

Production of CS and S in Comet Bradfield (1979 X)

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Summary. High and low resolution ultraviolet spectra of carbon monosulfide (CS) in Comet Bradfield (1979 X) were obtained with the IUE satellite. The high resolution rotational profile of the (0, 0) band at 257.5 nm can be fitted with a theoretical profile derived assuming a Boltzmann temperature of 70 K. Spatial plots of the low resolution data for both S and CS show that these emissions are concentrated toward the cometary nucleus. The results that have been obtained are consistent with a Haser model for CS and S where the parent molecule is CS₂. A very rapid variation of CS brightness with heliocentric distance is found.

Key words: comets – molecular ultraviolet spectroscopy – carbon monosulfide

1. Introduction

The first sulfur containing radical CS, discovered in comets was identified in ultraviolet emission of Comet West, by Smith et al., of Comet Seargent, Jackson et al., and Comet Bradfield (1979 X) (Feldman et al., 1980). The gas production rate from Comet Bradfield was sufficient in January 1980 so that high resolution spectra of CS could be obtained. Low resolution spectra of the comet were also obtained using the large spectrograph aperture at several heliocentric distances and these spectra show that both the CS and S emissions appear nearly point like. Three vibrational bands of the $A^1\Pi \rightarrow X^1\Sigma$ system of CS are clearly observed: 0–0, at 257.5 nm, 0–1, at 266.3 nm, and 1–0, at 250.7 nm. Krishna Swamy, (1981) has recently shown that the relative intensities of these vibrational bands, 1.0:0.1:0.05 respectively, are consistent with production via resonance fluorescence of sunlight. For purposes of analysis of gas production rates, only the strongest band, the 0–0 band, will be considered.

2. Observations

The details of the IUE satellite instrumentation have previously been described (Boggess et al., 1978) so that only the observational procedure will be outlined in this section. Three long wavelength high resolution spectra were taken at various times using the large (10" × 20") aperture of the spectrograph. The strong CS (0, 0) band appears similar in all three exposures. However, in two of the

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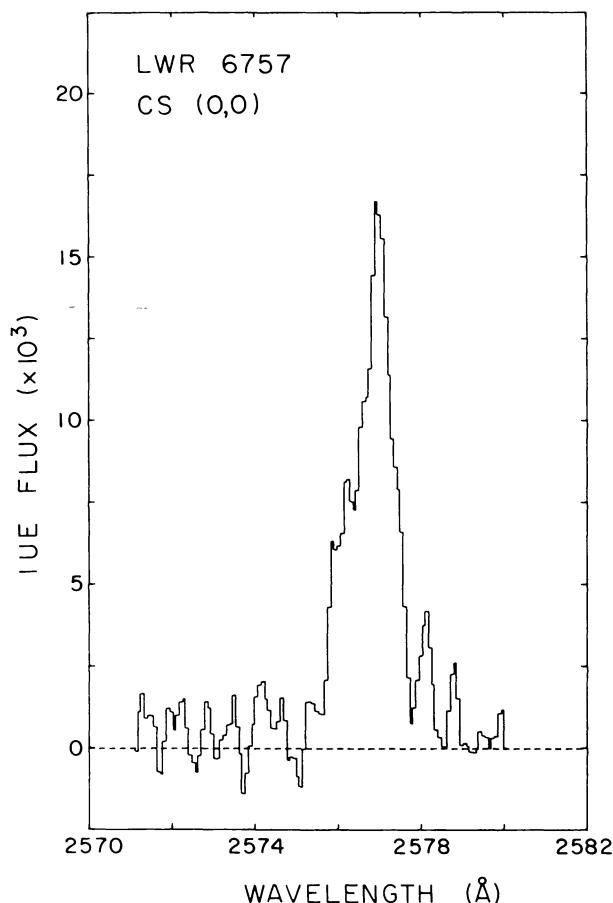


Fig. 1. High dispersion spectrum of the CS (0,0) band taken on 24 January 1980

spectra the exposure time was purposely kept short to prevent the OH (0, 0) band near 308.5 nm from saturating the camera, so that the CS (0, 0) band is rather weak. For analysis of the band lineshape, only the 144-min exposure obtained on 24 January 1980 (LWR 6757) was used. The CS (0, 0) band actually appears in two different orders in the spectrum, one of which occurs near the center of the camera and the other near the edge. The quality of the CS image near the edge of the camera is severely degraded by the variation in the grating efficiency across its blaze and is not used for analysis.

