

## WATER PRODUCTION MODELS FOR COMET BRADFIELD (1979 X)

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### ABSTRACT

*IUE* observations of comet Bradfield (1979 X) made in early 1980 allow a comprehensive study of the production of water by this comet. All three water dissociation products, H, O, and OH, were observed simultaneously with a spatial resolution of  $\sim 1000$  km and over a range of heliocentric distances from 0.71 to 1.55 AU. By comparing the observations to the predictions of two water models of the coma (Haser and vectorial), it is determined that these measurements support the idea of a comet composed principally of water ice. The vaporization of the water has a rather peculiar heliocentric variation, decreasing as  $r^{-3.7}$  over the entire range of observations.

*Subject headings:* comets — ultraviolet: spectra

### 1. INTRODUCTION

In 1951, Whipple (1950, 1951) proposed that water might be the dominant volatile constituent of the cometary nucleus. He postulated the existence of water ice in the nucleus mainly to explain the “nongravitational” accelerations experienced by some comets as they orbit the Sun, but he also pointed out that spectroscopic evidence seemed to support his hypothesis. Since then, the body of evidence accumulated in support of the water model of the cometary nucleus has been substantial, although of an indirect nature.

The small size of the nucleus is responsible for the lack of contrast between it and the surrounding gas and dust. As a consequence, the nucleus of a comet has probably never been observed. Furthermore, it is probable that none of the major constituent molecules of the nucleus have ever been observed since, after sublimating from the nucleus, they are transformed by various means into other molecules, atoms, or ions in the coma. Even relatively long-lived molecules might be hard to observe in the coma if they do not fluoresce strongly in the light of the Sun or if they are poor radiators of thermal energy (water satisfies both these conditions). Therefore, the composition of the nucleus must be inferred by indirect means. Basically, two methods may be employed; these methods are fundamentally different in approach. Detailed models of a hypothetical nucleus may be constructed, and predictions of its behavior can

be tested against observations of comets (Whipple 1950, 1951; Delsemme and Swings 1952; Delsemme and Wenger 1970; Delsemme and Miller 1970, 1971*a*, *b*). Alternatively, observations can be made of the comae of comets; then, by working backwards, it is possible to identify the molecules sublimating from the nucleus. Of course, any model of the nucleus would make definite predictions about the identity of species abundant in the coma, and observations of the coma could test the model. However, a model of the coma alone should place severe constraints on the identity of the progenitors of the coma species. These “parent” molecules are presumably sublimating from the nucleus and, thus, must comprise at least part of the nuclear composition. In this way, it is possible to identify the composition of the nucleus without considering its structure in detail. We do not attempt here to propose new models of the nucleus or even to discuss details of its physical nature. This paper emphasizes observations of the cometary coma and examines the clues these observations can provide concerning the parents of the dominant observed coma species.

Hydrogen (H), oxygen (O), and hydroxyl (OH) are all products of water photodissociation whose presence in the coma suggests water in the nucleus. In fact, if water ice is the main constituent of the nucleus, then H, O, and OH should be the most abundant species in the coma. The presence of oxygen in the coma was established by the discovery of the red oxygen doublet at 6300 and 6364 Å in ground-based spectra of comet

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Mrkos (1957 V) (Swings and Greenstein 1958). However, at that time most of the interest in this emission concerned its excitation mechanism, since the observed transition is electric-dipole forbidden, and it was not recognized that oxygen was a major constituent of the coma. Hydroxyl was first identified in a cometary spectrum by the presence of its (0,0) band in the head of comet Cunningham (1941 I) (Swings, Elvey, and Babcock 1941). Although the emission appeared to be weak, due to various experimental difficulties as well as the relatively small oscillator strength for the OH emission, it was recognized that OH must be at least as plentiful in the coma as the other observed molecules (e.g., CN, C<sub>2</sub>, and CH). From the first far ultraviolet observations of a comet in 1970, strong H Ly $\alpha$  and OH (0,0) band emissions were detected in *OAO 2* observations of comet Tago-Sato-Kosaka (1969 IX) (Code, Houck, and Lillie 1970). Later that year, *OAO 2* spectra of comet Bennett (1970 II) revealed that hydrogen and hydroxyl were by far more abundant in the coma than any of the species identified in visible spectra (Code, Houck, and Lillie 1972). The oxygen emission at 1304 Å was also tentatively identified in the spectrum of comet Bennett but was too weak for a quantitative analysis. The comet Kohoutek (1973 XII) observations in early 1974 provided the opportunity for a quantitative analysis of the oxygen emission. The derived production rates demonstrated for the first time that oxygen was approximately as plentiful in the coma as hydrogen and hydroxyl (Feldman *et al.* 1974; Opal and Carruthers 1977).

While it is necessary for the composition of the coma to be mainly H, O, and OH if the nucleus is primarily H<sub>2</sub>O, this qualitative condition alone is not sufficient for the proof of the hypothesis. For example, if certain other molecules (e.g., NH<sub>3</sub>, CH<sub>4</sub>, CO<sub>2</sub>, CO...) were present in sufficient numbers in the nucleus, their photodissociation might also provide the species observed in the coma. On the other hand, the problem then becomes one of trying to explain the relative obscurity of species other than H, O, and OH (e.g., C or N). In addition, an important argument favoring water as the primary source of coma constituents is the lack of a suitable alternative for the parent of OH (Festou 1981*b*).

There is other indirect evidence from comae observations for the water model of the nucleus. Analysis of the comet Bennett (1970 II) data showed that the H:OH abundance was roughly 2:1, and that the production rates of both species followed the same heliocentric variation, consistent with the assumption of a common water parent for both species (Keller and Lillie 1974). Also, analyses of the Ly $\alpha$  isophotes of comets Bennett (1970 II) (Keller and Thomas 1975) and Kohoutek (1973 XII) (Meier *et al.* 1976) and the *Copernicus* observations of the Ly $\alpha$  line shape in comet Kobayashi-Berger-Milon (1975 IX) (Festou *et al.* 1979) have demonstrated that the velocities of the hydrogen atoms in

the coma can be explained by considering the photodissociation of H<sub>2</sub>O and OH as the source of these atoms (although our knowledge of OH photodissociation is somewhat limited). A review of early UV observations supporting a dominant role for water in cometary phenomena can be found in Keller (1976).

