space. It was based on communication with scientists in America and Western Europe. The present author, who had participated in the earlier study, last year spent two months in India, three months in Japan and one month in Europe visiting laboratories and talking with research scientists and engineers. In addition, during the period since the first report was completed, he had made presentations at three international meetings in an attempt to stimulate interest in and suggestions for such experiments and others not involving free jets. This document reports on the results of these further attempts to identify worthwhile experiments. The harvest was rather lean but five interesting avenues of investigation were identified:

1. Natural Lasers and Transition State Spectroscopy. In the upper atmosphere the species OH is vibrationally very hot and rotationally very cold and thus invites attempts to obtain stimulated emission over very long path lengths. It might be rewarding to look very carefully at the infrared emission in the wings of excited OH. Because OH is formed by highly exothermic reaction of ozone and H atoms, any observed broadening could be interpreted in terms of the radiation occurring while the OH was still closely associated with the OOOH transition state complex.

2. Very Low Pressure Flames. It turns out that the volumetric flow rate of pre-mixed fuel and oxidant required to maintain a stable flame is inversely proportional to the pressure. The lowest pressures which have been reached on earth are of order one torr where the mean free path is only a micron. To reach much lower pressures one

must have very high pumping speeds, such as might be achieved on the Space Shuttle. One inviting prospect is that flame front structure could be resolved in much more detail than is now possible. Another is that collisional quenching times could be increased to the same order as radiation life times, thus giving rise to possibly interesting radiation effects.

3. Solid Propellant Combustion. For reasons similar to those involved in gaseous flames, achieving stable combustion of solid propellants at very low pressure also requires very high pumping speeds. There are a number of interesting and unanswered questions about low pressure deflagration of such propellants which might be answered by experiments at high pumping speeds.

4. Composition of Upper Atmosphere. In spite of many measurement attempts there are large uncertainties in the composition of the upper atmosphere which stem from difficulties in avoiding perturbations of the composition by the measuring instrument. Possibilities for overcoming these problems include velocity discrimination in sampling and laser sensing techniques.

5. Turbulence Effects on Aerosol Coagulation. Agglomeration or coagulation of colloidal particles due to Brownian motion is reasonably well understood. Agglomeration of larger particles in gaseous systems may be strongly affected by velocity fluctuations due to turbulence. Such effects may have had a profound influence on the composition of planets and other bodies formed by condensation from primordial gas. Interesting agglomeration experiments may be possible on the Space Shuttle in the absence of gravitational settling in gaseous suspensions of large particles.

# A SEARCH FOR EXPERIMENTS TO EXPLOIT THE SPACE SHUTTLE ENVIRONMENT

## I. Introduction

In 1976 Relay Development Corporation (RDC) undertook a study program for NASA-JPL aimed at identifying and evaluating worthwhile experiments which might be advantageously carried out in an environment to which the Space Shuttle promises to provide access. In particular, RDC's assignment was to consider experiments in which supersonic free jets would play a vital role. Such free jets have been rewarding objects of study because they comprise a rich source of phenomena which occur under conditions readily achieved in such jets but which are not otherwise obtainable. The attraction of the Space Shuttle Environment (SSE) consists in its ability to provide virtually unlimited pumping speed at relatively low background pressures. Such large pumping speed would make possible much higher source Reynolds numbers at lower background pressures than would be economically feasible at the bottom of the ocean comprising Earth's atmosphere. Large Reynolds numbers would permit experiments at relatively large scale and/or at large pressure ratios for the expansion.

The RDC Study culminated in a report which summarized the results of an extensive literature search, conversations with nearly 100 scientists and analysis of a number of *gedanken* experiments.[1] The essential conclusions were:

(1) No experiments emerged which in the sense of their scientific implications could be considered sufficiently critical to justify *ab initio* the investment of resources which would be required to carry them out aloft.

(2) There were some interesting and worthwhile experiments which, though not "critical", the SSE could expedite or enhance but there could be no assurance that clever earthbound investigators might not find ways to achieve equivalent results at lower cost and in less time.

(3) The prospectively most interesting experiments were spectroscopic in the sense that they all involved the interaction of molecules with photons. The principal basis for their appeal stems from the ability of the SSE to provide long optical paths in nearly collisionless gas. These long paths mean that there can be relatively large numbers of molecules in the field of view of a detector for relatively long times. The absence of collisions means that the states of the molecules do not change. Thus, initially non-equilibrium conditions can be maintained.

Since the appearance of that RDC report there has been renewed consideration of the so-called Molecular Wake Shield or MWS. This concept involves the disposition of an impermeable surface of relatively large frontal area on the Shuttle itself or on some outboard vehicle. The idea is that this shield would sweep the molecules of ambient atmosphere out of its path so that in its immediate wake the effective background pressure or density would be substantially lower than that of the ambient atmosphere through which the Shuttle is flying. Subject to some unknowns, e.g., the contribution to be expected from outgassing of shield and vehicle surfaces, it has been estimated that the effective background pressure for a typical orbit altitude and velocity would be reduced from about $10^{-6}$ torr in the free stream to the vicinity of $10^{-12}$ torr[2,3] in the wake of the shield. This ultra-high vacuum environment may make inviting some experiments which might not be feasible or interesting at the much higher background pressure presumed in the original study. Moreover, a corollary consequence of such a shield is the possibility of generating a collimated beam of molecules of ambient gas by means of a suitably shaped inlet aperture in the shield which would play the role of a skimmer in conventional nozzle beam systems. Oxygen atoms are the dominant atmospheric species at probable oribiting altitudes. For example, they are present at concentrations of nearly $10^{10}/cm^3$ at an altitude of 200 kilometers. An orbiting velocity of 8 km/s would thus give rise to a beam of oxygen atoms with an intensity near $8 \times 10^{15}/cm^2$-s. Such a beam, which would have a translational energy of about 5 eV, cannot now be readily generated in earthbound laboratories and would make feasible many interesting scattering experiments.

In sum, the SSE in conjunction with the MWS opens up possibilities not contemplated in RDC's original study.

Another limitation of the original RDC study concerned the scientists polled for ideas, suggestions and comments. Though their number was appreciable, they represented a community which was restricted geographically to North America and Western Europe and scientifically to those who had some research experience with molecular beams and/or rarefied gas dynamics. Moreover, good ideas frequently have fairly long gestation periods and many of the scientists who were approached had no previous occasion to consider the possibility of doing experiments in space. Consequently, it seemed appropriate to undertake an extension of the original survey. One objective would be to include a broader segment of the scientific community. Another would be to renew encounters with some of those who have been accosted earlier to see whether some seeds sown the first time around might have since germinated.

As it happened, one of the authors of the original RDC report, Professor John B. Fenn, was to be on leave from Yale University during the spring term of 1979. He had been invited to spend two months at the Indian Institute of Science in Bangalore and at the Institute of Space and Aeronautical Sciences of the University of Tokyo. In addition, he planned to travel a month in Europe visiting laboratories and attending the International Symposium on Molecular Beams beginning on 28 May at Riva del Garda in Italy. This itinerary appeared to provide an excellent opportunity for him to extend the scope of the original survey by seeking ideas from a broader segment of the scientific community than had been included in the earlier report. Moreover, he would have an opportunity for second encounters with some of the people who had been previously exposed to the idea of experiments in the Space Shuttle Environment. Perhaps some seeds sown then might have fallen on fertile ground. Professor Fenn was willing to pursue these goals during his travels and was commissioned to do so. This report summarizes his experiences and findings. Volume I includes a description of the possible experiments which emerged during the survey, a catalog of the scientists who were interviewed, and an account of the meetings at which formal presentations were made about the possibilities for Space Shuttle experiments. Volume II is essentially a travelogue describing the places which were visited. In the interests of informality and economy of words the writer will resort to the use of the vertical pronoun.

## II. The Results

The word about possibilities for experiments on board the Space Shuttle was spread substantially farther and wider in this survey than during RDC's initial study. Even so, the harvest of ideas was in some sense still disappointing. As in our earlier census, most responses fell into one of the following categories; usually expressed in more euphemistic terms than I will employ.

1. This is all so new and different that I will have to think about it.
2. It is too far from my regular research beat and I can't see any connection which would make it worth my while to give it much attention.
3. Clearly a boondoggle. I could make better use of the money in my lab on the ground.
4. You Americans have enough money to contemplate such experiments. We have to devote our resources and attention to more immediate problems.
5. What a great idea! You could do this, and this, and this,..., all the "thises" being fairly thoughtless and naive.
6. Sounds like a great opportunity but I can't think of any way to take advantage of it.

Amidst all this chaff, there were a few grains of wheat, some proposed experiments which seemed interesting enough to report. They are set forth in the following paragraphs of this section.

1. <u>Lasers Au Naturel and Transition State Spectroscopy</u>. After nearly twenty-five years of molecular beam reactive scattering experiments and maybe a decade of spectroscopy and photochemistry by lasers, today's chemists know more about the microscopic details of chemical reactions than Arrhenius and Bodenstein could have dreamt of. In particular, these modern techniques have led to so-called "state-to-state" chemistry which contemplates complete experimental specification of velocities, internal energy levels and even the orientation of reactant and product species immediately before and after a reactive encounter. What still eludes the most intrepid investigators is any direct observation of that construct, the "transition state"--a configuration of species which marks at once the end of their identity as reactants and the beginning of their identity as products. Of extremely short lifetime and perhaps in some cases not even identifiable or definable, this ephemeral species has existed thus far mainly in the minds of investigators. Whatever characteristics have been ascribable to its reality are largely based on deductions as to plausible bridges between reactant states and product states. Before the beam and laser era, most experimental data related to the initial state of reactants and the final state of products. We now have increasingly direct information on the final state of reactants and the initial state of products so the bridges to be built are much shorter and therefore less speculative in their design.

The direct experimental identification and description of the transition state has been called by John Polanyi the "last frontier" of chemical kinetics. Of late there have been a number of suggestions by theorists that extremely high powered lasers might be able to probe the transition state structure, and indeed, take advantage of its asymmetric nature by bringing about laser promoted reactions between reactants which in their symmetric initial configurations are not capable of absorbing photons.(4,5) The calculated power requirements are so large that many people are pessimistic about the outcome. Among the optimists is John Polanyi of the University of Toronto, and he sees the Space Shuttle, literally and figuratively, as a possible vehicle for experiments which might achieve the goal of direct observation of the transition state. After some discussion with me at the Riva meeting he wrote a letter summarizing his ideas. I know of no better way to present them than to reproduce his own words. What follows are essentially literal excerpts from his letter.

"The proposals for the skylab could be made to hinge on the observation of $OH^{\dagger}$ (vibrationally excited hydroxyl in its ground electronic state) and also Na* and Na** (electronically excited Na in the 3p and 4s states respectively). Since $OH^{\dagger}$ is emitting strongly from approximately 90 km and is hard to observe at ground level, I shall concentrate on that in setting forth the following two objectives:

(I) Look (for the first time) for evidence of what I termed in 1960 and 1961 publications, prior to the first laser, a "natural iraser" comprised of the upper atmosphere. The point was that vibrational temperature $T_{vib} \approx 10{,}000$ K and rotational temperature $T_{rot} \approx 230$ K. Hence hundreds of transitions in the P-branch of the fundamental ($\Delta v = 1$ at approximately 3 microns in the near infrared) have the potential for producing stimulated emission in view of the long path length.

The existence of "an inverse Frauenhofer effect" was postulated, i.e., the continuum emission from the sun should show narrow intervals of enhanced intensity when viewed through a long path-length of the upper atmosphere. (This, by the way, was the first time that $T_{vib} >> T_{rot} > 0$ had been noted to be a sufficient criterion for what was termed "partial population inversion"--a concept that underlies the $CO_2$ and CO vibrational lasers).

(II) A far more venturesome proposal which, however, requires a similar line of experimentation, is to look for infrared emission in the wings of the $OH^{\dagger}$ ($v \rightarrow v - 1$) fundamental, or the $OH^{\dagger}$ ($v \rightarrow v - 2$, $v \rightarrow v - 3, \ldots$) overtones, extending into the photographic region. This would constitute observations of a type of collision-induced broadening due to strong (high energy) collisions that could only be due to the fact that $OH^{\dagger}$ is produced chemically through $H + O_3 \rightarrow [HOOO]^{\ddagger} \rightarrow HO^{\dagger} + O_2$ (as is highly likely to be the case) and that one is observing the OH radical before it has moved out of range of the other product, $O_2$; i.e., one would have (for the first time) spectroscopic data bearing on the forces operating in $[HOOO]^{\ddagger}$ -- <u>spectroscopy of the transition state in a chemical reaction</u>.

Such an observation has the best chance of success if one can observe a very long column of reacting $H + O_3$, as is the case in the upper atmosphere. The low pressure ensures that there is no local depletion of H through rapid reaction with $O_3$, i.e., it solves the difficult problem of reagent mixing for fast reaction. Observation from space eliminates water absorption of radiation.

A similar experiment is possible for that part of Na* and Na** that is formed chemically in the upper atmosphere, naturally through reaction of $O + NaO^{\dagger} \rightarrow O_2 + Na^*$ (or Na**) or from the reaction of naturally-occurring atomic species with $Na_2$ injected into the surroundings from a supersonic orifice, thus $O + Na_2 \rightarrow NaO + Na^*$.

The ratio of concentrations of transition state to product species is $10^{-10} - 10^{-11}$ for $OH^{\dagger}$, and $10^{-4} - 10^{-5}$ for Na*. This renders the experiment very difficult, but not impossible in view of the fact that photons can be counted against a dark background. In the case that $Na_2$ is injected, interposition of a chopper blade in the $Na_2$ flow will permit subtraction of any background from signal.

We very much want to try feasibility studies on Objective II in our laboratory and are ready to do so as soon as we get the signal to go ahead.

2. Flames At Very Low Pressures. Flames have fascinated man ever since he began to control and use fire, probably even before. Until Galileo introduced the controlled experiment and launched the era of modern science, fire as manifested by flame was regarded with awe as an embodiment of godly magic. The Greeks assigned it a fundamental role in the composition of the real world. Along with earth, air and water, it was considered one of the four elements from which all things were made. Flames are rather spectacular consequences of a complex interaction between physical and chemical processes. The combustion which gives rise to them is still the major source of the heat from which prime movers derive the work that powers industrial society. For these reasons, flames have been the objects of intense scientific study for nearly two centuries. Investigators have tried to understand their phenomenology in terms of their physics and chemistry. They have sought to relate their speeds, structure and stability to the thermodynamics and kinetics of chemical reactions and the physical transport of mass energy and momentum. In recent years there has been increasing interest in the role of reactants and products which are present in amounts too small to effect flame behavior but large enough to have major environmental consequences. Growing concern about the depletion of oil and gas resources has renewed interest in achieving even small increases in the efficiency of all kinds of combustion systems.

One important and powerful variable in the experimental study of flames is pressure. In early experiments pressures were almost always atmospheric or higher, partly because such pressures were easy to achieve in the laboratory and partly because practical systems operated in this range. With the advent of high altitude flight internal combustion engines were required to perform at subatmospheric pressures. In the laboratory experimenters began to appreciate and exploit the fact that reaction zones in flames could be greatly extended and magnified by lowering the pressure and therefore the density of the reacting gases. In flames of premixed gases at one atmosphere much of the action occurs in a region somewhat less than a few tenths of a millimeter in thickness. At 25 torr this flame zone expands to a centimeter or more, depending upon the composition of the entering gas. This increase in thickness greatly improves the resolution of structure which can be achieved by various kinds of probes.

On a very elementary plane of flame phenomenology the question was often asked whether there was a limiting pressure below which a flame front could not propagate into unburned gas. In an attempt to answer this question and at the same time to increase the resolution of their spectroscopic probing of flame front structure, Gaydon and Wolfhard in 1950 carried out a then heroic effort to produce flames at very low pressures.[6,7] They found that there was in effect a characteristic Reynolds number below which stable flames could not propagate. In terms of more directly measurable quantities Reynolds number at a particular flame speed is proportional to the product of pressure and burner diameter. Thus, what Gaydon and Wolfhard found was that as long as this product was maintained at a characteristic value for a particular composition, they could lower the pressure as much as they wanted to as long as they increased the burner diameter correspondingly. They also found that for many fuel-oxidant combinations the burning velocity did not change appreciably with pressure. Thus, as the pressure was lowered the volumetric flow increased and they reached the limit of their available pumping speed at pressures of about one torr with a burner diameter of 10 cm. The pumping speed which they had available was not specified. They simply noted that they were using the largest available industrial vacuum pumps. With these low pressure flames and spectroscopic techniques, Gaydon and Wolfhard probed the species distribution in various flames. More recently, Wolfhard in collaboration with Vanpee, Hinck and Seamans examined the nature of OH radiation in flames at pressures down to about 10 torr on a burner 10 cm in diameter.[8] Their system was exhausted by a Roots pump with a speed of 300 liters/sec. Even more recently Vanpee has made observations on flames down to about one torr in a system whose pumping speed is about 2400 liters/sec.[9] None of these investigators apparently made any particular attempt to cool the burned gases before they arrived at the pump. Appropriate cooling together with judicious use of cryopumping when the exhaust gases are readily condensible could have greatly enhanced their effective pumping speeds. Even so, if one wanted to burn flames at pressures substantially lower than one torr it seems clear that it would be difficult and expensive to provide sufficient pumping speed because the required speed goes up with the inverse square of the pressure. To remove the gases from a flame at a pressure of one millitorr would require $10^6$ times as much pumping speed as would be required at one torr!