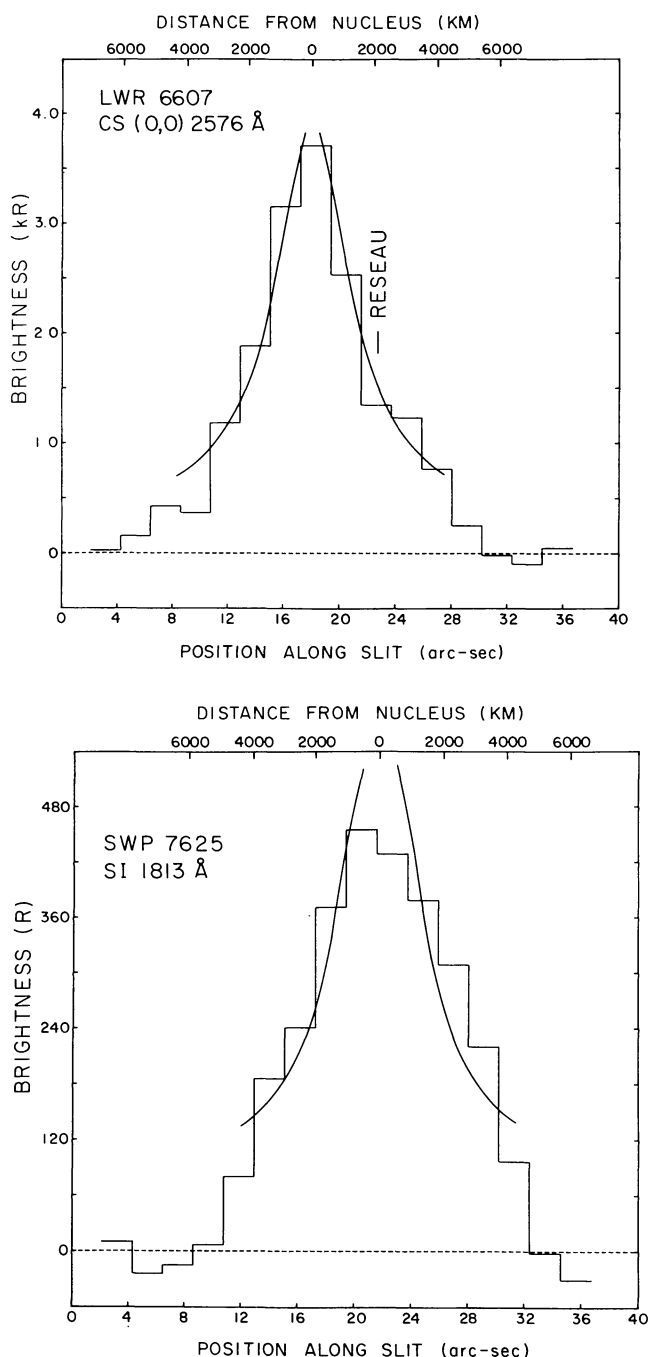


Fig. 2a and b. Brightness profiles along the long dimension ($20''$) of the IUE Spectrograph large aperture for **a** CS and **b** S I. The smooth curves show the expected profile from a Haser model with a CS_2 parent and production rates given in Table 1, folded with the approximate instrument response

A portion of the high resolution spectrum that was analyzed is shown in Fig. 1. The data have been smoothed using a three point running mean. The spectrum clearly shows a peak corresponding to the Q branch of the $(X^1\Sigma \rightarrow A^1\Pi)$ transition in CS and a shoulder corresponding to the R branch. The overall width of both bands is greater than 0.2 nm which is a factor of two to three times greater than the quoted instrumental bandwidth for an extended object.