Despite the references and arguments cited above, the case for water as the dominant constituent of the nucleus is still far from closed. The data from previous cometary observations have, in general, allowed only independent interpretations for the water dissociation products with little or no demonstrated correlation among all three linking them to a common water parent. In the early part of 1980, comet Bradfield (1979 X) was observed with the *International Ultraviolet Explorer* (*IUE*). These measurements are the first to allow a comprehensive study of all three water dissociation products, H, O, and OH, simultaneously. Furthermore, each species is studied with a spatial resolution which is the highest achieved in the ultraviolet ( $\sim 1000$  km) and over a wide range of heliocentric distances ( $0.71 \text{ AU} \leq r \leq 1.55 \text{ AU}$ ). A report on the data obtained during the first day of these observations, as well as a preliminary discussion of results derived from these data, has been given by Feldman *et al.* (1980). In this paper, we make use of the data covering the entire period of the *IUE* observations to address the question of water production by this comet. By comparing the *IUE* observations of comet Bradfield to the predictions derived from an H<sub>2</sub>O model, it is our intention to examine whether or not the data are consistent with the widely held assumption that water is the dominant constituent of the cometary nucleus.

## II. OBSERVATIONS

The *IUE* covers the entire spectral range from 1150 Å to 3400 Å by employing two separate spectrographs. For the comet Bradfield observations used in this analysis, each spectrograph was used in the low dispersion mode with the object placed in the large aperture. This aperture is  $\sim 10'' \times 20''$  and is roughly elliptical in shape. Used in this manner, the short wavelength spectrograph has a resolution of  $\sim 12$  Å and covers the spectral range from 1150 Å to 1950 Å, while the long wavelength spectrograph covers the range 1900 Å to 3400 Å at a resolution of  $\sim 18$  Å. Further details concerning the instrument have been given by Boggess *et al.* (1978).

Although the *IUE* aperture is  $\sim 10'' \times 20''$ , to facilitate comparisons with model predictions, only data from the rectangular portion of this aperture,  $\sim 10'' \times 15''$  in size, were used in this analysis. Thus, all surface brightnesses presented are actually averages over this reduced aperture. In addition, by making use of the line-by-line spatially resolved spectra provided as a part of the standard *IUE* data reduction package, the contamination of the spectra caused by camera blemishes (e.g.,

radioactivity in the phosphor, cosmic ray hits, and camera reseaux; all of which are confined essentially to one or two camera pixels corresponding to an angular size of  $\sim 2\text{--}4''$ ) is removed by the action of a seven-point running median filter which is passed over thirteen data points lying along a line of constant wavelength and centered on the dispersion line. Although not relevant for any of the species discussed here, it should be pointed out that this filter should not be used on emissions which do not uniformly fill the aperture, as it will then artificially alter the true aperture-average surface brightness.

The Fine Error Sensor (FES) on the *IUE* serves the purpose of a finder telescope, providing the observer with an image of up to a  $16' \times 16'$  field (resolution  $\sim 12''$ ) surrounding the object to be studied. The FES is sensitive to visible light with a peak sensitivity around  $4600 \text{ \AA}$ . An example of an FES image of comet Bradfield can be found on the cover of the 1980 July 10 issue of *Nature*. FES images of comet Bradfield revealed a well-defined spherical coma with no apparent dust tail. A slight trace of an ion tail was visible in the FES images of 1980 January 10 but was not seen during any of the later observations.

In order to permit display of the entire dynamic range of the instrument we show Figure 1, which is a composite spectrum at the cometary center from four *IUE* images taken on the same day (1980 January 10). The hydrogen Ly $\alpha$  emission at  $1216 \text{ \AA}$ , the (unresolved) oxygen triplet at  $1304 \text{ \AA}$ , and three hydroxyl bands, (1,0) at  $2811 \text{ \AA}$ , (0,0) at  $3064 \text{ \AA}$ , and (1,1) at  $3122 \text{ \AA}$  (wavelengths given are for band heads) are clearly evident. Spectra taken on succeeding observation dates showed no emissions other than those in Figure 1, but the intensities of all the features decreased, since the comet was moving farther from the Sun. In addition, the

observing program included exposures taken by offsetting the slit from the center of brightness by various distances in order to map the brightness variation across the coma for each species.

Table 1 summarizes the observational parameters for the data being considered here. In this table we include the observation date, the Sun-comet distance ( $r$ ), the earth-comet distance ( $\Delta$ ), and the comet's heliocentric velocity for each exposure used in this analysis. Some spatial imaging is possible within the  $10'' \times 20''$  *IUE* aperture, the resolution for a point source being  $\sim 5''$  (full width at half-maximum) perpendicular to the spectrograph dispersion line (i.e., along the  $20''$  dimension) (Boggess *et al.* 1978). The spatial resolution at the comet thus depends on its distance from the earth, and this value has been tabulated for each day of the *IUE* observations.

Accurate pointing at the center of brightness of the comet was verified by the presence of emissions which were confined essentially to the central portion of the aperture during such exposures. As an example, a photographic representation of a long wavelength spectrum taken on 1980 January 10 is shown in Figure 2. The continuum near  $2900 \text{ \AA}$  as well as the CS (0,1) band at  $2667 \text{ \AA}$  are emissions which are seen only near the center of brightness. During the offset exposures the telescope could be very precisely pointed and maintained at a specific position in the coma, a task achieved with an accuracy of  $\sim 1''$  over long exposure times (up to 190 minutes), since the telescope was programmed to track on the center of brightness of the comet.

### III. THE $\text{H}_2\text{O}$ PROBLEM

Water molecules sublimating from the cometary ice flow radially outward from the nucleus with a speed

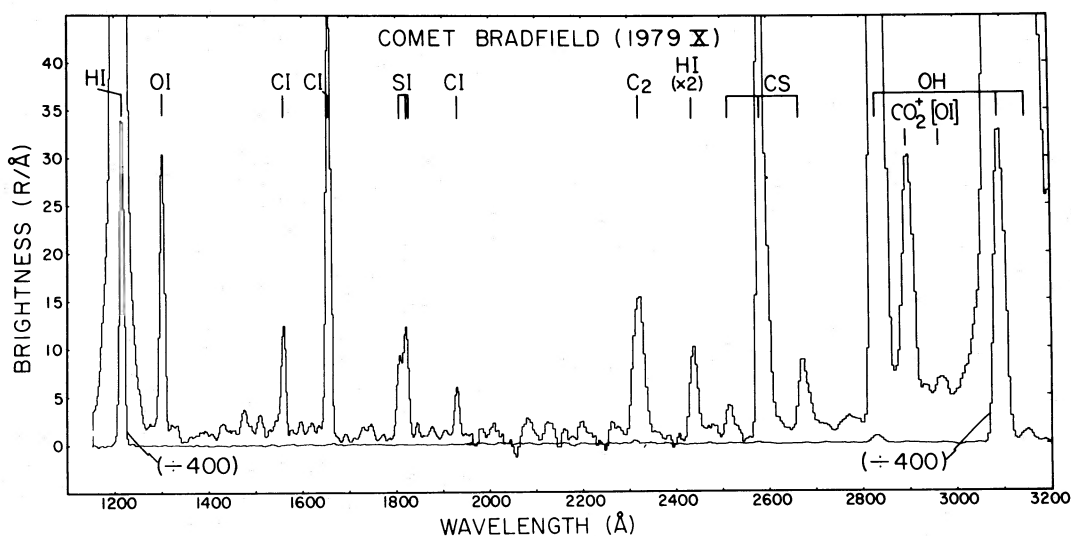


FIG. 1.—Composite spectrum at the cometary center from four *IUE* low dispersion images taken on 1980 January 10

