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Cometary Atmospheres:
Modeling the Spatial Distribution
of Observed Neutral Radicals

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I. Introduction

The primary goals of the research program are the inclusion and evaluation of the following processes which are ususally neglected in modeling cometary atmospheres: (1) dependence on heliocentric distance of initial comet expansion velocities and nucleus vaporization rates, (2) dependence on heliocentric velocity of photochemical lifetimes and photon emission rates where applicable, (3) the correct isotropic ejection of daughter radicals upon photodissociation of parent molecules, (4) solar radiation pressure, and (5) collisional effects on radical kinematics. The principal results of the modeling effort would be to generate the information necessary to reduce observed radical column abundances to radical production rates for CN, C_2, C_3, and OH. Secondary goals which would naturally follow would be a better quantitative understanding of the physical processes which are important in cometary atmospheres. In all instances, model development is constrained by the observed spatial distributions of these radicals already phblished in the literature, as well as by the best currently available photochemical data. In addition, the same models developed here could also be easily applied to analyze the new observed spatial distributions of cometary radicals.

A fairly large amount of the filter photometric data can be expected to be acquired during the 1985-1986 apparition of Comet P/Halley from the members of the Photometry/Polarimetry network organized under the International Halley Watch. The large amount of high quality data requires much more sophisticated models for analysis than are currently available.

The type of model developed is a many particle-trajectory Monte Carlo model. The facility and economy of using this type of model for treating the complex geometry and dependencies mentioned above has been discussed and demonstrated in the published literature (Combi and Delsemme 1980a,b; Combi 1980). The traditional approach initiated by Eddington's (1910) fountain model and continued in such later works by Haser (1957, 1966), Wallace and Miller (1958), Keller and Meier (1976) and Festou (1981) becomes computationally unmanageable for multi-dimensional time-dependent models. This is also true for the one-dimensional fluid models which have begun to model the physics correctly (Marconi and Mendis 1982, Huebner and Keady 1983).

Progress during the second year in the following areas will be discussed: (1) C_2 and CN spatial distributions and their heliocentric distance dependences, (2) C_3 and OH scale lengths, (3) incorporation of coma temperature into the Monte Carlo particle-trajectory model, and (4) collaboration in the analysis of Comet Halley CCD images and long slit spectra.

II. C_2 and CN in Comets

Attached in an appendix to this report is a reprint of the paper published in the Astrophysical Journal which deals with the spatial distributions and inferred production rates of the C_2 and CN radicals in comets.

The principal contents of the paper briefly enumerated are:

(1) new observations of C_2 brightness profiles,

(2) compilation of C_2 and CN scale lengths from previously published data, as well as their heliocentric distance dependences,

(3) re-evaluation of published filter photometry with the new scale length data which resolves the previously held anomalous C_2-to-CN production ratio's behavior with increasing heliocentric distance, and

(4) an analysis of sunward and antisunward C_2 profiles with the Monte Carlo particle-trajectory model which implies a total source (parent) lifetime of 3.1×10^4 s at 1 AU and an excess photolysis-energy ejection speed of 0.5 km s^{-1} for C_2 radicals.

III. C_3 and OH in Comets

Although the $({}^1\Pi_u - {}^1\Sigma_g^+)$ transition of the C_3 radical at ~ 4040 Å has been observed in cometary spectra for many years (see Swings and Haser 1956), and OH is believed to be the photodissociation product of water, surprisingly little has been done in the area of observing the spatial distributions of these two important species.

Other than qualitative descriptions of the apparent spatial distribution from long-slit and objective prism spectra (see A'Hearn 1982) that the C_3 radical was less spatially extended from the nucleus than C_2 and CN, little quantitative study of the C_3 coma had been done until the very recent paper by Cochran (1985) which presents six brightness profiles of C_3 in 5 comets covering a range of heliocentric distances from 0.74 to 1.58 AU. Her analysis involved fitting Haser models simultaneously to all six profiles where the parent and daughter scale lengths were assumed to vary with heliocentric distance according to r^n, where $n \sim 2$. These power laws were compared with those adopted by A'Hearn (1982) for photometric data reduction and that found by Newburn and Spinrad (1984) for only the C_3 parent. Cochran concluded on the basis of her analyses and comparisons that data for two of the profiles (Comets Crommelin at 0.74 AU and Austin at 0.78 AU) were best fit by the r^2 law of Newburn and Spinrad but that data for the other four profiles (Comets Tuttle at 1.02 AU, Stefan-Oterma at 1.58 AU, and Kopff at 1.58 and 1.81 AU) were best fit by a different r^2 law.

An alternative way of approaching this type of analysis, as has been adopted in this project, is to analyze each brightness profile separately and compare the resulting heliocentric distance dependences of best fit model parameters. The best-fit Haser model scale lengths for each of the six C_3 profiles are listed in Table 1. The dependences on heliocentric distance for the parent and daughter scale lengths are shown in Figure 1 a and b. For reference, the best-fit power laws are also plotted. The variations are not at all consistent with r^2 dependences, as might be expected, but are $r^{4.9}$ for the parent and $r^{3.4}$ for the daughter scale lengths. Such variations are inconsistent with straightforward photochemical production and decay as are appropriate for C_2 and CN. However, one must also keep in mind the fact that, when assuming a simple r^2 law for both parent and daughter scale lengths, A'Hearn (1982) finds C_3 production rates in proportion to those for dust (continuum), CN and OH.

The spatial distribution of OH has been observed by various satellite-based UV instruments, but sufficiently high quality observations are unfortunately not available over a wide enough range of heliocentric distance to enable a quantitative study of the heliocentric distance dependence to be made. Table 2 lists the results of fitting Haser's model to each of the available brightness profiles. If an r^2 law is assumed for both parent and daughter scale lengths (which may or may not be true), we find the following values at 1 AU:

$$\gamma \text{ (parent)} = (6.3 \pm 1.9) \times 10^4 \text{ km}$$
$$\gamma \text{ (daughter)} = (2.5 \pm 0.9) \times 10^5 \text{ km.}$$

These values are somewhat larger than those adopted by photometric observers, 4.1×10^4 km and 1.16×10^5 km for the parent and daughter, respectively (A'Hearn 1982).

IV. Coma Temperatures

Gas dynamic and dusty gas dynamic models of the cometary coma predict that the vaporized gas can in general be described as having a bulk outflow speed and a temperature (Marconi and Mendis 1982, 1984; Huebner and Keady 1983, Gombosi et al. 1985). The outflow speed and temperature are in general a variable function of the distance (r) from the nucleus. In previous Monte Carlo models, including those developed for this project, the outflow has simply been described as a single constant speed.

As part of another NASA project with AER (NASW-3966: Principal Investigator, William H. Smyth; Co-Investigator, Michael R. Combi), we have incorporated the Monte Carlo model developed under this project in another model which describes the production of cometary atoms H, C and O through the photodissociation of likely parent molecules (H, O, CO, and CO_2). One of the objects of that work is to see if the spatial distribution of the observed extended hydrogen coma of comets can be modeled by a physically based model which includes (1) time dependent lifetimes and production rates, (2) realistic photodissociation kinematics, (3) three-dimensional heliocentric atom trajectories with radiation pressure, and (4) collisional thermalization of hot H atoms.

Early attempts at modeling observed 2-dimensional Lyman-α isophotes show that the H atoms which are thermalized by a simple radially flowing parent gas introduce a very low speed component to the velocity distribution which is not present in the data. However, for reasonable outer coma gas temperatures of several hundred degrees, the thermal speed component of the thermalized H atom can be comparable to, or even larger than, the outflow speed.

This thermalization of H atoms, as well as the effect of the radial dependence of the coma temperature on the thermalization of all species is important for gaining insight into the physical conditions in the inner coma as well as determining the observed spatial distributions of neutral gases. Therefore, the outflow of parent molecules from the nucleus is more realistically described by a convected Maxwell-Boltzmann distribution rather than a simple single speed radial outflow. At some point in the coma, the gas flow of a parent molecule can be characterized by a bulk outflow speed, u, and a temperature, T. The speed distribution, f(v) dv, of molecules of mass, m, at temperature T is given by the Maxwell-Boltzmann distribution,

$$f(v)\,dv = \frac{4}{\pi^{1/2}}\frac{v^2}{v_m^3}\exp\left(-\frac{v^2}{v_m^2}\right)dv ,$$

where v_m is the most probable speed,

$$v_m = (2kT/m)^{1/2} .$$

In order to simulate this speed distribution on a microscopic level with the particle-trajectory model, we can use the principle of Monte Carlo. Since the Boltzmann distribution is a normalized probability density function, a simulated distribution can be generated from a random number sequence, R_i on the interval from 0 to 1 by solving for v_i in the equation,

$$\frac{4}{\pi^{1/2}}\frac{1}{v_m^3}\int_0^{v_i} v^2 \exp(-v^2/v_m^2)\,dv = R_i .$$

The integral in this equation is not analytical, but can be transformed into a single parameterized function by making the substitutions: $u \equiv v/v_m$, $u_i \equiv v_i/v_m$ and $du = \frac{1}{v_m}dv$. The equation then becomes

$$\frac{4}{\pi^{1/2}}\int_0^{u_i} u^2 e^{-u^2}\,du = R_i ,$$

which has been numerically solved and included as an interpolated table of the form, $u_i = u(R_i)$, in the model.

The effects of a thermal coma in the model will be investigated more fully in the third year of this project, and coma temperatures through the photochemical heating produced by the photodissociation of water molecules will be determined.

V. Distribution of Neutral Radicals in Comet P/Halley

A collaboration had been initiated last year with Dr. Uwe Fink of the University of Arizona to analyze both CCD filtered images and long slit spectra of Comet P/Halley. Late in this project year, the principal investigator traveled to Tucson for an extended stay to assess the entire data set and to begin the job of data reduction. Tables 3 and 4 show summaries of the radical images and the long slit spectra.

In Tucson, we went through the procedure of processing one pair of images including flat fielding, background subtraction and continuum subtraction. the images processed were those taken on May 11, 1986 with the filters at 9180 Å, which includes the (1-0) band of the CN red system, and at 8600 Å, which is a well-placed continuum filter. The relative weights associated with the two images were computed roughly from the filter transmission parameters and the system spectral response estimated from some of the long-slit spectroscopy data.

Figure 2 showns the two reduced but unsubtracted filter images and the resulting subtracted CN image. It is apparent that, On May 11, we are seeing one of the CN jets which have been reported by other observes (A'Hearn et al. 1986) and that, like other reports, there is no coincident continuum jet.

Because of the large amount of high quality data available from this observing program, only a selected set of the images can be reduced and analyzed under the limited scope of the project. This work will continue during the third project year. The emphasis will be placed upon the remainder of the May 11 data to test for the existence of jets in the emissions of the other radicals, and possibly on data from one or two other nights spanning a range of heliocentric distance. The existence of gas jets could have far-ranging implications as to the production mechanism(s) of cometary radicals, as evidenced by the suggestion of A'Hearn et al. (1986) that the CN and C_2 in the jets (~15% of the total) may be produced by the newly discovered CHON grains which are likely to be rich in hydrocarbons.

