ANALYSIS OF IUE OBSERVATIONS OF CS IN COMET BRADFIELD (1979 1)

W. M. Jackson and J. Halpern
Howard University
Washington, DC 20059

P. D. Feldman
Johns Hopkins University
Baltimore, MD 21218

J. Rahe
Laboratory for Astronomy and Solar Physics
Goddard Space Flight Center
Greenbelt, MD 20771

ABSTRACT

The CS high-resolution and low-resolution IUE data obtained on Comet Bradfield (1979 1) have been analyzed. The high resolution rotational band profiles can be fitted with theoretical band profiles which are derived using a Boltzmann temperature of 70 K. A very rapid variation with heliocentric distance, for the CS brightness has been found. The implications of these results for models of the coma along with the origin of the CS species are discussed.

INTRODUCTION

The first sulfur containing radical discovered in comets was observed in Comet West (1976 VI) during the rocket observations of Smith and Casswell (ref. 1). These initial results were later confirmed by IUE observations of Comet Seargent (1978 m) (ref. 2) and Comet Bradfield (1979 1) (ref. 3). The gas emission rate from Comet Bradfield (1979 1) was sufficient so that, contrary to the previous observations, high-resolution spectra of CS could be measured. Low-resolution spectra of the comet were obtained with the large aperture at different heliocentric distances and these spectra show that the CS emission appears as a point source.

OBSERVATIONS

The details of the IUE satellite instrumentation have previously been described (ref. 4) so that only the observational procedure will be outlined in this section. Several long wavelength high-resolution spectra were taken at various times using the large (10" x 20") aperture of the spectrograph. The comet was tracked on the center of its maximum brightness using the fine error sensor of the IUE. In all of the high-resolution spectra the photowrite images showed a darkening in the region of the CS bands but only two exposures were obtained which exhibit sufficient signal to noise ratios so that useful data could be extracted from the tape. The CS bands actually occur 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. Nevertheless, some indication of the presence of the CS band was obtained.

One of the two high-resolution spectra that were analyzed is shown in Figure 1. The data have been averaged using a five point running mean. The spectrum clearly shows two peaks corresponding to the Q and R branches of the $X^1\Sigma \rightarrow A^1\Pi$ transition in CS. The overall width of both bands is greater than 0.2nm which is a factor of two to three times greater than the quoted instrumental bandwidth for an extended object. The actual instrumental bandwidth is probably less than the quoted value of 0.08nm since as Figure 2 shows the CS emission does not completely fill the large aperture of the spectrograph. This increases the effective resolution of the instrument because the CS emission serves as a narrower slit.

HIGH RESOLUTION THEORETICAL PROFILES

In order to interpret the observed band profiles, theoretical band profiles based upon the known CS spectrum and rotational line factors as given in Herzberg (ref. 5) were calculated. The observed CS spectrum at 257.5nm is a $X^1\Sigma \rightarrow A^1\Pi$ transition and thus 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 have heads at 257.60 and 257.77nm, respectively while the P branch shows no head.

A perturbation exists in the CS spectrum at the J=15 level in the 0-0 band. This was neglected in the present calculations of the rotational line factors (ref. 5) since it is unlikely to lead to a serious error in the fitting of the rotational profile. Only one or two lines at relatively high values of J, will be affected by this perturbation so that only one or two lines in the total spectrum will be distorted.

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, the width of which equalled the slit width of the IUE spectrometer. The actual profiles were constructed on a PDP-11/03 computer with a VT 55 graphic display terminal. Theoretical profiles were calculated using a Lorentzian bandwidth varying from 0.001nm to 0.08nm. The best fit for the shape, wavelength and relative heights of the Q and R bandheads occurred when a HWHM bandwidth of 0.02nm was used. This is in reasonable agreement with the low-resolution results which show that HWHM of the intensity peak for the observed CS (0-0) band fills only ½ of the long side of the large aperture, corresponding to a true HWHM bandwidth of 0.02nm.

Figure 3 illustrates the comparison between the computed and observed spectra using a 0.02nm HWHM bandwidth for the three Boltzmann temperatures of 70, 80 and 90K. The points are the average value of the two runs and they are plotted with error bars which represent the average error between the runs. It is clear that the 80 K temperature gives the best fit to the observed data in terms of shape, peak wavelengths, and the relative heights of the observed rotational band. The fact that the observed data fits a Boltzmann temperature at 80 K implies that for the CS molecule there are enough collisions to support a "temperature". Infra-red radiative decay is not fast enough to allow the molecule to completely relax to its lowest rotational level, which is in complete contrast to all other cometary molecules which have allowed infra-red transitions. The "temperature" that is observed probably results from a competition between collisional pumping and radiative decay and thus does not correspond to any physical temperature associated with the nucleus or the coma. More detailed modeling which includes radiative decay will be required if a physically meaningful temperature is to be extracted.