TABLE 1  
COMET BRADFIELD (1979 X) OBSERVATIONAL PARAMETERS

Observation Date	Heliocentric Distance (AU)	Geocentric Distance (AU)	Heliocentric Velocity (km s <sup>-1</sup> )	Spatial Resolution at Comet (10 <sup>3</sup> km)
1980 Jan 10 ....	0.71	0.62	24.0	2.2
1980 Jan 16 ....	0.80	0.40	26.4	1.5
1980 Jan 24 ....	0.93	0.20	27.8	0.73
1980 Jan 31 ....	1.03	0.29	28.1	1.1
1980 Feb 7 ....	1.15	0.54	28.2	2.0
1980 Feb 13 ...	1.25	0.76	28.0	2.8
1980 Feb 20 ...	1.37	1.02	27.6	3.7
1980 Mar 3 ....	1.55	1.45	26.9	5.3

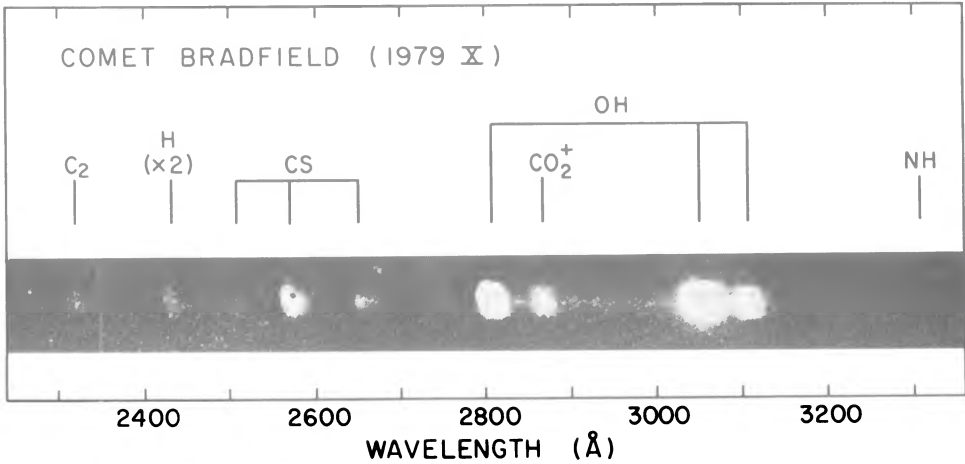


FIG. 2.—Uncorrected data from a 2 hour LWR exposure taken on 1980 January 10, shown as a photowrite image of the camera reconstructed from the digital data. Notice that the CS (0,1) band at 2667 Å and the continuum near 2900 Å do not fill the 10"×20" aperture. Their presence along the center of the spectrum indicates that the aperture was centered on the comet during the exposure. The CS (0,0) band and the three OH bands are saturated. An approximate wavelength scale is indicated on the figure.

which is characteristic of the temperature of the nucleus and the nature of the expansion of the gas. At a temperature of 200 K, the estimated temperature of a water ice nucleus (Delsemme and Miller 1971*a*), the water molecules will have an average velocity of  $\sim 0.5 \text{ km s}^{-1}$ . In a hydrodynamic description of the coma, Mendis, Holzer, and Axford (1972) have assumed supersonic flow (Shul'man 1970) and show that the radial expansion of the coma will increase the outflow speed of the water molecules to  $\sim 1 \text{ km s}^{-1}$ . The outflowing water molecules are subsequently destroyed by their interaction with the solar radiation. The theoretical photochemistry of water vapor under the influence of the solar photon flux has been investigated recently by Festou (1981*b*). The main results of this analysis will be summarized here.

Photodissociation is the main water destruction process. The photoionization rate is almost two orders of magnitude smaller than the photodissociation rate. Of

the  $\text{H}_2\text{O}$  molecules which are photodissociated,  $\sim 90\%$  produce  $\text{OH}(A^2\Sigma^+, X^2\Pi_i) + \text{H}(^2\text{S})$  and  $\sim 10\%$  are converted into  $\text{H}_2(X^1\Sigma_g^+) + \text{O}(^1\text{D} \text{ or } ^1\text{S})$  (the exact branching ratio depends strongly on the ratio of the solar Ly $\alpha$  flux to the 1300–1800 Å quasi-continuum). Since more energy is available (per incident solar photon) than is needed to dissociate the  $\text{H}_2\text{O}$  molecules, there is an energy excess which goes primarily into the kinetic energy of the dissociation products. By knowing the amount of this excess energy available, the velocities of the dissociation products can be determined. In  $\text{H}_2\text{O}$  photodissociation, the velocity of the H atoms is greater than  $18 \text{ km s}^{-1}$ , the velocity of the OH radicals lies in the range  $1.15\text{--}2 \text{ km s}^{-1}$ , and the O atoms are produced with a  $1.8 \text{ km s}^{-1}$  velocity (all values are valid in a frame of reference attached to the  $\text{H}_2\text{O}$  molecule).

The resultant OH is also photodissociated producing H and O, probably in their fundamental states, via a predissociation state. The computed lifetime of OH is



strongly dependent on the heliocentric radial velocity of the comet and varies between  $6.9 \times 10^4$  s and  $2.1 \times 10^5$  s at 1 AU (Jackson 1980). The velocity of the products is not known, but if the above predissociation occurs mainly from the  $A^2\Sigma^+$  ( $v'=2$ ) level, then 0.4 eV is available in the form of kinetic energy for the dissociation products. Consequently, in a frame of reference attached to the OH radical, the H and O atoms would have a velocity of 8.5 and 0.5 km s<sup>-1</sup>, respectively.

Besides these theoretical considerations, recent observations of bright comets have produced model independent measurements of some of the above-mentioned velocities. The OH velocity has been determined from radio observations of Despois *et al.* (1981) to be 1.5 km s<sup>-1</sup>. Huppler *et al.* (1975) measured the line profiles of the oxygen 6300 Å line and the hydrogen H $\alpha$  line in comet Kohoutek (1973 XII) and derive average outflow velocities of 1.8 km s<sup>-1</sup> and 7.8 km s<sup>-1</sup> for the oxygen and hydrogen atoms, respectively. However, one may question the validity of the O I measurements, since it is very likely that the 6300 Å line is contaminated by nearby NH<sub>2</sub> lines (Festou and Feldman 1981).

