

INFRARED MOLECULAR ABSORPTION FEATURES

S.P. Willner and R.C. Puetter
University of California, San Diego

Ray W. Russell
Cornell University

B.T. Soifer
California Institute of Technology

Spectra of infrared sources associated with molecular clouds have shown absorption features at wavelengths of 6.0 and 6.8 μm . We suggest that the 6.0 μm feature can be identified with the stretching vibration of C=O and the 6.8 μm feature with the bending vibrations of CH₂ and CH₃. The amount of carbon in the form of hydrocarbon molecules may be comparable to the amount in CO. This abundance of hydrocarbons is probably too large to be consistent with radio observations if the molecules are gaseous, but large abundances of hydrocarbons on the surfaces of grains may explain the infrared features, yet be unobservable in the radio.

OBSERVATIONS

Infrared sources associated with molecular clouds include compact HII regions and sources with much smaller or nonexistent thermal radio emission, often called "protostars". Spectra (typically with resolution $\lambda/\Delta\lambda \approx 60$) in the ground-based 2-4 μm and 8-13 μm windows of many examples of both classes of objects are available in the literature. The 8-13 μm spectra show evidence of silicate dust grains. The silicate feature is seen in emission in the Orion Trapezium, but most objects exhibit various amounts of silicate absorption, believed due to extensive overlying cold dust. In the 2-4 μm spectrum there is often an absorption feature having maximum depth at 3.1 μm ; this feature is usually attributed to water ice. The shape of the feature is, however, not entirely consistent with water ice absorption, in that there is significant optical depth between 3.3 and 3.5 μm (Merrill et al. 1976). Neither water nor ammonia ices would be expected to absorb sufficiently at these wavelengths to explain the observed shape of the feature. There is no correlation between the ice and silicate optical depths, except that if ice absorption is present, there is also finite silicate absorption present.

The Kuiper Airborne Observatory has recently made possible observations in the 4.5 to 8 μm spectral region. A total of 11 sources obscured by molecular cloud material have now been observed spectroscopically at these wavelengths (Russell et al. 1977, Puetter et al. 1979, Soifer et al. 1979, Puetter et al. 1980). All have depressions in the spectrum between 6 and 7 μm , and in most cases it can clearly be seen that there are two dips, centered near 6.0 and 6.8 μm . By far the strongest features were observed in the source W33A (Soifer et al. 1979), which also has the strongest silicate and 3.1 μm absorptions known (Capps et al. 1978). The spectrum of this source is shown in Figure 1. The 6.0 and 6.8 μm features are spectrally resolved and have