LOW-RESOLUTION ANALYSIS

A preliminary analysis of the low dispersion exposures at three different heliocentric distances is given in Table 1. Here, the brightness of the CS (0,0) band is averaged over a 10" x 15" aperture for comparison with model calculations. As the image of this feature is nearly point-like, no median filtering was applied. Also, no correction was made for the reseau mark that appears in the image and so the results given may be slightly in error. The production rate given in the table is derived by integrating the output of a Haser model over the given aperture size, and since the image is point-like, is extremely sensitive to the variation in geocentric distance. The model assumes a CS parent with a lifetime of 100 sec (at 1 a.u.), an outflow velocity of 1 km sec^{-1} and a g-factor for the (0,0) band of 7×10^{-4} photons sec^{-1} mol^{-1} at 1 a.u. The variation of production rate with heliocentric distance is very rapid, of the order of r^{-6}-r^{-7}, considerably faster than the variation for OH over the same period (ref. 8). Although the difference may well be real, one must use caution in applying a radial outflow model in this case as the parent scale length is within the collision region around the nucleus while the model is collisionless.

The most likely candidate as a parent for CS is the CS_2 molecule. This molecule is known to produce (ref. 6) CS via the following reactions

1. $CS_2\ (X^1\Sigma^+g) + h\nu \rightarrow CS(X^1\Sigma^+) + S(^3P)$

2. $\rightarrow CS(X^1\Sigma^+) + S(^1D)$

in the 190nm region. Recent work (ref. 7) suggests that at 193nm the CS is produced vibrationally excited to $v'' \leq 7$ and that the branching ratios for reactions (1) and (2) are 20% and 80%, respectively. The absorption coefficient for this band has been measured (ref. 9). When it is combined with the higher solar flux (ref. 10) in this region, one can compute a photochemical lifetime at 1AU of 103 sec. At the largest observed heliocentric distance and with a 1km/sec outflow velocity this corresponds to a scale length of 88 km, well below the resolution of the present observations.

DISCUSSION

The CS molecule is the first diatomic molecule with an allowed infrared transitions that shows any evidence that it has retained memory of the temperature at which it was formed. In light of the fact that CS is produced via photodissociation in high vibrational levels (ref. 7) it is likely that the observed "temperatures" are the result of radiative cascade from these higher levels. Thus one needs a detailed knowledge of the photodissociation dynamics to include the effect of these cascade processes in any radiative equilibrium model of the coma of the comet. Only when this is done will one be able to evaluate how collisions can contribute to the observed temperatures.

The photodissociation model of CS_2 can also explain the presence of S atoms in the comet since these atoms are the products of the photodissociation of both CS_2 and CS. Most of the S atoms are produced in the ^1D state which has a radiative lifetime (ref. 11) of 25 sec. However, because of this short lifetime and the relatively low sulfur abundance it is unlikely that ^1D atoms can be detected directly as in the case of carbon (the $^1D-^1P$ transition at 193.1nm) where the lifetime of the ^1D state is 3200 sec (ref. 12). It is possible that resonance fluorescence mechanism may excite the ($^1S \rightarrow ^1D$) transition at 7725Å since this transition has a lifetime of only 0.47 sec (ref. 11) and the analogous D atom transition has already been observed.

CONCLUSION

The detailed analysis of both the high- and low-resolution CS data obtained during the observation of Comet Bradfield (1979 l) suggests that this radical is produced by photodissociation of CS_2. The heliocentric variation of the CS brightness is consistent with this conclusion along with the presence of S atoms in comets. Further analysis of the data may reveal how important collisions are in the inner part of the coma.

ACKNOWLEDGEMENTS

The authors are grateful for the complete cooperation they received from the IUE observatory staff. W. M. Jackson would like to acknowledge the helpful conversations with M. A'Hearn and the support of the Planetary Atmospheres Program of NASA under grant number NSG 5071. The work at Johns Hopkins University was supported by NASA grant NSG-5393.

REFERENCES

1. Smith, A. M., and Casswell L., submitted to Astrohys. J. (1980).

2. Jackson, W. M., Rahe, J., Donn, B., Smith, A. M., Keller, H. U., Benvenuti, P., Delsemme, A. H., and Owen, T., Astron. Astrophys., 73, L 7 (1978).