Some results are model dependent. Ly $\alpha$  observations of two comets lead to the conclusion that two populations of H atoms exist, centered at 20 and 8 km s<sup>-1</sup> respectively (Keller 1976). These results are in agreement with the interpretation of Ly $\alpha$  linewidth measurements obtained with the *Copernicus* satellite on comet Kobayashi-Berger-Milon (1975 IX) (Festou *et al.* 1979). Also, numerous measurements of the OH lifetime are now available from UV observations (Blamont and Festou 1974; Keller and Lillie 1974; Festou 1981*b*), and all determinations lie in the range  $10^5$  to  $2 \times 10^5$  s at 1 AU.

Two models of the cometary coma are used in our analysis of the comet Bradfield data. For the sake of simplicity, a generalized Haser model (Festou 1981*a*) is used to compute density distributions for all three water dissociation products. This is a spherically symmetric model which assumes that all species flow radially outward from the nucleus with a constant speed. The input parameters for the model are the outflow velocities and lifetimes for each species. The calculated densities are then integrated along the line of sight, and the resulting column densities are related to measured surface brightnesses using an approximate radiative transfer calculation. The applicability of this model for the description of cometary comae has been examined in detail by Festou (1978, 1981*a*) and by Combi and Delsemme (1980). Both analyses show that under certain circumstances the Haser model can be used to describe the density distribution in the coma to reasonable accuracy (to within  $\sim 30\%$ ). Combi and Delsemme go a step further and prescribe a method for modifying the Haser formulas to obtain the correct density distribution even when the assumptions of the model are known to be

significantly in error. However, while Combi and Delsemme consider only "daughter" products of photo-destructive processes, Festou discusses "granddaughter" species as well. Furthermore, Festou considers the specific problem addressed here, namely, water production and the density distribution of the water dissociation products (except oxygen). Thus, under those circumstances in which it is clear that the Haser model gives an inadequate description of the coma, we also use Festou's vectorial model (Festou 1981*a*), which properly takes into account the directions of the excess velocities of the dissociation products, to calculate density distributions.

In light of the above discussion of the photochemistry of water and its dissociation products, we must make certain assumptions and choices in our model calculations. However, it is not the purpose of this paper to give precise values to the various model input parameters. There is still considerable uncertainty in our knowledge of many of these values. Moreover, as pointed out by both Festou (1981*a*) and Combi and Delsemme (1980), the "true" values of these parameters are not what should be used in the Haser formulas to obtain the closest approximation to the correct density distribution. The above discussion is used primarily to set the range within which the values of the various parameters probably lie. By considering various values within this range for our model calculations, the reader can estimate what other specific combinations of values for the parameters will also fit the data.

We consider two extreme cases for the water outflow velocity, 0.5 km s<sup>-1</sup> and 1 km s<sup>-1</sup>. The water lifetime against photodissociation at 1 AU is calculated to be  $8.2 \times 10^4$  s (Festou 1981*b*). Since it has been demonstrated that the lifetime of OH is highly dependent on the radial velocity of the comet, we use our own data to set a range of values for this parameter. An OH velocity of 1.15 km s<sup>-1</sup> is used in the Haser model calculation. This value is consistent with the average radial velocity for an OH molecule at  $\sim 10^4$ – $10^5$  km from the nucleus, as derived from the vectorial model (Festou 1981*a*). The production rate which is determined from the OH observations is the production rate of water, and this value is used in the interpretation of both the H I and O I data (if other parents are likely to exist for H and O, H<sub>2</sub>O seems to be the only acceptable candidate for OH). The present data are not suited to distinguish between the eventual different hydrogen populations. We assume that two populations exist with velocities of 20 km s<sup>-1</sup> (H from H<sub>2</sub>O) and 8 km s<sup>-1</sup> (H from OH). The H atom lifetime against photoionization and charge exchange with solar wind protons is  $2 \times 10^6$  s at 1 AU (Festou 1978). The optical depth effects are evaluated with the approximate radiative transfer calculation of Festou *et al.* (1979). The line center flux for the solar Ly $\alpha$  line is  $5.14 \times 10^{11}$  photons cm<sup>-2</sup> s<sup>-1</sup> Å<sup>-1</sup> as determined from

the measurements of the total flux in the line by Mount, Rottman, and Timothy (1980) using the empirical relation of Vidal-Madjar (1975) which relates this flux to the line center flux. The velocity of the O atoms is assumed to be  $1.8 \text{ km s}^{-1}$  for the component issued from  $\text{H}_2\text{O}$  and  $1.2 \text{ km s}^{-1}$  for the component produced by the dissociation of OH. The O I lifetime against photoionization and charge exchange with solar wind protons is  $1.2 \times 10^6 \text{ s}$  at 1 AU (Opal and Carruthers 1977; we have decreased the lifetime against photoionization by a factor of 2 relative to their value to take into account the effect of the solar cycle). An evaluation of the optical depth effects is conducted in the same way as for H. The line center flux for the solar O I line at  $1302.17 \text{ \AA}$  is  $1.8 \times 10^{10} \text{ photons cm}^{-2} \text{ s}^{-1} \text{ \AA}^{-1}$  using the line-integrated flux of Mount, Rottman, and Timothy (1980) and an effective width of  $\Delta\lambda = 0.26 \text{ \AA}$  (Strickland and Thomas 1975).

#### IV. OH

Since the velocity of the OH molecule is not too different from that of its assumed water parent, we would expect the Haser model to give reasonably accurate OH density distributions. Festou (1978, 1981a) has verified this, showing that the Haser and vectorial models give the same densities to within 5% for  $v_{\text{H}_2\text{O}} = 1 \text{ km s}^{-1}$  and to within  $\sim 20\text{--}30\%$  for  $v_{\text{H}_2\text{O}} = 0.5 \text{ km s}^{-1}$  (these numbers are valid for distances of  $\sim 10^4\text{--}10^5 \text{ km}$  from the nucleus and for  $\tau_{\text{OH}}$  in the range considered here). Thus, we are justified in using the Haser model to interpret the OH measurements.