Is there any good reason to go to such low pressures? The answer to this natural question is not entirely obvious. A number of reasons can be cited. How good they are is a matter of conjecture. We can give such conjecture a starting point by noting that an age old question in combustion circles has been whether there is really a low pressure limit to flame propagation. To the extent that simple extrapolation of past experience can be relied upon, the answer seems to be that one can maintain flames at as low a pressure as one wants provided only that one makes the diameter of the burner sufficiently large. Testing of this empirical rule to pressures well below one torr would be perhaps interesting but certainly not of overwhelming importance per se. However, upon more careful reflection some intriguing possibilities emerge. In the first place, it is to be recalled that some of the elementary exothermic reactions in many flames almost certainly involve atom and radical recombination which are thought to require three body encounters. At one torr these events are relatively scarce compared to binary collisions but still possibly numerous enough to allow ordinary flame reactions to proceed. Indeed, Wolfhard noted that in flames of carbon monoxide or hydrogen with oxygen there was a decrease in burning velocity with decreasing pressure which did not occur with hydrocarbons as fuels. He tentatively attributes this decrease in speed to the decrease in three body collisions but observed that another effect having to do with radiation could be involved.[10]

Flames clearly have fairly large populations of radiating species. Indeed, those that radiate in the visible portion of the spectrum are what make flames visible and attractive both esthetically and scientifically. The radiation lifetime of many of these species, especially those radiating in the infrared is much longer than the time between collisions at pressures as low as one torr. For example, radiation lifetimes for the various modes in $CO_2$ are all greater than three milliseconds. At one torr the time between collisions at flame temperatures is of the order of a microsecond. Thus, at that pressure the average $CO_2$ molecule undergoes several thousand collisions during its radiation lifetime, probably enough to insure thermalization of its internal energy. At substantially lower pressures, however, the possibility of radiation before thermalization becomes enhanced giving rise to a couple of provocative questions. Does the shift in mode of de-excitation for internally excited species make a difference in the structure and propagation characteristics of the flame? Is it possible that going to low pressures will greatly suppress collisional de-excitation so that population inversions capable of lasing might be achieved? It is to be remembered that in many exothermic reactions there is growing evidence that product molecules are formed in vibrationally or electronically excited states. It is this phenomenon which makes so-called chemical lasers possible. A possible advantage of flame systems for such lasers is that the reactants can be premixed because the relatively high activation energy of the initial flame reactions prevents the premixed reactants from reacting until they enter the flame front which is a region of very rapid rise in temperature and/or the concentration of free radicals and chain carriers which cause the reaction to occur very quickly. The other requirement for achieving and maintaining the inversion necessary for lasing is that collisional deactivation of the excited species must not occur too rapidly. It is this latter requirement that low pressures could make possible in flame systems.

Of course, even if effective high power chemical lasers could be developed around flame systems by using the high pumping speed available in space, it might represent something of a pyrrhic victory because there might not be much use for them up there. Nevertheless, exploration of the possibility by spectroscopic studies of very low pressure flames would seem to offer the prospects of some interesting science.

3. <u>A Variation on the Low Pressure Flame Theme</u>. Flames generated by the combustion of solid propellants as used in rocket motors also offer opportunities for study at pressures low enough to require very large pumping speeds. These propellants are of two general classes. So-called colloidal or double base propellants are based on dispersions of nitrocellulose in nitroglycerine, i.e., very similar to the smokeless powder or cordite used in guns. More popular in rocket motors are the so-called composite propellants which comprise a granular oxidizer, usually ammonium perchlorate, embedded in a matrix of resin boinder which also is the fuel. These formulations are molded into large monolithic "grains," usually cylinders with an axial cavity whose size and shape are determined by the burning characteristics of the propellant and the ballistic requirements of the motor. In designing the grain for a particular motor and mission it is extremely important to know and if possible to control the burning rate of the propellant and its dependence upon pressure. Moreover,

there are a number of concomitant phenomena such as combustion instabilities with which are associated violent pressure oscillations which must be taken into account in the design of a motor. For these reasons there has been a great deal of experimental and theoretical study of solid propellant combustion. Even so, the theory of solid propellant burning is in a much more primitive state than the theory of flames in premixed gaseous systems. The difficulties are due in part to the much greater chemical complexity of solid propellant systems and in part to the complications stemming from the phase change as the solid reactants become gaseous products. Much of the experimental study of solid propellant combustion aimed at developing a theoretical understanding of the process is done with relatively small samples of the propellant, usually in the form of rectangular or cylindrical prisms called "strands". These strands are placed in a bomb in which the ambient pressure can be controlled independently of the combustion behavior. All strand surfaces but the uppermost one are coated with an inhibitor. The exposed surface is ignited and the deflagration rate, i.e., the linear regression rate of the burning surface into the substrate propellant, is monitored. Of primary interest is the dependence of this rate on the ambient gas pressure and the temperature and composition of the strand. It is well known that for any particular strand composition and size, i.e., cross sectional area of the burning surface, there is a critical pressure below which a flame cannot be sustained. This so-called Low Pressure Deflagration Limit or LPDL is of some practical interest because of problems associated with extinguishing and re-igniting a solid propellant rocket motor at high altitudes. Of more fundamental interest is its use as a test of models for the combustion process. Any self respecting model should be able to predict and characterize the LPDL phenomenon.

Some years ago Roy Cookson and I carried out some experiments on LPDL in which we measured the pressure at which the flame was extinguished for a range of strand sizes, i.e., areas of burning surface.[11] We found that the LPDL varied directly with the hydraulic radius of the strand, i.e., the ratio of perimeter to cross sectional area. Consequently, we were able to make a straight line extrapolation to a zero value of this hydraulic radius which would correspond to an infinite burning area. Somewhat surprisingly we found that at this limit the LPDL was finite. That is to say, the flame would go out at a finite pressure even for a burning surface of infinite area. Most theories indicate that the LPDL is due simply to a heat loss by radiation from the surface and the hot gases. Our results suggest that some other mechanism may be involved because at zero pressure and infinite area of burning surface the flame front would be infinitely thick. It is not entirely clear that radiative heat loss could be significant under these circumstances. It would seem likely that as the pressure decreases the accompanying decrease in the number of three body collisions and the increase in the ratio of radiation life time to time between collisions might well be expected to play an important role in solid propellant flames as well as in the premixed gaseous flames discussed in the previous section.

I hasten to point out that the pumping speed which was available was only about 10 liters/sec and was just sufficient to cope with a strand about 2.5 cm in diameter for which the LPDL was 40 torr. It is a very long extrapolation from 2.5 cm to infinity! Because the deflagration rate is inversely proportional to pressure and the gas density decreases directly with pressure, the pumping speed required per unit area of burning surface is roughly constant. But the burning area increases with the square of strand diameter. Consequently, the required pumping speed also goes up with the square of diameter. Thus, to go from 2.5 cm to 100 cm would require a pumping speed of something like 16 thousand liters a second at a pressure somewhere between 5 and 25 torr. That would seem to require a very large and expensive rig in which to dump very dirty hot gas.

By going to much larger strand sizes than Cookson and I were able to accommodate in our rig, one could test our extrapolation out to much larger sizes. In addition, of course, lowering the pressure would spread out the flame zone and make possible much more effective probing by spectroscopy and sampling probes. Thus, the SSE might lend itself to some interesting studies of solid propellant combustion.

4. <u>On the Composition of the Space Shuttle Environment</u>. One of the items on which there was unanimous agreement of Professor James Mayer's ad hoc Committee on Experiments in Space was the need to characterize as completely as possible the composition of the gas through which the Space Shuttle would be flying. In addition, for many experiments, it would be important to know the composition of the gas actually "in" the laboratory or the immediate environs of the space craft. The obvious way to determine chemical composition of low density gas is with a mass spectrometer and it would seem to be almost a routine problem in the case of "in lab" atmosphere. For the free stream gas, however, there are substantial sampling problems. Contamination by outgassing from the vehicle is a serious problem. Moreover, because many of the free stream species are atomic and can undergo reaction upon collision with a surface, it becomes very difficult to be sure that the measured ion currents are truly characteristic of free stream gas and do not include contributions from species which have collided with a surface somewhere on the vehicle or even in the instrument. For these reasons there is substantial uncertainty as to the true composition of the outer atmosphere in spite of the many measurements which have been made with instruments on board sounding rockets and balloons. A further reason for pursuing the problem of composition measurement is that the composition is not uniform in time or space. Consequently, one would like a lot of data taken at various times and places in order to obtain information on the scale and intensity of the fluctuations in composition in order to learn more about the structure of the atmosphere.

In the course of my visits in Europe I learned about two projects relating to mass spectrometry measurements on board the shuttle. Although both of them are probably well known to JPL-NASA I will mention them briefly here for the sake of completeness in reporting my discussions. The German Space Group have access to some space on one of the early flights which one of its component companies (Dornier or Messerschmidt, I believe) committed itself to "rent" or "buy" when NASA accepted bids a few years ago. They have also obtained a spare of the gold plated mass spectrometer which von Zahn had designed for the Mars mission. They are now in the process of designing and building the auxilliary gear which will adapt this instrument for use in their "rented" space. For reasons which are not clear to me, this adaptation involves a major electronics development which is to cost several hundred thousand marks. Everyone seems to recognize that the sampling problems will not be solved in this experiment. They claim justification on the basis that they will get some hands on experience in carrying out an experiment in space. In particular, they hope to find out what kinds of problems they will have to solve before they can contemplate obtaining truly reliable mass spectrometric analyses of the free stream atmosphere.

A more advanced project has been proposed to NASA by Berndt Feuerbacher of the Space Science Department of the European Space Agency (ESTEC) at Noordwijk in the Netherlands. In a proposal responsive to NASA AO-OSS-2-78 he outlines a method for discriminating between free stream gas and any distortions due to outgassing or surface interactions in mass spectrometric analysis. This discrimination is achieved by forming a molecular beam using two skimmers aligned with the velocity vector of the shuttle and analyzing the beam with an integrated time-of-flight quadrupole mass spectrometer. Because the vehicle flight velocity is much higher than the thermal velocity of most species, contaminants from outgassing or reflection from surfaces will have markedly different velocities (both speed and direction) from the free stream species. Thus, fairly crude time-of-flight velocity analysis obtained by chopping the incoming beam can readily distinguish between free stream and contaminant species.

In my view this approach seems sound and I hope that NASA decides to support the proposed program. It should be noted that the proposed apparatus will also lend itself to experiments in which the incoming beam species can be deliberately scattered from various kinds of surfaces in order to study gas surface interactions. It has often been pointed out that the Shuttle can generate a reasonably intense highly collimated beam of O atoms with an energy of about 5 eV and a speed ratio of about 9 or 10. Such beams cannot now be readily produced in earthbound laboratories and would permit many kinds of interesting gas-gas and gas-surface scattering experiments. In particular gas-gas scattering experiments with hydrocarbons and other fuel molecules might provide much needed information on the chemistry of the flame combustion reactions in which O atoms are presumed to play an important role. Because these possibilities have been much discussed, I will not spend time and space in this report ruminating over them anew. I mention them at all by way of indicating that the Feuerbacher proposal would not be an isolated experiment but could be an important starting point for an extended series of interesting and worthwhile experiments.

There is one drawback to the use of mass spectrometers. They cannot readily provide information about the internal energy states of the species in the sample. In the lower atmosphere essentially all species are in the ground state. Because of its low density and exposure to the full intensity of solar radiation, the upper atmospheric gas can have substantial concentrations of internally excited species. Whether one wishes to carry out experiments in the SSE or whether one is concerned primarily with atmospheric structure and processes, it would be most valuable to know about the internal states of upper atmospheric species as well as their relative abundance. The availability of tunable lasers promises to make possible the acquisition of data on internal energy states. Two laser methods which have been fairly extensively investigated and which seem applicable to the SSE conditions are laser induced fluorescence and laser multiphoton ionization. These are both very sensitive but, of course, require lasers tunable in the absorption range of the species of interest. The former works better when the fluorescence is in the near visible or shorter wavelength range of the spectrum because the photons are higher energy and more readily detectable and because the radiation lifetimes are usually short so that emission will occur while the excited species are still in the field of view of the detector. The latter requires very high photon densities and consequently samples a very small volume of gas because the laser beam must be focused to a small area. If tunable lasers become available in the uv portion of the spectrum, single photons will become energetic enough to cause ionization and the requirement for photon beam intensity will be relaxed and the sampling volume will be correspondingly increased.

There is a third possibility for using tunable lasers to identify internal energy states which has recently been developed by Professor G. Scoles and his colleagues at the University of Waterloo and which seems worthy of note here. Scoles has been a long time devotee of the use of super conducting bolometers as molecular beam detectors. Bolometers respond to the total energy content of the incident molecular beam. Thus, he finds that he can cross a dc molecular beam with a laser beam which is chopped and obtain an ac signal from his detector at the frequency of the laser beam chopping. That is, when a beam molecule absorbs a photon, it deposits the photon energy on the detector along with any other internal or translational energy which it possesses at the time of the absorption. These other energies are dc so that by appropriate adjustments of chopping frequency and phase his detector output indicates only the absorbed photons. He tunes the laser over a frequency range and obtains signal corresponding to absorption when the laser frequency matches the absorption frequency of the molecule. In this way he has been able to do absorption spectroscopy at the very low densities characteristic of molecular beams.[12,13] Of course, the flight time of the excited molecule between the laser beam and the bolometer must be short relative to the radiation lifetime. This situation is quite characteristic of the infrared region of the spectrum so that his method becomes an admirable supplement to detection based laser induced fluorescence where long radiation lifetimes are a great handicap. Scoles estimates that with a bolometer sensitivity of $10^{-13}$ watts/hz$^{1/2}$ he can detect fluxes of $3 \times 10^6$ molecules/sec photon absorption in the near to middle infrared. If one could achieve an equivalent sensitivity for a detector surface area of one cm$^2$ and if the shuttle flight velocity is 8 km/s, then one could detect about 40 excited molecules/cc of sampled gas. Even if the photon absorption cross sections are very small, the effective sensitivity would be extremely high. Of course, this method like all laser methods depends upon the availability of tunable lasers over the spectral range of interest, but the tunable range is increasing steadily. Already, with color center lasers and other solid state devices there is a very wide range of infrared already within reach.

Quite clearly, the advantages of the Scoles detection method lends itself to many of the kinds of spectroscopic experiments which were discussed in the original RDC report. It further enhances the prospects of many kinds of scattering experiments which might be done with beams extranced from the flux of atmospheric gas by the spacecraft. For these reasons I sincerely hope that Scoles will receive the support necessary to develop further this most ingenious application of bolometer detectors.

5. Microgravity and Coagulation in Turbulent Aerosols. The opportunities for experiments to take advantage of the microgravity condition in the SSE have been recognized from the beginning, especially in the field of fluid mechanics. Indeed in the European plans for space lab there is a whole module devoted to fluid mechanics experiments. One area of interest is in the effects due to surface tension which can become very important when gravitational forces become negligible. There are prospective practical implications of these effects because they can be very influential in the process of drawing single crystals from melts, for example. The surface tension of such melts is very high and in the presence of temperature gradients it can cause strong convection currents, i.e., the so-called Marangoni effect. At the DFVLR-AVA Institute at Goettingen I ran across some very interesting research on this problem. Dr. Ch.-H. Chun has developed a technique for studying surface tension effects in an earth bound system. He minimizes distortions due to gravity by going to very small masses (i.e., volumes) of liquid so that the surface tension forces are large relative to the gravitational forces. He suspends a drop of liquid between the ends of two vertical copper rods 3 mm in diameter. Each rod can be rotated in either direction over a range of speeds and the temperature of each rod can be independently controlled. He induces Marangoni convection by providing a downward temperature gradient through the liquid, i.e., making the top rod slightly warmer than the bottom rod. Dispersed in the fluid is particulate material which is illuminated by a vertical sheet of light passed through the vertical axis of the drop so that only the particles in the plane of the sheet are illuminated. With an enlarging lens and a TV camera he projects the illuminated plane on a screen which very clearly displays the flow streamlines. He finds he can markedly affect the flow patterns if he rotates one rod with respect to the other. In a counter rotating mode at an appropriate differential velocity the Marangoni flow cell is completely inhibited. These experiments

are being done in anticipation of studies to be performed in the Fluid Dynamics Module. Thus, they are already tuned in to the Shuttle Program and need no further elaboration here. I report them simply because they were to me beautiful and interesting.

More appropriate to the purpose of this report are some experiments being carried out by Professor Hiroshi Sato at the Institute of Space and Aeronautical Studies at the University of Tokyo. He is addressing himself to the problem of how turbulence may affect the growth of droplets in a gas undergoing condensation. He mixes a stream of moist air with a stream of colder air and produces a stream of air with small droplets in it, i.e., a stream of fog. He then passes this stream vertically through grids of various sizes in order to induce varying degrees of turbulence. At various distances above the grid he probes the foggy stream with a hot wire in an anemometer configuration. The wire cools and gives a signal via resistance change when it is struck by a droplet. The size of the signal pulse is proportional to the size of the droplet. The frequency of pulses indicates the number density of droplets. Thus he obtains a measure of growth rate as a function of time by knowing the velocity of flow and comparing probe signal patterns at various heights in the stream. The apparatus has not yet been perfected but meaningful results are beginning to accumulate.

Professor Sato is convinced that an understanding of droplet agglomeration and growth by turbulence has important and far reaching implications. He seems particularly intrigued by the effects this phenomena may have had upon the composition of the planets during the condensation and accretion from initial primordial gas. He even thinks that it may have something to do with the fact that all planets rotate in the same direction. Of course, the coagulation of solid colloidal particles in liquids and the effects of stirring on the coagulation process have been studied for a long time. Smoluchowski of kinetic theory fame even did some theoretical analysis of the process many years ago. There seems to have been very little if any work done on gaseous dispersions of liquids. The diminution of gravitational effects which could be achieved in the SSE is obvious. Experiments like those which Sato is trying can deal only with particles small enough so that drag forces will keep them suspended in the gas. It is not entirely clear just how such experiments might be designed and carried out on the shuttle but they certainly would seem to deserve some careful consideration. Professor Sato himself has a great interest in pursuing this kind of work and assured me that he would be happy to cooperate in any project which might be undertaken in anticipation of performing such experiments.

