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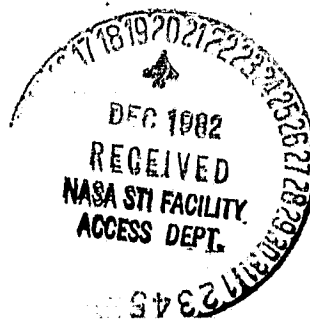
Molecular Emission Bands in the Ultraviolet Spectrum of
the Red Rectangle Star HD 44179

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ABSTRACT

New observations of the ultraviolet spectrum of HD 44179 are reported. Absorption due to the CO molecule is present in the spectrum with $N_{\text{CO}} \sim 10^{18} \text{ cm}^{-2}$. Emission due to either CO or a molecule containing $\text{C}\equiv\text{C}$, $\text{C}\equiv\text{N}$, $\text{C}-\text{C}$, and $\text{C}-\text{H}$ bonds (or both) is also present.

Key Words: ultraviolet: spectra - interstellar: molecules - nebulae:
individual - interstellar: matter

I. INTRODUCTION

Ever since its recent discovery by Cohen et al. (1975) the Red Rectangle and its associated central star HD 44179 have presented to astronomers a bewildering variety of spectroscopic properties. It is a strong source of infrared radiation and exhibits the emission bands at $3.3\mu\text{m}$, $6.2\mu\text{m}$, $7.7\mu\text{m}$, $8.6\mu\text{m}$, and $11.3\mu\text{m}$ (Russell, Soifer and Willner 1978, and sources therein) that are seen in a wide variety of astronomical objects (see Aitken 1981, for a brief review). In the visible the nebula has a very broad ($\sim 2000 \text{ \AA}$ wide) emission hump centered near 6500 \AA (Cohen et al. 1975), upon which are superimposed narrower emission features which Schmidt, Cohen, and Margon (1980) suggested might be due to molecules. Ultraviolet spectra obtained with the International Ultraviolet Explorer (IUE) satellite show a series of peculiar emission and absorption features unlike those seen in any other object (Sitko, Savage and Meade 1981, hereafter called SSM). To date HD 44179 is the only IR-band-emitting object known to possess these additional peculiar emission bands at shorter wavelengths. In addition, there is yet no positive identification of any of these features with a specific candidate. The origin of all of these features may be related, however.

Allamandola, Greenberg and Norman (1979) discuss the possibility of fluorescence emission in simple molecules as the source of the IR bands. Dwek et al. (1980), however, show that the necessary fluorescence efficiency might be too high, and that small heated grains, coated with some band-emitting material, would be efficient sources of the necessary IR flux. In particular, since the $3.3\mu\text{m}$ and $7.7\mu\text{m}$ bands are roughly coincident with the stretching and bending modes of C-H and H-C-H respectively, they suggested that the IR features may be caused by various atoms bonded onto chemically active sites on carbon-rich (perhaps graphite) grains. Another

possibility was suggested by Webster (1980) who pointed out that carbyne chains (...-C≡C-C≡C-...) might be at least partly responsible for some of these features. One of the strongest arguments against the presence of carbyne and carbyne-like chains in dust grains has been the high temperature (2600 K) necessary for direct condensation out of a carbon-rich gas (Whittaker 1978). However, Hayatsu et al. (1980) have shown that surface catalysis of CO with chromite yields CO₂ and solid carbon at temperatures as low as 600 K. There is also evidence that much of the carbon in carbonaceous chondritic meteorites is the form of carbyne chains (rather than graphite) and cyanoacetylenes (Whittaker et al. 1980, Hayatsu 1980), although the matter is still controversial [other investigators found only 2% of the carbon in the form of carbynes in their sample of one of the same meteorites (Smith and Busek 1981)].