The flexibility of the Monte Carlo particle-trajectory model will enable us to begin to model localized time-dependent multiple sources for cometary radicals for comparison with image data.

Table 1

Haser Model Scale Lengths for C_3[a]

Comet	r_H (AU)	γ_p (km)	γ_d (km)
Crommelin	0.74	1.4×10^3	3.3×10^4
Austin	0.78	1.5×10^3	3.7×10^4
Tuttle	1.02	3.2×10^4	1.5×10^5
Stephan-Oterma	1.58	7.7×10^4	9.9×10^5
Kopff	1.58	7.9×10^4	3.6×10^5
Kopff	1.81	1.0×10^5	4.8×10^5

[a]Cochran (1985)

Table 2

Haser Model Scale Lengths for OH

Comet	r_H (AU)	γ_p (km)	γ_d (km)
Kohoutek[a] (1973XII)	0.62	5.1×10^4	8.1×10^4
Bradfield[b] (1979X)	0.71	1.6×10^4	8.2×10^4
KBM[c] (1975IX)	0.82	4.8×10^4	1.2×10^5
Bennett[d] (1970II)	0.83	$< 7 \times 10^4$	1.4×10^5
Encke[e] (1980XI)	0.83	5.8×10^4	8.2×10^4
KBM[c] (1975IX)	0.87	2.7×10^4	4.8×10^5
Bradfield[b] (1979X)	1.03	2.29×10^4	$> 3 \times 10^5$

[a]Festou (1981)
[b]Weaver et al. (1981)
[c]Kobayashi-Berger-Milan, Festou (1981)
[d]Keller and Lillie (1974)
[e]Feldman et al. (1984)

Table 3

Summary of CCD Images of Neutral Radicals in Comet P/Halley

Date 1985-86	r AU	Δ AU	C_3 4060Å	C_2 5139Å	NH_2 5980Å	Cont 6250Å	Cont 8520Å	Cont 8600Å	CN 9180Å
Sep 23	2.45	2.30	-	1	-	-	1	-	-
Oct 19	2.10	1.46	-	1	2	1	-	1	1
Nov 14	1.73	0.76	1	2	2	1	-	2	2
Nov 16	1.71	0.72	2	4	3	3	1	3	2
Dec 7	1.39	0.69	1	3	2	2	1	3	3
Jan 8	0.90	1.29	-	-	-	2	-	2	2
Jan 13	0.83	1.37	3	2	2	3	-	-	-
Jan 19	0.75	1.46	-	-	-	3	-	2	2
Feb 28	0.71	1.29	-	-	-	3	-	1	1
Apr 17	1.42	0.47	-	2	-	3	-	-	-
Apr 18	1.44	0.48	1	2	2	1	-	2	2
May 10	1.76	1.08	-	-	-	1	-	-	1
May 11	1.78	1.11	1	1	2	1	-	1	1

Table 4

Summary of Long Slit Spectroscopy of Comet P/Halley

Date 1985-86	r AU	Δ AU	Number of Spectra
Aug 23	2.84	3.24	3
Aug 24	2.83	3.21	1
Sep 17	2.53	2.49	3
Sep 24	2.43	2.27	2
Oct 20	2.09	1.43	5
Oct 21	2.07	1.40	2
Nov 15	1.72	0.74	9
Dec 8	1.38	0.70	10
Dec 9	1.36	0.72	5
Jan 10	0.87	1.32	13
Jan 11	0.86	1.34	11
Jan 12	0.84	1.36	9
Mar 1	0.72	1.27	15
Mar 2	0.74	1.25	11
Mar 3	0.75	1.22	6
Mar 4	0.76	1.20	6
Mar 5	0.77	1.18	9
Apr 14	1.38	0.43	22
Apr 15	1.39	0.44	19
May 9	1.75	1.05	14
Jun 5	2.13	1.93	6
Jun 6	2.14	1.96	5

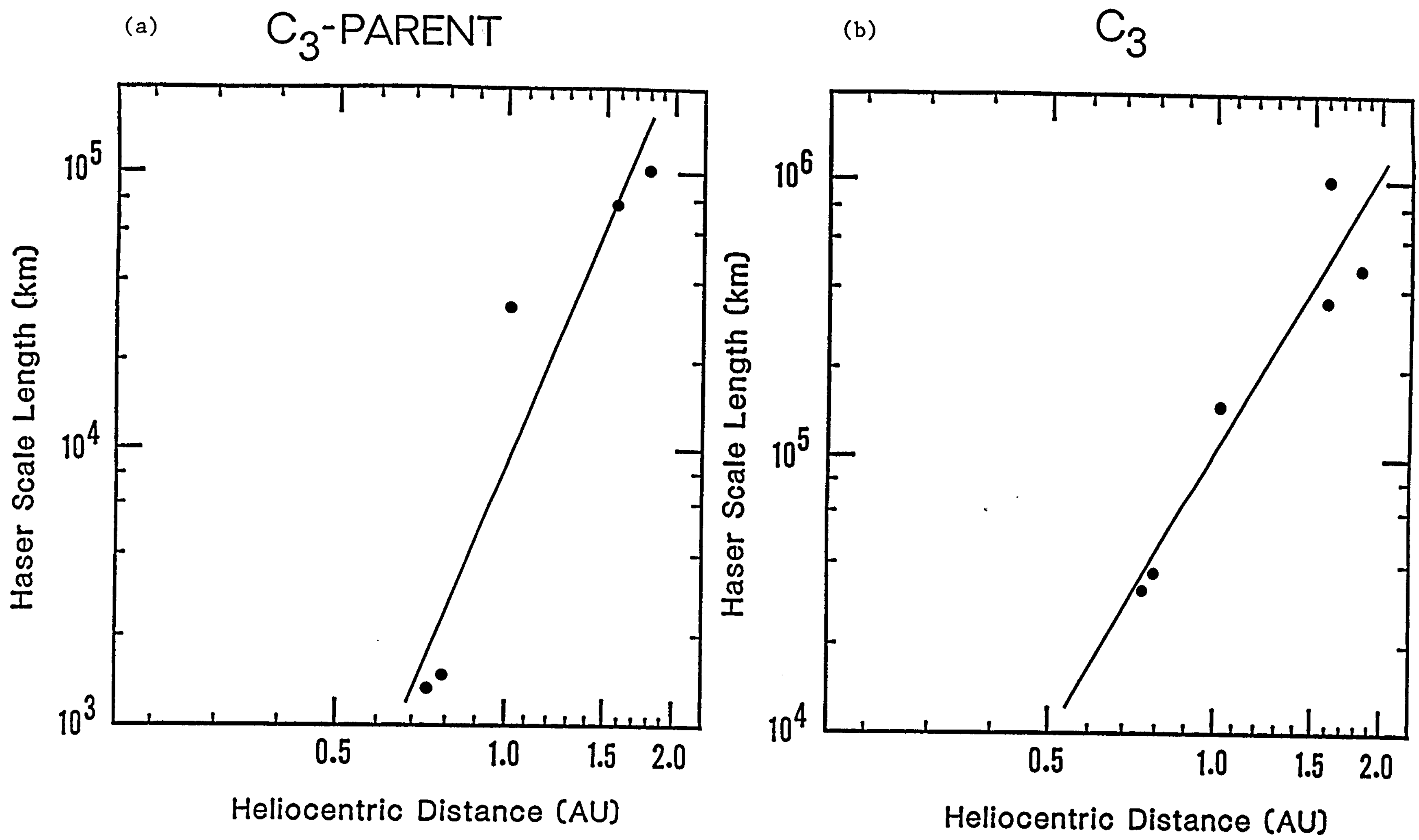
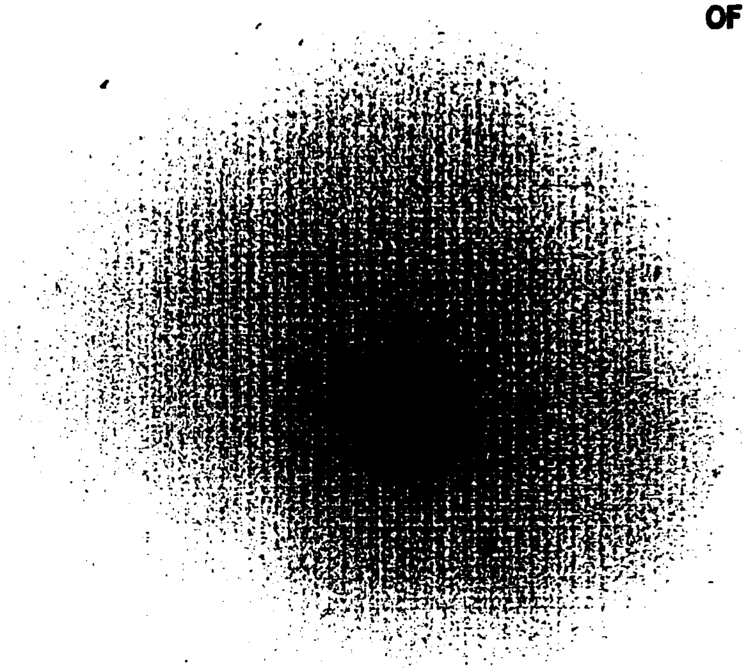
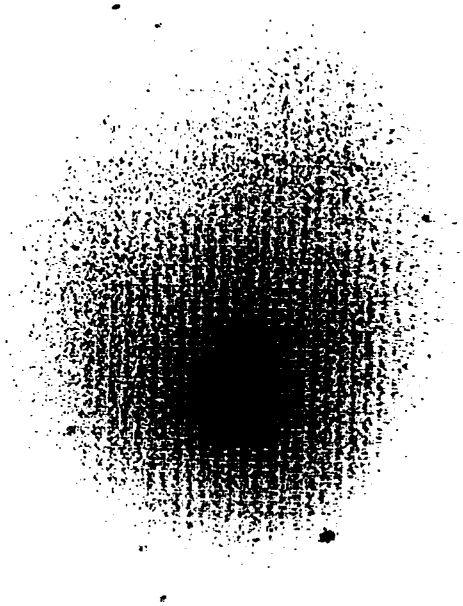


Figure 1. The Heliocentric Distance Dependence of Haser Model Scale Lengths for Cometary C_3.

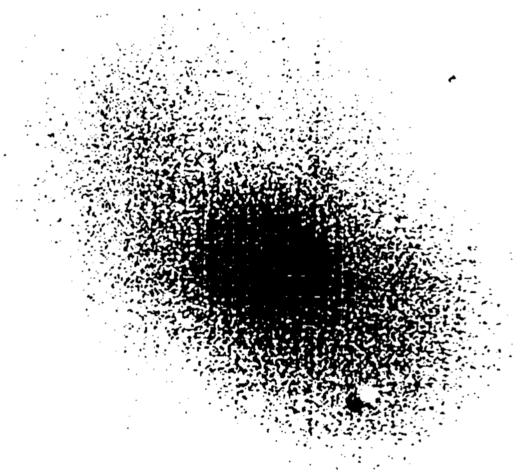
Part (a) gives the r dependence for the parent scale length and the best fit power law (r^n) where n = 4.9. Part (b) gives the r dependence for the daughter scale length and the best fit power law where n = 3.4.