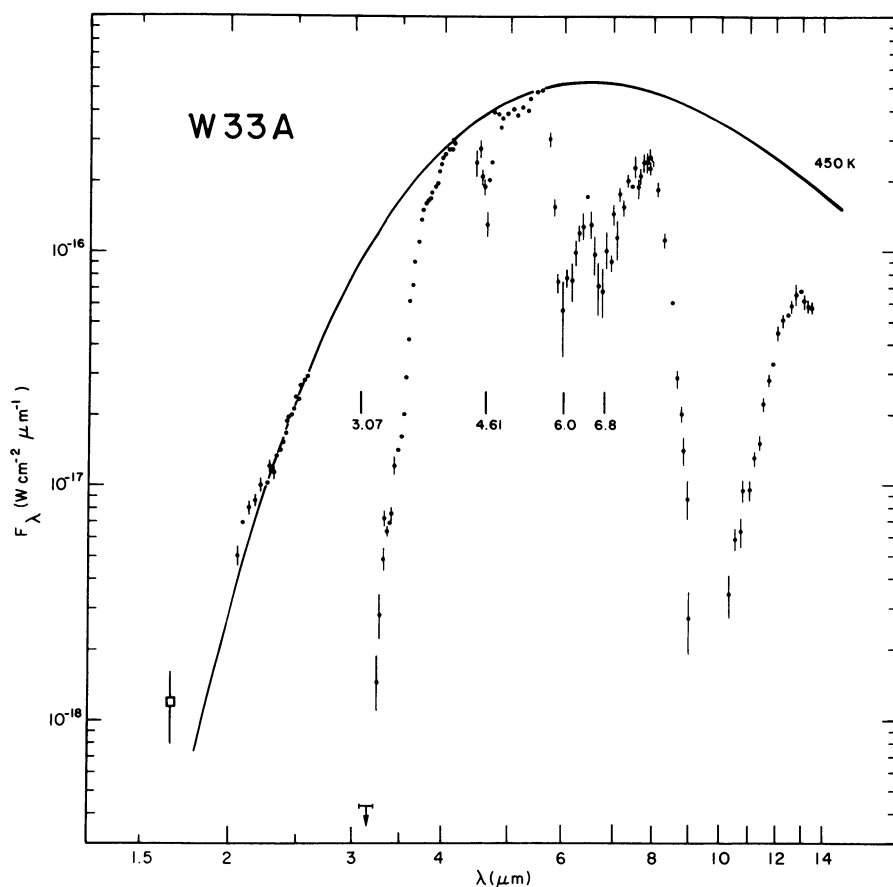


Fig. 1. The 2 to 13 μm spectrum of W33A. The 1.6–4 and 8–13 μm data are from Capps et al. (1978), and the 4–8 μm data are from Soifer et al. (1979). Error bars are shown when the statistical uncertainty exceeds 5%. The solid line represents the spectrum of a 450 K blackbody. Central wavelengths of 4 absorption features are marked.

widths of about 0.6 and 0.7 μm , respectively. The widths and positions of similar features are less easily determined in the spectra of other sources, but they are consistent with those in W33A. Table 1 gives the approximate peak optical depths of the features measured in 11 sources; the observations will be reported in more detail elsewhere. These numbers are, of course, strongly dependent on the choice of continuum level, which has generally been chosen as a blackbody fit through the spectrum at 4.5–5.5 μm and at 8.0 μm .

TABLE 1
PEAK ABSORPTION OPTICAL DEPTHS

Object	6.0 μm	6.8 μm
Becklin-Neugebauer	0.3	0.3
Sharpless 255	0.2	0.2
AFGL 989	0.3	0.4
W33A	1.9	1.5
AFGL 2136	0.3	0.3
AFGL 2591	0.2	0.2
AFGL 2884	0.5	0.3
NGC7538/IRS1	0.5	0.4
NGC7538/IRS9	0.6	0.4
W51/IRS2	0.5	0.5
K3-50	0.3	0.3

The 6.0 and 6.8 μm features were not seen in the line of sight to the galactic center (Willner et al. 1979). The features must therefore be characteristic of material in molecular clouds, rather than low-density interstellar material. The strengths of the features are not correlated with the strength of the silicate absorption and are only weakly correlated with the strength of the ice absorption.

DISCUSSION

It was first proposed that the 6.0 and 6.8 μm features were characteristic of hydrated or otherwise processed silicate minerals. Such features have been seen between 6 and 7 μm in the laboratory (Duley and McCullough 1977, Stephens and Russell 1979, Day 1978), although not at the exact wavelengths of the astronomical features. However, the features have not been seen to be as deep relative to the 10 μm band as in W33A. Moreover, the water of hydration band in silicates is usually at 6.1–6.2 μm rather than 6.0 μm and is only about half as wide as the astronomical absorption bands (Stephens and Russell 1979, Day 1978). Finally, the low temperatures of molecular clouds would seem more con-

ducive to the formation of ice mantles than hydrated grains, whereas in the envelope of an OH-IR star, where hydrated grains might be expected, no 6.0 or 6.8 μm features were found (Forrest et al. 1978). These arguments suggest that silicates are unlikely to be responsible for the 6.0 and 6.8 μm features.

Hydrocarbon bonds presently appear to be the most likely candidates for explaining the 6.0 and 6.8 μm features. The 6.0 μm band would be identified with the stretching vibration of the carbonyl group (C=O) with possibly some contribution from the stretch vibration of the C=C group. The 6.8 μm band would be identified with the scissors vibration in the methyl (CH_3) or methylene (CH_2) group. It is doubtful that any single molecule would be responsible for the observed absorptions, but rather, a large variety of molecules containing these groups would contribute to the observed bands. This is consistent with the broad absorptions that are observed, with the characteristic signatures of the functional groups in specific molecules being lost.