The instrumental bandwidth may be as small as 0.25 nm which is the point source bandwidth of the IUE telescope since as Fig. 2 shows, the CS emission does not completely fill the large aperture of the spectrograph. This increases the effective resolution of the instrument over the extended source resolution of 0.08 nm because the CS emission serves as a smaller slit.

3. Low Resolution Analysis

Of all the cometary emissions observed in the ultraviolet with IUE, as Fig. 2a and b show, only those from CS and S appear concentrated near the center of brightness. If the sulfur resulted solely from the dissociation of CS, its image would appear extended in the IUE large aperture. Thus, a common shortlived parent such as CS_2 is suggested. Fortuitously, the photochemical lifetime of CS_2 at 1 a. u. is 100 s, shorter than that of any other known cometary radical, which with an outflow velocity of 1 km s^{-1} , gives a scale length of 100 km. This distance is considerably smaller than the spatial resolution of the IUE spectrographs ($1\text{--}2 \cdot 10^3 \text{ km}$ at the geocentric distances of our observations), so that the spatial distribution of both CS and S will appear to be similar to that of a long-lived parent molecule, which is nearly point like.

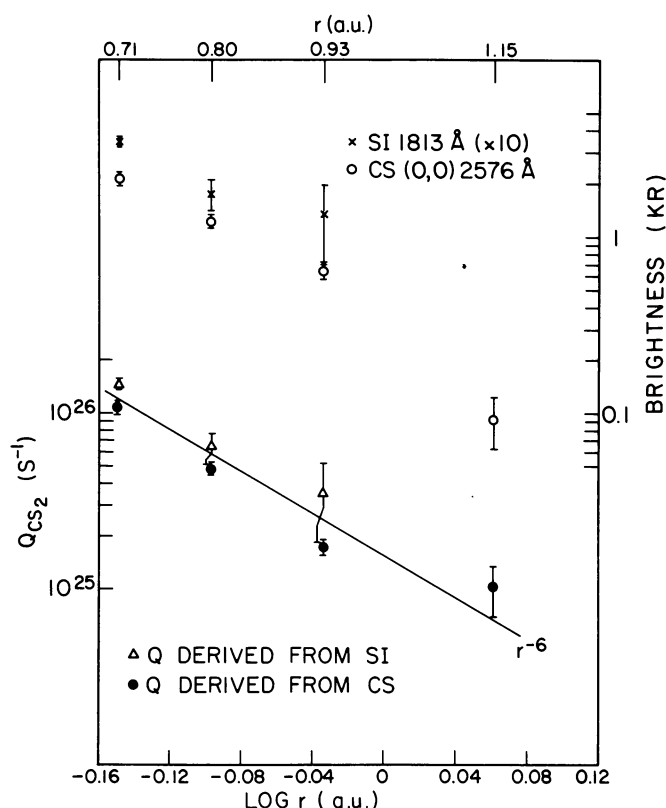
For the purpose of evaluating the parent production rate, a radial outflow Haser model, including a second daughter (Festou, 1981), was used with the parameters given above. The dissociation lifetime of CS was estimated to be 10^5 s at 1 a. u., but this parameter is not critical as the production of S from CS contributes only a small amount to the total S emission at the center of brightness. For comparison with the observed spatial profile, the brightness along the slit was calculated and smoothed with a triangular slit function of $5''$ FWHM to simulate the instrument resolution. The results for both CS and S are shown in Fig. 2. The agreement is quite good, the broader image in the case of S most likely due to tracking error (the exposure time was 120 min compared with 30 min for the CS image) and the relative weakness of the S image.