Recently, moderate resolution spectra have been obtained of the 7.7μm band (Russell et al. 1982) and of the red hump and its accompanying narrower features (Warren-Smith, Scarrott, and Murdin 1981). The IR spectrum showed that the 7.7μm band was not resolved into a band of narrow lines at $\frac{\lambda}{\Delta\lambda} \sim 800$ and Russell et al. suggested that the feature was probably not due to free molecules. The optical spectrum, at a resolution of $\frac{\lambda}{\Delta\lambda} \sim 6000$, show two distinct types of bands superimposed on the broad hump. One is a series of broad, diffuse, and roughly symmetric features. The other is a series of narrower emission features which are degraded to the red and resemble R-type molecular bands. In particular, Warren-Smith, Scarrott and Murdin noted that the pair of lines at λ5799 and λ6615 and the pair at λ5880 and λ6109 are separated by energies of 2127 cm⁻¹ and 638 cm⁻¹, respectively, and that these two energies corresponded to the vibration spectrum of dicyanoacetylene, one of a number of organic cations measured in the laboratory by Maier (1980). The linear carbon-chain structure of these cations is just that of a carbyne

chain with assorted other atoms or radicals at each end. It should be noted that even at the high resolution used by Warren-Smith, Scarrott and Murdin the R-type bands did not resolve into finer sets of lines.

In order to further constrain the available possibilities, HD 44179 was re-observed in the UV using the IUE satellite, and the earlier UV spectra were re-examined with the results of these recent investigations in mind.

II. OBSERVATIONS

HD 44179 was observed in the low-resolution mode of the IUE using both long and short wavelength cameras. These spectral images and those obtained earlier by SSM are tabulated in Table 1. Two new short-wavelength images, each exposed for 6 hours during low-radiation observing shifts, were obtained in order to further investigate the flux decline near 1600 Å first observed by SSM. The new short-wavelength spectra are shown in Figure 1.

III. DISCUSSION

As can be seen in Figure 1, the UV spectrum of HD 44179 is rich in strong emission and absorption features. The probable sources of these two sets of features, and their relationship, are discussed below.

A. The Absorption Bands

Below 1600 Å the UV flux of HD 44179 drops rapidly and is affected by a series of very strong absorption bands. If a wavelength shift of about +4 Å (+ 800 km/sec) is assumed, 5 strong features in the spectrum correspond to the $X^1\Sigma^+ \rightarrow A^1\Pi$ transitions of CO. Figure 2 shows this region in more detail. At least 4 more members of the vibration spectrum may also be present

as indicated in Figure 2. The strengths of the (0,0) and (1,0) lines indicate $N_{\text{CO}} \approx 10^{18} \text{ cm}^{-2}$. Using the tabulation of CO band heads in the UV of Wallace (1962) as a guide, the region below $\lambda \sim 1400 \text{ \AA}$ might be blanketed by the vibration spectrum of the $X^1 \Sigma^+ \rightarrow A^1 \Pi$ electronic transition of CO. These transitions from the ground state of CO alone may be sufficient to explain most of the sharp drop in flux below $\sim 1600 \text{ \AA}$ first noted by SSM. The spectrum in this region is very noisy, however, and other sources of absorption cannot be excluded. For example, CO_2 has an observed UV spectrum that consists of a series of broad continuous bands with diffuse narrower bands superimposed (Inn, Watanabe and Zelikoff 1953). The first two broad bands are blended and absorb strongly between 1600 \AA and 1220 \AA . For an A0 star (Cohen *et al.* 1975), the observed flux would indicate $N_{\text{CO}_2} \sim 10^{18} \text{ cm}^{-2}$ also. Many carbon-chain molecules absorb strongly in this region as well (Price and Walsh 1954, Connors, Roebber and Weiss 1974). Until higher quality data become available (Space Telescope is really needed), CO remains the best candidate due to the positive identification of its stronger vibration terms. But CO alone cannot be the only absorber, as witnessed by the structure within the (2,0) band.

The source of the strong absorption feature at 1925 \AA is still unknown. If it is the $X^1 \Sigma^+ \rightarrow a^3 \Pi_r$ (2,0) transition of CO, then the (1,0) and (0,0) bands will be at $\sim 1992 \text{ \AA}$ and $\sim 2063 \text{ \AA}$, respectively. Only weak absorptions are present at these wavelengths in Figure 6 of SSM.