The OH (0,0) band brightness at the nucleus was measured on all eight observation dates listed in Table 1. However, spatial brightness profiles were obtained for only three dates and these are plotted in Figure 3. The boxes represent the experimental values, while the curves are predicted brightnesses. The theoretical profiles have not been convolved to take into account the finite size of the IUE aperture. Rather, the model is fitted to the data by forcing the model to give the same aperture-averaged brightness as that measured for the observations in which the aperture is centered on the center of brightness of the comet. In addition, the theoretical profile must pass through the boxes which represent the offset measurements. In effect a convolution of the theoretical profile is performed near the nucleus, where a convolution is important, while an unconvolved profile is used at large distances from the nucleus, where a convolution will make only insignificant changes in the profile. The column densities computed from the model were converted to surface brightnesses assuming an optically thin emission and using excitation factors (the excitation or  $g$ -factor varies with the comet's heliocentric velocity) calculated by Schleicher and A'Hearn (1980). The labels A and B refer to the same (Haser) model but using different values for  $v_{\text{H}_2\text{O}}$  and  $\tau_{\text{OH}}$ . For a water velocity

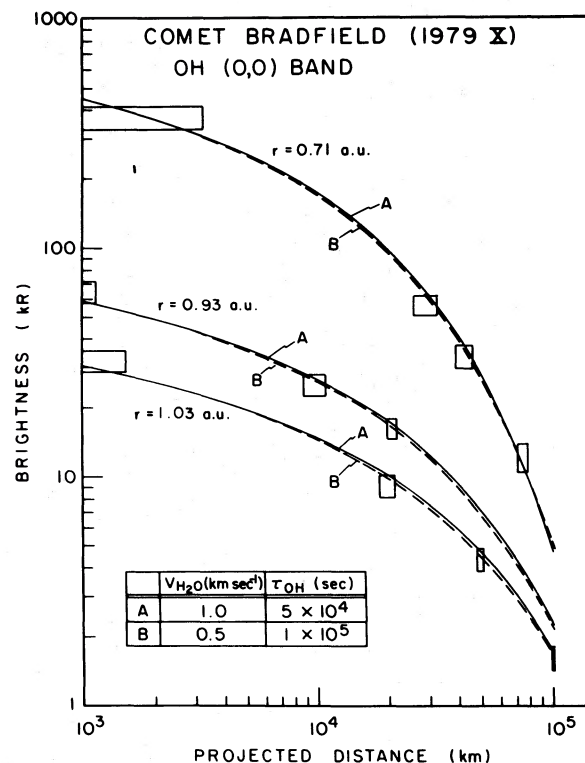


FIG. 3.—Comparison of OH (0,0) band brightness profiles with a radial outflow (Haser) model using the parameters defined in the inset. Data from 3 days are shown as rectangular boxes, the horizontal size being the projected length of the spectrograph slit (the  $15''$  dimension) on the comet and the vertical size the measurement uncertainty ( $2\sigma$  from noise plus 10% from absolute calibration).

of  $1 \text{ km s}^{-1}$  an OH lifetime (at 1 AU) of  $5 \times 10^4 \text{ s}$  is required to match the observed profiles, while for  $v_{\text{H}_2\text{O}} = 0.5 \text{ km s}^{-1}$  we require  $\tau_{\text{OH}} (1 \text{ AU}) = 1 \times 10^5 \text{ s}$  to fit the data. Both sets of curves fit the data for all three days as they are virtually indistinguishable at these values of projected distance. Unfortunately, therefore, we cannot use the OH measurements to distinguish the two cases.

The OH (0,0) band emission was determined to be optically thin by considering the optical depth at line center for the strongest rotational line in the band. By using the average of the most recently measured values of the oscillator strength for the entire band ( $f_{00} = 8 \times 10^{-4}$ ; Grevesse and Sauval 1973), we determined the oscillator strength for the strongest line to be  $f_{\text{max}}^{\text{rot}} = 2 \times 10^{-4}$ . The populations of the rotational levels were determined assuming fluorescence equilibrium (Schleicher and A'Hearn 1980) with the result that no more than approximately one-half of the OH molecules can be in any one rotational level. For a Doppler-broadened absorption profile with a most probable velocity for the OH molecules of  $\sim 1 \text{ km s}^{-1}$ , we have determined

TABLE 2  
MODEL PARAMETERS AND DERIVED WATER PRODUCTION RATES

Model	$v_{\text{H}_2\text{O}}$ (km s $^{-1}$ )	$\tau_{\text{OH}}(\text{s})^a$	$Q_{\text{H}_2\text{O}}$ (mol s $^{-1}$ ) <sup>b</sup>
Haser A .....	1	$5 \times 10^4$	$2.3 \times 10^{29}$
Haser B .....	0.5	$1 \times 10^5$	$1.2 \times 10^{29}$
Vectorial A ...	1	$6 \times 10^4$	$1.4 \times 10^{29}$
Vectorial B ...	0.5	$1.6 \times 10^5$	$1.0 \times 10^{29}$

<sup>a</sup> At 1 AU.

<sup>b</sup> ( $r=0.71$  AU).

$\tau_0^{\text{max}} \approx 0.09$  for our observations of the first day, justifying the assumption of negligible optical depth.

The derived water production rates ( $Q_{\text{H}_2\text{O}}$ ) also depend on the input parameters used in the model. The values derived on the first day of observations (1980 January 10) are displayed in Table 2. As a check on the accuracy of the Haser model calculations, we also performed a vectorial model analysis of the OH brightness profile for the first day of observations. These numbers are also given in Table 2. As pointed out by Festou (1981a), the Haser model underestimates the OH lifetime. However, the derived water production rates are nearly identical, in agreement with what was said earlier. We can therefore use the Haser model values for  $Q_{\text{H}_2\text{O}}$  in our calculations involving hydrogen and oxygen.

The study of the heliocentric variation of the water production rate produced some interesting and rather surprising results. Figure 4 shows  $Q_{\text{H}_2\text{O}}$  as a function of heliocentric distance for the entire range of IUE observations ( $0.71 \text{ AU} \leq r \leq 1.55 \text{ AU}$ ). Also shown are the OH (0,0) band brightnesses from which these production rates were derived. Our result that  $Q_{\text{H}_2\text{O}}$  decreases as  $r^{-3.7}$  is quite different from the results derived from OAO 2 observations of comets Bennett (1970 II) and Tago-Sato-Kosaka (T-S-K) (1969 IX) (Keller and Lillie 1974, 1978). For comet Bennett, Keller and Lillie derive an  $r^{-2.3}$  decrease in water production over the entire range of heliocentric distances for which observations were made ( $0.77 \text{ AU} \leq r \leq 1.26 \text{ AU}$ ). Their results for comet T-S-K show a rather peculiar heliocentric variation:  $r^{-3.3}$  for  $0.78 \text{ AU} \leq r \leq 0.84 \text{ AU}$  and  $r^{-1.5}$  for  $0.90 \text{ AU} \leq r \leq 1.03 \text{ AU}$ , but it should be kept in mind that the two sets of measurements span relatively small intervals of heliocentric distance. (Note: Although Keller and Lillie actually show graphs of  $Q_{\text{OH}}$ , the heliocentric variation for  $Q_{\text{H}_2\text{O}}$  will be the same, since it is always assumed in these models that the two quantities differ by only a constant factor.) It is significant that our measurements of comet Bradfield include the same range of heliocentric distance covered by the comets Bennett and T-S-K observations, and that we use virtually the same model for the cometary coma to derive water production rates. Since it has already been shown that the Haser model is fairly accurate in predicting water

production rates derived from OH brightness profiles, it is unlikely that a better model of the coma would significantly alter our result. Furthermore, ground-based observations of comet Bradfield (1979 X) in the visible (A'Hearn, Millis, and Birch 1981) show that the production rates of  $\text{C}_2$ ,  $\text{C}_3$ , and CN display a steep heliocentric variation similar to that of water, although the production rates of these three species are less than 1% of that of  $\text{H}_2\text{O}$ . It seems clear that the heliocentric distance dependence of water production varies significantly from comet to comet.