CN + Continuum
(9180Å)



Continuum
(8600Å)



CN

Figure 2

CCD Images of Comet P/Halley on May 11, 1986. Shown are the two direct images (above) and the subtracted image (below) which shows the distribution of CN alone. An apparent CN jet can be seen in the contrast-enhanced reduced image below.

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APPENDIX

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NEUTRAL COMETARY ATMOSPHERES. V. C_2 and CN IN COMETS

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ABSTRACT

Brightness profiles of C_2 in comets Bennett 1970 II and Kohoutek 1973 XII are presented. Model analysis of these profiles yields radial Haser scale lengths for production and destruction of C_2 which, when combined with other scale length determinations in the literature, are shown to vary as the *square* of the heliocentric distance. This is consistent with photochemical production and destruction. Also presented is an updated compilation of CN scale lengths, which shows that the mean parent scale length law varies as $r^{+1.5}$. A reanalysis of published cometary photometry, using the new scale length laws, yields a C_2 to CN ratio which is *independent* of heliocentric distance. The previously documented drop-off in C_2 production rate relative to other neutral species for heliocentric distances larger than $\sim$1.5 AU was a simple artifact of the previously assumed scale length variations.

Analysis of the sunward-tailward distortion of the brightness profiles with a Monte Carlo particle-trajectory model shows that C_2 is released from its parent molecule with an ejection speed of $\sim$0.5 km s^{-1}, owing to the excess photolysis energy. This result also implies that the photochemical lifetimes for the C_2 parent and C_2 respectively are 3.1×10^4 s and 1.2×10^5 s at 1 AU.

Subject headings: comets — molecular processes

I. INTRODUCTION

The Swan system ($d\ ^3\Pi_g$–$a\ ^3\Pi_u$) of C_2 dominates the emission spectra of most comets at visible wavelengths. Furthermore, the detection of C_2 along with C_3 has suggested the possible presence of hydrocarbons in comets. Thus, although it is really one of the minor components of the comae of comets, C_2 has been the subject of considerable study. Despite this effort, though, there are still many unanswered questions regarding both its production mechanism(s) and its detailed excitation mechanism.

Although it has been long accepted that the excitation of C_2 emission bands is through resonance fluorescence with solar light (Swings 1941), and much progress has been made in modeling the observed Swan band intensity distribution (Arpigny 1966; Krishna Swamy and O'Dell 1977, 1979; A'Hearn 1978; Lambert and Danks 1983), fundamental unknowns still exist. The ground state of C_2 is $x\ ^1\Sigma_g^+$; therefore, intercombination transitions must play an important role. Krishna Swamy and O'Dell (1979) had assumed an intercombination transition of $a\ ^3\Pi_u$–$x\ ^1\Sigma_g^+$ with a rate, $A \approx 10^{-3}$ s^{-1}, which was later found to be consistent with the Mulliken ($d\ ^1\Sigma_u^+$–$x\ ^1\Sigma_g^+$) system intensity discovered by A'Hearn and Feldman (1980). However, more recent studies by Johnson, Fink, and Larson (1983) and Lambert and Danks (1983) do not favor this ad hoc assumption and point to the likely importance of intercombination transitions involving excited triplet states.

A principal method for studying the production and destruction mechanisms for observed cometary radicals has been the observation and model analysis of their spatial distributions. Modeling has generally been done with Haser's (1957) model, which provides radial scale lengths for production and decay. These can be related to true photochemical lifetimes if the ejection velocity of the daughter radical and the expansion velocity of the parent molecule are known (Combi and Delsemme 1980*a*, hereafter Paper I).

We present here revised sunward and antisunward brightness profiles of the C_2 (0–0) band of the Swan system in Comet Bennett 1970 II and a pair of profiles in Comet Kohoutek 1973 XII. Haser model scale lengths determined for these profiles are then compared with those found by other investigators to examine their heliocentric distance dependence. The separate sunward and antisunward profiles are then analyzed with the Monte Carlo particle-trajectory model, as described in Paper I and used similarly by Combi (1980, hereafter Paper III) for pairs of CN profiles. Since the solar radiation pressure on C_2 radicals can be calculated, the sunward-antisunward distortion can be modeled to deduce photochemical lifetimes from the spatial distribution. The newly revised C_2 scale length laws and those determined from an updated compilation of CN observations are then used to reexamine the production rates as determined from filtered photometry. Finally, possible sources of C_2 are discussed in the light of the other results presented in this paper.

II. MODELING THE SPATIAL DISTRIBUTIONS OF NEUTRAL RADICALS

There are active today three major, broadly defined approaches to modeling the spatial distributions of neutral cometary species. The traditional method is, of course, that put forth in the model of Haser (1957), which considers observed daughter radicals to be produced at a constant rate from a source of exponentially decaying parent molecules streaming radially from a point source nucleus. The radicals continue to

[1] Work was begun while a Postdoctoral Research Associate at the University of Toledo.

move radially and decay exponentially themselves. The two decay times are related to scale lengths by the assumed radial velocity. A closed form expression for the column density can be written in terms of simple integrals of modified Bessel functions. The two scale lengths give the model enough parameter flexibility such that it can be fitted to almost any observed radial brightness profile. Unfortunately, early attempts to identify suspected parent molecules by comparing observed scale lengths with photochemical lifetimes (Potter and DelDuca 1964; Delsemme and Moreau 1973) generally found cometary scale lengths to be too short to be explainable by photochemistry alone.

At this point, two other possible sources of dissociation or ionization of parent molecules had been suggested. These were gas phase chemistry (Aitken 1974; Oppenheimer 1975), particularly fast ion-molecule reactions, and an internal ionization source created by the interaction between solar wind flow through the cometary plasma (Ip and Mendis 1975, 1976*a*, 1977) in combination with chemistry. These ideas evolved through large, complicated chemistry models having more than 100 species and more than 1000 gas phase and photochemical reactions (see Huebner, Giguere, and Slattery 1982; and Mitchell, Prasad, and Huntress 1981) finally into multifluid chemical-dynamic models which address the feedback of photochemistry and radiative transfer on the energy balance of the inner coma (Marconi and Mendis 1982, 1983; Huebner and Keady 1983). The former of these two schemes, a one-dimensional chemistry model, has been adopted by Cochran (1982, 1985*a*) to analyze observations of cometary radicals. This model calculates the nonequilibrium chemistry occurring in a single fluid parcel of cometary gas moving radially away from the nucleus's surface at a constant velocity and expanding, of course, as r^2. Results for CN (Cochran 1982) and C_2 (Cochran 1985*a*) are apparently consistent with photochemical production of these two species. In fact, the earlier results of this type of chemical model generally underproduced radicals which could not be produced by a one- or two-step photodissociation (Giguere and Huebner 1978).

A third general approach to the question of modeling the spatial distribution of cometary radicals was developed simultaneously with the chemical models and is based on the principal weakness of the simple Haser model. That is, when a radical or atom is produced during the photodissociation of its immediate parent molecule or radical, there is in general some excess energy which is divided between the internal energy of the fragments (i.e., rotationally, vibrationally, or electronically excited states) and translational energy. This translational energy can impart extra nonradial velocities to the newly created fragments which are of the same order or even much larger than the typical outflow velocities of the parent molecules of 0.3 to 1.0 km s^{-1} (Whipple 1980; Delsemme 1982), e.g., 1.2–1.5 km s^{-1} for OH from H_2O, ~ 20 km s^{-1} for H from H_2O, ~ 8 km s^{-1} for H from OH, ~ 1 km s^{-1} for CN from HCN, 3–7 km s^{-1} for C and O from CO and CO_2 (Huebner and Carpenter 1979; Festou 1981*b*).

The vectorial model (Festou 1978; Festou *et al.* 1979; Festou 1981*a*, *b*) addressed the nonradial radical velocities in a way similar to Haser's model, i.e., in terms of a closed-form multiple-integral expression for the space or column density of an observed radical. Festou successfully applied the vectorial model to the distributions of OH as well as H in the inner ($\leq 10^5$ cm) coma. The vectorial model requires at least a triple numerical integration to calculate the column density for single-parent outflow and daughter ejection velocities.

Work by the authors (Combi 1979; Papers I, III; Combi and Delsemme 1980*b* hereafter Paper II) addressed the same question of nonradial radical velocities in two different ways. One was the Average Random Walk Model (ARWM), which was based on a simple geometric reinterpretation of Haser model scale lengths as radial projections of true nonradial scale lengths. The second was the introduction of a Monte Carlo model, which simulates the actual photochemical kinetics by calculating explicit particle trajectories for many individual radicals. We successfully applied the ARWM to show that 16 symmetric brightness profiles (i.e., average of sunward-antisunward pairs) of CN in comets Bennett 1970 II and West 1976 VI could be explained by the photodissociation of cometary HCN but not CH_3CN. Paper III went on to explain the observed distortion in the sunward-antisunward pairs of CN brightness profiles in terms of the expected excess velocity imparted to CN during the photodissociation of HCN combined with the radiation pressure force using the Monte Carlo model.

Whereas the optical data (see above, and Cochran 1982) are consistent with HCN as the parent of observed CN, recent radio observations provide conflicting evidence. Irvine *et al.* (1984) presented the results of radio observations of two comets (1983d and 1983e) from 14 observatories. Observations of the 1–0 transition of HCN in comet *IRAS*-Araki-Alcock 1983d were made at the National Radio Astronomy Observatory (NRAO) and the Five College Radio Astronomy Observatory (FCRAO) on 1983 UT May 8.6 and 10.1, respectively. The NRAO observations yielded a tentative detection indicating a production rate for HCN of $\sim 3 \times 10^{25}$ s^{-1}, which is roughly equivalent to the optical production rate for CN. On the other hand, the FCRAO observation only two days later provided only an upper limit which was an order of magnitude lower.

The principal qualitative results found in both studies of non-radial radical motion were that the use of the Haser model resulted in a measurement, in fact, of a radial projection of the true scale length and thus would always give smaller values than one might suspect from photochemical lifetimes, and that the effect of nonradial motion is both measurable and important. Furthermore, the cases of H and OH from H_2O and CN from HCN can in fact be understood in terms of purely (but geometrically correct) photochemical models, for generally large comets with supposedly well developed collision zones and ionospheres.