The absorption spectrum of HD 44179 appears to be dominated by bands of CO. Such strong CO bands are presently unknown in other stars of similar spectral type ($\sim \text{A0}$). Strong CO absorption is expected in some degenerate stars but even the carbon-rich C_2 white dwarfs L 97-3 and L 145-141 do not exhibit these bands (Weidemann, Koester and Vauclair 1980, 1981).

The unusual " $\lambda 4135$ " white dwarf Grw +70°8247 does show a strong flux decline at $\sim 1600 \text{ \AA}$ (Greenstein and Oke 1982) which could be due to highly broadened CO bands. If true the narrower lines in HD 44179 would indicate a lower atmospheric pressure and presumably lower surface gravity. Even if the star were unreddened, at a distance of $\sim 300 \text{ pc}$ (Cohen et al. 1975) the integrated flux between 1200 \AA and 2000 \AA alone is $\sim 0.2 L_{\odot}$, much in excess of normal white dwarfs, and indicating a significantly larger radius.

If the CO absorption is not stellar, but circumstellar in origin, then the breadth of the bands indicates either large (1000 km/sec) turbulent velocities or a large velocity gradient in a nearby gas flow. Such an interpretation may be supported by the emission band spectrum described below. HD 44179 is very unusual in that the column density of CO is very much in excess of what would be expected by its apparent reddening of $E(B-V) \sim 0.5 \text{ mag}$ (SSM, Figure 7). The star $\zeta \text{ Oph}$ with $E(B-V) = 0.32 \text{ mag}$ has $N_{\text{CO}} < 10^{16} \text{ cm}^{-2}$ (Morton 1975). Thus the abundance of CO implies peculiar dust characteristics or a large gas to dust ratio, compared to the average interstellar line of sight. Geometry alone cannot explain the data for a "normal" mixture of gas and dust.

B. The Emission Bands

With the possible exception of the $\lambda 1655$ feature, which could arise partly from the UV2 multiplet of CI, none of the emission features in the UV spectrum of HD 44179 could be confidently identified with plausible atomic transitions and SSM suggested a molecular origin for these bands. Because of the possible existence of long carbon-chain molecules in the surrounding nebula (Warren-Smith, Scarrott and Murdin 1981) and because molecules as complex as HC_{11}N have been observed in circumstellar shells (Bell et al. 1982), a comparison of the strengths and wavelengths of the emission bands in HD 44179 was made with the UV absorption features of cyanogen (C_2N_2), cyanoacetylene (HC_3N), dicyanoacetylene (C_4N_2), and dicyanodiacetylene (C_6N_2) measured in the

laboratory by Connors, Roebber and Weiss (1974). No convincing correspondences with the strengths and wavelengths in the electronic-vibration absorption spectra of these molecules was found. However, a strong resemblance between the energy spacings of these lines and those expected from $C\equiv C$, $C\equiv N$, $C-C$, and $C-H$ stretching vibrational energies of carbon-chain molecules with alternating single and triple bonds does exist. The resemblance is summarized in Figure 1 and Table 2. The $C\equiv C/C\equiv N$ and $C-C$ modes at $\sim 2100\text{ cm}^{-1}$ and $\sim 600\text{ cm}^{-1}$ are the same ones suggested by Warren-Smith, Scarrott and Murdin (1981) as the source of some of the optical emission bands in the nebula. The observed emission spectrum is consistent with the bands originating primarily from electronic transitions from the ground vibrational level of an excited electronic state to various vibrational levels of a lower (ground?) electronic state. If the strongest band ($\lambda 1655$) is the (0,0) transition then the vibrational structure of the upper electronic state is not readily visible, except perhaps for the feature at 1600 \AA (whose structure differs from the other lines). Part of this may be due to the large amount of absorption present at shorter wavelengths, but such an interpretation may not be required, since similar behavior is seen in the molecular emission of other objects. The (1,0) emission band of OH is many times weaker than the (0,0) band in the UV spectrum of Comet Bradfield, for example (A'Hearn et al. 1981). In GL 2688, a bipolar nebula which may be similar to the Red Rectangle, the (0,0) and (0,1) transitions of C_2 are present in emission, but (1,0) and (1,1) not detected (Zuckerman et al. 1976, Crampton, Cowley and Humphreys 1975). In both objects the primary source of the emission is fluorescence (A'Hearn et al. 1981, Cohen and Kuhl 1980). On the other hand, the $\lambda 1600$ feature might be a self-absorbed (0,0) band. A wavelength of 1600 \AA is close to the $(0,0)\ ^1\Sigma_u^{+a} \leftrightarrow ^1\Sigma_g^{+}$ band of C_4N_2 , with an f-value in excess of unity and an observed laboratory wavelength of $\lambda 1613\text{ \AA}$. The next two bands due to the vibration level of the upper state would lie inside the (0,0) and (2,0) bands of CO. Unless the observed wavelengths