To convert the observed brightnesses to gas production rates the fluorescence scattering efficiencies, or “ g -factors” are also needed. For the CS (0,0) band a g -factor of $7 \cdot 10^{-4} \text{ photons s}^{-1} \text{ mol}^{-1}$ at 1 a. u. was derived using a oscillator strength, $f_{00} = 0.01$ (Hines and Brophy, 1979), a Franck-Condon factor of 0.75 (Suchard, 1977) and a solar flux of $1.6 \cdot 10^{12} \text{ photons cm}^{-2} \text{ s}^{-1} \text{ \AA}^{-1}$ (Broadfoot, 1972). This represents an average g -factor neglecting the Swings effect which can cause large changes in the fluorescence absorption with the comet’s heliocentric velocity due to structure in the solar spectrum (Kohl et al., 1978). A g -factor of $7 \cdot 10^{-5} \text{ photons s}^{-1} \text{ atom}^{-1}$ for the S I triplet was used, similar to the value adopted by Smith et al. (1980).

The results at four different heliocentric distances are given in Table 1 and Fig. 3. The brightnesses tabulated represent an average over the central $10'' \times 15''$ of the IUE spectrograph large apertures. No median filtering was applied to the data, nor was any correction made for the camera reseau mark that appears towards the edge of the CS image so that the CS brightness is slightly underestimated. The details of the data reduction have been given by Weaver et al. (1981). The parent production rate is determined by integrating the Haser model over the same field-of-view and adjusting the rate to match the observed brightness. Because of the nearly point-like nature of the emissions, the conversion from brightness to production rate is very sensitive to the large variation in geocentric distance over the period of the observations, as can be seen in Fig. 3. The error bars given in both Table 1 and Fig. 3

Table 1. Average brightness^a of the CS and S emissions

Date	Distance r (a.u.)	Distance r (a.u.)	Average brightness ^b (kR)		Production rate ^b (10^{26} s^{-1})	
			CS	SI	From CS	From SI
10 Jan. 1980	0.71	0.615	2.15 ± 0.19	0.35 ± 0.09	1.08 ± 0.09	1.48 ± 0.09
16 Jan. 1980	0.08	0.40	1.21 ± 0.10	0.18 ± 0.04	0.49 ± 0.04	0.65 ± 0.13
24 Jan. 1980	0.925	0.20	0.64 ± 0.06	0.14 ± 0.06	0.18 ± 0.02	0.35 ± 0.17
7 Feb. 1980	1.15	0.54	0.09 ± 0.03	—	0.10 ± 0.03	—

^a In central $10'' \times 15''$ of IUE spectrograph large aperture^b Measurement uncertainty only (see text)**Fig. 3.** Average Brightness of the CS and SI emissions and the derived parent production rates for four days of observation of Comet Bradfield (1979 X). The line only illustrates an r^{-6} variation and does not represent a fit to the data. The error bars indicate the measurement uncertainty only

represent the measurement uncertainty *only* and are included to facilitate the comparison between data taken on different days. Additionally, there is approximately 10% absolute calibration uncertainty in the brightness value and perhaps a factor of two in the derived production rates. The close agreement between parent production rates derived independently from the CS and S data considering the uncertainties in the g -factors and other model parameters, provides further strong evidence for a common parent, such as CS_2 , for these two species. One should note that the variation of production rate with heliocentric distance is very rapid, of the order of r^{-6} , which is considerably faster than the variation of OH (and presumably H_2O) over the same range of

distance (Weaver et al., 1981). Also, comparison with the OH data shows that this production rate is always less than 10^{-3} of that of water, so that CS_2 is truly a minor constituent in the cometary ice.

4. High Resolution Profiles

In order to interpret the observed band profiles, theoretical band profiles based upon the known CS spectrum as measured by Bergeman and Cossart were calculated. The observed CS spectrum at 257.5 nm is a ($X^1\Sigma \rightarrow A^1\Pi$) transition and shows P , Q , and R branches. Because of the small rotational constant of CS, the lines are closely spaced, especially in the Q branch, where many lines are bunched together near the origin. The R and Q branches both form heads which are responsible for the principal features observed in the high resolution spectra. The P branch forms no head and the lines are spread out so that they are difficult to identify above the background noise level.