The single-fluid-one-dimensional chemistry models (e.g., Giguere and Huebner 1978; Mitchell, Prasad, and Huntress 1981; Cochran 1982, 1985*a*), of course, cannot easily address the problem of nonradial motion. Huebner and Keady (1983) have used our ARWM to approximate the transition from collision-dominated flow to free flow in vacuum in their multi-fluid chemical dynamic models. They are currently working on a more fundamental treatment of the transition region (Huebner 1985). Finally, a two-dimensional multi-fluid model (one fluid for each observed species) that treats this transition zone in a proper way would be required to attack the problem of the radiation pressure distortion, which is quite apparent for C_2 and CN for heliocentric distances less than 1 AU.

Let us enumerate a few points regarding these various modeling efforts:

1. That chemical reactions (especially the fast ion-neutral reactions) occur in the inner regions ($r < 1000$ km) of comets with large gas production rates for heliocentric distances 1 AU or less is not questioned. The rates for the reactions involving particular species may well dominate photochemical rates in

the inner coma regions. A major reshuffling of ion species may in fact occur, and the special case of observed $C(^1D)$ may be produced by dissociative recombination. However, the situation is complicated by the fact that a gas parcel only spends on the order of 1000 s in this region, and all the gas phase chemistry must occur in that time scale.

2. Photochemical reaction rates vary from 10^{-4} to 10^{-6} s^{-1}. However, since the rates depend only on the square of the heliocentric distance and in some cases on the heliocentric velocity, they have no time constraint and should generally dominate in the long run.

3. The impressively large base of information gathered by A'Hearn and his collaborators over the last 12 yr in the form of photometric observations of the major visible radicals and dust has demonstrated that there are no systematic compositional differences between the gas composition of the comae of large and small gas-producing comets. This corresponds to gas production rates (and collision zone radii) varying by well over two orders of magnitude. The only consistently anomalous behavior has been that of the apparent fall-off in the C_2 abundance relative to all other species for heliocentric distances larger than 1.2 AU, and even this behavior seems to be independent of the comets' gas production rates (A'Hearn and Cowan 1980; A'Hearn 1982; see § IV below). The uniformity seems also to be evident in the growing base of ultraviolet data, especially from *IUE* [again with the exception of $C(^1D)$, Weaver *et al.* 1981; Feldman 1982].

4. Even the results of Cochran (1982, 1985*a*), which used a single-fluid, one-dimensional, constant outflow velocity, nonequilibrium chemistry model, point to photodissociation of parent molecules as by far the dominant source of the observed radical species.

5. The simple single-fluid, constant outflow velocity chemistry models are clearly inappropriate outside the collision zone. Here, exothermic nonthermal nonradial velocities and radiation pressure dominate the kinematics and either photodissociation, photoionization, or charge exchange impact with the solar wind dominate the radical production and decay processes.

6. In the case of negligible impact by gas phase chemistry in this type of chemistry model, the density distribution of a radical should be virtually identically reproduced by a sum of either simple Haser models for the case of several single-step photodissociations or, at worst, some type of multiple-step grandparent-parent model, such as was introduced by Malaise (1966). For example, Cochran (1985*b*) has recently fitted Haser models to observed C_2, C_3, and CN profiles which had been previously analyzed with a one-dimensional chemistry model (Cochran 1982, 1985*a*).

7. A major weakness of almost all modeling efforts is the fact that the principal shaping factor of the outer radical coma (i.e., the daughter scale length region $\sim 1\text{–}2 \times 10^5$ km) may in fact be the sporadic activity of the nucleus's vaporization. This was suggested some time ago by Malaise (1970) and was borne out by the measured Haser scale lengths for CN decay determined for comets Bennett 1970 II and West 1976 VI (Paper II). Figure 1 shows the variation of the two Haser scale lengths for observed CN brightness profiles. We have added points from Combi (1978); Cochran (1982); Delsemme and Combi (1983, hereafter Paper IV); and Johnson, Fink, and Larson (1983) to our original data. Although the variation of the parent scale lengths is not inconsistent with a simple r^2 law (owing to the large amount of scatter), the best power-law fit is actually proportional to $r^{1.5}$. On the other hand, we found no measurable trend in the Haser scale length for CN decay as a function of heliocentric distance, as we had for the Haser scale length for decay of the CN parent (HCN). Rather, we found a fairly random distribution of values generally greater than 10^5 s. Simply put, this means that whereas a steady state vaporization rate for time scales 10^4 s or less may make it possible to identify parent molecule decay rates (or at least Haser scale lengths or source region sizes), either sporadic or periodic variations in the vaporization rate on time scales of $1\text{–}5 \times 10^5$ s may make it at least very difficult to model full observed brightness distributions. It should also be mentioned here that Cucchiaro and Malaise (1982) and Keller and Meier (1980) have attempted some models with time-dependent outbursts in production rate to explain observed spatial distributions.

8. Finally, the results of a chemical model run depend critically on many rate constants, nearly half of them poorly known, and on the initial assumed composition of the nucleus's volatile mix (which is exactly what is unknown). The problem, of course, cannot be uniquely inverted even if all the rate constants are precisely known. The agreement of the model profiles with observations is a necessary but not a sufficient condition for having the correct nuclear mix. Furthermore, some of the dominant photolytic rates used in these models are approximations derived from Haser model fits to observed brightness profiles.

In conclusion, since there has yet to be demonstrated a reasonable case for the production of any of the principally observed neutral cometary species—with the possible exception of $C(^1D)$—by gas phase chemical reactions, it seems reasonable to choose some combination (or sum) of the exospheric photochemical models with which to attempt to understand the observations of the spatial distributions of neutral cometary species. A method we (Papers I, II, III) have used still remains quite viable. This is to use the Haser model, realizing that the scale lengths may have no direct physical meaning (even for pure photochemistry) to characterize the spatial extent and heliocentric distance dependence of the source region. From this point, one can then move on to the ARWM interpretation of the scale lengths; or to explicit modeling with the Monte Carlo particle-trajectory models (PTM) which can handle radiation pressure, collisions, velocity distributions, and time dependencies as necessary; or to both.

Note that the simplest version of the particle-trajectory model, i.e., with nonradial ejection of photodissociated radicals, is *fundamentally equivalent* to the vectorial model (Festou 1981*a*). Also, even though neither the vectorial nor the particle-trajectory model is as directly invertible as Haser's we are still left with only a handful of parameters, such as lifetimes and velocities, to specify, and we do not have to prespecify the identity of a proposed parent but simply find the best-fit lifetimes and velocities for a given data set.

III. BRIGHTNESS PROFILES OF C_2

The brightness profiles of C_2 (0–0) presented here were determined from microdensitometer scans of spectrograms of comet Bennett 1970 II and comet Kohoutek 1973 XII. The details regarding the observations and the principal data reduction have been discussed at length in earlier papers for both the Toledo plates of comet Bennett (Delsemme and Combi 1979; Paper II) and the Lick plates of comet Kohoutek (Paper IV), and will not be pursued further in this paper. See

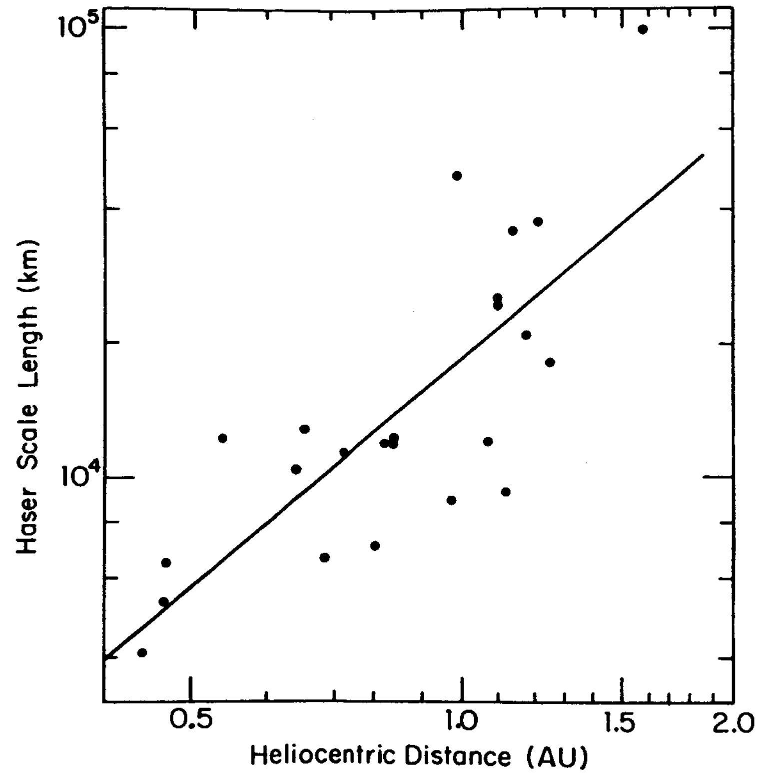

FIG. 1*a*

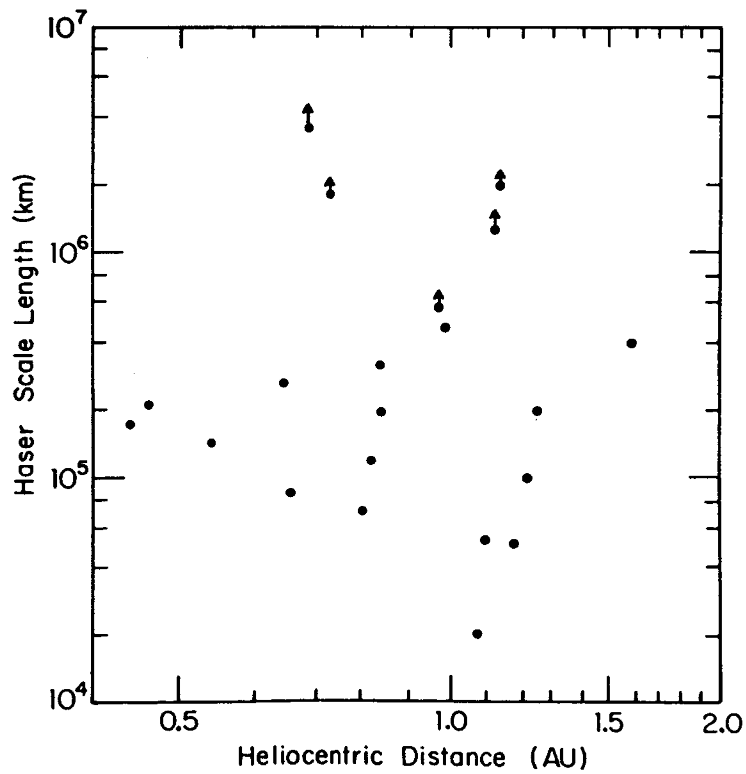

FIG. 1*b*

FIG. 1.—Variation of CN Haser (*a*) parent and (*b*) daughter scale length with heliocentric distance. *Circles*, values which result from Haser model fits to whole brightness profiles. In (*a*) the line shows the best-fit power law of $1.6 \times 10^4\, r_H^{1.5}$ km. In (*b*) the daughter scale lengths exhibit no obvious trend but likely reflect only coma activity (Combi and Delsemme 1980*b*).

