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SPECTROSCOPY OF THE 3.4 MICRON EMISSION FEATURE IN COMET HALLEY

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ABSTRACT

Infrared spectra in the 3–5 μm region have been obtained of comet Halley after perihelion, at heliocentric distances of 1.6 and 2.0 a.u. A broad emission feature, peaking near 3.4 μm and containing some spectral substructure, was observed, while at longer wavelengths only a featureless blackbody emission spectrum was seen. The emission feature probably arises from UV-pumped infrared fluorescence of organic molecules which are either in the gas phase or are embedded in very small grains. In the former interpretation the molecules must be quite large. These results lend support to the idea that comets formed out of interstellar grains whose molecular ice mantles largely consist of nonvolatile complex organic molecules.

Subject headings: comets — infrared: spectra — molecular processes

I. INTRODUCTION

Comets are believed to be the most pristine objects in the solar system. Because they undergo little or no chemical change after their formation out of interstellar matter in the solar nebula, their composition must reflect the physical and chemical nature of interstellar grains rather well. The appearance of a bright comet, such as P/Halley, thus provides a unique opportunity to study the properties of interstellar grains in the solar neighborhood.

Cometary nuclei are inaccessible to direct detailed observations. Much of our present knowledge of a comet's composition is inferred indirectly by analyzing emission lines in the surrounding coma. The interpretation of these spectra, due both to parent molecules and to photodissociated and ionized fragments, in terms of parent molecules relies on models and assumptions concerning the fluorescence excitation mechanisms and the lifetimes against dissociation and ionization. Furthermore, the sublimated molecules and fragments can be modified by chemical reactions taking place in the collision zone near the nucleus. Also, the molecular constituents of the dust, which is emitted at a rate comparable to the gas, cannot be observed in this way.

An alternative method to derive the composition of a comet is to follow the evolution of interstellar grains, from which a comet is formed, through the pre–solar nebula phase. One of the most detailed current models, which is capable of explaining hard-to-understand phenomena such as cometary outbursts at large solar distances, has been developed by Greenberg (1982). His model predicts large relative abundances of complex organic molecules, which are inevitably formed when grain mantles are photolyzed in interstellar space and occasionally raised to higher temperatures. Such organic molecules have strong characteristic transitions near 3.3 μm, due to C—H stretch vibrations.

The recent reports of a broad and strong emission feature in the spectrum of comet Halley at 3.4 μm (e.g., Wickramasinghe and Allen 1986; Combes *et al.* 1986; Knacke, Brooke, and Joyce 1986) give strong general support to the Greenberg model. Because only low spectral resolution instruments were used in the initial measurements of the emission feature, we were motivated to observe it in as much spectral detail as possible.

II. OBSERVATIONS AND RESULTS

Comet Halley was observed in 1986 April 25 and May 24 at the United Kingdom infrared 3.8 m telescope on Mauna Kea. The spectra were obtained using a seven-channel cooled grating spectrometer (Wade 1983) with a circular aperture of diameter 5″. Standard chopping and nodding practices were employed, using a beam separation of 60″. During the first night, three wavelength ranges 3.15–3.60, 3.55–4.10, and 4.50–5.00 μm were covered. The resolving power of the spectrometer ranges from ~ 400 in the short-wavelength band to ~ 800 in the long-wavelength band. In May, the 3 μm flux received from the comet had dropped by roughly a factor of 5, and only the wavelength range 3.15–3.60 μm was remeasured. Table 1 summarizes the relevant observational parameters and comet properties (heliocentric distance, topocentric distance, and radius of the coma seen within our aperture) for both nights.

The final spectra were obtained by co-adding many individual spectra. The final 3.15–3.60 and 3.55–4.10 μm spectra obtained in April were flux-calibrated by dividing by the spectrum of BS 4094 (K4 III) and multiplying by a blackbody spectrum corresponding to a color temperature of 4000 K. The 4.50–5.00 μm spectrum was divided by the spectrum of BS 4786 (G5 III) and multiplied by a blackbody spectrum of 5200 K. The 3 μm spectrum obtained in May was reduced using a spectrum of BS 3994 (K0 III, 4600 K). The resultant spectra are insensitive to the exact blackbody temperatures used. At these moderate resolutions, UKIRT spectra of G stars show no features in the 4.5–5.0 μm band, and 3–4 μm spectra of K stars show only the weak overtone band heads of

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TABLE 1

COMET HALLEY OBSERVATIONAL PARAMETERS

Date (UT)	Wavelength (μm)	R (a.u.)	Δ (a.u.)	Aperture	r (km)
1986 Apr 25	3.15–3.60 3.55–4.10 4.50–5.00	1.56	0.65	5″	1276
1986 May 24.......	3.15–3.60	1.97	1.56	5	3062

SiO at 4.0 μm and beyond. We are confident that except for the 4.0–4.1 μm interval the divided spectra correctly represent the intrinsic spectra of comet Halley.