There are several strong perturbations in the CS ($A^1\Pi$) state. Bergeman and Cossart have identified the amount of perturbative mixing for each state. Only one or two lines at relatively high values of J , will be strongly affected by this perturbation so that only one or two rotational lines in the total spectrum will be distorted. Since the population of these strongly perturbed states is very small at temperatures below 100 K, we have not adjusted the Honl-London factors to take account of the perturbation.

The rotational line strengths used in this calculation neglected the two strong perturbations in the CS ($A^1\Pi$) state, while the line positions, calculated from the measured term values of Bergeman and Cossart took them into account. This was believed to be reasonable as the perturbations lie at relatively high rotational quantum numbers ($J=12$ for the perturbation reflected in the Q branch and $J=15$ for that seen in the P and R branches). These states will thus not be greatly populated at temperatures less than 100 K.

It was assumed that the rotational energy could be described in terms of a Boltzmann temperature. Spectral profiles were built up using a Lorentzian form for each individual line. Theoretical profiles were calculated for a range of bandwidths from 0.001 nm to 0.08 nm but the best fit for the shapes, wavelengths and relative heights of the Q and R bandheads occurred when a FWHM bandwidth of 0.04 nm was used. This is reasonable in view of the previous discussion of the IUE instrumental bandwidth of 0.08 nm when the slit is filled and 0.02 nm for a point source. It has already been shown in Fig. 2 that the CS emission fills only about one half of the slit. Decreasing the bandwidth of course leads to well defined rotational lines while increasing the bandwidths distorts the shape

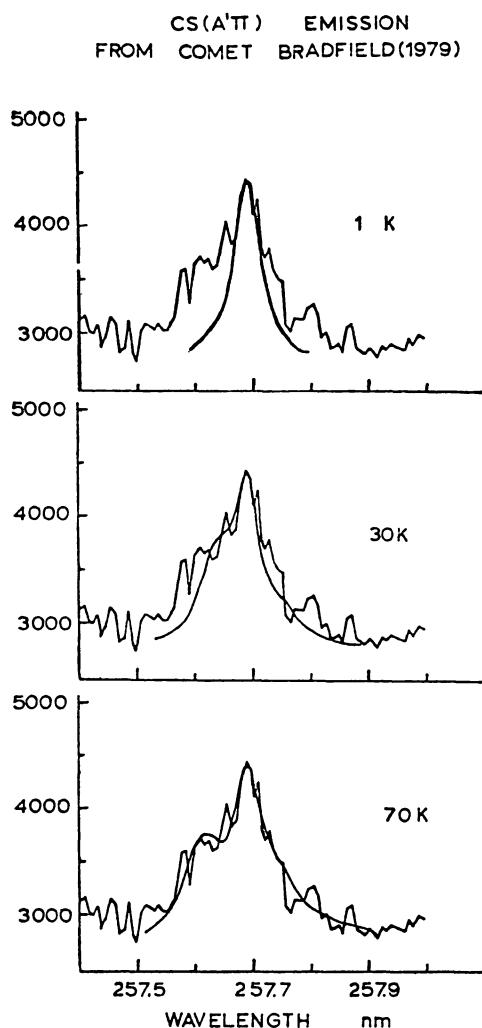


Fig. 4. The heavy solid curve is the computed rotational profile for CS assuming various rotational temperatures. As the temperature rises the profile broadens and the small feature that occurs on the short wavelength side disappears

and relative heights of the q and R bandheads compared to the observed spectra.

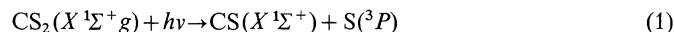
Figure 4 illustrates the comparison between the computed and observed spectra using a 0.04 nm FWHM bandwidth for the three Boltzmann temperatures of 1, 30 and 70 K. The spectra that are illustrated were calculated by assuming the radical was excited by solar radiation with the wavelength profile corresponding to illustrated were calculated by assuming the radical was excited by (1978) and corrected for the Doppler shift. The observed and calculated spectra were normalized to each other at their points of greatest intensity. It is clear that the 70 K temperature gives the best fit to the observed data in terms of shape, peak wavelengths, and the relative heights of the observed rotational bandheads. Higher temperatures result in a broadening of the calculated spectra and a poorer fit.