TABLE 1

OBSERVATIONAL DATA

Comet	UT	r^a (AU)	Δ^b (AU)	ϕ^c
Kohoutek 1973 XII	1974 Jan 9 0260	0.465	0.846	85°5
Bennett 1970 II	1970 Apr 18 0960	0.841	1.054	62.5
	1970 Apr 26 0960	0.970	1.247	51.8
	1970 Apr 27 0960	0.986	1.271	50.7

[a] Heliocentric distance.
[b] Geocentric distance.
[c] Sun-comet-Earth angle.

TABLE 2

C_2 PARENT AND DAUGHTER SCALE LENGTHS FROM HASER'S MODEL

Observer	Comet	r_H (AU)	$\log \gamma_{p_H}$ (km)	$\log \gamma_{d_H}$ (km)
O'Dell and Osterbrock 1962	Burnham 1960 II	1.00	...	4.93
Delsemme and Miller 1971	Burnham 1960 II	1.00	4.10[b]	4.95
Kumar and Southall 1976	Tago-Sato-Kosaka 1969 IX	1.25	4.40	5.09
Malaise 1976[a]	Bennett 1970 II	0.664	3.61	4.83
	Bennett 1970 II	0.713	3.95	5.08
Cochran 1985[a]	1980 XIII P/Tuttle	1.019	4.25[b]	5.11[b]
	1980 X P/Stefan-Oterma	1.58	4.62[b]	5.68[b]
	Meier 1980 XII	1.755	4.72[b]	5.59[b]
This work	Kohoutek 1973 XII	0.465	3.69	4.29
	Bennett 1970 II	0.841	4.05	4.78
	Bennett 1970 II	0.970	4.08	4.97
	Bennett 1970 II	0.986	4.23	4.92

[a] Scale length was computed by Combi 1978 from the original data.
[b] Determined from the data for this paper.

also Delsemme and Combi 1979) for a discussion of the earlier C_2 profiles deduced from these plates of comet Bennett by Delsemme and Moreau (1973). A systematic error in the original data reduction by Delsemme and Moreau, due to unsuspected vignetting in the spectrograph, was the reason for reanalyzing the CN data in Paper II and the C_2 data in this paper. We had cautioned in Paper II that a revision for the original C_2 scale lengths (similar to that for CN) was also likely. Relevant information concerning comet parameters for each observation are given in Table 1. The brightness profiles are shown in Figures 2–5. As noted in the figure legends, the profiles are exactly sunward and antisunward for the Bennett plates but are 51° from the true projected radius vector for the Kohoutek plate.

Parent and daughter scale lengths were determined with Haser's (1957) model using the same non-linear least-squares method as in Paper II (see also Combi 1979) for the average symmetric profiles and are listed as part of Table 2. Also in Table 2 is a compilation of other measured Haser scale lengths determined for C_2 profiles in different comets from whole brightness profile observations only. Newburn and Spinrad (1984) have computed Haser model parent scale lengths for C_2, C_3, and CN from two-point spectrophotometry of five different comets. They determined column densities within a 4″ diameter aperture centered on the nucleus and displaced 17″5 and 35″ from the nucleus. From the nucleus value and one displaced point, they determined a parent scale length and a production rate. In order to do this, they had to assume the value for the daughter scale lengths as adopted by A'Hearn (1982)

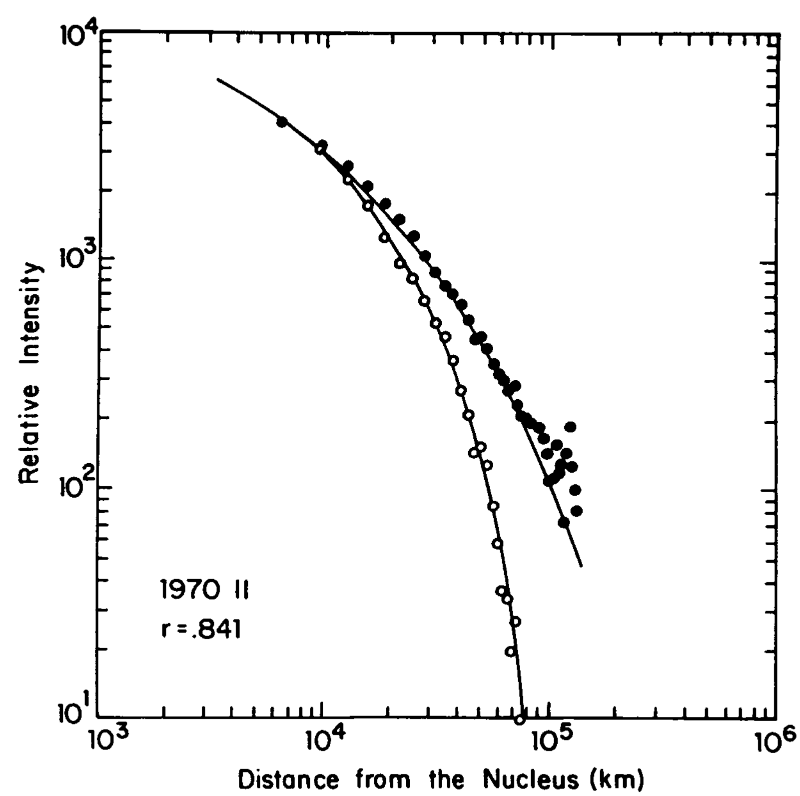

FIG. 2.—Brightness profiles of C_2 in comet Bennett 1970 II. The circles show the data taken on 1970 April 18, and the solid lines show the best-fit Monte Carlo particle-trajectory model with radiation pressure acceleration. *Open circles*, sunward; *filled circles*, antisunward.

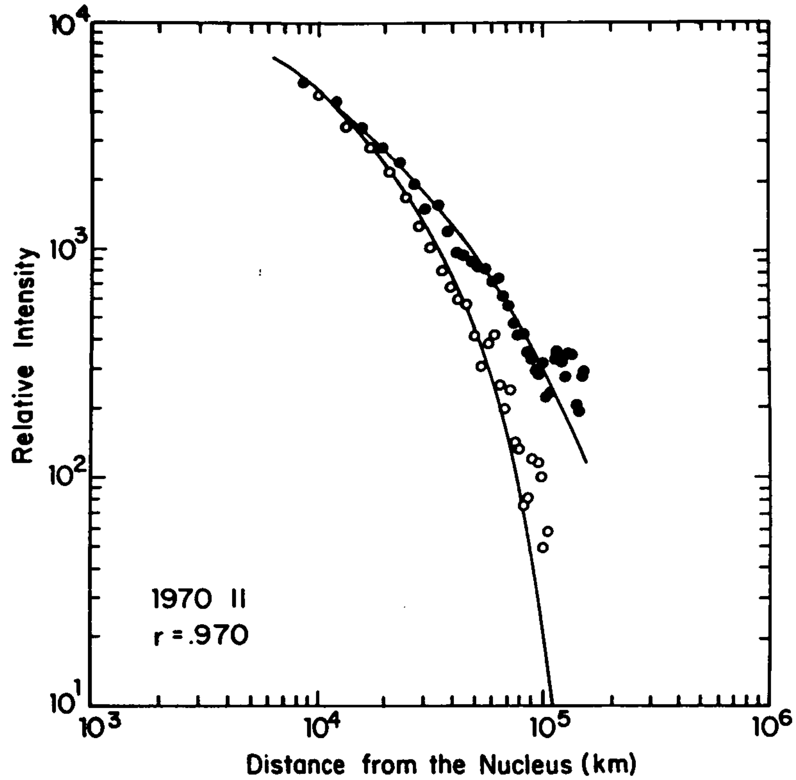

FIG. 3.—Same as Fig. 2, for 1970 April 26

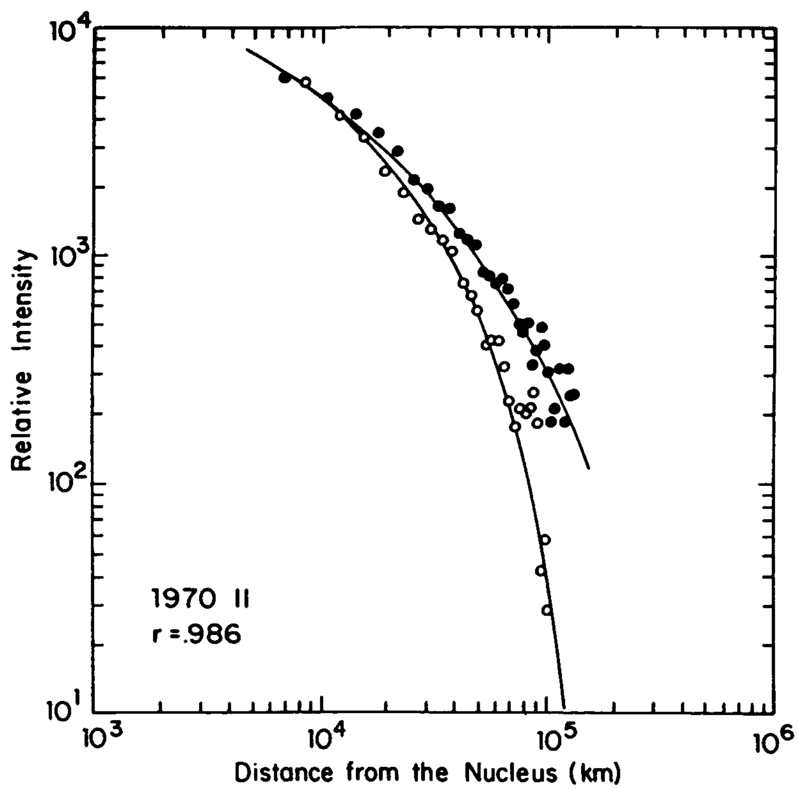

FIG. 4.—Same as Fig. 2, for 1970 April 27

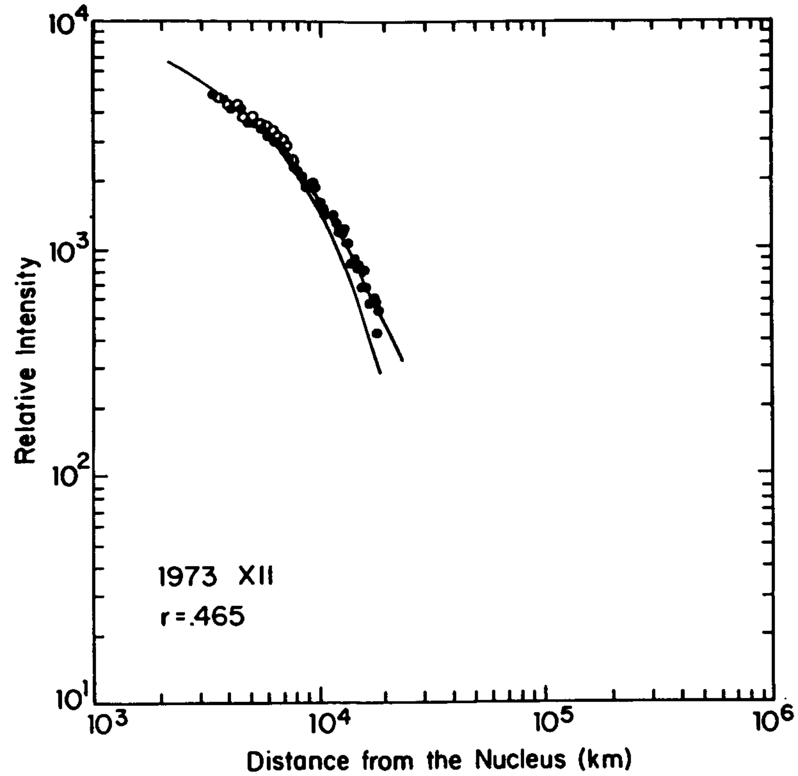

FIG. 5.—Brightness profiles of C_2 in comet Kohoutek 1973 XII; symbols as in Fig. 2. The points marked sunward and antisunward are actually 51° from the true directions. Because of the limited spatial extension, especially sunward, no asymmetric profile information could be extracted. However, the corresponding Monte Carlo PTM (*solid lines*) were computed for this observational geometry with model parameters scaled appropriately from the other pairs of profiles.