## III. Conclusions and Recommendations

I talked to many people from many disciplines. The response was somewhat less than overwhelming but I did glean a few ideas which seem to merit further consideration and analysis. Moreover, I was able to identify some capable investigators who are not now associated with a space program but who are interested in pursuing possibilities for extending their studies to take advantage of the Space Shuttle Environment:

1. Professor John C. Polanyi of the Department of Chemistry at the University of Toronto is keenly interested in high resolution spectroscopy of species native to or introduced into the upper reaches of the atmosphere.

2. Professor Marcel Vanpee of the Department of Chemical Engineering at the University of Massachusetts would be very interested in a spectroscopic study of ephemeral but kinetically important species in low pressure flames and tube reactors taking advantage of the high speed pumping that SSE offers.

3. Professor Giacinto Scoles of the Department of Chemistry at the University of Waterloo in Waterloo, Ontario is eager to develop his laser-bolometer detector system for use in the analysis of atmospheric species and the determination of their internal energy levels.

4. Professor Hiroshi Sato of the Institute of Space and Aeronautical Sciences wants very much to cooperate in any project which might extend his study of aerosol coagulation by turbulence, possibly taking advantage of the low gravity forces in orbiting laboratories.

If NASA gets to the point where it can seriously entertain proposals for research projects toward any of these goals, it would do well to get in touch with these investigators.

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## APPENDICES

### "Spreading the Word"

This section attempts to provide some dimension to the extent of my evangelistic activities. Section A comprises a list of all those with whom I have had direct conversations in the past year on possible SSE experiments. In addition to these "person-to-person" encounters, I also described the opportunity and the advantages of the spacecraft environment for experiments to audiences of various sizes in the course of lectures and seminars presented during my travels. On three occasions I made organized presentations on the subject to relatively large groups. At the 1978 Conference on Dynamics of Molecular Collisions at Asi lomar, California in June 1978 and at the Eleventh International Symposium on Rarefied Gas Dynamics at Cannes in July 1978, I made oral presentations with slides and transparencies. These meetings were prior to the term of the contract for which this document is the final report, but they were subsequent to the report on the original RDC study. Therefore, to indicate the extent of exposure to the idea of Space Shuttle experiments, Section B is an attendance list for the Asilomar Conference and Section C is a list of participants at the Cannes meeting.

The third occasion for a selected audience was the International Symposium on Molecular Beams which was at Riva del Garda, Italy in June 1979. At that meeting the message was presented in a Poster Session which remained on display throughout the week of the symposium. During scheduled Poster Sessions I was on hand for discussion. Unfortunately, I do not have an attendance list for that meeting but I am including a program in Section D. Because most scientists have to present papers if they are to qualify for travel support from their sponsors, this program provides a fairly representative census of those in attendance. Needless to say it also includes authors who stayed home, but maybe they got the word by hearsay from their colleagues.

APPENDIX A

People Engaged in Direct Conversation

(Numbers in parentheses refer to key for Fields of Interest at end of II-A)

Akamatsu, Professor Teruaki
Dept. of Mechanical Engr.
Kyoto University
Yoshida Honmachi, Sakyo-ku, Kyoto

Anderson, Professor J. B.(4,11,23,10,70)
Dept. of Chemistry
Pennsylvania State Univ.
University Park, Pa. 16802

Andres, Professor R. P.(4,11,14,70,71)
Dept. of Chemical Engr.
Princeton Univ.
Princeton, NJ

Balasubramanian, Professor D.(22,23,37,47)
Dept. of Chemistry
Univ. of Hyderabad
Hyderabad, India

Becker, Professor E. W.(4,11,69,70)
Institut f. Kernverfahrenstechnik
Kernforschungzentrum
D-7500, Karlsruhe, W. Germany

Bernstein, Professor R. B.(6,11,21,23)
Dept. of Chemistry
Columbia University
New York, NY 10027

Bose, Professor T. K.(24,26)
Aeronautical Engr. Dept.
Indian Inst. of Technology
Madras, India

Brooks, Professor Philip R.(6,11,21,23)
Chemistry Dept.
Rice University
Houston, TX 77001

Brusdeylins, Dr. G.(4,11,12,13)
Max Planck Inst. f. Strömingsforsch.
Postfach 867, Böttingerstrasse 4/8
3400 Göttingen, W. Germany

Campargue, Dr. Roger(4,11,70)
C.E.N. Saclay, SCPH
Lab. Jets Moleculaires
BP 2, 91190, Gif-sur-Yvette, France

Cassuto, Dr. A.(5,17,18,19,34)
CNRS Laboratoire M. Letort
Rt. de Vandoeuvre
54600 Villers, Nancy, France

Chandrasekahr, Professor (35,45)
Liquid Crystal Group
Raman Inst.
Bangalore, India

Chun, Dr. C. H.
DFVLR-AVA
Bunsenstrasse 10
3400 Göttingen, W. Germany

Chupka, Professor William(6,23,37,69)
Dept. of Chemistry
Yale Univ.
New Haven, CT 06520

Cross, Professor R. J., Jr.(6,12,11,23)
Dept. of Chem.
Yale Univ.
New Haven, CT 06520

Deshpande, Professor S.M.(24,26,27)
Aeronautical Engr.
Indian Inst. of Science
Bangalore, India

deVries, Dr. A. E. (6,11,12,21)
FOM Inst. for Atomic & Molec. Physics
Kruislaan 407
Amsterdam-Oost, The Netherlands

Ding, Dr. A. (11,12,37,68)
Hahn-Meitner Inst. f. Kernforschung
Berlin GMBH
D-100 Berlin 39, W. Germany

Ehrfeld, Dr. W. (4,11,69,70)
Institut f. Kernverfahrenstechnik
Kernforschungszentrum
D-7500, Karlsruhe, W. Germany

Faubel, Dr. M. (6,11,12,23)
Max Planck Inst. f. Strömungsforsch.
Postfach 867, Böttingerstrasse 4/8
3400 Göttingen, W. Germany

Feuerbacher, Dr. Berndt (11,18,19,69)
Space Science Dept.
European Space Agency, ESTEC
Noordwijk, The Netherlands

Franck, Professor Ulrich (22,16,22,37)
Inst. for Physical Chemistry
Univ. of Karlsruhe
Karlsruhe, W. Germany

Fujiwara, Professor Toshi (2,24,20)
Dept. Aeronautical Engr.
Nagoya University
Furo-cho, Chikusa-ku, Nagoya

Fukuda, Professor Kuniya (20,23,37,54)
Dept. of Engr. Physics
Kyoto University
Yoshida Honmachi, Sakyo-ku, Kyoto

Gentry, Professor W. R. (6,12,11,20,21)
Chemistry Dept.
Univ. of Minnesota
Minneapolis, MN 55455

Govinda-Raju, Professor G. R.(55,56,57,59)
High Voltage Engr.
Indian Inst. of Science
Bangalore, India

Gowariker, Dr. V. R. (25,26)
Chemicals and Materials Group
Vikram Sarabhai Space Center
Trivandrum, India

Greene, Professor E. F. (2,6,11,18)
Dept. of Chemistry
Brown University
Providence, RI 02912

Grover, Dr. James R. (11,23,72)
Dept. of Chemistry
Brookhaven National Lab
Upton, NY 11973

Gspann, Dr. J. (4,11,70,71)
Institut f. Kernverfahrenstechnik
Kernforschungszentrum
D-7500, Karlsruhe, W. Germany

Hagena, Dr. Otto (11,14,70,71)
Inst. f. Kernverfahrenstechnik
Kernforschungszentrum
D-7500, Karlsruhe, W. Germany

Herschbach, Professor D. R. (5,6,11,20,21,2
Dept. of Chemistry
Harvard University
Cambridge, MA 02138

Hishinuma, Professor Naoshi (11,68)
Inst. of Physics
College of General Education,
Univ. of Tokyo
Komaba, Meguro-ky, Tokyo

Hulpke, Dr. G. (11,18,19)
Max Planck Inst. f. Strömungsforsch.
Postfach 867, Böttingerstr. 4/8
3400 Göttingen, W. Germany

Jain, Professor S. R. (29,30,31)
Aeronautical Engr.
Indian Inst. of Science
Bangalore, India

Katayama, Professor Mikio (23,37,21)
Dept. of Pure & Applied Science
College of Gen. Education., Univ. of Tokyo
Komaba, Meguro-ku, Tokyo

Kaufman, Professor F. (5,6,23,37,49,66)
Dept. of Chemistry
Univ. of Pittsburgh
Pittsburgh, Pa. 15261

Kitagawa, Professor Taiji (5,11,12,37)
Faculty of Pharmaceutical Sciences
University of Medical and Pharm. Sci.
Toyama

Kobayashi, Professor Yasunori (3,4)
Inst. of Applied Physics
Univ. of Tsukuba
Sakura, Niihari, Ibaraki 300-31, Japan

Kodera, Professor K. (Emeritus)
Dept. of Chemistry
Kyoto University
Yoshida Honmachi, Sakyo-ku, Kyoto

Kolb, Dr. C. E. (5,6,11,12,23,37)
Aerodyne Research Inc.
Crosby Dr.
Bedford, MA 01730

Kondow, Dr. Tamotsu (22,23,65,66,67)
Dept. of Chemistry
Univ. of Tokyo
Hongo, Bunkyo-ku, Tokyo

Kotake, Professor Susumu (11,14,32)
Inst. of Space & Aeronautical Sci.
Univ. of Tokyo
Komaba, Meguro-ku, Tokyo

Kuchitsu, Professor Kozo (22,23,65,66,67)
Dept. of Chemistry
Univ. of Tokyo
Hongo, Bunkyo-ku, Tokyo

Kumar, Professor R. (41,42,43)
Chemical Engr. Dept.
Indian Inst. of Science
Bangalore, India

Koppenwallner, Dr. G. (4,1,18)
DFVLR-AVA
Bunsenstrasse 10
3400 Göttingen, W. Germany

Kupperman, Professor Aron (5,6,11,65)
Dept. of Chem.
California Inst. of Technology
Pasadena, CA 91125

Kuratani, Professor Kenji (24,25,26,20)
Inst. of Space & Aeronautical Sci.
Univ. of Tokyo
Komaba, Meguro-ku, Tokyo

Lai, Professor Hon-Ming (23,46,58)
Dept. of Physics
Chinese University of Hong Kong
Shatin, N.T., Hong Kong

Lee, Professor Y. T. (5,6,11,21,69)
MMRD - 70A-4414
Lawrence Berkeley Labs
Berkeley, CA 94720

Legge, Dr. H. (4,11,15)
DFVLR-AVA
Bunsenstrasse 10
3400 Göttingen, W. Germany

Leung, Professor Alfred F. (35,37)
Dept. of Physics
The Chinese Univ. of Hong Kong
Shatin, N.T., Hong Kong

Lang, Dr. H. (4,9,12,15)
Max Planck Inst. f. Strömungsforsch.
Postfach 867, Böttingerstr. 4/8
3400 Göttingen, W. Germany

Miller, Professor D. R. (4,6,11,13,18)
Dept. of Applied Mech. & Engr. Sci.
University of California
San Diego, Ca.

Murakami, Dr. M. (10,15,32,64)
Inst. of Space & Aeronautical Sci.
Univ. of Tokyo
Komaba, Meguro-ku, Tokyo

Oguchi, Professor Hakuro (2,3,4,9,10)
Inst. of Space & Aeronautical Sciences
Univ. of Tokyo
Komaba, Meguro-ku, Tokyo

Onji, Dr. A. (2,4,11,18)
National Aerospace Laboratory
Mitaka, Tokyo

Oshima, Professor Koichi (1,2,3,4,9,32)
Inst. of Space & Aeronautical Sciences
Univ. of Tokyo
Komaba, Meguro-ku, Tokyo

Nair, Dr. K. Narayanan (52,53,58)
Space Physics Division
Vikram Sarabhai Space Center
Trivandrum

Narasimha, Professor R. (1,2,3,4,28)
Aeronautical Engr.
Indian Inst. of Science
Bangalore, India

Polanyi, Professor J. C.
262 Lash Miller Chem. Lab.
Univ. of Toronto
Toronto, Ontario, M5S 1A1

Prasad, Professor K. K. (2,3,4,44)
Mechanical Engr. Dept.
Indian Inst. of Science
Bangalore, India

Raghunandan, Dr. B. N. (24,26,32)
Aeronautical Engr.
Indian Inst. of Science
Bangalore, India

Rao, Professor C. N. R. (34,36,37,38)
Solid State and Structural Chem.
Indian Inst. of Science
Bangalore, India

Rao, Professor K. H. (36,39,37,40)
Solid State & Structural Chemistry
Indian Inst. of Science
Bangalore, India

Rao, Dr. P. V. M. (50,51,52,59)
Space Physics Div.
Vikram Sarabhai Space Center
Trivandrum, India

Rao, Dr. U. R. (60,61,62)
Director
ISRO Satellite Center
Peenya, Bangalore, India

Rebrov, Professor A. K. (4,13,14)
Inst. of Thermophysics
Novosibirsk-90
USSR

Reddy, Dr. C. A. (49,50,51)
Space Physics Division
Vikram Sarabhai Space Center
Trivandrum, India

Reuss, Professor J. (6,11,14,20,71)
Fys. Lab. Kath. Univ.
Toernooiveld, Driehuizerweg 200
Nijmegen, The Netherlands

Riley, Professor S. J.
Chemistry Dept.
Yale Univ.
New Haven, CT 06520

Rothe, Professor E. W. (5,6,11,21,67)
RIES, College of Engineering
Wayne State University
Detroit, MI 48202

Sano, Professor Taeko (3,11,14)
Inst. of Industrial Science
Tokai University
Kita-kaname, Hiratsuka, Japan

Sato, Professor Hiroshi (1,3,27,28)
Inst. of Space & Aeronautical Sciences
Univ. of Tokyo
Komaba, Meguro-ku, Tokyo

Schumacher, Professor Ernst (6,11,20,23)
Inst. for Physical Chemistry
Univ. of Bern
Bern, Switzerland

Scoles, Professor G. (11,18,20)
Dept. of Chemistry
Univ. of Waterloo
Waterloo, Ontario

Professor A. K. Srikante (1,3,4)
Dept. of Aeronautical Engineering
Indian Institute of Science
Madras, India

Takayanagi, Professor Kazuo (9,12,13,54)
Inst. of Space & Aeronautical Sciences
Univ. of Tokyo
Komaba, Meguro-ku, Tokyo

Teshima, Dr. Koji (2,11,18)
Dept. of Aeronautical Engr.
Kyoto University
Yoshida Honmachi, Sakyo-ku, Kyoto

Toennies, Professor J. P. (2,4,11,12,23)
Max Planck Inst. f. Strömungsforschung
Postfach 867, Böttingerstrasse 4/8
3400 Göttingen, W. Germany

Tsuchita, Professor Soji (12,13,21,22)
Dept. of Pure & Applied Sciences
College of General Education, Univ. of Tokyo
Komaba, Meguro-ku, Tokyo

Vanpee, Professor Marcel (24,25,37)
Dept. of Chemical Engr.
Univ. of Massachusetts
Amherst, Mass.

Vasagam, Dr. R. M. (32,33)
Director, Ariane Passenger Payload Exp.
ISRO Satellite Center
Peenya, Bangalore, India

Venugopalan, Dr. S. (37,45)
Liquid Crystal Group
Raman Institute
Bangalore, India

Wharton, Professor Lennard (6,11,18,20,23)
James Franck Inst., Univ. of Chicago
5640 S. Ellis Ave.
Chicago, IL 60637

Wolfhard, Dr. H. G. (23,24,25,37)
Inst. for Defense Analysis
400 Army Navy Drive
Arlington, Va.