We also point out that our result is in disagreement with the intuitive assumption, based on the concept that the comet's absorption of solar radiation controls the vaporization of gas from the nucleus, that the heliocentric variation in the gas production rate should vary

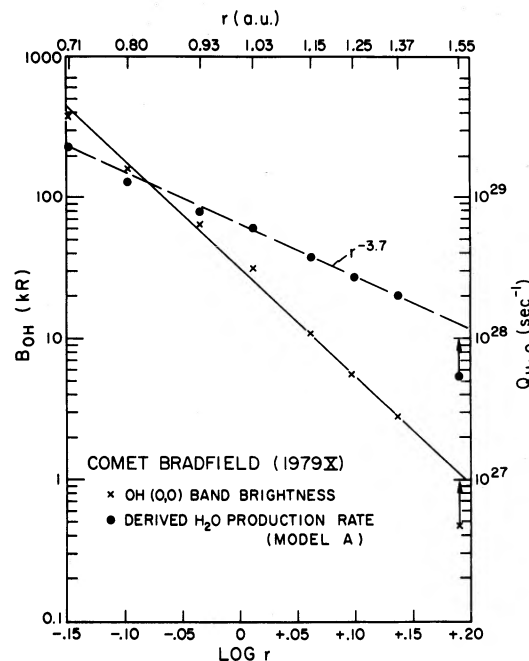


FIG. 4.—Brightness of the OH (0,0) band as a function of heliocentric distance. Also shown is the derived water production rate using Haser model A. Model B reduces the production rate by a factor of 2 for each measurement but leaves the slope unchanged.



as  $r^{-2}$ . In fact, present models of the cometary nucleus predict a rate of vaporization of gas with roughly an  $r^{-2}$  dependence within  $\sim 1.5$  AU from the Sun (A'Hearn, Thurber, and Millis 1977). This heliocentric dependence is somewhat sensitive to the choice of visible and infrared albedo for the nucleus. Delsemme (1973) derives  $Q_{H_2O} \propto r^{-n}$  with  $2.4 < n < 2.9$  for a "reasonable" range of albedos. However, it should be recognized that all of these models assume, among others things, a spherically symmetric and homogeneous nucleus with no provision for effects due to the coma, i.e., a nucleus which may have little connection with reality. Although the result may not be applicable to comet Bradfield, which apparently produced little dust (A'Hearn, Millis, and Birch 1981), recent modeling of comet Halley indicates that the presence of a dust coma significantly steepens the heliocentric variation in the gas production rate (Weissman and Kieffer 1981). Furthermore, numerous other factors, such as surface inhomogeneities, "seasonal" effects, dust mantles, etc., may be important in controlling the vaporization of gas. Our results indicate that these models need to be reconsidered.

One other comment should be made concerning the heliocentric variation of  $Q_{H_2O}$ . The rapid decrease in the OH (0,0) band brightness observed at  $r=1.55$  AU is almost certainly *not* real. During this final day of observations the visual brightness of the comet was sufficiently faint as to make the comet practically indiscernible on the FES image. As a consequence, placing the aperture precisely at the center of brightness was virtually impossible. For the exposure in which we measured

the OH brightness we repositioned the telescope by  $\sim 1'$  ( $\sim 6.3 \times 10^4$  km at the comet) after  $\sim 1$  hr of exposing (total exposure time = 190 minutes) because we did not think we were on the center of brightness. An examination of our earlier OH brightness profiles (Fig. 3) shows that with such an offset, the OH brightness decreases considerably from its value at the nucleus. Therefore, our OH measurement was not representative of the true OH brightness at the nucleus, and we have underestimated the corresponding water production rate. Further evidence to justify this conclusion comes from an examination of the Ly $\alpha$  brightness for the same day (see Fig. 5) which does *not* show a similar decrease. Since the Ly $\alpha$  brightness does not vary as rapidly with distance from the nucleus as the OH brightness, we would expect that the pointing of the telescope is not as critical for the Ly $\alpha$  measurement as for the OH measurement. Finally, ground-based photometry of C<sub>2</sub>, C<sub>3</sub>, and CN indicate a constant decrease in the brightness of these species for increasing heliocentric distances up to  $r=1.63$  AU (A'Hearn, Millis, and Birch 1980). For these reasons we conclude that the water production rate varied as  $r^{-3.7}$  uniformly to  $r=1.55$  AU.

#### V. H I

While the OH emission is optically thin, this is not the case for the Ly $\alpha$  emission of atomic hydrogen. For our measurements at the center of brightness during the first day of observations, the optical depth at line center is  $\tau_0 \approx 3$ . An approximate radiative transfer calculation is used to relate column densities to surface brightnesses (Festou *et al.* 1979). In this calculation we assume no shielding of the incident solar flux by the constituents of the coma, but we do take into account absorption of scattered photons along our line of sight through the medium. The two H I velocity distributions are distinguished from each other by the different widths of their absorption profiles, and this is also incorporated into the calculations.

Due to the high velocities of the hydrogen atoms relative to their parents (H<sub>2</sub>O and OH), we would expect that the Haser model would seriously underestimate H I densities within  $\sim 10^4$  km from the nucleus. Using water production rates derived from the OH measurements, the Haser model predictions for the brightness at the nucleus are too low by a factor of 3 to 4 from the measured values. On the other hand, the vectorial model more closely follows the observed values, as shown in Figure 5. Once again, curves A and B refer to the same (vectorial) model but using different values for  $v_{H_2O}$  and  $\tau_{OH}$ . These values are listed in Table 2. As the calculations are very lengthy, they were performed for only three values of heliocentric distance, and these are marked on the graph. Nevertheless, the trend seems clear, since these three points span our entire period of observations, and we have drawn a