from our earlier papers (Delsemme and Moreau 1973; Paper II). In a few cases, they determined scale lengths using each displaced point in combination with the nucleus values, and differences up to a factor of 2 resulted. When using entire brightness profiles, both scale lengths can be determined with uncertainties of only 10%–25%, so we limit our study to this type of data (see Table 2 for references). Figures 6*a* and 6*b* show the variation with the comet's heliocentric distance of the C_2 parent and the C_2 radial Haser length respectively. Simple power-law fits to the data imply the following expressions for the C_2 parent and C_2 scale lengths:

$$\gamma_H(C_2 \text{ parent}) = 1.6 \times 10^4 r_H^{2.0 \pm 0.3} \text{ km} ,$$

$$\gamma_H(C_2) = 1.1 \times 10^5 r_H^{2.0 \pm 0.3} \text{ km} ,$$

where r_H is the comet's heliocentric distance. The scatter of values in Figures 6*a* and 6*b* likely results from both the 10%–25% uncertainties in the Haser model fitting procedure as well as temporal fluctuations in the vaporization rate of the cometary nucleus.

It is worth noting here that if we include the C_2 parent scale lengths determined by Newburn and Spinrad (1984), the overall power-law fit is not changed much, although their data do deviate much more from the mean power law. This is also true when comparing their CN results with the results from whole profiles (Fig. 1).

IV. THE PRODUCTION RATES OF C_2 AND CN IN COMETS

A'Hearn, Thurber, and Millis (1977, hereafter ATM) have published an extensive set of filter photometric observations of C_2, C_3, and CN over a wide range of heliocentric distance for comet West 1976 VI. In Paper II we rereduced their CN data with the updated scale lengths and scale length laws and found a CN production rate law consistent with that of C_3 as determined by ATM. Both of these pointed to a dependence on the heliocentric distance consistent with an inverse square law out to $r_H \approx 2.5$ AU. The case for C_2, on the other hand, has been different.

ATM assumed both C_2 and CN parent scale lengths varying as $r_H{}^{+1}$. Subsequent papers (A'Hearn, Millis, and Birch 1979; A'Hearn and Cowan 1980; A'Hearn and Millis 1980) used this same scale length law for C_2 but now use our revised values for CN. In Table 3 we present the rereduced C_2 and CN production rates, assuming the new Haser scale length laws as well as the corrected g-factor for C_2 (0–0) (i.e., 4.5×10^{-13} ergs s^{-1} per radical; A'Hearn 1985).

The production rates for both C_2 and CN in comet West now vary almost exactly as $r_H{}^2$. The steep drop-off in C_2 production rate from an $r_H{}^2$ law for $r_H \geq 1.5$ AU has been eliminated. A plot of the C_2/CN ratio versus r_H for comet West is shown in Figure 7. A very slight downward trend remains apparent for most points where $r_H = 2.5$ AU. Since it appears that some irregularity occurred in the production rate curves for C_2, C_3, CN, and solids in comet West near $r_H \gtrsim 1.5$ AU (A'Hearn and Cowan 1980), we should examine the behavior of the C_2/CN ratio in other comets as a function of heliocentric distance. A'Hearn and Millis (1980) found that this apparent relative depletion of C_2 at larger heliocentric distances occurred in many comets, both periodic and new. A'Hearn and Cowan (1980) attributed this to the hypothesis that the C_2

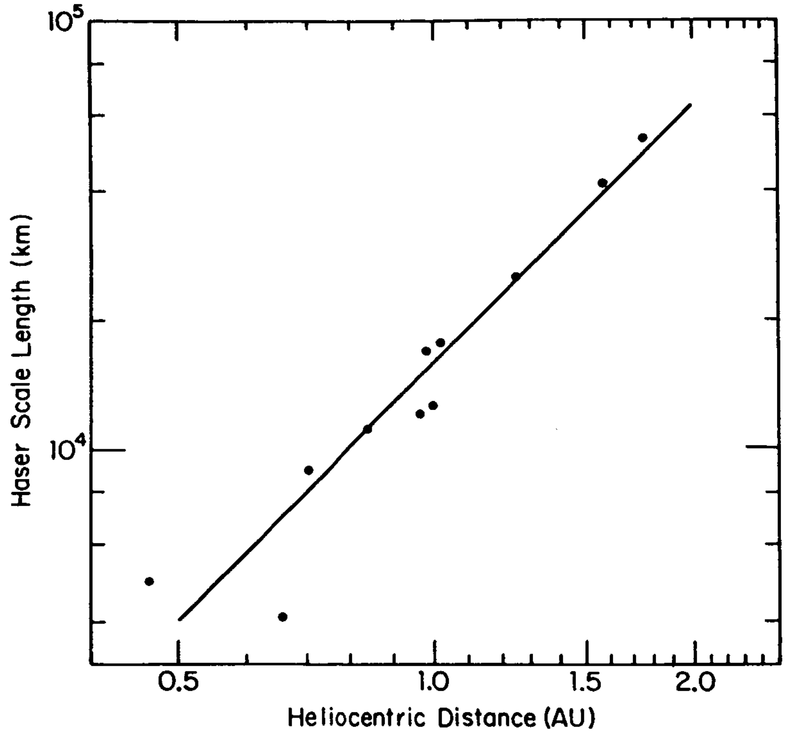

FIG. 6*a*

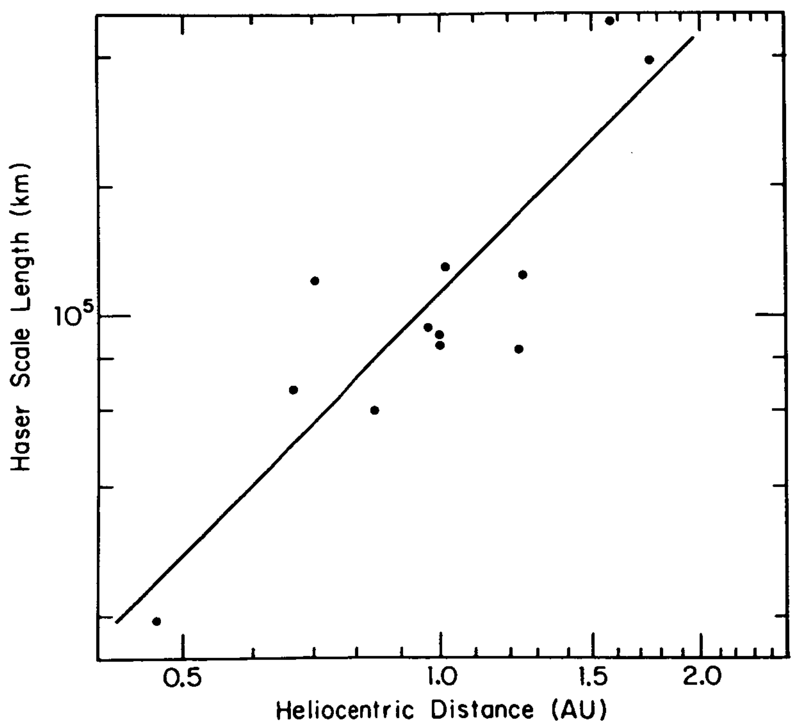

FIG. 6*b*

FIG. 6.—Variation of C_2 Haser (*a*) parent and (*b*) daughter scale lengths with heliocentric distance. *Circles*, values in Table 2; *lines*, best power-law fit of $r_H^{2.0}$.

TABLE 3

PRODUCTION RATES[a] OF C_2 AND CN IN COMET WEST 1976 VI

r (AU)	log Q_{C_2} (s^{-1})	log Q_{CN} (s^{-1})
0.468......	27.675	27.707
0.522......	27.662	27.790
0.522......	28.757	27.782
0.522......	27.664	27.733
0.600......	27.483	27.495
0.651......	27.560	27.567
0.773......	27.295	27.340
0.820......	27.432	27.426
0.899......	27.206	27.208
1.044......	27.203	27.129
1.406......	26.665	26.640
1.443......	26.535	26.645
1.443......	26.544	26.625
1.554......	26.688	26.722
1.767......	26.738	26.814
1.852......	26.683	26.837
1.852......	26.666	26.844
2.002......	26.439	26.604
2.146......	26.417	26.554
2.209......	26.157	26.403
2.497......	26.255	26.182
2.540......	26.097	26.243
2.550......	26.281	26.388

[a] Recalculated from the photometry of ATM with the new revised Haser scale length laws.

parent is embedded in grains of a less volatile component than water, whose vaporization turns off at a higher temperature than the bulk vaporization of the nucleus. They constructed a model which quantitatively explains the data. This explanation now no longer seems necessary.

We have also rereduced all the photometry of six comets, observed by A'Hearn and Millis (1980) for C_2 and CN, and find similar results, as shown in Table 4. The values of the ratios of the production rates have been categorized in a way similar to that done by A'Hearn and Millis, in two groups: those with a heliocentric distance less than 1.5 AU, and those greater than 1.5 AU. These results are summarized in Table 5. Using the old scale length laws, a sizeable depletion (45%) of C_2 relative to CN for $r > 1.5$ AU was found as in the case for comet West, but with the revised scale lengths laws this depletion again disappears.

Thus we have explained the apparent drop of C_2 production rate for larger heliocentric distance to be simply an artifact of an inappropriate Haser scale length law.

V. RADIATION PRESSURE ON C_2

Paper III showed that the difference between the sunward and antisunward brightness profiles of a cometary radical due to solar radiation pressure could be quantitatively modeled and used to disentangle the velocity and lifetime from the decay scale length. The same many-particle Monte Carlo coma model has been used to analyze the profiles of C_2 as was used in Paper III for CN.