The 3.15–3.60 μm spectrum obtained in April is shown in Figure 1. The error bars shown are typical for data points in the spectral subintervals in which they are located, except for the one at 3.32 μm, where very strong telluric absorption occurs. The broad emission feature is seen to extend from 3.25 to 3.55 μm. The total flux in the feature is 4.2 ($\pm$0.4) $\times$ 10^{-19} W cm^{-2} in the 5″ beam. In Figure 2 the April spectrum is reproduced at much lower resolution along with the one that was obtained 1 month later. Note that the May spectrum has been scaled up by a factor of 5. The factor of 4 decrease in the strength of the emission feature between April and May implies a dependence on heliocentric distance of $R^{-2.2}$ if the dependence on geocentric distance is Δ^{-1}. This suggests that the production rates of the emitting material were similar at the times of the two observations. In view of the rapid variations in the IR flux that have been reported for comet Halley (e.g., Knacke, Brooke, and Joyce 1986), this result is probably not significant.

The flux densities of the continua in the April spectra increase to longer wavelengths, even in the 3 μm band; therefore, at that time the continuum must have had a significant thermal component. However, the decrease in the slope of the 3 μm continuum in May implies that scattered radiation was the dominant contributor then. Note that the strength of the emission feature relative to the continuum increased between April and May. This change is similar to, although smaller than, that found by Knacke, Brooke, and Joyce (1986) between 1986 March and April. Clearly the emission feature is not coupled to the thermal continuum.

The spectra obtained at longer wavelengths are not reproduced here, since they appear to be featureless. A blackbody curve with a temperature of 250 K provides the best fit to the spectra between 3.6 and 5.0 μm. This value is consistent with the results obtained by Tokunaga *et al.* (1986*a*). Between 3.2 and 3.6 μm, the blackbody flux density increases by a factor of 4, whereas in the April spectrum only a factor of ~ 1.5 increase is observed. This demonstrates quantitatively that the continuum in the short-wavelength region of the April spectrum (Fig. 1) has a large scattered light component.

The emission feature in Figure 1 appears to consist of several partially blended features which are well above the noise level and are therefore believed to be real. Most prominent is the bright, central emission which peaks near 3.36 μm (2990 cm^{-1}). There also are subsidiary emission peaks centered at 3.28 μm (3040 cm^{-1}) and 3.52 μm (2840 cm^{-1}). Although considerably less prominent than the central feature, each of these consists of several independent and adjacent data points which lie above the background level. Both features also appear to be present in the lower resolution spectrum of Knacke, Brooke, and Joyce (1986). There may be a weak absorption at 3.22 μm; it is detected in both halves of the April data when they are reduced separately. It is not clear if the remaining spectral structures (e.g., those on the shoulders of the central feature) are caused by absorption bands which are superposed on a smooth and broad emission band (as is suggested by the possible presence of the isolated

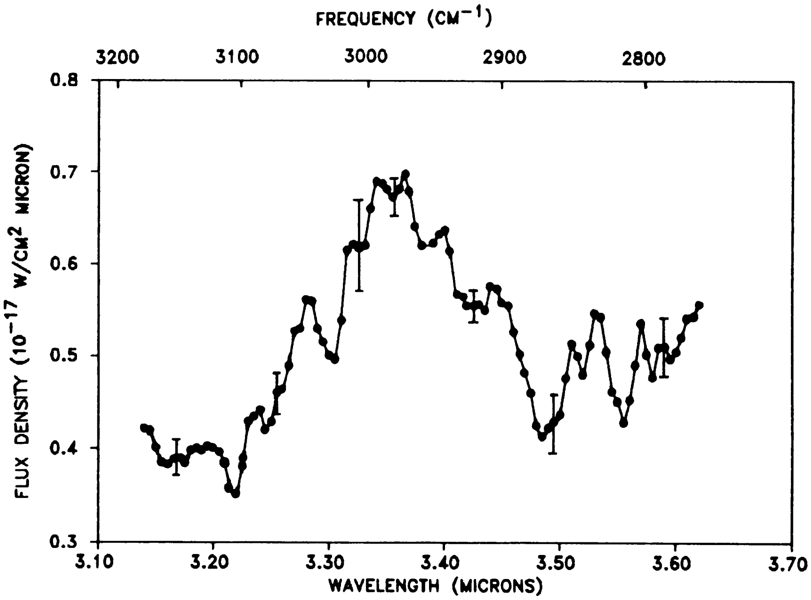

FIG. 1.—Spectrum of comet Halley obtained on 1986 April 25. The resolution is 0.008 μm. The error bars ($\pm 1\sigma$) shown are typical for data points in their respective spectral subintervals, except for the one at 3.32 μm.