3. Feldman, P. D., Weaver, H. A., Festou, M. C., A'Hearn, M. F., Jackson, W. M., Donn, B., Rahe, J., Smith, A. M., and Benvenuti, P., accepted for publication, Nature (1980).

4. Boggess, A. et al. Nature, 275, 377-385 (1978).

5. Herzberg, G., Diatomic Molecules, D. Van Nostrand, New York, (1950), 128.

6. Filseth, S. V., Advances in Photochemistry, 10, John Wiley and Sons, (1977) 1.

7. Yang, S. C., Freedman, A., Kawasaki, M., and Bersohn, R., J. Chem. Phys., 72, 4058 (1980).

8. Weaver, H. A.; Feldman, P. D.; and Festou, M. C.: Water Production Models for Comet Bradfield (19791). The Universe in Ultraviolet Wavelengths: The First Two Years of IUE. NASA CP-2171, 1980: this compilation.

9. Rabalais, J. W., McDonald, J. M., Scherr, V., and McGlynn, S. P. Chem. Rev., 71, 73 (1971).

10. Huebner, W. F., and Carpenter, C. W. Los Alamos report LA-8085-MS 1979.

11. Okabe, H., Photochemistry of Small Molecules, John Wiley and Sons (1978) 156.

TABLE 1

Heliocentric Variation of the Average Brightness of the CS (0,0) Band

Heliocentric Distance, r (a.u.)	Geocentric Distance, Δ(a.u.)	Average Brightness (kR)	Derived CS Production Rate (sec^{-1})
0.71	0.615	2.1	1×10^{26}
0.80	0.40	1.2	5×10^{25}
0.925	0.20	2.6	1.6×10^{25}