The model discussed in detail in Paper I correctly models photochemical kinematics by taking into account the isotropic

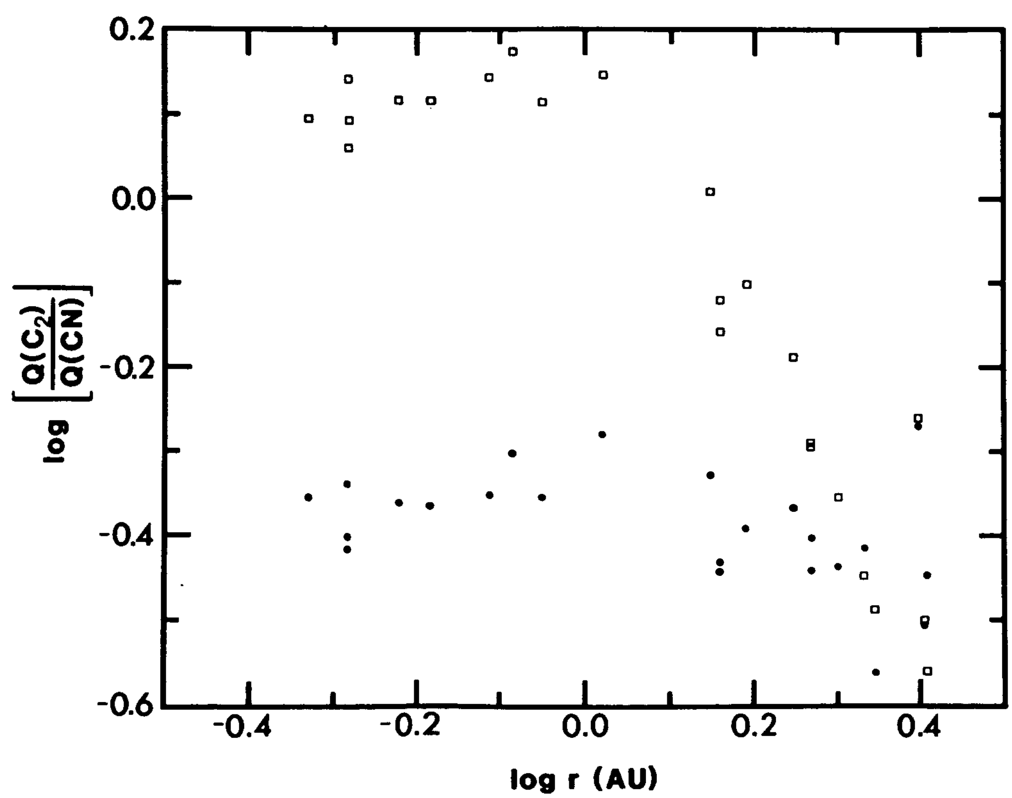

FIG. 7.—Ratio of the production rates of C_2 to CN in comet West 1976 VI. *Open squares*, reduction of photometric band fluxes determined by ATM and reduced with the Haser scale lengths adopted by A'Hearn and Cowan (1980). *Filled circles*, our reduction of the photometric band fluxes reduced with the new Haser scale length laws as presented in this paper.

TABLE 4

PRODUCTION RATES[a] OF C_2 AND CN IN SIX COMETS

r (AU)	log $Q_{C_2}(s^{-1})$	log $Q_{CN}(s^{-1})$
1978 XIV P/Ashbrook-Jackson		
2.349......	25.31	...
2.347......	24.92	25.05
2.344......	25.02	24.79
2.288......	24.95	24.74
1978 XI P/Wild 2		
1.803......	25.19	25.18
1.497......	25.62	25.44
1.495......	25.63	25.49
1.495......	25.64	25.43
1.493......	25.62	25.42
1.493......	25.68	25.48
Meier 1978 XXI		
2.858......	26.72	25.57
2.587......	26.93	26.69
2.553......	27.00	26.73
2.553......	27.14	26.73
2.222......	<25.15	26.79
2.211......	...	26.82
1978 XX P/Haneda-Campos		
1.777......	24.66	23.88
Bradfield 1979c		
0.960......	24.83	24.84
0.978......	24.84.	24.88
Meier 1979i		
1.479......	25.19	24.87

[a] Recalculated from the photometry of A'Hearn and Millis 1980 with the new revised Haser scale length laws.

ejection of the daughter radicals. In the model, the trajectories of many radicals (usually 10^5) are actually calculated, and the column and space densities are found by counting the number of radicals in grids and bins of known area and volume respectively. This is in contrast to the usual cometary free-flow models which compute densities by numerical integration of emission flux functions.

Haser's model can be fitted to data in terms of three independent parameters: the ratio of Q (production rate) to v (radial outflow speed), and the two scale lengths (one for production and one for decay of the daughter radical). In contrast, the Monte Carlo PTM without radiation pressure (and the vectorial model), owing to the isotropic ejection directions of daughter radicals, introduces two extra free parameters, which are the parent outflow and the radical ejection speeds. However, if a sizeable radiation pressure acceleration is present and can be independently calculated, and the distorted coma can be observed, the two additional parameters become constrained. Therefore, if one can determine the radiation pressure acceleration from the total solar fluorescence efficiency (g-factor) and can measure sunward and antisunward brightness profiles (or a 2-dimensional mapping), then the velocities and lifetimes can be completely deconvolved.

The response of modeled sunward and antisunward profiles to the relative speeds of the radical and the parent is illustrated in Figure 8. The location of the sunward limit is set approximately by the maximum radial speed v_{max} (i.e., the scalar sum

TABLE 5

C_2 TO CN PRODUCTION RATIO FOR SIX COMETS

RANGE OF HELIOCENTRIC DISTANCE (AU)	log (Q_{C_2}/Q_{CN})[a]	
	Current[b] Scale lengths	New Scale Lengths
$r < 1.5$......	+0.072	+0.176
$r > 1.5$......	−0.088	+0.178

[a] Q_{C_2} and Q_{CN} are the respective C_2 and CN production rates.

[b] As adopted by A'Hearn and Millis 1980.

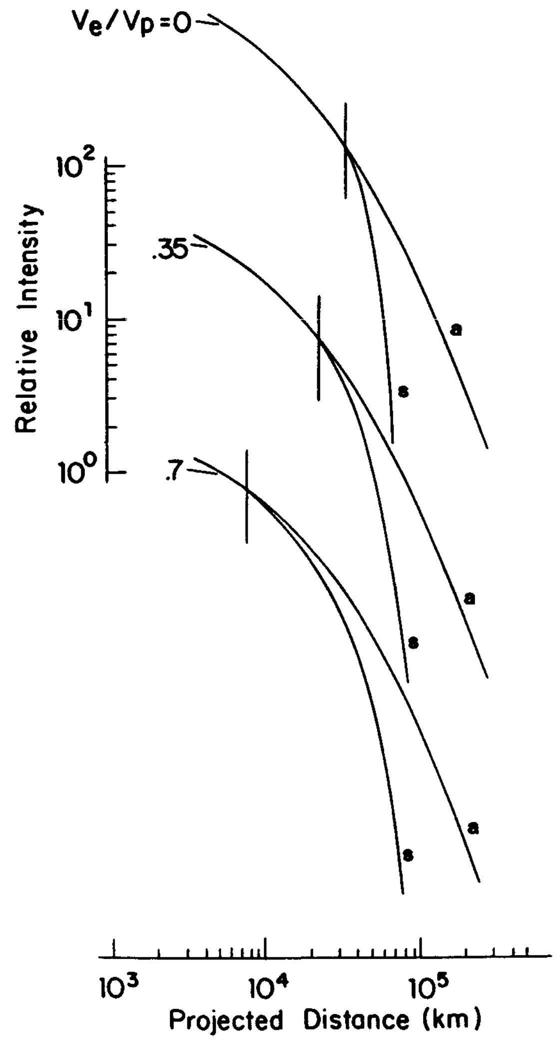

FIG. 8.—Effects of radical ejection velocity on the modeled radiation pressure asymmetry. Three pairs of profiles are shown as modeled with the Monte Carlo particle-trajectory model. All three exhibit the same symmetric radial scale lengths, as determined with the ARWM, but have different velocity ratios of radical ejection to parent outflow. As the radical ejection velocity is increased, the location where the sunward and antisunward profiles diverge from one another moves backward toward the nucleus. This response yields an effective method for disentangling velocities and lifetimes from observed scale lengths.

of the parent and radical ejection speeds) and the radiation pressure acceleration a as a $v_{max}^2/2a$ envelope. The distance from the nucleus where the sunward and antisunward profiles diverge is set by the relative parent outflow and the radical ejection speeds. All three sets of model profiles in Figure 8 have the same radial (Haser) scale lengths, with the appropriate lifetimes being set using the ARWM. They also have the same sunward limit set by the maximum velocity and the acceleration. As radical speed increases, the location where the two profiles diverge moves back toward the nucleus.

The radiation pressure on a C_2 radical at 1 AU can be calculated from the fluorescence efficiency of the (0–0) band of the Swan System (4.5×10^{-13} ergs s^{-1}; A'Hearn 1975) and the observed relative band ratios for the rest of the system (A'Hearn 1985). We find a value of 0.81 cm s^{-2}. There are other spectroscopic systems which may contribute to the radiation pressure, principally the singlet Phillips ($A\ {}^1\Pi_u$–$X\ {}^1\Sigma_g{}^+$) and Mulliken ($d\ {}^1\Sigma_u{}^+$–$x\ {}^1\Sigma_g{}^+$) systems. This raises the question of whether intercombination transitions are important. It appears that two alternate scenarios can be envisioned: either intercombination transitions are not important and we have two populations of C_2 radicals, triplets and singlets, coexisting in the ratio of ~20 to 1 (Johnson, Fink, and Larson 1983; Davis *et al.* 1984); or intercombination transitions are important and we have one population of C_2 radicals spending ~95% of their time in triplet states and ~5% in singlet states. In either case, total C_2 abundances determined from the Swan band observations would be underestimated by ~5%. In the former case, contributions to the radiation pressure on the triplet population of C_2 radicals would result from triplet (mainly Swan) transitions only. Here also, singlet and triplet populations of C_2 would be accelerated at different rates. In the latter case, the radiation pressure would be determined by the triplet transitions 95% of the time and by the singlet transitions only 5% of the time, and thus the effective acceleration on all C_2 radicals would be the same and a few percent less than that determined from the triplet g-factor alone. Such a difference could be tested observationally from the comparison of the spatial distributions of triplet and singlet C_2 emissions. One should expect significantly less distortion from circularity for the isophotes of a separate population of singlet C_2 radicals than for triplet C_2 radicals (the former case), and identically distorted isophotes from a mixed population (the latter case). However, we are concerned with Swan band (triplet) observations, and there is a large uncertainty in the absolute g-factor which may be as large as 40% (A'Hearn 1985). Therefore, a value near 0.81 cm s^{-2} is quite reasonable for our purposes.