Yamashita, Dr. M. (11,14,20)
Inst. of Space and Aeronautical Sciences
Univ. of Tokyo
Komaba, Meguro-ku, Tokyo

Yamazaki, Dr. Satoshi (2,5,13,11)
Toyota Central Res. & Development Labs.
Hisakata, Tempaku-ku,
Nagoya, 408

Yoshikawa, Professor Kenneth K. (4,9,10)
Inst. of Applied Physics
Univ. of Tsukuba
Sakura, Niihari, Ibaraki 300-31, Japan

Zare, Professor R. N.(6,11,18,20,21,37,70)
Dept. of Chemistry
Stanford University
Stanford, CA 94305

## Field of Interest Key

1. Fluid Mechanics
2. Shock Tubes
3. Gas Dynamics
4. Rarefied Gas Dynamics
5. Chemical Kinetics

6. Molecular Dynamics
7. Thermodynamics
8. Statistical Mechanics
9. Kinetic Theory
10. Monte Carlo Methods

11. Molecular Beam Experiments
12. Molecular Energy Transfer
13. Relaxation Rates
14. Nucleation-Condensation
15. Vaporization Studies

16. Physical Organic Chemistry
17. Heterogeneous Catalysis
18. Molecule Surface Scattering
19. Surface Physics
20. Laser Spectroscopy

21. Laser Induced Chemistry
22. Physical Chemistry
23. Chemical Physics
24. Combustion
25. Liquid Rocket Propellants

26. Solid Rocket Propellants
27. Propulsion Dynamics
28. Turbulence
29. Astronautics
30. Orbital Mechanics

31. Satellite Trajectory Analysis
32. Heat Transfer
33. Molecular Structure
34. Surface Chemistry
35. Solid State Physics

36. Solid State Chemistry
37. Spectroscopy
38. Structural Chemistry
39. Amorphous Materials
40. Solution Chemistry

41. Chemical Engineering
42. Chemical Process Dynamics & Control
43. Chemical Reaction Engineering & Reactor Design
44. Gas Dynamic Lasers
45. Liquid Crystals

46. Theoretical Physics
47. Biochemistry
48. Biophysics
49. Meterology
50. Ionospherics

51. Radio Wave Propagation
52. Geomagnetics
53. Ultrasonic Acoustics
54. Plasma Physics
55. Power Transmission

56. High Field Phenomena
57. Dielectric Materials
58. Properties of Materials
59. Electrostatics
60. Astro Physics

61. UV Astronomy
62. X-Ray Astronomy
63. Electronics
64. Heat Pipes
65. Low Energy Electron Scattering

66. Photochemistry
67. Excited Atom Chemistry
68. Charge Exchange
69. Mass Spectrometry

70. Isotope Enrichment
71. Molecular Clusters
72. Synchroton Radiation Spectroscopy

Participants
1978 Conference on Dynamics of Molecular Collisions
Asilomar, California
June 26-30, 1978

Dr. O. William Adams
Dept. of Energy
Washington, DC 20545

Professor Millard H. Alexander
Dept. of Chemistry
University of Maryland
College Park, Maryland 20742

Prof. James B. Anderson
152 Davey Laboratory
Dept. of Chemistry
Pennsylvania State Univ.
University Park, PA 16802

Dr. Roger W. Anderson
Natural Sciences II
University of California
Santa Cruz, CA 95064

Brian Kitfield Annis
Oak Ridge National Lab.
P. O. Box X
Oak Ridge, Tenn. 37830

Prof. Vincenzo Aquilanti
Dipartimento di Chimica
Universita 'degli Studi
06100 Perugia (ITALY)

Prof. Daniel J. Auerbach
Dept. of Chemistry
Johns Hopkins University
Baltimore, MD 21218

Dr. Michael Baer
Soreq Nuclear Research Center
Yavne, ISRAEL

Prof. Thomas L. Bailey
Dept. of Physics
University of Florida
Gainesville, Florida 32601

Dr. Andre D. Bandrauk
103 Lewis Hall
University of California
Berkeley, CA 94720

Dr. John R. Barker
SRI International
Menlo Park, CA 94025

Mr. Chris Becker
MMRD - 70A-4429
Lawrence Berkeley Lab.
Berkeley, CA 94720

Prof. R. B. Bernstein
Dept. of Chemistry
Columbia University
New York, NY 10027

Dr. Normand C. Blais
MS-732
Los Alamos Scientific Lab.
Los Alamos, NM 87545

Dr. Stephen M. Bobbio
Chemistry Dept.
University of Georgia
Athens, Georgia 30602

Dr. Dietrich Brandt
University of Toronto
Chemistry Dept.
80 St. George St.
Toronto, CANADA

Prof. Philip R. Brooks
Chemistry Dept.
Rice University
Houston, TX 77001

Dr. John H. Brophy
Room 2-045, Chemistry Dept.
M.I.T.
Cambridge, Mass. 02139

Nancy J. Brown
E & E Division
Lawrence Berkeley Laboratory
Berkeley, CA 94720

Dr. Brunetto Brunetti
Dipartimento Di Chimica
Dell'Universita-Via Elce
Di Sotto, 06100 Perugia (ITALY)

Mr. Richard Buss
MMRD - 70A-4425
Lawrence Berkeley Laboratory
Berkeley, CA 94720

Dr. Piergiorgio Casavecchia
MMRD - 70A-4429
Lawrence Berkeley Laboratory
Berkeley, CA 94720

Miss Sylvia Ceyer
MMRD - 70A-4418
Lawrence Berkeley Laboratory
Berkeley, CA 94720

Prof. Sally Chapman
Dept. of Chemistry
Barnard College
Columbia University
New York, NY 10027

Dr. David C. Clary
IBM Research Laboratory
K34/281, 5600 Cottle Road
San Jose, CA 95193

Dr. Michael J. Coggiola
SRI International
Menlo Park, CA 94025

Dr. Ronald B. Cohen
Aerospace Corporation
P. O. Box 92957
Los Angeles, CA 90009

Dr. J.N.L. Connor
Dept. of Chemistry
University of Manchester
Manchester, M13 9PL, ENGLAND

Dr. Robert D. Coombe
Science Center
Rockwell International
1049 Camino Dos Rios
Thousand Oaks, CA 91360

Dr. William H. Cramer
Chemistry Division
National Science Foundation
1800 G St. NW
Washington, DC 20550

Prof. R. James Cross, Jr.
Dept. of Chemistry
Yale University
New Haven, Conn. 06520

Dr. John B. Cross
CNC-2, MS-732
Los Alamos Scientific Lab.
Los Alamos, NM 87545

Prof. Paul J. Dagdigian
Dept. of Chemistry
The Johns Hopkins University
Baltimore, Maryland 21218

Dr. Sheldon Datz
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, Tenn. 37830

Dr. Adalbert Ding
Hahn-Meitner-Institut fur
Kernforschung Berlin GmbH
D-1000 Berlin 39, GERMANY

Dr. Thomas H. Dunning
Argonne National Laboratory
Chemistry Division
Argonne, Illinois 60439

Dr. Rudolf M. Duren
Max-Planck-Institut fur
Stromungsforschung
Bottingerstr.4-8
D3400 Gottingen, WEST GERMAN

Dr. Marie Durup
Lab. de Resonance electron.
et ionique, Univ. de Paris
91405 Orsay, FRANCE

Dr. Michael B. Faist
Chemistry Dept.
Brookhaven National Laboratory
Upton, NY 11973

Prof. James M. Farrar
Dept. of Chemistry
Univ. of Rochester
Rochester, NY 14627

Prof. John B. Fenn
Mason Laboratory
Yale University
New Haven, Conn. 06405

Dr. Andrew Freedman
Havemeyer Hall
Columbia University
New York, NY 10027

Prof. Jean H. Futrell
Dept. of Chemistry
University of Utah
Salt Lake City, Utah 84112

Dr. Bruce C. Garrett
Dept. of Chemistry
Univ. of Minnesota
Minneapolis, MN 55455

Prof. W. R. Gentry
Chemistry Dept.
University of Minnesota
Minneapolis, MN 55455

Dr. Dieter Gerlich
MMRD - 70A-4405
Lawrence Berkeley Laboratory
Berkeley, CA 94720

Dr. Anna Giardini-Guidoni
C.N.E.N. Divisione N. Attivita
C.P. 65 - 00044 Frascati
(Rome), ITALY

Prof. Clayton F. Giese
Tate Laboratory of Physics
University of Minnesota
Minneapolis, MN 55455

Dr. Robert G. Gilbert
Dept. of Theoretical Chem.
University of Sydney
N.S.W. 2006, AUSTRALIA

Dr. Keith T. Gillen
Molecular Physics Laboratory
SRI International
Menlo Park, CA 94025

Dr. Graham P. Glass
Chemistry Dept.
Rice University
Houston, TX 77001

Dr. David M. Golden
SRI International
Menlo Park, CA 94025

Prof. Robert J. Gordon
Dept. of Chemistry
University of Illinois
Chicago, Illinois 60680

Dr. Thomas R. Govers
Lab. de Resonance
Electronique et Ionique
Univ. Paris-SUD
91405 Orsay, FRANCE

Prof. E. F. Greene
Chemistry Dept.
Brown University
Providence, RI 02912

Dr. James R. Grover
Dept. of Chemistry
Brookhaven National Lab.
Upton, New York 11973

Dr. Hellmut Haberland
Fakultat fur Physik
der Universitat Freiburg
Hermann-Herder-Strasse 3
7800 Freiburg, WEST GERMANY

Prof. William L. Hase
35 Chemistry
Wayne State University
Detroit, MI 48202

Dr. Raymond F. Heidner
The Aerospace Corp.
Bldg. 130 - Room 145
El Segundo, CA 90245

Dr. Irving Philip Herman
155 Monte Cresta Ave. #203
Oakland, CA 94611

Prof. Dudley Herschbach
Dept of Chemistry
Harvard University
Cambridge, Mass. 02138

Prof. Peter Hess
Dept. of Chemistry
University of California
Berkeley, CA 94720

Prof. Peter M. Hierl
Chemistry Department
Kansas University
Lawrence, Kansas 66045

Dr. Tomohiko Hirooka
MMRD - 70A-4418
Lawrence Berkeley Laboratory
Berkeley, CA 94720

Prof. William M. Jackson
Dept. of Chemistry
Howard University
Washington, DC 20059

Prof. F. Kaufman
Department of Chemistry
University of Pittsburgh
Pittsburgh, PA 15261

Prof. James L. Kinsey
Room 6-229
M.I.T.
Cambridge, MA 02139

Prof. Fritz S. Klein
Isotope Dept.
Weizmann Institute
Rehovot, ISRAEL

Prof. Kumasaburo Kodera
31-2 Shimogamokitazonocho
Sakyoku, Kyoto 606
JAPAN

Dr. Herbert F. Krause
Oak Ridge National Lab.
4500 W, F-17
Oak Ridge, TN 37830

Prof. John R. Krenos
Dept. of Chemistry
Douglass College
Rutgers University
New Brunswick, NJ 08903

Prof. Aron Kuppermann
Dept. of Chemistry (127-72)
California Inst. of Technology
Pasadena, CA 91125

Dr. George H. Kwei
Mail Stop 732
Los Alamos Scientific Lab.
Los Alamos, NM 87545

Dr. Neil Lang
Lawrence Livermore Laboratory
Livermore, CA 94550

Prof. Y. T. Lee
MMRD - 70A-4414
Lawrence Berkeley Laboratory
Berkeley, CA 94720

Prof. Stephen R. Leone
JILA, Nat. Bureau of Standards
University of Colorado
Boulder, Colorado 80309

Dr. William Lester
NRCC
Lawrence Berkeley Laboratory
Berkeley, CA 94720

Prof. Jacob J. Leventhal
Dept. of Physics
University of Missouri
St. Louis, MO 63121

Dr. M. C. Lin
Code 6110
Naval Research Laboratory
Washington, DC 20375

Dr. Hans J. Loesch
Universitat Bielefeld
Fakultat fur Fhysik
Universitatsstrasse
D-4800 Bielefeld 1, W GERMANY

Prof. Dr. J. Los
FOM-Inst for Atomic &
Molecular Physics
Kruislaan 407, Amsterdam
THE NETHERLANDS

Dr. Alan C. Luntz
IBM Research Laboratory
5600 Cottle Road
San Jose, CA 95193

Miss Elizabeth R. Manzares
Radiation Laboratory
Univ. of Notre Dame
Notre Dame, Indiana 46556

Prof. R. A. Marcus
174 Noyes Lab.
University of Illinois
Urbana, Illinois 61801

Dr. Raymond P. Mariella Jr.
Allied Chemical Co., MRC
P. O. Box 1021R
Morristown, NJ 07960

Prof. Richard M. Martin
Dept. of Chemistry
University of California
Santa Barbara, CA 93106

Dr. Chang-Chi Mei
Dept. of Chemistry
University of Calif.
Berkeley, CA 94720

Prof. C. Bradley Moore
Dept. of Chemistry
University of Calif.
Berkeley, CA 94720

Dr. John Moseley
Molecular Physics-106B
SRI
Menlo Park, CA 94025

Dr. James T. Muckerman
Chemistry Dept.
Brookhaven Nat. Laboratory
Upton, NY 11973

Prof. M. Menzinger
Lash Miller Chemical Laborator
80 St. George Street
Toronto, CANADA, M5S 1A1

Prof. J. Douglas McDonald
366 Noyes Laboratory
University of Illinois
Urbana, Illinois 61801

Dr. Charles A. McDowell
Dept. of Chemistry
University of British Columbia
2075 Wesbrook Place
Vancouver, BC, CANADA

Prof. David McFadden
Dept. of Chemistry
Boston College
Chestnut Hill, MA 02167

Dr. Robert K. Nesbet
IBM Research Laboratory
San Jose, CA 95193

Dr. Roy H. Neynaber
IRT Corporation
7650 Convoy Court
San Diego, CA 92111

Dr. Cheuk-Yiu Ng
Dept. of Chemistry
Iowa State University
Ames, IA 50011

Dr. Nikitin
Institute of Chemical Physics
Academy of Sciences
Moscow, V-334, U.S.S.R.

Dr. Jean B. Ozenne
3192 Bryant St.
Palo Alto, CA 94306

Dr. Eric K. Parks
Bldg. 200
Argonne National Laboratory
Argonne, Illinois 60439

Dr. Christopher A. Parr
Univ. Texas at Dallas
BE 2.6, P.O. Box 688
Richardson, TX 75080

Prof. John M. Parson
Chemistry Dept, OSU
140 W. 18th Avenue
Columbus, OH 43210

Prof. Dr. Hans Pauly
Max-Planck-Institute
Bottingerstr 4-8
D3400 Gottingen, WEST GERMANY

Dr. James R. Peterson
Molecular Physics Lab-106B
SRI International
Menlo Park, CA 94025

Prof. Norman C. Peterson
Polytechnic Institute
333 Jay Street
Brooklyn, NY 11201

Prof. Leon F. Phillips
Department of Chemistry
University of Canterbury
Christchurch, NEW ZEALAND

Prof. J. C. Polanyi
262 Lash Miller Chem. Lab.
University of Toronto
Toronto, Ontario, CANADA

Dr. Eli Pollak
Dept. of Chemistry
Columbia University
New York City, NY 10027

Dr. Lise Lotte Poulsen
Institute for Chemistry
University of Copenhagen
Copenhagen, DK-2200 N, DENMARK

Dr. Jack M. Preses
Division of Basic Energy Sci.
U.S. Dept. of Energy
Washington, DC 20545

Prof. David E. Pritchard
Room 26-231
M.I.T.
Cambridge, Mass 02139

Dr. Alfred T. Pritt
Rockwell International
P. O. Box 1085
Thousand Oaks, CA 91360

Dr. J. Gary Pruett
Dept. of Chemistry
University of Pennsylvania
Philadelphia, PA 19104

Dr. Martin Quack
Institut fur Physikalische
Chemie, der Universitat
Tammanstrasse 6
3400 Gottingen, WEST GERMANY

Dr. Lionel M. Raff
Dept. of Chemistry
Oklahoma State University
Stillwater, Oklahoma 74074

Prof. Gene P. Reck
35 Chemistry
Wayne State University
Detroit, MI 48202

Prof. Stephen J. Riley
Chemistry Department
Yale University
New Haven, Conn. 06520

Prof. John Ross
Room 6-123
M.I.T.
Cambridge, Mass 02139

Prof. Erhard W. Rothe
RIES, College of Engineering
Wayne State University
Detroit, MI 48202

Prof. George C. Schatz
Dept. of Chemistry
Northwestern University
Evanston, IL 60201

Prof. Christoph Schlier
Fakultat fur Physik
der Universitat
78 Freiburg, WEST GERMANY

Mr. Peter A. Schulz
MMRD - 70A-4418
Lawrence Berkeley Laboratory
Berkeley, CA 94720

Prof. G. Scoles
Facolta di Scienze
Universita di Trento
Povo(Trento) ITALY

Prof. H. K. Shin
Dept. of Chemistry
Univ. of Nevada
Reno, Nevada 89557

Dr. Kosuke Shobatake
MMRD - 70A-4435
Lawrence Berkeley Laboratory
Berkeley, CA 94720

Dr. Joel A. Silver
Aerodyne Research Inc.
Crosby Drive
Bedford, Mass. 01730

Prof. Peter A. Siska
Dept. of Chemistry
Univ. of Pittsburgh
Pittsburgh, PA 15260

Prof. James G. Skofronick
Dept. of Physics
Florida State University
Tallahassee, Florida 32306

Dr. James J. Sloan
National Research Council
Division of Chemistry
100 Sussex Drive
Ottawa, CANADA

Dr. Thompson M. Sloane
Physical Chemistry Dept.
General Motors Research Lab.
Warren, Michigan 48090

Dr. Ian W.M. Smith
Dept. of Physical Chemistry
Univ. Chemical Laboratories
Lensfield Road
Cambridge, ENGLAND

Mr. Randal K. Sparks
MMRD - 70A-4435
Lawrence Berkeley Laboratory
Berkeley, CA 94720

Prof. Leonard D. Spicer
Chemistry Dept.
University of Utah
Salt Lake City, UT 84112

Dr. Richard C. Stern
L-468
Lawrence Livermore Laboratory
Livermore, CA 94550

Dr. Steven Stolte
University of Nymegen
Physics Dept.
Toernooiveld, Nymegen
HOLLAND

Dr. Michael Stuke
Max-Planck-Institut
Postfach 968
3400 Gottingen, W. GERMANY

Prof. William C. Stwalley
Dept. of Chemistry
University of Iowa
Iowa City, IA 52242

Dr. Shen Y. Tang
IRT Corporation
P. O. Box 80817
San Diego, CA 92138

Dr. William L. Taylor
Monsanto Research Corp.
P. O. Box 32
Miamisburg, OH 45342

Dr. Peter W. Tiedemann
MMRD - 70A-4418
Lawrence Berkeley Laboratory
Berkeley, CA 94720

Prof. Dr. Juergen Troe
Inst. fur Physik. Chemie
Universitaet Goettingen
D-3400 Goettingen, W GERMANY

Prof. Donald G. Truhlar
Dept. of Chemistry
University of Minnesota
Minneapolis, Minn. 55455

Prof. Trina Valencich
1370 Palms Blvd.
Venince, CA 90291

Dr. James J. Valentini
Dept. of Chemistry
Harvard University
Cambridge, Mass. 02138

Dr. Jochen Wanner
Projektgruppe fur Laserforschung der Max-Planck-Gesellschaft, D-8046
Garching/Munich, WEST GERMANY

Dr. Sol Wexler
Argonne National Laboratory
9700 S. Cass Ave.
Argonne, Illinois 60439

Prof. Lennard Wharton
James Franck Inst.
University of Chicago
5640 S. Ellis Ave.
Chicago, IL 60637

Dr. John Wiesenfeld
Dept. of Chemistry
Cornell University
Ithaca, NY 14853

Prof. John Winn
Dept. of Chemistry
University of California
Berkeley, CA 94720

Prof. Daniel H. Winicur
Chemistry Dept.
Univ. of Notre Dame
Notre Dame, Indiana 46556

Dr. Francis J. Wodarczyk
Rockwell International Science
Center, P.O. Box 1085
Thousand Oaks, CA 91360

Dr. Charles Edward Young
CHM 200-A101
Argonne National Laboratory
Argonne, Illinois 60439