of Connors, Roebber and Weiss are in error by as much as 500 cm^{-1} , a large ($\sim 2400 \text{ km s}^{-1}$) velocity shift is required. A column density of 10^{15} - 10^{16} cm^{-2} would also be required. If the $\lambda 1600 \text{ \AA}$ feature is the weak band of HC_3N observed by Connors, Roebber and Weiss, the strongest HC_3N absorption band would be at $\sim 1450 \text{ \AA}$, inside the (3,0) CO band.

The possible identification of the UV emission band structure as being due to either HC_3N or C_4N_2 is speculative. However, the coincidence of the UV emission bands and 4 optical emission bands with the vibration energy spacing of linear carbon-chain molecules suggests the presence of molecules with similar vibration structures around HD 44179, although a specific candidate is not available at this time.

Due to the universal character of Murphy's Law, however, another source of the emission lines is possible. Because the $\text{C}\equiv\text{O}$ vibration energy in the CO molecule is $\sim 2100 \text{ cm}^{-1}$, the UV emission bands could be largely due to this molecule. In particular, if an average shift of $\sim +3 - +4 \text{ \AA}$ ($+600 - +800 \text{ km s}^{-1}$) is assumed (i.e. the same as the absorption bands), then $\lambda\lambda 1655, 1670, 1714, 1733, 1753, 1780, 1800$ and 1816 correspond to the (0,2), (1,3), (0,3), (1,4), (2,5), (0,4), (1,5), and (2,6) $A^1\Pi \rightarrow X^1\Sigma^+$ transitions of CO (Figure 1). These transitions would naturally arise from radiative pumping of the $A^1\Pi$ state due to the absorptions from the ground state, observed at $\lambda < 1600 \text{ \AA}$. The $\lambda 1600$ feature might then be self-absorbed (0,1), and the absorption features just redward of the (1,0) and (2,0) band cores would be (2,1) and (3,1), indicating population of the first excited vibrational state of CO. The poorest-fitting line is the (1,5) line near 1800 \AA , but this may be affected by the nearby camera reseaux mark.

At the present time there is insufficient information to confidently distinguish between these alternatives. The lack of a good specific carbon-chain

molecule that reproduces the observed spectrum is a serious difficulty for the first explanation. Only a few such molecules have been studied in the UV, and one that gives a good match to the energy spacings (Maier 1980) and that has been observed in circumstellar shells (see Winnewisser and Walmsly 1979) is cyanodiacetylene (HC_5N). Such molecules would also explain the energy spacings of many of the optical emission bands. Such molecules would also be a natural by-product of carbon-chain production by catalytic conversion of CO, known to be present near HD 44179 (while the other product of the reaction, CO_2 , may be present as well).

On the other hand, CO as the source of the emission has the advantage that it is an identifiable molecule present in the system that can produce the UV emission lines by a specific process (radiation-induced fluorescence). Recently, it has also been observed in emission in the nebula in the $\Delta v = 2$ system near $2.3\mu\text{m}$ by Thronson (1982). But it does not adequately explain the observed optical bands. And while the existence of CO around HD 44179, in the light of both UV and infrared detections, is virtually certain, it cannot extend very far from the central source. The $J = 1-0$ ^{12}CO line was searched for over a 250 km s^{-1} region with the NRAO 11m telescope, with a resulting upper limit of $T_A < 0.1 \text{ K}$, implying column densities as low as 10^{13} cm^{-2} if it is optically thin (as in high-velocity bipolar flows) or 10^{17} cm^{-2} if it is optically thick, assuming the emission fills the beam (Blitz 1982). Either the large velocity dispersion of CO broadens the radio line beyond the bandwidth of the NRAO system, or the emission is confined to a very small solid angle, or both. An attempt will soon be made to detect the possibly broadened $J = 1-0$ line with a more suitable detector system.