An alternate approach to constraining the model parameters would be to adopt the parent outflow speed law of Delsemme (1982). From the compilation of halo expansion velocities measured by Bobrovnikoff (1954) and Beyer (1961), Whipple (1980) has suggested that the initial radial velocity of parent molecules expanding from the nucleus is given approximately as $0.535 r_H^{-0.6}$ in km s^{-1}. Delsemme (1982) has added to this data set the result of Malaise (1970), who deduced outflow velocities near the nucleus using the Swings-Greenstein effect on CN rotational lines. Furthermore, Delsemme has provided a simple theoretical argument that, since a temperature law of $T = T_0 r_H^{-1}$ is expected, the true radial velocity expansion law should now be given as

$$v = (0.58 \pm 0.03) r_H^{-0.5} .$$

The change in the power-law exponent is due to the fact that Bobrovnikoff's and Beyer's data beyond 3 AU must clearly reflect vaporization of gases more volatile than water; the constant shift corresponds to a factor of 1.25, yielding an average molecular weight of 28 for these gases. Either CO or a mixture of CO_2 with lighter gases could explain this shift.

If we adopt this parent speed law, then the best-fit models to the observed profiles will yield both lifetimes, the radical outflow speed *and* the radiation pressure acceleration. It was found that the best fits to all three of the pairs of C_2 profiles (shown as the solid lines in Figs. 2, 3, and 4) in comet Bennett were obtained with an ejection velocity of ~0.5 km s^{-1}. The corresponding profiles for the limited comet Kohoutek profiles have also been calculated and are shown in Figure 5. The numerical results of the Monte Carlo PTM analysis of the three pairs of C_2 profiles in comet Bennett are summarized as follows:

Assumptions:

1. v (parent) $= 0.58/r^{1/2}$ km s^{-1}
2. $C_2X + h\nu \rightarrow C_2 + X$ + energy

Results at 1 AU:

$v_e(C_2)$	0.5 km s^{-1}
τ(parent)	3.1×10^4 s
τ(daughter)	1.2×10^5 s
a(rad. pr.)	0.70 cm s^{-2}

A value for the radiation pressure acceleration of 0.70 cm s^{-2}, found from the model analysis, compares rather favorably with the value calculated from the g-factor (0.81 cm s^{-2}). In fact, this is well within the 40% uncertainty expected for the g-factor. The self-consistency in the results lends confidence in the model, the g-factor, and a parent outflow speed of ~0.6 km s^{-1} near 1 AU. Of course, since we have observations over only a narrow range of heliocentric distance (0.84–1.0 AU), we really can neither confirm nor deny the validity of the Delsemme velocity law.

VI. POSSIBLE SOURCES OF C_2

We now turn to the question of examining the possible C_2 source(s) in comets in terms of the deduced production lifetime (i.e., destruction of the parent), found to be $\sim 3.1 \times 10^4$ s at $r_H = 1$ AU and the ejection speed of 0.5 km s^{-1}. The uncertainty in this lifetime can be crudely estimated from the uncertainties in the (0–0) band g-factor (40%), the parent velocity law (6%), and the effective scale length fitting procedure ($\lesssim$ 15%). Since the spatial distortion is in effect set by a $v^2/2a$ paraboloid envelope, uncertainties in the inferred velocities enter as the square root of those in the radiation pressure acceleration (the g-factor). Therefore, a total uncertainty of ~20% in the determined parent lifetime is expected if one relies on the parent velocity law and of ~35% if one relies on the g-factor.

C_3 once seemed like a viable candidate for at least a major source of cometary C_2, but the g-factor for the λ4040 band has been revised upward by a factor of 40 (A'Hearn 1982). Thus, the C_3 production rate is now believed to be nearly two orders of magnitude less than those of C_2 and CN.

In their extensive work on solar photochemical radiation rates, Huebner and Carpenter (1979) had calculated the photochemical lifetimes of C_2H_2 and C_2H_4. The following reactions which may ultimately produce C_2, shown with the lifetime of the original reactant, are:

1. $C_2H_4 + h\nu \rightarrow C_2H_2 + H_2$, $\tau = 2.1 \times 10^4$ s (Huebner and Carpenter 1979);
2. $C_2H_2 + h\nu \rightarrow C_2H$, $\tau = 3.1 \times 10^4$ s (Huebner and Carpenter 1979);
3. $C_2H + h\nu \rightarrow C_2 + H$, τ theoretically unknown.

TABLE 6

C_2H_2 PHOTOCHEMISTRY

Reaction	Rate[a] (s^{-1})	E_{excess} (eV)	v_{heavy} ($km\ s^{-1}$)	Branching Ratio
$C_2H_2 + h\nu \rightarrow C_2H + H$ ...	1×10^{-5}	3.2	0.97	0.79
$\rightarrow C_2 + H_2$	2.7×10^{-6}	3.1	1.4	0.21
Total C_2H_2	1.27×10^{-6}			1.0
Old C_2H_2	3.1×10^{-5}			1.0
$C_2H + h\nu \rightarrow C_2 + H$	Unknown	...	...	...

[a] New reaction rates from Huebner (1985); old reaction rate from Huebner and Carpenter 1979.

It seems that with a total parent lifetime of 3.1×10^4 s found in this paper (i.e., "total" meaning all steps of a multiple-step process added up to yield a simple effective parent lifetime), C_2H_4 can probably be eliminated as a principal parent. Furthermore, even C_2H_2 would only be possible if the lifetime for reaction (3) were very short. This would be precisely the same conclusion reached with the chemical model by Cochran (1985*a*), who placed a value of 2000 s on the lifetime for C_2H in order for acetylene to be the primary parent frozen in the cometary nucleus. However, new information regarding the C_2H_2 photodissociation has become available (Huebner 1985), which revises the lifetime of C_2H_2 upward (or the reaction rate downward) by more than factor of 2. These new data are given in Table 6. The reaction rate for photodissociation of the C_2H radical is still unknown. A photochemical lifetime of 7.9×10^5 s and the large ejection speeds would appear to eliminate C_2H_2 as the only or principal primary parent for C_2.

However, the determination of photodissociation rates from solar spectral fluxes and laboratory-measured photoabsorption cross sections is not a simple problem. Even in cases where a complete absorption spectrum has been measured, the validity of this approach is complicated by (1) the multiline nature of the solar UV spectrum, (2) the relatively low wavelength resolution of the experiments (~ 10 Å) and, most importantly, (3) the high density and high internal temperature (~ 270 K) of the target gas. As cometary molecules leave the collision-dominated inner region, they naturally undergo rapid radiative cooling, leaving them in their lowest rotational and vibrational levels ($T < 100$ K). Actual photodissociation cross sections (and the major branching ratios) can be more than two orders of magnitude different from values measured in the laboratory (Jackson 1982).

These difficulties can be best illustrated by the widely varying total solar photodissociation rates quoted for C_2H_2 over the years in the literature: 1.6×10^5 s by Potter and DelDuca (1964); 5.7×10^3 s by Jackson (1976); 3.1×10^4 s by Huebner and Carpenter (1979); and 7.9×10^4 s by Huebner (1985). Finally, Huebner (1985) has suggested that C_2 may be produced by a combination of many sources, possibly including C_2H_2. In any event, the effective lifetime of the C_2 source(s) has been determined empirically here to be $\sim 3.1 \times 10^4$ s.

The case for attempting to identify the parent(s) of cometary C_2 is a perfect example of the dangers in trying to use complicated chemical models for routine analyses of observed spatial distributions of cometary radicals. Revisions by factors of 2–5 are to be expected as better laboratory measurements and ab initio calculations of gas phase chemical and photochemical reactions are made. In this case, a revision by a factor of 2.5 *in only one out of more than* 1000 *reactions* completely reversed an interpretation. (Furthermore, the same interpretation would have been drawn using the old reaction rate and the Haser and Monte Carlo model approach adopted in this paper.)

VII. SUMMARY

1. Brightness profiles of C_2 in comets Bennett 1970 II and Kohoutek 1973 XII have been presented.

2. Radial (Haser) scale lengths for production and destruction of C_2 have been determined from these profiles, and when compared with those determined from other brightness profiles in the literature are found to be consistent with both scale lengths varying as the square of the heliocentric distance r. An updated compilation of the CN Haser scale lengths yields an $r^{1.5}$ for the CN parent.

3. The production rates of C_2 and CN as determined from the photometry of ATM and A'Hearn and Millis (1980) have been recalculated using Haser's model and the new scale length r-dependences. The drop in production rate of C_2 relative to CN (and presumably other species) for heliocentric distances greater than 1.5 AU is now eliminated. Furthermore, the production rates of both C_2 and CN is comet West vary almost precisely as the inverse square of the heliocentric distance.

4. Monte Carlo particle-trajectory models which take into account the radiation pressure acceleration on C_2 were fitted to the sunward and antisunward pairs of profiles for comet Bennett. These results yield a photochemical lifetime of 3.1×10^4 s at 1 AU for the parent(s) of C_2 and an ejection velocity of ~ 0.5 km s^{-1} for C_2 upon dissociation and a radiation pressure acceleration consistent with that expected for solar fluorescence, if one assumes a parent outflow of ~ 0.6 km s^{-1} (Delsemme 1982). A photochemical lifetime of 1.2×10^5 s for C_2 was found. This interpretation is consistent with the radiation pressure acceleration as determined by the total C_2 solar fluorescence rate.

5. We have examined the possible molecular sources for cometary C_2 in terms of the parent lifetime of 3.1×10^4 s at 1 AU. C_2H_4 in a multiple-step process seems unlikely as an ultimate source. C_2H_2 as the sole or even primary source is also inconsistent with the recently updated photodissociation rates for C_2H_2 (Huebner 1985).

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Note added in proof.—It has been pointed out by M. F. A'Hearn that, whereas a C_2 triplet-to-singlet ratio of 20 to 1 was implied by the results of Johnson, Fink, and Larson (1983), as discussed in § V, A'Hearn and Feldman (1980) found a value closer to 6 to 1. Nonetheless, the value is large and as such has no effect on the content of the discussion in § V.

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16. Abstract

Progress during the second year of a program of research on the modeling of the spatial distributions of cometary radicals is discussed herein in several major areas. New scale length laws for cometary C_2 and CN have been determined which explain that the previously-held apparent drop of the C_2/CN ratio for large heliocentric distances does not exist and that there is no systematic variation. Monte Carlo particle trajectory model (MCPTM) analysis of sunward and anti-sunward brightness profiles of cometary C_2 has been completed. This analysis implies a lifetime of 3.1×10^4 seconds for the C_2 parent and an ejection speed for C_2 of ~0.5 km/s upon dissociation from the parent. A systematic reanalysis of published C_3 and OH data was begun. Preliminary results find a heliocentric distance dependence for C_3 scale lengths with a much larger variation than for C_2 and CN. Scale lengths for OH are generally somewhat larger than currently accepted values. The MCPTM has been updated to include the coma temperature. Finally, the collaborative effort with the University of Arizona programs has yielded some preliminary CCD images of Comet P/Halley.

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