Prof. Richard N. Zare
Dept. of Chemistry
Stanford University
Stanford, CA 94305

Dr. Reinhard Zellner
Inst. fur Physik. Chemie
Universitat Gottingen
3400 Gottinge, W. GERMANY

# APPENDIX C

## Attendance List 11th International Symposium on Rarefied Gas Dynamics, Cannes, July 3-8, 1978

DR. A.S. ABBASS
DEPT. OF PHYSICS - COLLEGE OF SCIENCE
UNIVERSITY OF BAGHDAD - ADHAMIYA
BAGHDAD
IRAQ

PROFESSOR J.R. ANDERSON
DEPT. OF CHEMISTRY
PENNSYLVANIA STATE UNIV.
UNIVERSITY PARK, PA. 16802
USA

T. ABE
INST. SPACE AND AERON. SCI.; TOKYO UNIV.
KOMABA;MEGURO-KU
TOKYO
JAPAN

DR. K. AOKI
DEPT. OF AERON. ENGIN. ;KYOTO UNIV.
7 MATSU-MACHI,MORIGUCHI
OSAKA 570
JAPAN

PROF. G. ADOMEIL
INSTIT. F. ALLG. MECHANIK , TECHN. HOSCHULE
TEMPIERGRABEN
51 AACHEN
RFA

DR. G. ARMAND
C.E.N. SACLAY; BAT. 62
BP N•2
91190 GIF SUR YVETTE
FRANCE

DR. M. ALEXANDRE
C.E.N. SACLAY; D.G.I./SEPCP
B.P. N• 2
91190 GIF SUR YVETTE
FRANCE

MADAME HUETZ-AUBERT
CNRS GR 14
ECAM
92290 - CHATENAY MALABRY
FRANCE

PROFESSOR B.V. ALEXEJEV
MOSCOW AVIATION INSTITUTE
MOSCOW A-80
VOLOKOLAMSCOJE HIGHWAY 4
USSR

PR. S.P. BAKANOV
DEPT. SURF. PHENOM.- INST. PHYS. CHEM.
USSR ACAD. OF SC.
LENINSKI PROSPECT, 31
MOSCOW, B-71 - USSR

PR. J.A. ANDERSON
DEPT. OF CHEMISTRY
152 DAVEY LAB.-PENNSYLV. STATE UNIV.
UNIVERSITY PARK, PENNSYLVANIA 16802
USA

DR. A.G. BASHKIROV
USSR NATIONAL COMMITTEE
ON THEORETICAL & APPLIED MECHANICS
VERNADSKOVO PROSPECT, 101
117526 MOSCOW B-526 - USSR

PROFESSOR R.P. ANDRES
DEP. OF CHEMICAL ENGINEERING
PRINCETON UNIVERSITY
PRINCETON, NEW JERSEY 08540
USA

PROFESSOR E.W. BECKER
KERNFORSCHUNGSZENTRUM
7500 KARLSRUHE
POSTFACH 3640
RFA

DR. J. ANDRE
UNIV. DE PROVENCE - U.E.R. DE PHYSIQUE
CENTRE DE ST-JEROME - SERVICE 232
13397 MARSEILLE CEDEX 4
FRANCE

PROFESSOR J.J.M. BEENAKKER
RIJKSUNIVERSITEIT LEIDEN - HUYGENS LAB.
WASSENAARSEWEG 78
LEIDEN 2405
THE NETHERLANDS

PROFESSOR N. BELLOMO
POLIT. DI TORINO, IST. DI MECC. RAZ.
CORSO DUCA DEGLI ABRUZZI, 24
10129 TORINO
ITALIA

PROFESSOR G.A. BIRD
DEPARTMENT OF AERONAUTICS
THE UNIVERSITY OF SYDNEY
SYDNEY, N.S.W. 2006
AUSTRALIA

PROFESSEUR J.J. BERNARD
UNIV. P. ET M. CURIE; LAB. AEROTHERMIQUE
4 TER, ROUTE DES GARDES
92190 MEUDON
FRANCE

DR. P. BLEY
INST. FUER KERNVERFAHRENSTECHNIK DER
UNIV. UND DES KERNFORSCHUNGSZENTRUMS
D-7500 KARLSRUHE
RFA

PROFESSOR S.B. BERNDT
ROYAL INST. OF TECHNOLOGY ; K.T.H.
S-10044
STOCKHOLM 70
SWEDEN

PROFESSOR G. BOATO
FAC. DI SCIENZA MATEMATICHE
UNIVERSITA DI GENOVA
GENOVA
ITALY

DR. H.C.W. BEYERINCK
PHYSICS DEPARTMENT
EINDHOVEN UNIV. OF TECHNOLOGY
EINDHOVEN - P.O. BOX 513
THE NETHERLANDS

DR. R. BOETTGER
HAMBURG UNIV.; MPJ FUR KERNPHYS.
POSTFACH 103980
69 HEIDELBERG 1
R.F.A.

PROF. DR. ALFRED E. BEYLICH
TECHNISCHE HOCHSCHULE
5100 AACHEN

RFA

DR. VICINIO BOFFI
LAB. DI INGEGNERIA NUCLEARE
16, VIA DEI COLLI
BOLOGNA 40137
ITALY

DR. G.K. BIENKOWSKI
GAS DYNAMICS LABORATORY
FORRESTAL CAMPUS PRINCETON UNIV.
PRINCETON, NEW JERSEY 08540
USA

DR. PETEK BRAŃKO
LJUBLJANA UNIV.;PHYSICS DEPT.

61000 LJUBLJNA
YUGOSLAVIA

PR. DR. K. BIER
INST. FUER TECH. THERM. & KALT.
DER UNIV. KARLSRUHE
75 KARLSRUHE 1
RFA

DR. B. BRIGOLI
C.I.S.E.
P.O.B. 3986
20100 MILANO
ITALY

DR. N.S. BIRAJDAR
DEPT. OF MATHEMATICS
YESHAWANT COLLEGE
NANDED (431602)
INDIA

DR. GIAN PAOLO BRIVIO
IST. DI FISICA DELL'UNIV.
GRUPPO SOLIDI
VIA CELORIA, 16, MILANO
ITALY

PROFESSOR C.L. BRUNDIN
OXFORD UNIVERSITY
DEPT. OF ENG. SC.-PARKS ROAD
OXFORD OX1 3PJ
ENGLAND

DR. C.D. CANTRELL
LOS ALAMOS SCIENTIFIC LABORATORY
LOS ALAMOS
NEW MEXICO 87545
USA

PROFESSEUR R. BRUN
UNIV. DE PROVENCE; LAB. DYNAM. THERMOPH. FLUIDES
CENTRE ST-JEROME
13397 MARSEILLE CEDEX 4
FRANCE

DR. M. CATHALA
SNIAS
B.P. N•52
06322 CANNES LA ROCCA
FRANCE

DR. G. BRUSDEYLINS
MAX-PLANCK-INST. FUER STROMUNGS-
FORSCHUNG - BOTTINGER STR. 6-8
D 3400 GOETTINGEN
RFA

DR. T.D. MC CAY
ARO, INC. AEDC DIVISION
A SVERDRUP CORP. COMPANY
ARNOLD AIR FORCE STATION,
TENNESSEE 37389 - USA

DR. MANFRED BECKER
D.F.V.L.R.
INSTITUT FUER ANGEWANDTE GASDYNAMIK
5000 KOLN 90 - POSTFACH 90 60 58
RFA

PROFESSOR CARLO CERCIGNANI
ISTITUTO DI MATEMATICA
20133 MILANO
PIAZZA LEONARDO DA VINCI, 32
ITALY

PROFESSOR E.A. BRUN
MEMBRE DE L INSTITUT
8-10 PLACE DU COMMERCE
75015 PARIS
FRANCE

MADAME SYLVIE CHABAUTY
CNRS - INFORMASCIENCE
CENTRE DE DOC. SCIENT. & TECH.
26, RUE BOYER
75971 PARIS CEDEX 20 - FRANCE

PROFESSOR H. CABANNES
UNIVERSITE PARIS VI
MECANIQUE THEORIQUE - TOUR 66
4, PLACE JUSSIEU
75005 - PARIS, FRANCE

DR. ASHOK U. CHATWANI
INST. FUER THERM. & FLUIDDYNAMIK
RUHR-UNIVERSITAET BOCHUM
BOCHUM
RFA

DR. R. CAMPARGUE
CEN SACLAY;SCPH
LAB. JETS MOLECULAIRES
BP 2 91190 GIF SUR YVETTE
FRANCE

DR. K.Y. CHIEN
NAVAL SURFACE WEAPONS CENTER
SILVER SPRING
MARYLAND 20910
USA

DR. D.H. CAMPBELL
UNIV. OF SOUTHERN CALIFORNIA
LOS ANGELES,
CALIFORNIA 90007
USA

A.A. CHIKHAOUI
LAB. DYN. THERMOPHYS. FLUIDES
CENTRE DE ST. JEROME
13397 MARSEILLE CEDEX 4
FRANCE

DR. P. CODA
C.N.E.N.
S.P.ANGUILLARESE KM 1+300
ROMA
ITALY

DIPL. PHYS. C. DANKERT
DFVLR, AERO. VERSUCHSANSTALT
I. F. DYN. VERDUENNTER GASE
BUNSENSTR. 10, 3400 GOETTINGEN
RFA

DR. G.T. COLEMAN
ROYAL AIRCRAFT ESTABL.; AERODYNAMICS DEPT.

FARNBOROUGH; HAMPSHIRE
G.B.

DR. J. DARROZES
ENSTA
32, BD VICTOR
75015 PARIS
FRANCE

DR. R. COLE
BOLOGNA UNIVERS.;LAB. NUCLEAR ENGIN.
VIA DEI COLLI,16
40136 BOLOGNA
ITALY

DR. R. DAVID
J.G.V. DER KERNFORSCH. JUELICH
KFA JUELICH/JGV
5170 JUELICH, POSTFACH 1913
R.F.A.

PROFESSOR GEORGE COMSA
I.F. GRENZFLAECHENFORSCHUNG
UND VAKUUMPKYSIK
POSTFACH 1913, 5170 JUELICH 1
RFA

MADAME C. DEGEN
CNRS - INFORMASCIENCE
CENTRE DE DOC. SCIENT. & TECHN.
26, RUE BOYER
75971 PARIS CEDEX 20 - FRANCE

PROFESSOR NOEL CORNGOLD
APPLIED SCIENCE DEPT.
CAL. INSTITUTE OF TECHNO.
PASADENA, CALIF, 91125
USA

DR. S.M. DESHPANDE
DEPARTMENT OF AERON. ENG.
INDIAN INSTITUTE OF SCIENCE
BANGALORE
INDIA

DR. C. CREEMERS
FYSICO-CHEMISCH LABORATORIUM
VAN DE K.U. LEUVEN
CELESTIJNENLAAN 200 G
B - 3030 HEVERLEE - BELGIUM

DR. F. M. DEVIENNE
LAB. PHYSIQUE MOL. DES HAUTES ENERGIES
BP N•2
06530 PEYMEINADE
FRANCE

DR. J. CUVELLIER
C.E.N. SACLAY; PHYS. ATOMIQUE
B.P.N•2
91190 GIF SUR YVETTE
FRANCE

DR. I. DIMICOLI
C.E.N. SACLAY; D.R.A./SIRMA
BP N•2
91190 GIF SUR YVETTE
FRANCE

DR. A.E. DABIRI
MECHANICAL ENGIN. DEPT.
ARYA MEHR UNIV. OF TECHNOLOGY
P.O. BOX 3406 - TEHRAN
IRAN

PROFESSOR J. DORNING
LAWRENCE LIVERMORE LABORATORY
UNIVERSITY OF CALIFORNIA
P.O. BOX 808 - LIVERMORE, CA 94550
USA

DR. C. DREVET
C.E.A.
3, CLOS PEROULT
91200 ATHIS-MONS
FRANCE

DR. X. DE L EPREVIER
D.R.E.T.
26 BD VICTOR
75996 PARIS ARMEES
FRANCE

DR. D. DREYFUSS
M.I.T.
R.M. 37-438
77 MASSACHUSETTS AV., CAMBRIDGE MA 02139
U.S.A.

DR. EROFEEV
COMP. CENTER OF ACAD. OF SC. OF USSR
VAVILOVA 40
MOSCOW 117333
USSR

DR. ANIONI DROBNIK
POLITECHNIKA LODZKA
INSTYTUT FIZYKI
UL. WOLCZANSKA 219
93-005 LODZ - POLAND

DR. M. EYB
DORNIER SYSTEM GMBH
POSTFACH 1360
7990 FRIEDRIECHSHAFEN
RFA

DR. B. DUBORGEL
C.E.N. LIMEIL
BP N•27
94190 VILLENEUVE ST GEORGES
FRANCE

DR. U. EHRFELD
KERNFORSCHUNGSZENTRUM
7500 KARLSRUHE
POSTFACH 3640
RFA

DR. RICHARD EDWARDS
DEPARTMENT OF AEROSPACE ENGINEERING
UNIVERSITY OF SOUTHERN CALIFORNIA
LOS ANGELES, CALIFORNIA 90007
USA

DR. ALAN MC FALL
DIV. 5735 - SANDIA LABORATORIES
BOX 5800
ALBUQUERQUE NM 87115
USA

DR. W. EHRFELD
KERNFORSCHUNGSZENTRUM KARLSRUHE GMBH
INSTITUT FUER KERNVERFAHRENSTECHNIK
POSTFACH 3640 - D 7500 KARLSRUHE 1
RFA

DR. JEAN FARGES
GROUPE DES AGREGATS MOLECULAIRES
BAT. 210 - UNIV. PARIS-SUD
91405 ORSAY CEDEX
FRANCE

DR. T. ENGEL
INST. FUER PHYS. CHEMIE
UNIVERSITAET MUENCHEN
SOPHIENSTR. 11, D-8000 MUENCHEN 2
RFA

PROFESSOR A. FAVRE
DIRECTOR, I.M.S.T.
12, AVENUE DU GENERAL LECLERC
13003 MARSEILLE
FRANCE

DR. HIROSHI ENJOJI
THERMONUCLEAR FUSION LABORATORY
INST. OF PHYS. & CHEM. RESEARCH
2-1, HIROSAWA, WAKO-SHI, SAITAMA 351
JAPAN

PROFESSOR JOHN B. FENN
YALE UNIVERSITY - MASON LABORATORY
9 HILLHOUSE AVENUE
NEW HAVEN, CONN. 06520
USA

PROFESSOR M. FIEBIG
RUHR UNIV., BOCHUM,
INSTITUT FUR THERMO-FLUID DYNAMIK
RUHR UNIVERSITAT BOCHUM
463 BOCHUM - RFA

DR. ROBERT J. GALLAGHER
8321, FLUID MECHANICS DIVISION
SANDIA LABORATORIES
LIVERMORE, CALIFORNIA 94550
USA

PROFESSOR S. S. FISHER
UNIVERSITY OF VIRGINIA
ENGINEERING AND APPLIED SCIENCE
CHARLOTTESVILLE, VA 22901
USA

PRIV. DOZ. DR. ING. B. GAMPERT
UNIVERSITAET ESSEN - GESAMTHOCHSCHULE
FACHBEREICH 12 - MASCHINENTECHNIK
4300 ESSEN 1 - POSTFACH 6843
RFA

PROFESSOR W. FISZDON
INST. OF FUND. TECH. RES.
DEPT. OF FLUID DYNAMICS
SWIETOKRZYSKA 21,
00-049 WARSZAWA, POLAND

DR. R. GATIGNOL
LABORATOIRE DE MECANIQUE THEORIQUE
UNIVERSITE P. & M. CURIE
TOUR 66 - 4 PLACE JUSSIEU
75230 CEDEX 05 PARIS - FRANCE

PROFESSOR MARC FITAIRE
LAB. DE PHYSIQUE DES PLASMAS
BATIMENT 212
91405 ORSAY CEDEX
FRANCE

DR. P. GAUCHEREL
LAB. D'AEROTHERMIQUE DU CNRS
4 TER ROUTE DES GARDES
92190 MEUDON
FRANCE

DR. D. FRADKIN
LOS ALAMOS SC. LAB.
P.O. BOX 1663 M.S. 565
LOS ALAMOS NEW MEXICO 87545
U.S.A.

DR. M. A. GAVEAU
CEN SACLAY,SCPH
LAB. JETS MOLECULAIRES
BP 2 91190 GIF SUR YVETTE
FRANCE

PROFESSOR J.B. FRENCH
INST. FOR AEROS.STUDIES-UNIV. OF TORONTO
4925 DUFFERIN ST.
DOWNSVIEW, ONTARIO
M3H 5T6 - CANADA

DR. G. GEORGANTOPOULOS
PATRAS UNIVERSITY; MECHANICS DEPT.