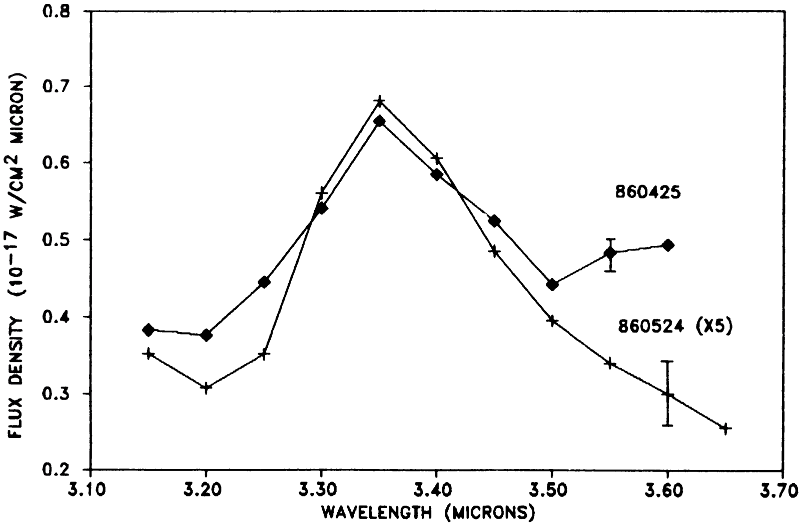

FIG. 2.—Block-averaged spectra of comet Halley from 1986 April 25 and May 24. The latter spectrum has been scaled up by a factor of 5. Typical error bars are shown.

3.22 μm absorption feature), or by structure in the emission spectrum which is intrinsic to the radiating molecule(s).

The weak emission peaks at 3.28 μm and 3.52 μm are close in wavelength to the well-known 3.3 μm and 3.5 μm unidentified emission features, which have been observed by Baas *et al.* (1983), Geballe *et al.* (1985), and de Muizon *et al.* (1986) at resolutions comparable to the present comet Halley spectra. However, neither the peak wavelengths nor the shapes of these features are precisely the same as those in the comet. The bright 3.36 μm emission feature in Halley has no emission counterpart in other astronomical objects. In terms of wavelength proximity and width it bears some resemblance to the 3.4 μm absorption feature observed in the interstellar medium towards the galactic center (Butchart *et al.* 1986); however, the profiles of the two features have little in common. Except for a low-resolution, apparently featureless 3 μm spectrum of the (bare) nucleus of comet *IRAS*-Araki-Alcock (Hanner *et al.* 1985), and a 3 μm spectrum of comet West (Oishi *et al.* 1978), in which a weak 3.4 μm emission feature may possibly be present, no 3 μm spectra of other comets have been published. A low-resolution 3 μm spectrum of comet Halley prior to perihelion passage also does not show an emission feature (Tokunaga *et al.* 1986*b*). To summarize, the present 3 μm spectrum of comet Halley does not closely resemble the spectrum of any known astronomical object.

III. DISCUSSION

Several authors (e.g., Yamamoto 1982; Crovisier and Encrenaz 1983; Weaver and Mumma 1984) have investigated whether infrared line emission from cometary parent molecules would be detectable and have concluded that emission lines from a number of simple molecules should be observable above the continuum background in bright comets. Of the candidate molecules, methane (CH_4) and carbon monoxide (CO) have strong bands within the spectral intervals we have observed (centered at 3.31 μm and 4.67 μm, respectively). However, neither of these molecules are detected in our spectra. Instead, a broad and structured feature stands out at 3.4 μm. The shape and position of this feature is indicative of resonance radiation due to hydrocarbon molecules. The resonance wavelength of the —C—H stretch vibration in saturated and aldehydic compounds is typically in the 3.4–3.5 μm range but shifts to shorter wavelengths when unsaturated double and triple bond structures are present. Depending on the nature of neighboring atoms, the =C—H stretch is usually seen between 3.2 and 3.3 μm.

A strong and broad emission feature, centered at 7.5 μm, has been detected in comet Halley by the *Vega I* spacecraft (Combes *et al.* 1986) and has been interpreted as representative of the presence of C—C bonds in the region observed. The absence of a peak around 6 μm, caused by the C=C stretch mode, is somewhat puzzling, however, and indicates that the molecules must have a center of symmetry in the C=C bond. In fact, the spectrum obtained by *Vega I* is more consistent with the symmetric C—H bending modes of $—CH_3$, but contributions from different subgroups, such as —CN,—NO, and $—NO_2$ cannot be ruled out. Based on present spectroscopic data, no definite assignment of even the molecular subgroups emitting at 3.4 and 7.7 μm can be made.