C. Other Problems

In the above discussion no mention was made of three important properties of HD 44179 and its nebula: the source of the very broad optical hump seen in the nebular spectrum, the anomalous character of the broad 2200 Å absorption feature (SSM), and the source of the geometry of the nebula.

First, since molecular emission is present in the object, such emission is a likely candidate for the red hump. The bandwidth in cm^{-1} of the red hump is similar to that of the CO_2 UV absorption bands and might result from re-emission into or out of the excited state producing those bands [to date, only one such diffuse emission band has been observed, at ~ 4200 Å, (Dixon 1963)]. Furthermore, the observed energy absorbed from 1100 Å-1600 Å is $\sim 3 \cdot 10^{-18} \text{ W cm}^{-2}$ while the data of Cohen et al. (1975) indicate that the integrated flux across the red hump for the entire nebula is $\sim 2 \cdot 10^{-17} \text{ W cm}^{-2}$. If $A_V \sim 2$ for the star (Oke and Greenstein 1977) then $E_{\text{DUST}}(1600 \text{ Å}-6500 \text{ Å}) \sim 3.7 \text{ mag}$ for normal interstellar dust (Savage and Mathis 1979). Although the dust around HD 44179 is peculiar (see below), a value of $E_{\text{DUST}}(1600 \text{ Å}-6500 \text{ Å}) \gtrsim 2$ is probably reasonable. If $E_{\text{DUST}}(1600 \text{ Å}-6500 \text{ Å}) \gtrsim 2$, then the UV absorption at $\lambda < 1600 \text{ Å}$ is sufficient to power the red hump. Second, the shape of the mid-UV extinction ($\lambda \sim 2200 \text{ Å}$) seen in HD 44179 is broader than that seen in the general interstellar medium or in other hot stars with circumstellar dust (see SSM).

A collection of organic molecules with extinction maxima near 2200 Å (Hoyle and Wickramasinghe 1977, 1979) or predissociation or preionization bands of some yet unspecified molecule or group of molecules might be responsible. However grains composed of carbyne-like chains that have not attained temperatures necessary to transform them to graphite (Whittaker et al. 1980) are likely candidates (an extinction feature at $\sim 2200 \text{ Å}$ is present in the carbonaceous

material from the Murchison meteorite (Sakata et al. 1977) although the shape of this feature is somewhat different than that in HD 44179). This transformation may explain the lack of the $3.3\mu\text{m}$ band inside the Orion HII region when it is present at the HII region - molecular cloud boundary (Sellgren 1981). The presence of the IR band features at $T \geq 200\text{ K}$ (where it may be produced) and its absence much higher temperatures (where it is transformed to graphite) is consistent with this hypothesis. If so, there should be a correlation between the shape of the 2200 \AA extinction feature and the presence of the IR bands along any given line of sight.

Finally, the strong geometrical properties of the nebula indicate a process that confines the nebular flow through some mechanical process. Geometries of this kind can naturally arise from flows originating in accretion disks (Davidson and McCray 1980, Icke 1981). The lack of lines arising from highly ionized atoms in the UV spectrum of HD 44179 and the lack of detectable X-ray emission (a limit of $\sim 10^{-13}\text{ erg cm}^{-2}\text{ s}^{-1}$, Pravdo 1982) indicate the lack of a large shock-heated region of the kind that is observed in many binary systems with mass flows.

IV. CONCLUSIONS

The UV spectrum of HD 44179 indicates substantial amounts of the molecule CO, with $N_{\text{CO}} \geq 10^{18}\text{ cm}^{-2}$. At least 5 and possibly as many as 9 absorption bands due to the $X^1\Sigma^+ \rightarrow A^1\Pi$ electronic transition of CO are present.