PATRAS
GREECE

PROFESSOR DR. A. FROHN
INSTITUT FUER THERMODYNAMIK
DER LUFT-UND RAUMFAHRT UNIV. STUTTGART
7 - STUTTGART 80 (VAIHINGEN)
RFA

DR. D.P. GIDDENS
SCHOOL OF AERO. ENG.
GEORGIA INST. OF TECH.
ATLANTA, GA. 30332
GEORGIA - USA

DR. INZ. PIOTR GAJEWSKI
INSTYTUT TECHNIKI LOTNICZEJ
I MECHANIKI STOSOWANEJ
NOWOWIEJSKA 24
00-665 WARSZAWA - POLAND

DR. GERSTENKORN
LAB. AYME COTTON - CNRS II
CAMPUS D ORSAY
91405 ORSAY CEDEX
FRANCE

DR. VON HALLE
UNION CARBIDE CORP. OAK RIDGE GAS DIF.
PLANT K-25 - P.O. BOX P
OAK RIDGE, TENNESSEE 37830
USA

PROFESSOR Y. K. HSU
BANGOR COMMUN. COLL. UNIV. OF MAINE AT ORONO
ROOM 111 BANGOR HALL
BANGOR MAINE 04401
USA

DR. B.B. HAMEL
THERMAL & FLUID SCI. GR. DREXEL UNI.
32ND AND CHESTNUT STREET
PHILADELPHIA, PENNA 19104
USA

PROF. DR. H. HULSMAN
DEPT. NATUURKUNDE,
UNIV. INSTELLING ANTWERPEN
B-2610 WILRIJK
BELGIUM

DR. P.J. HARBOUR
CULHAM LABORATORY
ABINGDON OXON, OX 14 3 DB

ENGLAND

PROFESSOR FRANKLIN C. HURLBUT
DEPT. OF MECH. ENGINEERING
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720
USA

DR. J.K. HARVEY
IMPER. COL. OF SC. & TECHNOLOGY
DEPT. OF AERONAUTICS
PRINCE CONSORT ROAD,
LONDON SW7 2BY - ENGLAND

DR. A. E. LE JEUNE
CEN SACLAY; DGI/SEPCP
BP N•2
91190 GIF SUR YVETTE
FRANCE

DR. L.J.F. HERMANS
HUYGENS LABORATORIUM
RIJKSUNIVERSITEIT LEIDEN
LEIDEN
THE NETHERLANDS

DR. E.A. JOHNSON
DEPARTMENT OF PHYSICS
UNIV. OF SURREY, GUILDFORD
SURREY, GU2 5XH
ENGLAND

DR. G. HERMAN
AMSTERDAM UNIVERSITY; NATUURKUNDIG LAB.
VALCKENIERSTRAAT 65
AMSTERDAM
THE NETHERLANDS

DR. NIKOS KAFOUSIAS
PATRAS UNIVERSITY; DEPT MECHANICS
PATRAS

GREECE

DR. A. HOAREAU
UNIV. CLAUDE BERNARD LYON I
43 BD. DU 11 NOV. 1918
69621 VILLEURBANNE
FRANCE

PROFESSOR K. KARAMCHETI
DEPT. OF AERO. & ASTRONAUTICS
STANFORD UNIVERSITY
STANFORD, CALIFORNIA 94305
USA

PROFESSOR HEINRICH HORA
DEPT. OF THEORETICAL PHYS.
THE UNIV. OF NEW SOUTH WALES
KENSIGTON NSW 2033 - P.O. BOX 1
AUSTRALIA

PROFESSOR GERALD R. KARR
UNIVERSITY OF ALABAMA
P.O. BOX 1247
HUNTSVILLE, ALABAMA 35807
USA

DR ROBERT G. GILBERT
DEPT. OF THEOR. CHEMISTRY
UNIVERSITY OF SYDNEY
N.S.W. 2006
AUSTRALIA

PROFESSOR A.E. GROSSER
DEPARTMENT OF CHEMISTRY
MC GILL UNIV.,
801 SHERBROOKE STREET WEST
MONTREAL H 3A 2K6 - CANADA

DR. A. GINZBERG
HEBREW UNIVERSITY
EINSTEIN ST. 25/A
HAIFA
ISRAEL

DR. R. DE GRYSE
GENT STATE UNIVERSITY; SOLID STATE LAB.
S1 KRIJGSLAAN 271
9000 GENT
BELGIUM

DR. GIUSEPPE GOBBINI
MASSACHUSETTS INST. OF TECHNOLOGY
DEPT. OF AERONAUTICS & ASTRONAUTICS
CAMBRIDGE, MASSACHUSETTS 02139
USA

DR. J. GSPANN
I.F. KERNVERFAHRENSTECHNIK
KERFORSCHUNGSZENTRUM
7500 KARLSRUHE - POSTFACH 3640
RFA

DR. G. GODEFROY
C.E.N. LIMEIL
BP N•27
94190 VILLENEUVE ST GEORGES
FRANCE

DR. F. GUENTHER
SIEMENS AG
8000 MUENCHEN

RFA

DR. L. GOTTESDIENER
LABORATOIRE D'AEROTHERMIQUE DU CNRS
4 TER ROUTE DES GARDES
92190 MEUDON
FRANCE

DR. F. GUNTHER
INST. FUER TECH. CHEMIE DER TECHN.
UNIVERSITAET HANNOVER
CALLINSTR. 3
3000 HANNOVER - RFA

PROFESSOR C. GOUDAS
PATRAS UNIVERSITY; MECHANICS DEPT.

PATRAS
GREECE

DR. M. GILBERT
CEN SACLAY ; SCPH
BP N•2
91190 GIF SUR YVETTE
FRANCE

PROFESSOR T.E. GOUGH
GUELPH-WATERLOO CENTRE FOR
GRADUATE WORK IN CHEMISTRY
UNIV. OF WATERLOO, ONTARIO
N2L 3G1 - CANADA

DR. H. HABERLAND
FAK. FUER PHYSIK DER UNIVERSITAET
78 FREIBURG I. BR.
HERMANN-HERDER-STRASSE 3
RFA

PROFESSOR R. GRICE
THEORETICAL CHEMISTRY DEPARTMENT
CAMBRIDGE UNIVERSITY
CAMBRIDGE CB 2 1EW
ENGLAND

PROF. DR. O.F. HAGENA
I.F. KERNVERFAHRENSTECHNIK
KERNFORSCHUNGSZENTRUM
7500 KARLSRUHE, PF. 3640
RFA

DR. M.D. KARTALEV
INST. OF MATH. AND MECHAN.
P.O. BOX 373
SOFIA 1000
BULGARIA

DR.J. KORVING
LEIDEN UNIV.; HUYGENS LAB.
WASSENAARSEWEG 78
2300 RA LEIDEN
THE NETHERLANDS

DR. H. KIESEWETTER
RWTH AACHEN ABTLG PHYSIOLOGIE
MELATENERSTR. 211
51 AACHEN
RFA

DR. Y.A. KOSHMAROV
MOSCOW AVIATION INSTITUTE
MOSCOW

USSR

PROFESSOR F. KLEIN
WEIZMANN INST. OF SCIENCE; ISOTOPE RES. DEPT.

REHOVOT
ISRAEL

DR. S. KOSOWSKI
INST. OF FUND. TECHNOLOGY RES.
UL. PERECA 2 M 1214
00-849 WARSAW
POLAND

PROFESSOR H.F. P. KNAAP
LEIDEN UNIV.; HUYGENS LAB.
WASSENAARSEWEG 78
2300 RA LEIDEN
THE NETHERLANDS

DR. K. KOURA
NATIONAL AEROSPACE LAB.
1880 JINDAIJI-MACHI CHOFU
TOKYO
JAPAN

PROFESSOR E. KNUTH
5531 BOELTER HALL
UCLA
LOS ANGELES, CALIFORNIA 90024
USA

DR. MIROSLAV KRANYS
DEPARTEMENT DE PHYSIQUE
UNIVERSITE DE MONTREAL
MONTREAL - CASE POSTALE 6128
CANADA

DR. A. KOCIC
INST. OF NUCL. SC. BORIS KIDRIC
11001 BEOGRAD
P.O. BOX 522
YUGOSLAVIA

DR. G. KRIEG
KERNFORSCH.ZENTR. KARLSRUHE
POSTFACH 3640
75 KARLSRUHE
R.F.A.

PROFESSOR M.N. KOGAN
COMP. CENTER OF ACAD. OF SC. OF USSR
VAVILOVA 40,
MOSCOW 117333
USSR

DR. J.G. KUHRY
C.R.NUCL. DE STRASBOURG
23 RUE DU LOESS
67037 STRASBOURG CEDEX
FRANCE

DR. G. KOPPENWALLNER
DFLVR - INST. DYN. VERD. GASE
3400 GOETTINGEN
BUNSENSTRASSE 10
RFA

DR. A. KULICKI
INST. OF HEAT ENGINEERING
WARSAW TECHN. UNIVERSITY
UT. NOWOMIEJSKA 25
00-665 WARSAW - POLAND

DR. JOSEF KUNC
WARSAW TECHNICAL UNIVERSITY
NOWOWIEJSKA 25
00-665 WARSAW
POLAND

DR. LANG
MAX-PLANCK-INST. FUER STROMUNGS-
FORSCHUNG - BOTTINGER STR. 6-8
D 3400 GOETTINGEN
RFA

PROFESSOR IVAN KUSCER
UNIVERSITAET KAISERSLAUTERN
6750 KAISERSLAUTERN
POSTFACH 3049
RFA

DR. J. LAPUJOULADE
C.E.N. SACLAY; PHYS. ATOM. BAT.62
BP N•2
91190 GIF-SUR-YVETTE
FRANCE

PROFESSOR S.S. KUTATELADZE
CORR. MEMBER OF THE USSR AC. OF SC.
DIRECTOR - INST. OF THERMOPHYSICS
NOVOSIBIRSK-90, 630 090
USSR

DR. A.R. LARSON
UNIV. OF CALIF.,LAS. SCIENT. LAB.
P.O. BOX 1663 LOS ALAMOS
NEW MEXICO 07545
USA

DR. K. KYNEFORS
GOTEBORG UNIV., PHYS. CHEM. DEPT.
FACK; S-402 20 GOTEBORG

SWEDEN

DR. S. LEACH
CNRS-LAB. DE PHOTOPHYSIQUE
BATIMENT 213
FACULTE DES SCIENCES
91405 ORSAY - FRANCE

DR. F. LABERNEDE
C.E.N. LIMEIL
BP N•27
94190 VILLENEUVE ST GEORGES
FRANCE

DR. A. LEBEHOT
CEN SACLAY ; SCPH
LAB. JETS MOLECULAIRES
BP 2 91190 GIF SUR YVETTE
FRANCE

DR. WOLTERBEEK LAMBERT
TWENTE UNIV. OF TECHNOLOGY
AFD. TN , T.H.TWENTE POSTBUS 217
ENSCHEDE
THE NETHERLANDS

PROFESSOR J.H. DE LEEUW
UNIVERSITY OF TORONTO
30 VALLONCLIFFE ROAD
TOWNHILL, ONTARIO
CANADA

DR. J.A.C. LAMBREGTS
LIMBURG UNIV.;BIOMEDL.CENT. MED.FACULTY
BEELDSNIJDERSDREEF 101
6216 EA MAASTRICHT
THE NETHERLANDS

PROFESSOR Y.T. LEE
LAWRENCE BERKELEY LABORATORY
UNIV. OF CALIFORNIA - BERKELEY
CALIFORNIA 94720
USA

DR. M. LAMPIS
IST. DI MATEM. DEL POLIT. DI MILANO
PIAZZA LEONARDO DA VINCI, 32
20133 MILANO
ITALY

DR. D. LEGUILLON
LAB. DE MECAN. THEOR.
UNIVERSITE P. & M. CURIE
TOUR 66 - 4 PLACE JUSSIEU
75230 CEDEX 05 PARIS - FRANCE

DR. Y. LEJAY
C.E.N. SACLAY; PHYS. ATOM. BAT.62
BP N•2
91190 GIF SUR YVETTE
FRANCE

DR. J.C. LEMONNIER
CEN SACLAY;SCPH
LAB. JETS MOLECULAIRES
BP 2 91190 GIF SUR YVETTE
FRANCE

MONSIEUR JC. LENGRAND
CNRS-LAB. D'AEROTHERMIQUE
4 TER. ROUTE DES GARDES
92190 MEUDON
FRANCE

PROFESSOR V.B. LEONAS
SPACE RESEARCH INST. USSR ACAD. SCI.
68. PROFSOYUZNAJA ST.
117810 GSP 312, MOSCOW
USSR

PROFESSOR L.L. LEVENSON
DEPARTMENT OF PHYSICS
UNIV. OF MISSOURI-ROLLA
ROLLA, MISSOURI 65401,
USA

PROFESSOR CLARK H. LEWIS
VIRGINIA POLYT. INST. & STATE UNIV.
AEROS & OCEAN ENGR.
BLACKSBURG
VIRGINIA 24061 - USA

DR. C.P. LI
APPLIED MECHANICS DEPARTMENT
LOCKHEED ELECTRONICS CO., INC.
HOUSTON, TEXAS 77058
USA

PROFESSOR J. LOS
FOM INST. FOR ATOM.& MOL. PHYS.
KRUISLAAN 407
AMSTERDAM-OOST
THE NETHERLANDS

DR. P. LOUVET
CEN SACLAY; SCPH
BP N•2
91190 GIF SUR YVETTE
FRANCE

DR. D.Y.S. LOU
DEPT. OF MECH. & AEROS. ENGIN.
UNIVERSITY OF DELAWARE
NEWARK, DE 19711
USA

DR. A. LUBBERT
INST. FUER TECH. CHEMIE DER TECHN.
UNIVERSITAET HANNOVER
CALLINSTR. 46, EINGANG 3 -
D 3000 HANNOVER - RFA

DR. J.W.L. LEWIS
ARO, INC. AEDC DIVISION
A SVERDRUP CORP. COMPANY
ARNOLD AIR FORCE STATION
TENNESSEE 37389 - USA

PROFESSOR R.J. MADIS
DEPT. OF PHYSICAL CHEMISTRY
UNIVERSITY OF MUNICH
MUNICH
RFA

DR. N.K. MAJUMDAR
SAHA INST. OF NUCLEAR PHYSICS
CALCUTTA

INDIA

PROFESSOR J.R. MANSON
CENS - SERVICE DE PHYS. ATOMIQUE
INTERACTIONS GAZ-SOLIDES
B.P. NO. 2
91190 GIF-SUR-YVETTE - FRANCE

DR. C. MANUS
CEN SACLAY ; DPH.G/ PA
BP N•2
91190 GIF SUR YVETTE
FRANCE

DR. D. MARETTE
CEN SACLAY;SCPH
LAB. JETS MOLECULAIRES
BP 2 91190 GIF SUR YVETTE
FRANCE

DR. D.R. MILLER
UNIV. OF CALIFORNIA, SAN DIEGO
DEPT. OF APPL. MECHAN.& ENG. SC.B-010
LA JOLLA, CALIFORNIA 92093
USA

DR. K. M. MARTENSSON
A.B. ATOMENERGI

61101 NYKOPING
SWEDEN

DR. N.K. MITRA
INSTITUT FUER THERMO-UND FLUIDDYNAMIK
463 BOCHUM-QUERENBURG
POSTFACH 2148
RFA

DR. J.P. MARTIN
CNRS - ECOLE CENTRALE (050014)
GRANDE VOIE DES VIGNES
92290 CHATENAY MALABRY
FRANCE

PROF. V. MOLINARI
BOLOGNA UNIV.; LAB. NUCL. ENG.
VIA DEI COLLI 16
BOLOGNA
ITALY

DR. NATAKEYAMA MASAYUKI
TOKYO MET. COLLEGE AERON. ENGEN.
8-53-1 MINAMISENJU
ARKAWA-KU TOKYO
JAPAN

DR. R. MONACO
ISTITUTO DI MECCANICA RATIONALE-POLITECH. TORINO
CORSO DUCA DEGLI ABRUZZI 24
TURIN
ITALY

PROF. D. MASSIGNON
CEN SACLAY; SCPH
BP N•2
91190 GIF SUR YVETTE
FRANCE

DR. G. MONNOM
LAB. PHYS. MOL. DES HAUTES ENERGIES
BP N•2
06530 PEYMEINADE
FRANCE

DR. P. MENGER
EINDHOVEN UNIV. OF TECHNOLOGY
PO BOX 513
EINDHOVEN
THE NETHERLANDS

DR. G. MONNON
LAB. PHYS. MOL. DES HAUTES ENERGIES
BP N•2
06530 PEYMEINADE
FRANCE

MR. S.C. METCALF
HEAD, HIGH SPEED FLOWS SECT. AER. DEPT.
ROYAL AIRCRAFT ESTABLISHMENT
FARNBOROUGH/HANTS
ENGLAND

DR. J.P. MORERA
CEN F.A.R.; DPH/PFC
BP N•6
92260 FONTENAY AUX ROSES
FRANCE

PROFESSOR HISASHI MIKAMI
RESEARCH LAB. OF NUCL. REACTOR
TOKYO INSTITUTE OF TECHNOLOGY
O-OKAYAMA, MEGURO-KU
TOKYO - JAPAN

DR. A. MORTELETTE
AEROSPATIALE-CANNES
BP 52
06322 CANNES LA BOCCA
FRANCE

PROFESSOR E.P. MUNTZ
UNIV. OF SOUTH. CALIFORNIA
DEPT. OF AERO. ENG. UNIV. PARK
LOS ANGELES, CALIFORNIA 90007
USA

PROFESSOR W.H. MILLER
DEPT. OF CHEM. LAWRENCE BERKELEY LAB.
UNIVERSITY OF CALIFORNIA
BERKELEY, CA 94720
USA

PROFESSOR RODDAM NARASIMHA
DEPARTMENT OF AERONAUTICAL ENG.
INDIAN INSTITUTE OF SCIENCE
BANGALORE
INDIA

PROF. H. NEUERT
HAMBURG UNIV.; INST. EXPER. PHYSICS
36 JUNGRUNSTR.
2000 HAMBURG
R.F.A.