5. Discussion

One of the most significant features of the observations of CS and S in Comet Bradfield is that both of these features appear to be

nearly point-like rather than extended, and show a similar spatial distribution. This suggests that they are intimately connected and probably come from the same parent. The most likely candidate as a parent for CS and S is the CS₂ molecule. The vapor pressure of CS₂ is much higher than the vapor pressure of water so it should be carried along easily as the ice in nucleus evaporates.

This molecule is known to produce CS in the 190 nm region via the following reactions (Filseth, 1977):



Recent work (Yang et al., 1980) suggests that at 193 nm the CS is produced vibrationally excited to $v''=7$ and that the branching ratios for reactions (1) and (2) are 20% and 80%, respectively. The absorption coefficient for this band has been measured (Rabalais et al., 1971). When it is combined with the higher solar flux (Huebner and Carpenter, 1979) in this region, one finds a photochemical lifetime at 1 a.u. of 103 s. At a typical heliocentric distance of 1 a.u. and with a 1 km s⁻¹ outflow velocity, this corresponds to a scale length of about 100 km, well below the resolution of the present observations (about 1000 km at a geocentric distance of 0.2 a.u.).

The high resolution spectra were fitted with a "temperature" of approximately 70 K. The CS radical is produced primarily in a zone where collisions are still occurring so it is possible that this represents the Boltzmann temperature of this region of the coma. However, it is also possible that the CS "temperature" that is being observed is a result of radiative equilibrium. To determine whether radiative or collisional equilibrium is responsible for the observed "temperature" a detailed knowledge of the photochemistry is required. To obtain this detailed knowledge, laboratory work on CS₂ similar to Yang et al. (1980) would have to be done throughout this molecule's first absorption band which extends from 185 to 210 nm. It should be noted that the observation that the vibrational bands of the A'' Π \rightarrow X'' Σ system are consistent with a fluorescence excitation model does not mean that the rotational profile of the band is determined by this mechanism. It is possible that the system can be vibrationally relaxed, say, by radiation but not yet rotationally relaxed.

Malaise (1965) and Arpigny (1974) have done detailed calculations on radiative and collisional excitation of the rotational levels for cometary spectra. Arpigny points out, however, that in all of the observed cometary spectra, there appear to be some residuals that cannot be explained with a radiative equilibrium model. Radiative relaxation is faster for those radicals that have hydrogen atoms because they have a larger rotational spacing and hence higher transition probability. For example, the rotational constant, B_v , in OH is 18 cm⁻¹ whereas in CS it is 0.8 cm⁻¹. Since both radicals have about the same transition dipole moment, the relative values of the radiative lifetime for a pure rotational transition is inversely proportional to the cube of these B_v values. In CS, then the rotational relaxation rate via radiative decay, is very slow and since the CS molecule is produced within the collision region there is a high probability that the radicals can be rotationally equilibrated by collisions. The other radicals that are observed in comets are formed at larger distances and therefore, they are less likely to be rotationally equilibrated by collision.

6. Conclusion

The analysis of both the high and low resolution CS data obtained during the observation of Comet Bradfield (1979 X) suggests that

both CS and S are produced by photodissociation of a very short lived parent. The CS₂ molecule that is known to photodissociate at 200 nm to give both of these products has a photochemical lifetime at 1 a. u. of 103 s. This is one to three orders of magnitude shorter than the lifetime of other proposed parents of cometary atoms and radicals. It is, therefore, highly likely that this molecule is the parent for CS and S.

In this paper we have also shown that the parent of CS and S is a minor constituent of the cometary nucleus, with a production rate that is 10^{-3} of the production rate of water. The short photochemical lifetime of CS₂ means that most of the CS and S are formed in the collision zone of the coma so that these species may serve as an ideal probe of that region.

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