An important question that must be addressed is whether the emission is caused by resonance scattering from molecules in the gas phase or originates from molecules either in the gas phase or embedded in warm grains and pumped by some other mechanism. Following Yamamoto (1982) the observed photon flux from molecules which scatter incident solar radiation resonantly is given by

$$F = gN/4\pi\Delta^2 \tag{1}$$

with

$$N = Qt_L f(x), \tag{2}$$

where g represents the number of photons emitted per molecule per second at distance R from the Sun, and N the number of molecules seen in a given aperture. N is a function of the sublimation rate, Q, and the lifetime, t_L, of the molecules in question. The geometrical factor, $f(x)$, depends on the ratio between the aperture and scale length of the emitting molecules.

An estimate for the flux from (gaseous) CH_4 can be obtained using a sublimation rate of 2×10^{29} s^{-1} for H_2O at $R = 1.56$ a.u. and a relative abundance of 0.07 for CH_4 (Krankowsky *et al.* 1986). The resulting flux is 3×10^{-20} W cm^{-2} for a g factor of 1.51×10^{-4} at $R = 1.56$ a.u., which is not only a factor of 10^2 smaller than predictions made by Yamamoto (1982), mainly because of our small aperture, but is still an overestimate since LTE is valid in the aperture observed by us. This result not only explains why CH_4 was not detected by us, but it also implies that the observed 3.4 μm emission band cannot be caused by resonance scattering, because the band strengths of hydrocarbon groups in common molecules are not likely to exceed the strength of the ν_3 band in CH_4 by a large factor, and the abundance of the emitters cannot be taken to be much larger than that assumed for CH_4 without running into conflict with relative abundances. The same conclusion was drawn by Combes *et al.* (1986) for the 7.5 μm feature present in the *Vega I* spectra.

Infrared line emission from molecules in cometary dust is another possibility that must be explored. Thermally pumped infrared fluorescence in grains has been the subject of a paper by Dwek *et al.* (1980), who discussed the subject in an attempt to explain the high ultraviolet to infrared photon conversion efficiency by grains in regions of high ultraviolet photon intensity. In their model, vibrational transitions of embedded molecules greatly enhance the emissivity Q_{bb} of a grain at specific wavelengths. High values for the line-to-continuum ratio $Q_{\mathrm{line}}/Q_{\mathrm{bb}}$ can be obtained this way even when using modest f-values for the transition. Thus, by itself, the April 25 spectrum might be explained using this model, because the 3.4 μm feature is superposed on a reasonably strong thermal continuum background. The spectrum obtained in May is inconsistent with this picture, however, because relative to the feature the thermal background is greatly decreased. It might be possible that the grain size distribution drastically changed between the two observations, and that the emission bands and the thermal radiation are not due to the same class of dust particles. However, the high f-value that is required to explain the emission feature flux in May makes this explanation unlikely.

There remains the possibility of UV-excited infrared fluorescence from large molecules (or very small grains). This subject has been discussed extensively in recent literature in connection with the possibility of infrared emission from large polycyclic aromatic hydrocarbon molecules (e.g., Leger and Puget 1984; Allamandola, Tielens, and Barker 1985). At ultraviolet wavelengths high f-values (approaching unity) are quite common for large organic molecules. For comparison, the f-value for the strong OH resonance line at 308.5 nm in cometary spectra is only 0.001. For $f = 1$, each molecule would emit 0.1–1 infrared photons per second at $R = 1$ a.u. Assuming a scale length much larger than the radius sampled by our aperture $[f(x) = 1]$, then, for $g = 0.1$ (at $R = 1.56$ a.u.) an abundance of only $\sim 0.15\%$ relative to the observed H_2O abundance in comet Halley would be required for the unknown molecule(s) to account for the observed flux in the 3.4 μm feature in our spectra. Thus, although the specific molecules are not identified, infrared fluorescence appears to be the most viable means of producing the 3.4 μm emission feature. Complex organic molecules, especially those with conjugated bands, will also fluorescence efficiently in the visible, probably forming a weak and broad quasi-continuum. This process might at least in part be the cause of the continuum in comets appearing redder than the solar spectrum (A'Hearn 1982).

IV. CONCLUSION

Spectroscopy of comet Halley in the 3–5 μm interval indicates that its 3.4 μm emission band is due to ultraviolet-pumped infrared fluorescence of complex hydrocarbons which are either free-floating or occur in very small grains. It appears likely that the 7.5 μm emission feature observed by *Vega I* was produced by the same mechanism. These complex molecules probably were sputtered or evaporated off the cometary grains. Therefore, it is likely that in these emission features we are seeing the fingerprints of the cosmic dust from which the comet was formed, a large fraction (by mass) of which, according to the grain model of Greenberg (1982), should consist of nonvolatile organic compounds.

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