DR. MICHIO NISHIDA
DEPT. OF AERON. ENGIN.
KYOTO UNIVERSITY
KYOTO
JAPAN

DR. W. OBERT
KERNFORSCHUNGSZENTRUM KARLSRUHE GMBH
INST. FUER KERNFAHRENSTECHNIK
POSTFACH 36 40 - D 7500 KARLSRUHE
RFA

DR. M.J. OFFERHAUS
FOM-INST. VOOR ATOOM-EN MOLEC.
KRUISLAAN 407
AMSTERDAM
THE NETHERLANDS

PROFESSOR HAKURO OGUCHI
I. OF SPACE & AERONAUTICAL SCIENCE
UNIVERSITY OF TOKYO
KOMABA, MEGURO-KU
TOKYO, JAPAN

PROFESSOR D.C. PACK
UNIV.OF STRAT.-DEPT. OF MATHEMATICS
LIVINGSTONE TOWER
26 RICHMOND STREET
GLASGOW G1 1XH, SCOTLAND

DR. G. C. PANDE
UNIV. PATRAS ; DEPT. MECHANICS
PATRAS

GREECE

PROFESSOR H. PAULY
MPI F. STROEMUNGSFORSCHUNG
3400 GOETTINGEN
BOETTINGERSTR. 6/8
RFA

DR. T. PLATKOWSKI
WARSAW UNIV., DEPT. MATH. & MECHANICS
WARSAW P.KI. N.
WARSAW
POLAND

DR. P. PLURIEN
CEN SACLAY ; DGI
BP N•2
91190 GIF SUR YVETTE
FRANCE

DR. B.T. PORODNOV
URALS POLYTECHNICAL INSTITUTE
PHYSICAL & TECHN. FACULTY
620002, SVERDLOVSK K-2
USSR

DR. J. LEITH POTTER
VON KARMAN GAS DYNAMICS FAC. ARO, INC.
ARNOLD AFS
TENN. 37389
USA

MME. C. POUX
SOPEMEA
18 RUE EDOUARD BELIN
31029 TOULOUSE
FRANCE

PROFESSOR I. PRIGOGINE
PRIX NOBEL DE CHIMIE
UNIVERSITE LIBRE DE BRUXELLES
BRUXELLES
BELGIUM

PROF. Y. RIJOV
MOSCOW AVIATION INSTITUTE
VOLOKOLAMSKOJE ROAD 4
MOSCOW A-80
USSR

DR. STEFAN RADEV
INST. OF MATHEMATICS & MECHANICS
ACADEMY OF SCIENCES
KV. GEO MILEV, UL. 36, BL. 8
SOFIA 1113 - BULGARIA

MR. MILTON ROGERS
6309 PEARCE AVE.
BALTIMORE
MARYLAND
USA

DR. S.M. RAMACHANDRA
HINDUSTAN AERONAUTICS LIMITED
POST BOX 1789
BANGALORE 560017
INDIA

DIPL. ING. F. ROMANI
LEHRSTUHL FUER ALLG. MECHAN.
AN DER RHEIN. WESTF. TECHN. HOCHSCHULE
5100 AACHEN
RFA

DR. A.K. RAY
2012, HOLYBROOK CRESCENT
OTTAWA KIJ7Y6
ONTARIO
CANADA

PROFESSEUR A. RO[illegible]GARD
CEN SACLAY; SCPH
BP N•2
91190 GIF SUR YVETTE
FRANCE

PROFESSOR A.K. REBROV
INSTITUTE OF THERMOPHYSICS
SIBERIAN BRANCH OF THE USSR AC. SCI.
NOVOSIBIRSK-90
USSR

DR. G. PITTION-ROSSILLON
CEN LIMEIL
BP N•2
94190 VILLENEUVE ST GEORGES
FRANCE

DR. R. REICHENBACH
EUROPEAN RESEARCH OFFICE; US ARMY
223 OLD MARYLEBONE ROAD
LONDON NW1 5TH
U.K.

DR. J.C. ROUSTAN
LAB. PHYS. MOL. DES HAUTES ENERGIES
BP N•2
06530 PEYMEINADE
FRANCE

PROFESSOR J. REUSS
FYS. LAB. KATH. UNIV.
TOERNOOIVELD, DRIEHUIZERWEG 200
NIJMEGEN,
THE NETHERLANDS

DR. B. ROWE
LAB. D'AEROTHERMIQUE DU CNRS
4 TER ROUTE DES GARDES
92190 MEUDON
FRANCE

DR. P. RIGNY
CEN SACLAY; DGI/SEPCP
BP N•2
91190 GIF SUR YVETTE
FRANCE

PROFESSOR OLEG RYZHOV
COMPUTING CENTER
USSR ACAD. OF SCI.
40 VAVILOV ST. - 117333 MOSCOW
USSR

DR. W.C. SCHIEVE
CENTER FOR STAT. MECH. & THERM.
THE UNIV. OF TEXAS AT AUSTIN,
AUSTIN, TEXAS 78712
USA

DR. E. SCHMID
KERNFORSCH.ZENTR. KARLSRUHE ABT. : IKVT
POSTFACH 3640
D 75 KARLSRUHE
RFA

PROFESSOR G. SCOLES
LIBERA UNIV. DEGLI STUDI DI TRENTO
FACOLTA DI SCIENZE
38050 POVO (TRENTO)
ITALY

LT.COL. D. W. SEEGMILLER
US AIR FORCE EUROP. OFFICE SCIENT. RES. & DEVEL.
EOARD, 223 OLD MARYLEBONE RD.
LONDON NW1
UK

DR. M. SEIDL
DORNIER SYSTEM GMBH
7990 FRIEDRICHSHAFEN
POSTFACH 1360
RFA

DR. F. SEILER
INST. F. STROM. & STROMUNGSMASCH.
UNIVERSITAET KARLSRUHE
D-7500 KARLSRUHE
RFA

DR. P.J. SEVERIN
PHILIPS RESEARCH LABORATORIES
EINDHOVEN

THE NETHERLANDS

DR. E.M. SHAKHOV
COMPUTING CENTER
USSR ACADEMY OF SCIENCES
MOSCOW
USSR

DR. R.G. SHARAFUTDINOV
INSTITUTE OF THERMOPHYSICS
SIBERIAN BRANCH OF THE USSR AC. SC.
NOVOSIBIRSK-90
USSR

PROFESSOR FREDERICK SHERMAN
DEPT. OF MECHANICAL ENGINEERING
UNIVERSITY OF CALIFORNIA
BERKELEY CALIFORNIA 94720 TM01
USA

DR. STEVEN J. SIBENER
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720
USA

DR. D. SIEGELMAN
AVCO SYSTEMS DIV.
201 LOWELL ST.
WILMINGTON, MA 01887
USA

DR. R.E. SMALLEY
DEPT. OF CHEMISTRY - RICE UNIVERSITY
P.O. BOX 1892
HOUSTON, TX 77001
USA

DR. T. SOGA
DEPARTMENT OF AERON. ENG.
NAGOYA UNIVERSITY
CHIKUSA-KU NAGOYA 464
JAPAN

PROFESSOR YOSHIO SONE
DEPARTEMENT OF AERONAUTICAL ENG.
KYOTO UNIVERSITY
KYOTO 606
JAPAN

DR. V.M. SOUNDALGEKAR
DEPT. OF MATHEMATICS
INDIAN INST. OF TECH. POWAI
BOMBAY -400076
INDIA

PROFESSOR GILBERT D. STEIN
GASDYNAMICS LABORATORY
DEPT. OF MECH. ENG. & AST. SC.
NORTHWESTERN UNIVERSITY
EVANSTON, ILLINOIS 60201 - USA

ACAD. V.V. STRUMINSKII
DEPT. OF MECH. OF HETEROG. MEDIA
USSR ACAD. OF SCIENCES
125040 MOSCOW A-40
LENINGRADSKII PROSP. 7 - USSR

PROFESSOR L. TALBOT
UNIVERSITY OF CALIFORNIA
MECHANICAL ENGINEERING
BERKELEY, CALIFORNIA 94720, TM01
USA

DR. S.P. TANG
TRW - DEFENSE & SPACE SYST. GRP ONE
SPACE PARK R1-1196
REDONDO BEACH, CALIFORNIA 90278
USA

PROFESSOR C.M. TCHEN
2 STORSKOVSVEJ
4682 TUREBY

DENMARK

PROFESSOR J.G. THEOBALD
FAC. DES SCIENCES
LAB. SPECT. HERT. & D'ELECTRONIQUE
F-25030 BESANCON CEDEX
FRANCE

PROFESSOR L.B. THOMAS
PHYSICAL CHEMICAL LABORATORY
UNIVERSITY OF MISSOURI
COLUMBIA, MISSOURI 65201
USA

PROFESSOR DR. J.P. TOENNIES
MAX-PLANCK-INST. F. STROEMUNGSFORSCH.
D 3400 GOETTINGEN
POSTFACH 867, BOETTINGERSTRASSE 4/8
RFA

DR. G. TORCHET
GROUPE DES AGREGATS MOLECUL.
UNIVERSITE PARIS SUD
91405 ORSAY
FRANCE

DR. K.J. TOURYAN
FLUID & THERMAL SCIENCES DEPT. 1260
SANDIA LABORATORIES, P.O. BOX 5800
ALBUQUERQUE, NEW MEXICO 87115
USA

PROFESSOR L. TRILLING
AERONAUTICS AND ASTRONAUTICS
MASSACHUSETTS INST. OF TECHNOLOGY
CAMBRIDGE, MASSACHUSETTS 02139
USA

PROFESSOR J. VALENSI
LABORATOIRE DE MECANIQUE DES FLUIDES
1, RUE HONORAT.
13000 - MARSEILLE
FRANCE

DR. Y. VENDENBOOMGAERDE
CEN LIMEIL
BP N•27
94190 VILLENEUVE ST GEORGES
FRANCE

PROFESSOR DR. N.F. VERSTER
TECHN. HOGESCHOOL TE EINDHOVEN
INSULINDELAAN 2
EINDHOVEN
THE NETHERLANDS

DR. H. VESTNER
INSTITUT F. THEORETICAL PHYSIK
DER UNIVERSITAET ERLANGEN - NUERNBERG
852 ERLANGEN, GLUECKSTRASSE 6
RFA

PROFESSOR Y. WACHMAN
MASSACHUSETTS INST. OF TECHN.
DEPT. OF AERO. & ASTRONAUTICS
CAMBRIDGE, MASSACHUSETTS 02139
USA

PROFESSOR L. WALDMANN
INST. F. THEORETISCHE PHYSIK
UNIV. ERLANGEN-NUERNBERG
8520 ERLANGEN
GLUECKSTRASSE 6 RFA

DR. Z. WALENTA
FLUID MECH. DEPT.; INST. FUNDTL. TECHNOL. RES.;AC
SWIETOKRZYSKA 21
00-049 WARSAW
POLAND

DR. G.H. WEGDAM
UNIVERSITEIT VAN AMSTERDAM
LABORATORIUM VOOR FYSICHE CHEMIE
NIEUWE PRINSENGRACHT 126
AMSTERDAM - THE NETHERLANDS

PROFESSOR J.F. WENDT
VON KARMAN INST. FOR FLUID DYNAMICS
CHAUSSEE DE WATERLOO 72
B - 1640 RHODE-ST-GENESE
BELGIUM

PROFESSOR LENNARD WHARTON
THE J. FRANCK INST.,UNIV. OF CHICAGO
5640 ELLIS AVE.
CHICAGO, ILLINOIS 60637
USA

PROFESSOR DR. M.M.R. WILLIAMS
NUCL. ENGIN. QUEEN MARY COLLEGE
LONDON UNIVERSITY
LONDON
ENGLAND

DR. KLAUS WINKELMANN
MAX-PLANCK-INST. FUER STROMUNSFORSCH.
3400 GOETTINGEN
BOETTINGERSTRASSE 6/8
RFA

DR. A. WISNIEWSKI
WARSAW TECHNICAL UNIVERSITY
UL.ZWYCIEZCOW 13 M.7
03-936 WARSAW
POLAND

DR. H. WITEK
INT. FUR MOLPHYS.-FREIE UNIV. BERLIN
BOLTZMANNSTRASSE 20
1000 BERLIN 33
RFA

PROFESSOR CURT WITTIG
UNIVERSITY OF SOUTHERN CALIFORNIA
DEPARTMENT OF ELECTRICAL ENGINEERING
LOS ANGELES, CALIFORNIA 90007
USA

PR. G. WORTBERG
LEHRSTUHL FUER ALLG. MECH.
TECHNISCHEN HOCHSCHULE AACHEN
5100 AACHEN
RFA

PROFESSOR DR. W. WUEST
DFVLR-INST. DYN. VERDUENNTER GASE
3400 GOETTINGEN.
BUNSENSTRASSE 10
RFA

DR. KYOJI YAMAMOTO
DEPT. OF MECHANICAL ENGINEERING
SCHOOL OF ENGINEERING, OKAYAMA UNIV.
OKAYAMA
JAPAN

PROFESSOR SHEE-MANG YEN
UNIVERSITY OF ILLINOIS
AT URBANA-CHAMPAIGN
URBANA, ILLINOIS 61801
USA

DR. KENNETH K. YOSHIKAWA
NASA-AMES RESEARCH CENTER N 230-3
MOFFETT FIELD
CALIFORNIA 94035
USA

PROFESSOR TOR YTREHUS
NTH-INSTITUTT FOR MEKANIKK
NORGES TEKNISKE HOGSKOLE
7034 TRONDHEIM-NTH
NORWAY

Dr. Bernard Zappoli
Societe Europ de Propulsion
27207 Vernon, B.P. 802
France

APPENDIX -D Program - 7th International Symposium on Molecular Beams
Riva del Garda (Trento. Italy) 5/28/79

MONDAY - INELASTIC SCATTERING

8.30 * K. Bergmann (Kaiserslautern)
LASER SPECTROSCOPY AND INELASTIC COLLISIONS

9.00 ** U. Buck (MPI - Göttingen)
MOLECULAR SCATTERING FROM NON-SPHERICAL POTENTIALS

10.00 * D. Beck, U. Ross, W.Schepper (Bielefeld)
ON THE BULGE EFFECT OF MOLECULAR SCATTERING

10.30 COFFEE BREAK

MINISYMPOSIUM ON ELASTIC SCATTERING

11.00 * J.J.H. v.d.Biesen, E.H.v.Veen, F.A.Stokvis, C.J.N.v.d. Meijdenberg (Leiden)
MEASUREMENT OF THE GLORY STRUCTURE IN THE TOTAL CROSS SECT. OF AR-KR, KR-KR, KR-XE AND XE-XE

11.30 U. Buck, G.Mäneke, J.Schleusener (MPI - Göttingen),R.A. Aziz (Waterloo) G.Scoles (Waterloo - Trento) U.Valbusa (Waterloo)

ON THE QUESTION OF THE WELL DEPTH OF THE HeAr INTERATOMIC POTENTIAL

11.45 F. Torello, M.G. Dondi (Genova)
A NEW $H-H_2$ SPHERICAL POT. FROM HIGH RES. MOL.BEAM EXPERIMENTS

12.00 B. Brunetti, G. Liuti, E.Luzzatti, F.Pirani, F.Vecchiocattivi (Perugia)
ABSOLUTE TOTAL CROSS SECT. FOR $O - O_2$, $O_2 - O_2$, $O - N_2$, $O_2 - N_2$ COLLISIONS

12.15 R. Düren; H.O.Hoppe, H.Tischer (MPI - Göttingen)
OBSERVATIONS OF THE "ORBITING" PHENOMENON AS A BACKWARD PEAK IN THE DIFFERENTIAL CROSS SECTION

12.30 U. Schwalm, J.P. Toennies (MPI - Göttingen)
ORBITING RESONANCES IN THE SCATT. OF H ATOMS FROM MOLECULES

12.45 H.C.W. Beijerinck,P.M.A. v.d.Kam, N.F. Verster (Eindhoven)
THE SMALL ANGLE DIFF. CROSS-SECTION FOR AN INVERSE POWER POTENTIAL.

MINISYMPOSIUM ON NON SPHERICAL POTENTIALS

17.00 G. Rotzoll, A. Lübebrt (Hannover)
FITTING OF TOTAL DIFFERENTIAL ATOM-MOLECULE CROSS SECT. WITH ANISOTROPIC POTENTIALS

* = Invited paper

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| 17.15 | H. Thuis (Nijmegen)<br>ANISOTROPY OF NO-INERT GAS SYSTEMS |
| 17.30 | W.P. Kraemer (MPI - München)<br>QUANTUMCHEMICAL SCF AND CI CALCULATIONS OF THE ENERGY HYPERSURFACE FOR THE SYSTEM He-CO |
| 17.45 | A.Kuppermann, M.Kiel, J.T.Slankas, G.A.Parker (Caltech)<br>ANISOTROPIC POTENTIALS FOR HELIUM BEAMS BY CROSSED MOLECULAR BEAMS OF $N_2$, $O_2$, NO, CO AND $CO_2$ |
| 18.00 | V.N. Khromov, V.B. Leonas (Moscow)<br>ON THE USE OF SCATTERING DATA AS A TEST OF THE ACCURACY OF AB INITIO CALCULATIONS OF ANISOTROPIC POTENTIALS |
| 18.15 | W.R. Gentry, M.A. Hoffbauer, C.F.Giese (Minnesota)<br>PULSED MOL. BEAM STUDIES OF STATE-RESOLVED ROT. EXCITATION |
| 18.30 | J. Andres, U.Buck, F.Huisken, J.Schleusener, F.Torello (MPI - Göttingen)<br>STATE RESOLVED DIFFERENTIAL CROSS SECTIONS FOR $0 \rightarrow 2$ ROTATIONAL TRANSITIONS IN $D_2$ + Ne COLLISIONS |
| 18.45 | J. Schaefer (MPI - München)<br>RECENT RESULTS OF He - $H_2$ (HD) CROSS SECT. FOR EL. AND INELASTIC SCATTERING BELOW 1.5 eV CENTER OF MASS ENERGY |
| 19.00 | L. Monchick (Johns Hopkins), J.Schaefer (MPI - München)<br>AB INITIO CALCULATIONS OF THE TRANSPORT CROSS-SECTION OF $H_2$ |
| 19.15 | CHAIRMAN'S REMARKS : G.P. TOENNIES (MPI - Göttingen) |

## - T U E S D A Y -

REACTIVE SCATTERING

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| 8.30 | * | R. Grice (Manchester)<br>REACTIVE SCATTERING OF A SUPERSONIC OXYGEN AYOM BEAM |
| 9.00 | ** | Y.T. Lee (Berkeley)<br>RECENT ADVANCES IN STATE TO STATE REACTIVE SCATTERING |
| 9.45 | ** | J.C. Polanyi (Toronto)<br>CHEMICAL DYNAMICS; THEORY VS. EXPERIMENT |
| 10.30 | | COFFEE BREAK |

- T U E S D A Y -

MINISYMPOSIUM ON INELASTIC SCATTERING

11.00 S.B. Ryali (Connecticut), G.E.Kolb (Aerodyne Corp.),J.B. Fenn (Yale)
VIBRATIONAL EXCITATION OF $CO_2$ BY COLLISIONAL T-V EXCHANGE

11.15 F.A. Gianturco, U.T.Lamanna, D.Ignazzi (Bari)
VIB. EXCITATION OF SIMPLE MOLECULES BY COLLISION WITH PROTONS : A THEORETICAL STUDY ON CO TARGETS

11.30 J.A.D. Stockdale, R.J. Warmack (Oak Ridge)
COLLISIONAL IONIZATION OF Cs AND K BY $O_2$

11.45 M.J.P. Maneira, U.Weigmann, A.M.C. Moutinho, K.Lacmann(H.M.I. - Berlin)
DOUBLE DIFF. CROSS SECT. FOR K FORMATION IN K + $SnCl_4$ COLL.