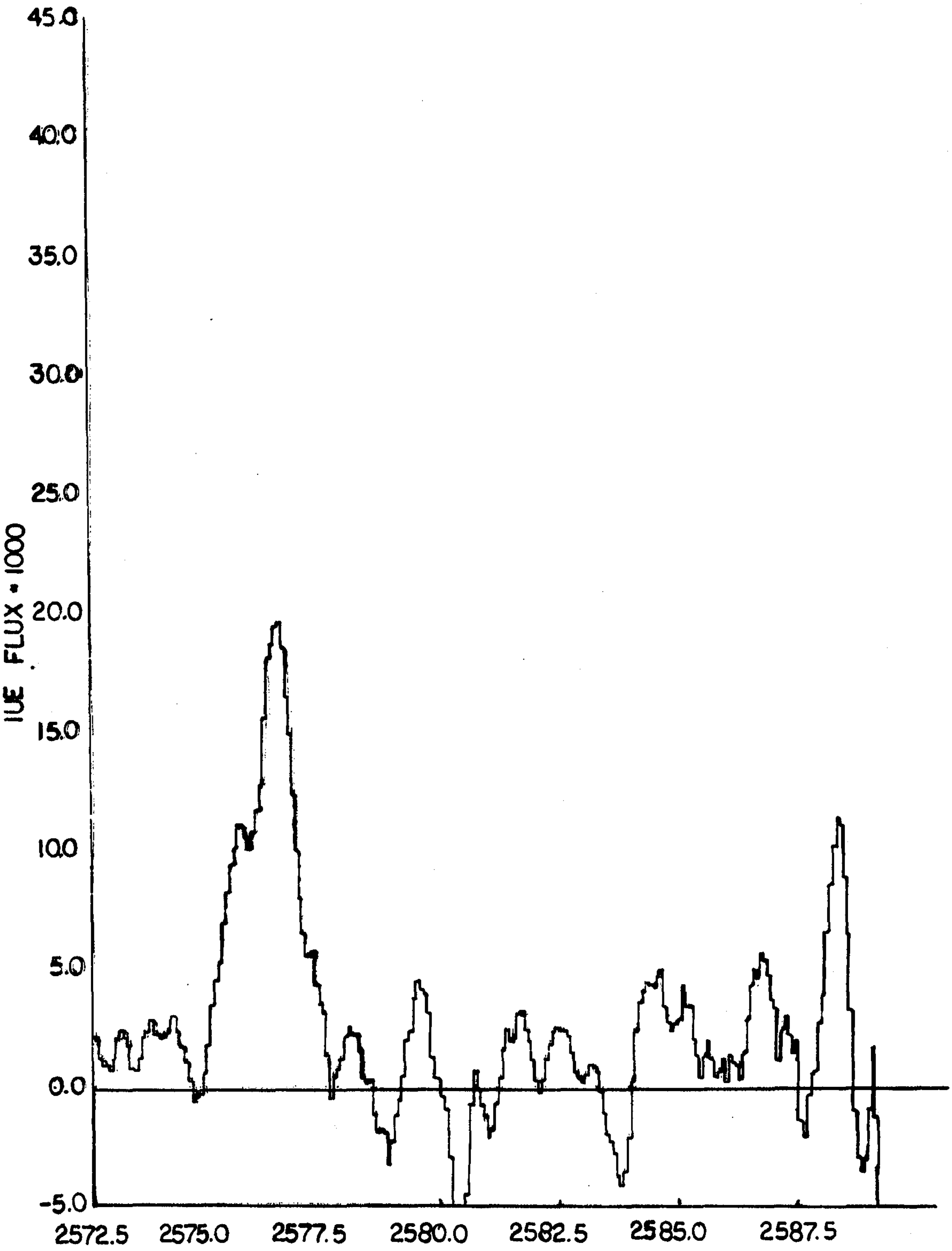

Figure 1.

High-resolution IUE Spectra of Comet Bradfield (1979 1) in the CS region.

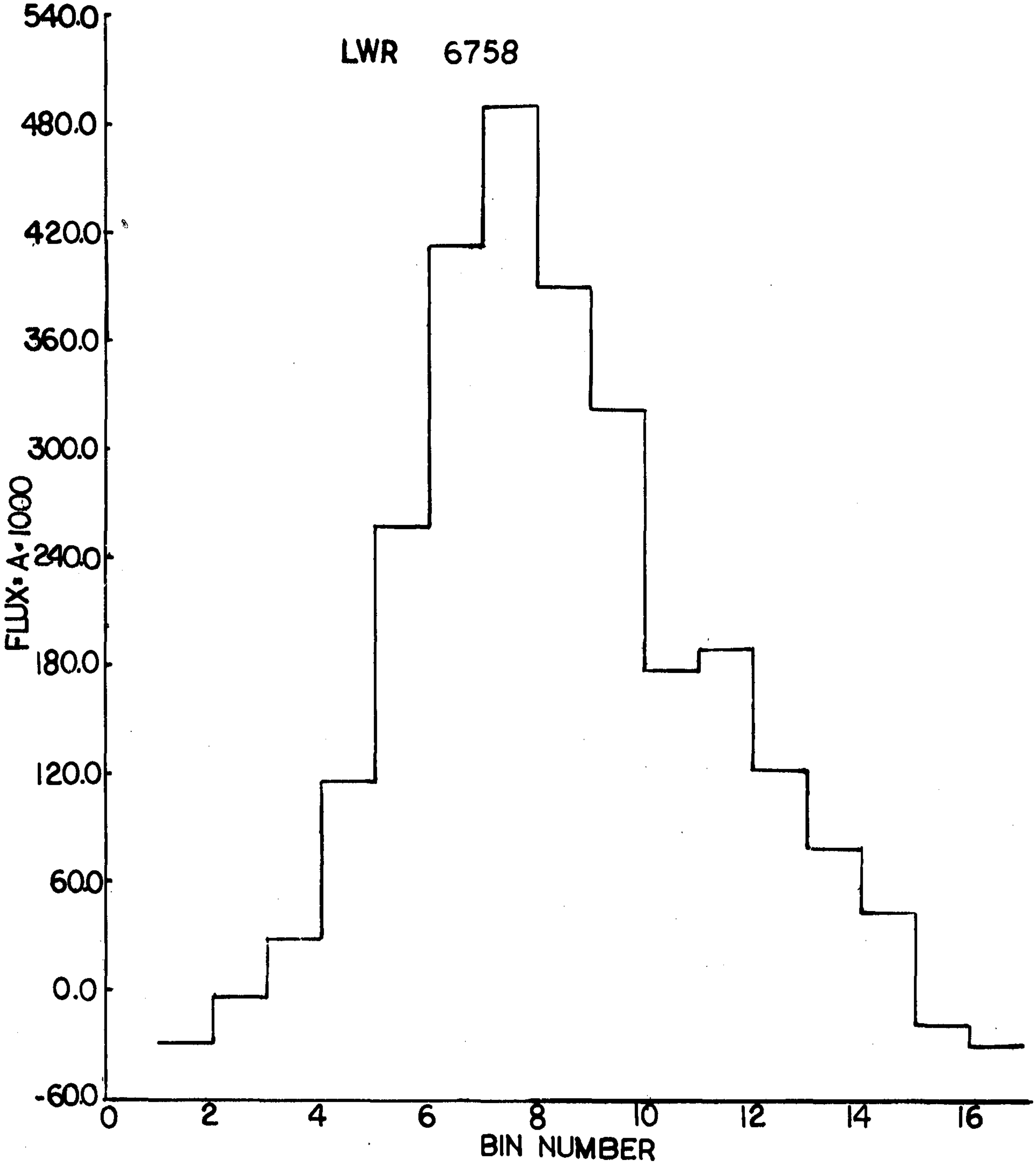

Figure 2.