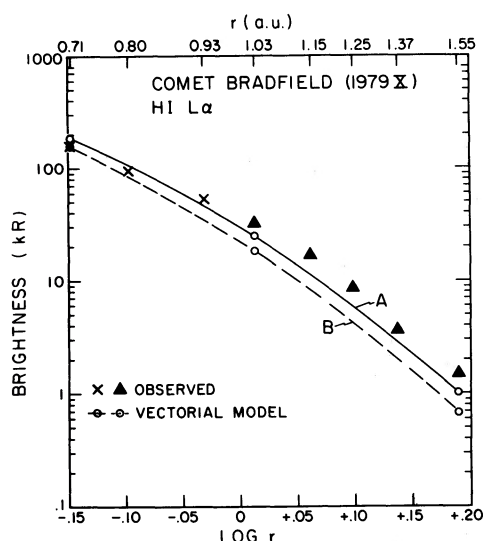


FIG. 5.—Predicted H I Ly $\alpha$  brightness at the nucleus as a function of heliocentric distance using vectorial models A and B. Smooth curves are drawn between the three calculated points. Of the measured points, the filled triangles include a subtraction of geocoronal Ly $\alpha$ , while the X's do not.



smooth curve connecting the three points to emphasize this fact. Also shown are the measured  $\text{Ly}\alpha$  brightnesses, some of which include subtraction of geocoronal  $\text{Ly}\alpha$  when it was not negligible relative to the cometary emission (the geocoronal measurements were made by offsetting  $\sim 2 \times 10^6$  km from the center of brightness, where there is vanishing contribution from the comet, and measuring the  $\text{Ly}\alpha$  signal).

The fact that the predicted intensities agree reasonably well with the measured values lends support to the water model. However, since the predicted absolute intensities depend critically upon the value of the solar  $\text{Ly}\alpha$  flux at line center, and since this number is uncertain to some extent, it is also important to be able to predict the slope of the heliocentric brightness variation. Although we use only three points for the model calculations, the sketched curves should give a good approximation to the true values. Assuming this to be true, we see that the slope of the predicted curve is about right for  $r \gtrsim 1.025$  AU but is too steep for  $r < 1.025$  AU. Since the  $\text{Ly}\alpha$  emission becomes optically thick for  $r < 0.92$  AU, we suspect that the lack of agreement in this region is due to our approximate treatment of the radiative transfer. We do not attempt to rectify this situation here, because the important point, namely that the hydrogen comes mainly from  $\text{H}_2\text{O}$  and OH, appears to be established by the magnitude of the observed brightness data. Finally, notice that once again the measurements do not allow us to choose between the different sets of input parameters, A or B.

## VI. O I

In principle we can use oxygen to distinguish between cases A and B, since a factor of 2 difference in  $\tau_{\text{OH}}$  produces a significant difference in the oxygen density profile. But the oxygen problem is complicated by other factors. First, the oxygen emission is optically thick ( $\tau_0 \approx 8$  for our measurements at the nucleus for the first day), requiring an approximate radiative transfer calculation similar to the one used for the H I  $\text{Ly}\alpha$  emission. For this calculation we must know the value of the solar flux at the cometary absorption wavelength. However, the absorption wavelength is Doppler-shifted into a steeply sloped portion of the solar line, making this determination highly uncertain. Also, since the absorption takes place from a  $^3P$  term, it is necessary to know the relative populations of the fine-structure levels of the ground state.

As far as the density model is concerned, we expect the case of oxygen to be similar to that of OH. The oxygen velocities are low enough that the Haser model should give a reasonably accurate approximation to the true density profile. However, as discussed above, our ability to relate these densities to absolute surface brightnesses is somewhat limited. Since collisions are not important, and since the scattering efficiency of the

oxygen atoms is small, we assume that all the atoms are in the lowest fine-structure level. We have examined the shape of the solar oxygen line at 1302.2 Å in an attempt to take into account the Doppler shift of the cometary line. *Skylab* measurements made in 1973 indicate that the solar flux at the center of the cometary absorption line is reduced by a factor of  $\sim 2.4$  from its value at line center (Feldman *et al.* 1976). Moreover, the width of the line appears to be consistent with the effective width of 0.26 Å quoted by Strickland and Thomas (1975) and used in § III of this paper. However, the *Skylab* measurements taken were made near solar minimum conditions, while the comet Bradfield observations were made during solar maximum. Preliminary data from the *Solar Maximum Mission* experiment (high spatial resolution measurements taken near the center of the solar disk and near the solar limb; Woodgate 1981) indicate a solar line of approximately the same width but asymmetrical about line center so that the solar flux at the Bradfield absorption wavelength may be reduced by a factor of  $\sim 4$  or more from its value at line center. Until a further analysis of the *Solar Maximum Mission* data can be accomplished, we attempt to correct for the Doppler shift of the cometary line by dividing our value of the solar flux at line center by a factor of 3.5. Although this specific value is chosen to give good agreement between the calculated and measured O I brightness when  $r = 0.71$  AU, the choice does not appear to be too unreasonable.

Oxygen brightnesses were measured only during the first three observation dates. Figure 6 shows the results of our calculations as well as the measured brightnesses for these three days. A number of points can be made concerning the graphs. First, the predicted brightness profiles appear to be too flat relative to the observed profiles. This is not an optical depth effect, since the column density profiles, from which we derive the brightness profiles, are also relatively insensitive to projected distance from the nucleus. Two ways to create steeper brightness profiles would be either to decrease the oxygen lifetime or to increase the contribution to the oxygen population from the direct dissociation of water. Both of these changes might be possible if the solar conditions were different at the time of the Bradfield observations than what is assumed here. Further comment concerning these points will be made in the next section. However, we point out that the Haser model may simply be inadequate in describing the oxygen density profile. Festou's vectorial model would certainly predict steeper brightness profiles since, unlike the Haser model, it takes into account the filling of the inner coma with dissociation products. Notice also that the procedure prescribed by Combi and Delsemme (1980) for modifying the Haser formula (choose smaller velocities and shorter scalelengths than the "true" values) would result in steeper brightness profiles as well.