12.00 J. Krenos (Rutgers)
CHEMICAL DYNAMICS OF ENERGY TRANSFER : FORMATION OF $Ne^*$ IN COLLISIONS OF He ($2^1S$) WITH GROUND-STATE Ne.

12.15 H. Haberland, P. Oesterlin (Freiburg)
THE PUMPING PROCESS OF THE HeNe-LASER, STUDIED IN DETAIL IN A CROSSED MOLECULAR BEAM EXPERIMENT

12.30 R. Düren; U. Krause, G. Moritz (MPI - Göttingen)
ELECTRONIC EXCIT. IN COLLISIONS OF Na, K and Rb WITH Hg

12.45 CHAIRMAN'S REMARKS : V. AQUILANTI (Perugia)

MINISYMPOSIUM ON REACTIVE SCATTERING

17.00 D. Brandt, J.C.Polanyi (Toronto)
MICROSCOPIC BRANCHING IN REACTIONS H+FY (Y=Cl, Br, I)$\rightarrow$HF (v', J') + Y

17.15 J.R. Grover, D.E.Malloy, J.B.A. Mitchell (Brookhaven)
APPLICATIONS OF RADIOACTIVE MOL. BEAMS : (1) THE CHEMISTRY OF ASTATINE; (2) THE MEAS. OF ABSOLUTE DIFF. CROSS. SECT.

17.30 K.K. Verma, W.C. Stwalley (Iowa)
THE PRODUCTION OF OH ($A\ ^2\Sigma^+$) FROM COLL. OF SUPERTHERMAL H ATOMS WITH $H_2O$ AND $O_2$

17.45 A.C. Luntz, P. Andresen (IBM - San José)
DYNAMICS OF THE CHEMICAL REACTIONS OF O ($^3P$) WITH SATURATED HYDROCARBONS

18.00 S. Chapman (Columbia)
THEORETICAL STUDY OF Be + HF $\longrightarrow$ BeF + H

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| 18.15 | | E. Vietzke, M.Erdweg, J.Heuschkel, L.Matus, G. Stöcklin (Jülich)<br>CROSSED BEAM KINETICS : ABSTRACTION AND SUBSITU TION IN THE REACTION OF Br WITH $CH_3I$ AND $(CH_3I)_2$ |
| 18.30 | | R. Dirscherl, H.U. Lee (Stuttgart)<br>MOLECULAR BEAM KINETICS : REACTIVE SCATT. OF Sm WITH $O_2$ AND LASER FLUORESCENCE STUDY OF YbBr. |
| 18.45 | | E.K. Parks, S. Wexler (Argonne)<br>COLLISION-INDUCED DISSOC. OF THE CESIUM HALIDES BY RARE GAS ATOMS AND $SF_6$ MOLECULES |
| 19.00 | | W.L. Hase, R.J. Wolf (Wayne State)<br>CHEMICAL DYNAMICS OF $C_2H_5$ DECOMPOSITION |
| 19.15 | | CHAIRMAN'S REMARKS : R.B. BERNSTEIN (Columbia) |

## - W E D N E S D A Y -

BEAMS OF CLUSTERS

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|---|---|---|
| 8.30 | * | E. Schumacher, W.H.Gerber, A.Herrmann, M.Hoffmann, S.Leutwyler, L.Wöste (Bern)<br>SPECTROSCOPY OF METAL CLUSTERS IN MOLECULAR BEAMS |
| 9.00 | ** | D. Herschbach (Harvard)<br>MOLECULAR CLUSTER BEAMS |
| 10.00 | * | Dr. F.M.Devienne, M. Teisseire (Peymeinade)<br>METAL AGGREGATES FORM. BY HIGH ENERGY MOL. BEAMS BOMBARDMENT |
| 10.30 | | COFFEE BREAK |

MINISYMPOSIUM ON CLUSTERS

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| 11.00 | | K. Sattler, J.Mühlbach, A.Reyes Flotte, E.Reckna - gel (Konstanz)<br>A SOURCE FOR METAL ATOM AGGLOMERATES OF UNIF. MASS |
| 11.15 | | S. Romano, E. Clementi (Donegani)<br>MONTE CARLO SIMULATION OF SMALL ION-WATER CLUSTERS |
| 11.30 | | G.L. Griffin, J.Kratsios, R.P.Andres (Princeton)<br>PRODUCTION AND SIZE ANALYSIS OF MOL. BEAMS OF ME - TAL CLUSTERS |
| 11.45 | * | R. Monot, E.R.Dietz, A.R. George, W.D.Knight (Berke ley)<br>BEAM OF POTASSIUM CLUSTERS : STERN-GERLACH EXPERI MENT. |

12.15 J. Gspann, H.Vollmar (Karlsruhe)
METASTABLE CLUSTERS

12.30 M. Cavallini, G. Grillo (Assoreni)
TWIN MOL. BEAM STUDY OF OXIDATION REACTIONS ON TRANS.METALS

12.45 L. Holmlid, J.O. Olsson (Göteborg)
SURFACE CATALYZED REACTIONS ON CARBON COVERED Pt(8%W)

## MINISYMPOSIUM ON ION AND MUONIUM CHEMISTRY

11.00 * D.M. Garner, D.G. Fleming (Vancouver)
MUONIUM REACTION KINETICS : HYDROGEN ISOTOPE EFFECTS AND CHEMICAL DYNAMICS IN STUDIES OF Mu + $X_2$ AND Mu+ HX

11.30 J.N.L. Connor, A.Laganà (Manchester)
QUASICLASSICAL DYNAMICS OF LIGHT HEAVY-HEAVY ATOM REACTIONS - THE REACTIONS Mu + $F_2$ AND Mu + $Cl_2$

11.45 H. Schmidt, M. Konrad, F. Linder (Kaiserslautern)
CROSSED-BEAM MEASUREMENTS OF CHARGE TRANSFER REACTIONS FOR $He^+$ + $N_2$ AND $He^+$ + $O_2$ IN THE 1 eV COLLISION ENERGY RANGE.

12.00 I. Kusunoki, Ch. Ottinger (MPI - Göttingen)
CHEMILUMINESCENT ION-MOLECULE REACTIONS : ROT.-VIB. STATE DISTRIBUTIONS OF $CH^+$ (A )FROM $C^+$ + $H_2$ ($D_2$) COLLISIONS.

12.15 W. Lindinger, E. Alge, H.Villinger, H.Störi (Innsbruck); D.L. Albritton, F.C.Fehsenfeld (Boulder)
DEPENDENCE OF ION-MOLECULE REACT. ON THE ION VIB. ENERGY

12.30 * A. Ding, A.Redpath, U.Steinmetzger (H.M.I. Berlin)
INFRARED CHEMILUMINESCENCE FROM ION MOLECULE REACTIONS

## - T H U R S D A Y -

### SURFACE SCATTERING

8.30 * F. Tommasini (Genova), U.Valbusa (Waterloo)
ATOMIC HYDROGEN SCATTERING FROM CRYSTAL SURFACES

9.00 ** V. Celli (Virginia)
THE DYNAMICS OF GAS-SURFACE INTERACTIONS

9.45 ** L. Wharton (Chicago)
SURFACE REACTIONS AND MOLECULAR BEAMS

10.30 COFFEE BREAK

11.00 POSTER SESSION (in alph. order of 1st author)

D.H.H. Al-Amiedy, D.E.Dugdale, D.C.Lainé (Keele)
ELECTROSTATIC STATE SELECTION OF MOLECULES EMPLOYING A SINGLE WIRE HELIX.

E. Alge, H. Villinger, H.Helm, W.Lindinger (Innsbruck), D.L. Albritton, F.C. Fehsenfeld (Boulder)
DRIFT TUBE MEAS. : THE LINK BETWEEN THERMAL RATE CONST. AND CROSS SECT. OBTAINED IN BEAM EXPERIMENTS.

B. Andresen (Copenhagen), S.Hultberg, B.Jelencovic, L.Liljeby, S.Mannervick, E. Veje (Stokholm)
DISSOCIATION AND EXCITATION OF SMALL MOLECULES UPON PASSAGE THROUGH THIN FOILS

D. Bassi (Trento), M. Cavallini, G. Grillo (Assoreni)
THE CATALYTIC OXIDATION OF CO ON PALLADIUM SURFACES

D. Bassi, A. Boschetti, S.Marchetti, M.Zen(Trento), T.E.Gough, R.E. Miller (Waterloo), G. Scoles (Waterloo & Trento)
I.R. SPECTROSCOPY OF SUPERSONIC MOL. BEAMS WITH TUNABLE DIODE AND COLOR CENTRE LASERS

K.Bergmann, R.Engelhardt, U.Hefter, P.Hering (Kaiserslautern)
MOL. BEAM DIAGNOSTIC WITH INTERNAL STATE SELECTION : PERPENDICULAR VEL. DISTRIBUTION IN A NA/NA SUPERSONIC BEAM

G. Brusdeylins, R.B.Doak (M.P.I. Göttingen)
TOTAL INTEGRAL CROSS SECTIONS FOR He - CO

U.Buck, L.Mattera, D.Pust (M.P.I. Göttingen), D. Haaks (Wuppertal)
ULTRAVIOLET EMISSION IN Xe + Xe COLLISIONS NEAR THRESHOLD

J.M.Calo (Princeton)
CRYOGENIC DEPOSITION AND DESORPTION STUDIES OF STRATOSPHERICALLY RELEVANT SPECIES

G. Caracciolo, T.H.Ellis, G.O.Este, G.Knight, G.Scoles, U. Valbusa (Waterloo)
SCATTERING EXPERIMENTS WITH H ATOMS. NON-SPHERICAL SYSTEMS : H + $C_2H_6$, H + $C_3H_8$, H + $CO_2$, H + CO.

M.A.A.Clyne, SJ.Davis, M.C.Heaven, I.S. McDermid (Queen Mary Coll.)
QUANTUM-RESOLVED DYNAMICS IN DIATOMIC HALOGENS AND INTERHALOGENS, USING DOPPLER-LIMITED LASER EXCITATION.

C.Dankert, H.Legge (Göttingen)
INVESTIGATION OF A BEAM SKIMMED AT SMALL KNUDSEN NUMBERS

A.Ding (H.M.I. Berlin)
A SEMICLASSICAL INVERSION PROCEDURE FOR STUECKELBERG OSCILLATIONS

E.N.Evlanov, Y.V. Lebedev, V.B. Leonas (Moscow)
"COLD" BEAM OF HYDROGEN ATOMS

J.D. Ganière, R.Monot, R.Rechsteiner (Lausanne)
BEAMS OF NA CLUSTERS : TIME OF FLIGHT MASS SPECTROMETRY

F.A. Gianturco, U.T.Lamanna, A.Attimonelli
A SCATTERING-ORIENTED POTENTIAL ENERGY SURF. STUDY FOR VIB-ROT EXCITATIONS OF DIATOMICS BY $H^+$.

H. Helm, K.Stephan, T.D.Märk (Innsbruck)
MASS SPECTROMETRIC INVESTIGATION OR RARE GAS DIMER BEAMS

M.Hofmann, S.Leutwyler, E.Schumacher (Bern) W.Schulze (Berlin)
MATRIX SPECTROSCOPY OF NA AND K CLUSTERS FORMED IN A SUPERSONIC MOLECULAR BEAM

A.P. Kalinin, V.N. Khromov, V.B.Leonas (Moscow), R.W. Wiynaendts van Resandt, J.Los (Amsterdam)
DIFFERENTIAL SCATTERING OF $Li^+$ IONS ON $N_2$ MOLECULES

P.M.A. van der Kam, H.C.W. Beijerinck, N.F. Verster (Eindhoven)
MONTE CARLO CALCULATION OF ANGULAR RESOLUTION FUNCTIONS

M.E.Koch, W.C.Stwalley (Iowa)
MULTIPHOTON IONIZATION OF $Li_2$

M.J.P. Maneira, A.J.F. Praxedes, A.M.C.Moutinho (Lisboa)
DIFF. CROSS. SECT. FOR ION PAIR FORM. IN K+$CCl_4$ COLLISIONS

D.Menzel, V.Ramakrishan (Garching)
THERMAL ACCOMODATION OF HELIUM AND NEON ADSORBATE-COVERED TUNGSTEN SURFACES.

R.A.R. Porter, A.E.Grosser (McGill)
$CH_2$ MOLECULAR BEAM SOURCE

W.C.Stwalley, R.W.H. Webeler, R.F.Ferrante, Yea-Hwang Uang (Iowa)
A PROPOSED BEAM METHOD FOR PRODUCTION OF SPIN-ALIGNED HYDROGEN

P.G.A. Theuws, C.E.E.Pernot, H.C.W.Beijerinck, N.F.Verster (Eindhoven)
EXCITATION AS A DETECTION MECHANISM FOR GROUND STATE PARTICLES

P.G.A.Theuws, C.E.E.Pernot, H.C.W. Beijerinck, D.C.Schram, N.F. Verster (Eindhoven)
PRODUCTION OF METASTABLES IN A HOLLOW CATHODE ARC DISCHARGE

J. Verberne (Nijmegen)
SPECTROSCOPY ON $(H_2)_2$ DIMERS

A.E.Zarvin, R.G. Sharafutdinov (Novosibirsk)
DIRECT EXP. VERIFICATION OF SUPERSONIC MOL. BEAM FORMATION MODEL

MINISYMPOSIUM ON GAS-SURFACE INTERACTIONS

17.00 * M.J.Cardillo (Bell Labs.)
THE DIFFRACTION OF He ATOMS FROM Si SINGLE CRYSTALS

17.30 H.Conrad, G.Ertl, J.Küppers, S.W.Wang (München), K.Gérard, H. Haberland (Freiburg)
PENNING IONIZATION ELECTRON SPECTROSCOPY OF CLEAN AND CO-COVERED METAL SURFACES

17.45 E. Ficocelli-Varracchio (Bari)
FIELD-THEORETIC APPROACH TO SCATTERING OFF SOLID SURFACES

18.00 A.C. Levi (Genova and Trento)
DEBYE-WALLER FACTOR AND INELASTIC ATOM-SURFACE SCATTERING

18.15 A.Armand, J.Lapujoulade, Y.Lejai, N. Papanicolau (Saclay)
THERMAL DEPENDENCE OF THE SPECULAR PEAK OF HELIUM SCATTERED FROM (100) COPPER

18.30 E. Semerad, E.M. Hörl (Seibersdorf)
DEBYE-WALLER FACTOR IN Ne-BEAM SCATT. BY A LiF SURFACE

18.45 G. Boato, P. Cantini, C.Guidi, R.Colella (Genova)
CHARGE DENSITY WAVES OBSERVED BY MOL. BEAM DIFFRACTION

19.00 L. Greiner, H.Hoinkes, H. Wilsch (Erlangen)
CORRELATION OF SPEC. AND DIFF. INTENSITY AT SELECTIVE ADSORPTION EXP. INVESTIGATIONS WITH D ON LiF (001)

19.15 CHAIRMAN'S REMARKS : G. BOATO (Genova)

BEAM-PHOTON INTERACTIONS

8.30 * W.R. Gentry, M.A. Hoffbauer, C. Giese (Minneapolis)
PHOTODISSOCIATION OF v.d. WAALS DIMERS IN PULSED MOL.BEAMS

9.00 ** V.S. Letokhov (Moscow)
MULTISTEP PHOTOIONIZATION OF MOL. BEAMS BY LASER LIGHT

9.45 ** J. Durup (Orsay)
PHOTODISSOCIATION

10.30 COFFEE BREAK

MINISYMPOSIUM ON PHOTOIONIZATION AND PHOTODISSOCIATION

11.00 * N.J.A. van Veen, M.S. de Vries, A.E. de Vries (F.O.M. Amsterdam)
PHOTOFRAGMENTATION OF DIATOMIC HALOGEN COMPOUNDS

11.30 R.B. Bernstein (Columbia)
LASER MULTIPHOTON IONIZ. AND FRAGMENT. OF MOL. BEAMS

11.48 R.K. Sparks, L.R. Carlson, K.Shobatake, M.L. Kowalczyk, Y.T. Lee (Berkeley)
DYNAMICS OF PHOTODISSOCIATION OF $O_3$

12.06 S. Leutwyler, M. Hoffmann, E. Schumacher (Bern)
SEQUENTIAL TWO-PHOTON-IONIZATION OF NaK AND $K_2$ IN SUPERSONIC MOLECULAR BEAMS

12.24 I.M. Beterov, Yu.V.Brzhazovskii, V.P.Chebotaev, A.K.Rebrov, B.E. Semyachkin, A.A. Vostrikov
INFLUENCE OF $CO_2$ LASER RADIATION ON $SF_6$ CONDENSATION AND MOLECULAR BEAM INTENSITY.

12.42 J.R. Grover, J.B.A. Mitchell (Brookhaven)
A VERSATILE USER-ORIENTED ATOMIC AND MOL. BEAM APPARATUS FOR USE WITH THE NAT. SYNC. LIGHT SOURCE.