The column densities of the appropriate absorbers can be crudely estimated using observed equivalent widths and laboratory integrated band intensities (Puetter et al. 1979, Wexler 1967). These column densities, compared either to silicate or to radio CO column densities, generally indicate an amount of carbon comparable to but less than that in the form of CO.

The stretching vibration of the C-H bond is centered at 3.1-3.4 μm , depending on the specific group involved. The absorption is expected to be somewhat greater than that of the 6.8 μm band, and it could even be strong enough to explain all of the observed absorption between 2.9 and 3.5 μm . It is possible that some of the absorption is actually due to ice, but a major portion must be due to hydrocarbons. There will probably be no difficulty explaining the observed shape of the absorption with an appropriate mixture of molecules, either with or without ice.

Radio observations have shown the presence of quite complex hydrocarbons in molecular clouds (e.g., Kroto et al. 1978, Winnewisser and Walmsley 1978), but the derived abundance of known hydrocarbons is considerably smaller than that indicated here (Allen and Robinson 1977 and references therein). The lack of radio detection of such large abundances of hydrocarbons could be explained if most of the molecules are coated onto grains, where the lack of freedom to rotate would prevent radio emission. Such a situation would not be surprising at the low temperatures characteristic of molecular clouds (Watson and Salpeter 1972).

If large abundances of hydrocarbons in molecular clouds can be confirmed, it will probably require that their formation rates be higher than presently believed. Most of the available calculations include only gas-phase reactions, but for a full understanding of molecular clouds, it may be necessary to consider the far more complex subject of surface reactions.

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DISCUSSION FOLLOWING WILLNER

Thaddeus: It does not seem to me that you are talking about an unreasonable amount of carbon in C=O bonds. We only see a fraction of the total carbon in molecules like CO, and the rest has to be somewhere.

Willner: Yes. There must be a family of molecules with C=O bonds because the spectral features are resolved even with our low resolution, and no one particular molecule would make features as broad as that. If ~10% of the carbon is in the form of CO, another 10% in the form of hydrocarbons would be more than enough to account for the observations. The implied abundance is, however, much higher than suggested for individual hydrocarbons in the radio.

Greenberg: Earlier the point was made that there is as much oxygen

in H₂O as in CO, as if this were an awful lot of H₂O. I figured out that this would mean that at most 10% of all the oxygen is in H₂O. If what you say is true about CO relative to H₂O, then there is a further reduction by a factor of 4, so there is not such a large amount of H₂O compared to what we find in dust.

Willner: The data show considerable scatter, but the 3.1 μm absorption is roughly 10 times as strong as the 6.0 μm absorption. If the absorption efficiency per bond for OH stretch is as great as for C=O stretch, half as much oxygen in OH bonds as in CO would account for the 3.1 μm feature. If I have interpreted them correctly, Hagen's data suggest that OH stretch is a more efficient absorber than C=O, so an even smaller number of OH bonds would suffice.

Allamandola: I will take the bait early. What are your reasons for attributing the 6.0 μm feature to hydrocarbons and not, say, water of hydration or the H-O-H bend or H-N-H bend in the classic dirty ice? This vibration shifts considerably from its uncomplexed position at 1600 cm⁻¹ toward 1700 cm⁻¹ (6.0-6.2 μm), and undergoes substantial broadening when it complexes.

Willner: We are not aware of the possible shift in wavelength or the suppression of the 11.3 μm ice feature. There are a few sources, such as OH 0739-14, where the 3.1 μm absorption has returned to the continuum level by 3.3 μm, and the 11.3 μm absorption is present, and we felt that these characteristics indicated the presence of ice. Most sources do not look like this, and it seemed natural to suggest something other than ice. Also, the 3.1, 6.0, and 6.8 μm features occur together, and would probably be the strongest absorptions for hydrocarbon molecules.