Spatial profile of low-resolution spectra of CS scanned along the long dimension of the slit.

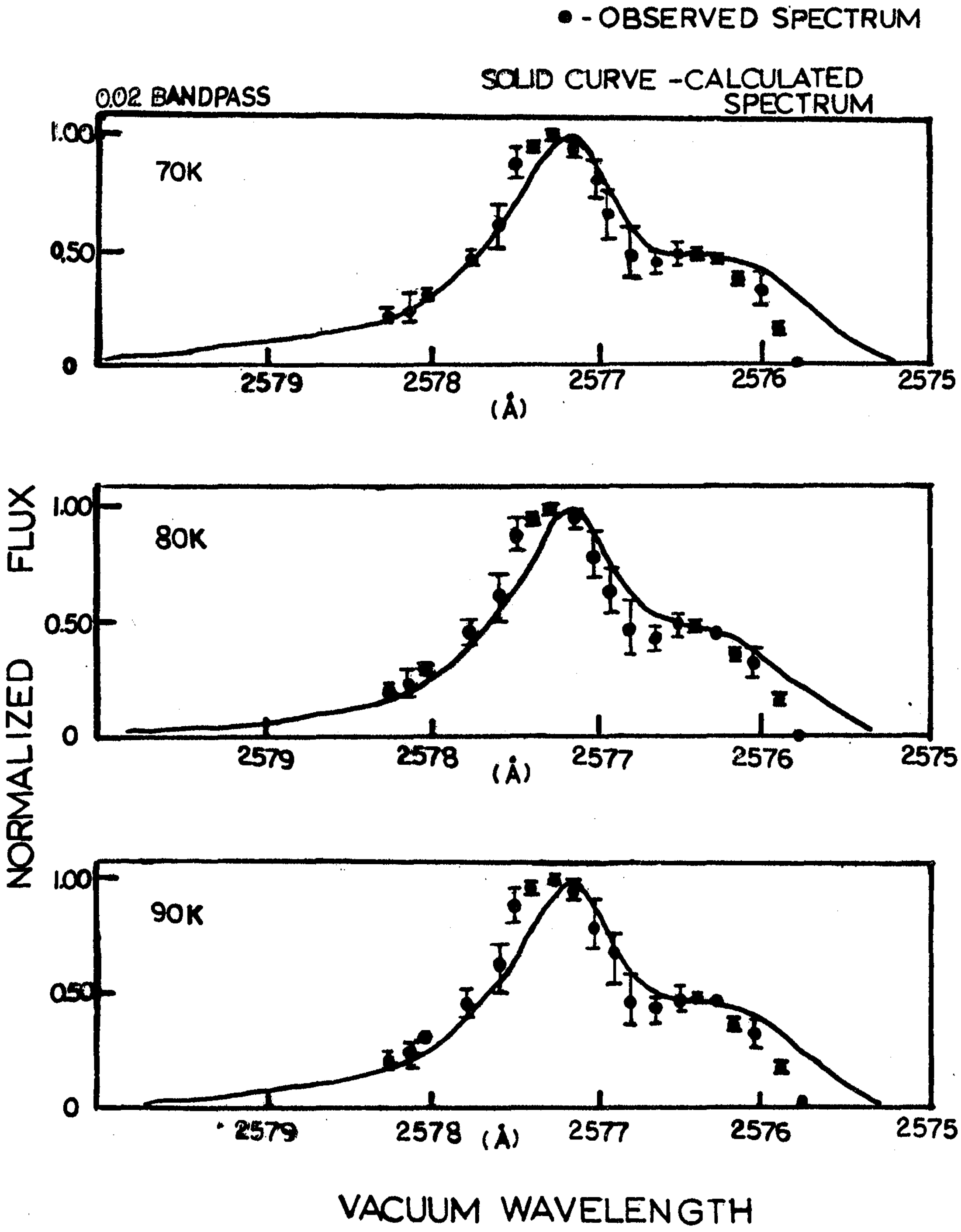

Figure 3.

Comparison between observed and theoretical CS band profiles for 0.02nm HWHM bandpass and at temperatures of 70, 80, and 90 K.