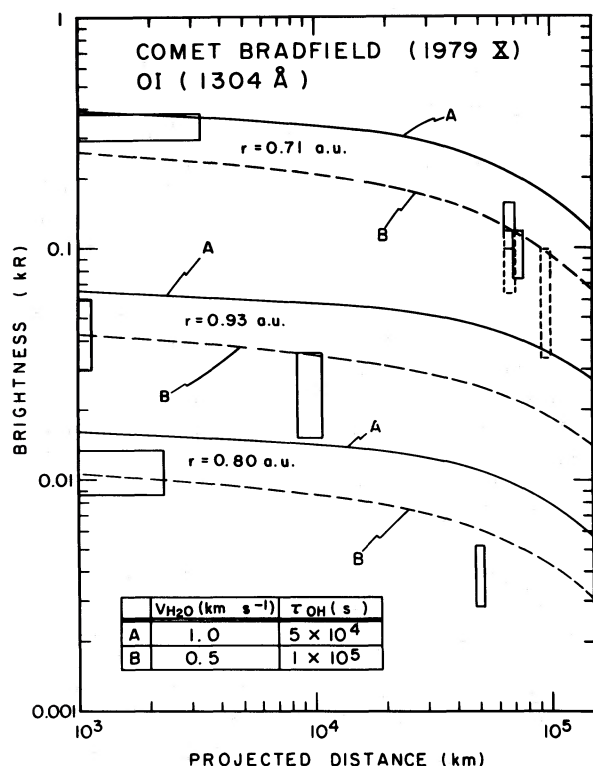


FIG. 6.—Comparison of the O I (1304 Å) brightness profiles with Haser model predictions for 3 days of observations. The rectangular boxes and A and B labels have the same significance as in Fig. 3. The data for  $r=0.71$  AU indicate a significant sunward (solid line)–tailward (dashed line) brightness asymmetry (Greenstein effect). The data and curves for  $r=0.80$  AU are shown a factor of 10 lower for clarity.

An interesting feature in the brightness profile obtained 1980 January 10 is the sunward–tailward brightness asymmetry shown at  $\sim 7 \times 10^4$  km from the nucleus. Although the boxes overlap, this is because the uncertainties due to the absolute calibration ( $\pm 10\%$ ) are included in the error estimates. If only the measurement error is considered, then it becomes clear that there is a real asymmetry. This asymmetry is apparently due to a “Greenstein” effect (Greenstein 1958) in which the absorption of radiation by atoms in the sunward coma is Doppler-shifted toward the center of the exciting solar line (where the flux is higher) relative to the absorption of the atoms in the tailward coma (see Meier 1975 for a discussion of this effect). Since the models used here assume spherical symmetry, the predicted brightness profiles cannot possibly display this effect.

Despite our inability to match the oxygen brightness profiles exactly, we appear to be able to predict the absolute intensities fairly well for all three days. Of course, the value of the exciting solar flux was chosen to give agreement between model and observation on the first day ( $r=0.71$  AU), but agreement on the other days is not due to such a fit. The apparent systematic increase

in the model prediction relative to the observed values as the comet moves farther from the Sun is in the same direction as what would be expected considering that the same value of exciting solar flux is used for all three days, while the comet’s heliocentric velocity is increasing during this time. Also, as discussed earlier in this section, our choice of solar flux is not so arbitrary as to render the agreement on the first day meaningless. As a consequence, it appears that the abundance of oxygen in the coma is consistent with the photodissociation of  $H_2O$  and OH as the source of these atoms. However, given the uncertainties involved in the value of the exciting solar flux, it would seem to be inappropriate to use the present data to choose between the different sets of input parameter, A and B.

## VII. CONCLUSION

The IUE observations of comet Bradfield made in early 1980 have allowed us to examine in detail whether or not the observed hydrogen, oxygen, and hydroxyl in the coma can be related to the production of water at the nucleus. Our results indicate that the observed brightnesses of H, O, and OH are certainly consistent with a common water source for all three species. The good agreement between the OH(0,0) band spatial brightness profiles and the model predictions (Fig. 3), along with arguments ruling out alternative parents, strongly support the hypothesis that  $H_2O$  is indeed the only parent of OH. However, uncertainties in the model parameters and in the values of the solar flux (see below) prevent us from excluding small contributions to the production of H and O from parent molecules other than  $H_2O$ . The uncertainties are particularly large for oxygen, but we note that two of the most likely alternatives, CO and  $CO_2$ , cannot contribute more than  $\sim 30\%$  to the total oxygen production (Festou and Feldman 1981).

The water production rate derived from these observations shows an unexpectedly strong heliocentric variation, decreasing as  $r^{-3.7}$  for  $0.71 \text{ AU} \leq r \leq 1.55 \text{ AU}$ . The value of the water production rate depends on the assumed water velocity and OH lifetime. We derive  $Q_{H_2O} \approx 1\text{--}2.4 \times 10^{29} \text{ mol s}^{-1}$  for  $r=0.71$  AU.

One of the major problems encountered in trying to model the cometary coma is the uncertainty in our knowledge of the absolute values of the solar flux. In addition to their importance in predicting the absolute brightness of the resonantly scattered light, these numbers are used in determining the branching ratios into the various water dissociation channels and the lifetimes of the coma constituents (Oppenheimer and Downey 1980). For example, depending on the ratio of the solar Ly $\alpha$  flux to the flux at  $\sim 1700$  Å, we would have  $\sim 20\%$  of the  $H_2O$  molecules dissociating into  $H_2 + O$  instead of our assumed value of  $\sim 10\%$ . With such a change we would obtain a steeper oxygen brightness profile, which

would give a better fit to the data. A shortening of the O I lifetime would produce the same effect. Also, depending on the solar flux, we could have as many as  $\sim 25\%$  of the OH molecules with  $v_{\text{OH}} \approx 1.8 \text{ km s}^{-1}$  (we use  $v_{\text{OH}} = 1.15 \text{ km s}^{-1}$ ) and as many as  $\sim 25\%$  of the hydrogen atoms with  $v_{\text{H}} \approx 30 \text{ km s}^{-1}$  (we assume  $50\%$  with  $v_{\text{H}} = 20 \text{ km s}^{-1}$  and  $50\%$  with  $v_{\text{H}} = 8 \text{ km s}^{-1}$ ). These changes would affect some of the results of the calculations, but the magnitude of the changes would probably be too small to affect our basic conclusion that water is the dominant source of the major species observed in the coma.

Another area where we have made approximations is in the radiative transfer analysis. Implicit in our formulas is the assumption that the atoms and molecules in the coma absorb and emit light with a Doppler profile. This means that we have assumed an isotropic, Maxwellian distribution of velocities for the scatterers. This is not only inconsistent with the Haser model approach but also clearly wrong. (In fact, the vectorial model arose from an attempt to correctly model the velocity distribution of the coma constituents.) Also, we assume that the solar flux which excites the observed resonance lines is constant over the cometary linewidth. This is approximately correct for the H Ly $\alpha$  emission but is certainly not true for the oxygen emission. The

extent to which the radiative transfer approximation affects our results has not yet been investigated.

Clearly, there are many free parameters in our model. We should therefore be cautious and refrain from attaching too much significance to the quantitative results. However, we are confident that we have made reasonable assumptions which are based either on sound physical principles or on standard practice within the field. Certainly our results from comet Bradfield can be compared to those based on studies of other comets. The heliocentric variation in the production rate of gas, for example, apparently distinguishes comet Bradfield from the other comets for which such data exist. Beyond the comparative studies, however, this analysis presents convincing evidence that the vaporization of water determines the primary composition of the coma and, thus that water is the main constituent of the cometary nucleus.

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