The origin of the many emission bands observed in the UV remains ambiguous. They might arise either from electronic transitions in an as yet unspecifiable linear carbon-chain molecule, from radiation-induced fluorescence of CO, or both. At the low resolution available with the IUE for such a faint object, the

(0,v''), (1,v''), and (2,v'') $A''\Pi \rightarrow X^1\Sigma^+$ transitions of CO effectively mimic the energy spacings of a combination of $C\equiv C$, $C\equiv N$, $C-C$, and $C-H$ bands. If the bands are due to a linear carbon-chain molecule it suggests that much of the dust in the nebula may be in the form of carbynes and that this may be the source of the anomalous mid-UV absorption feature. Carbynes might be produced through catalytic conversion of CO, known to be present in the system in substantial quantities. Another product of this reaction is CO_2 , which may also be present.

The source of the broad emission hump seen in optical spectra of the nebula remains a mystery, although diffuse emission similar to that observed at shorter wavelengths in the spectrum of CO_2 is possibly responsible.

The presence of substantial molecular emission and the lack of lines due to highly ionized species of atoms suggests the lack of a hot spot in any accretion disk that may govern the outflow geometry of the nebula.

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Table 1

Data for IUE Exposures of HD 44179¹

DATE (UT)	Image	Exposure Time (min)
1979 April 15	SWP 4944	180
	SWP 4945	60
	LWR 4273	70
	LWR 4274	25
1982 January 8	SWP 15990	360
January 10	SWP 16014	360
	SWP 16015	60
January 11	LWR 12323	30

¹All exposures are low resolution, large aperture

Table 2

Molecular Emission Features in the Ultraviolet Spectrum of HD 44179

Observed Wavelength (Å)	Energy (cm ⁻¹)	Observed Energy Differences (cm ⁻¹)	Line Origins	
			Carbon-Chain Molecule ²	¹ CO A Π → X ¹ Σ ⁺ [Predicted Wavelengths] ³
1655	60420	- 540	Zero Vibration, C≡C, C≡N	(0,2), ((3,4)) [1653, (1648)]
1670	59880	- 1180	C-C	(1,3) [1670]
1688	59240	- 2080	C-C?, C-H??	(2,4) [-1686]
1714	58340	- 640	C≡C, C≡N	(0,3), ((3,5)) [1712, (1705)]
1733	57700	- 1300	C-C	(1,4) [1729]
1753	57040	- 2160	C-C, C-H	(2,5) [1747]
1780	56180	- 620	C≡C, C≡N	(0,4) [1775]
1800	55560	- 1110	C-C	(1,5) [1792]
1816	55070		C-C, C-H	(2,6) [1811]

1. Estimated error $\pm 35 \text{ cm}^{-1}$ ($\Delta\lambda \sim 1 \text{ Å}$ at $\lambda \sim 1700 \text{ Å}$).

2. Using vibration spectra of Maier (1980).

3. From Wallace (1962) except for (2,4) which should occur at the wavelength shown.

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Figure Captions

Figure 1 The ultraviolet spectrum of HD 44179 from 1200 Å to 2000 Å. The images SWP 15990, SWP 16014, and SWP 16015 were combined to produce a single spectrum of high quality. Data dropouts indicate the presence of camera fiducial marks. The brackets above the spectrum indicate the predicted spacings of the $C\equiv C/C\equiv N$, C-C, and C-H vibration levels, using an average value of 2100 cm^{-1} , 600 cm^{-1} , and 3300 cm^{-1} , respectively. The notation below the spectrum indicates the predicted transitions of CO with a shift of approximately +4 Å. The resonance absorptions ($v',0$) of CO, which are seen in absorption, are indicated separate from the higher order (v',v'') terms.

Figure 2 The ultraviolet spectrum of HD 44179 from 1200 Å to 1600 Å. Log flux is plotted to enhance the low flux region of the spectrum at $\lambda < 1450\text{ Å}$. The transitions of CO are plotted using a shift of approximately +4 Å. Also shown are the predicted positions of the strongest transitions of C_2 and HC_3N with the same shift.

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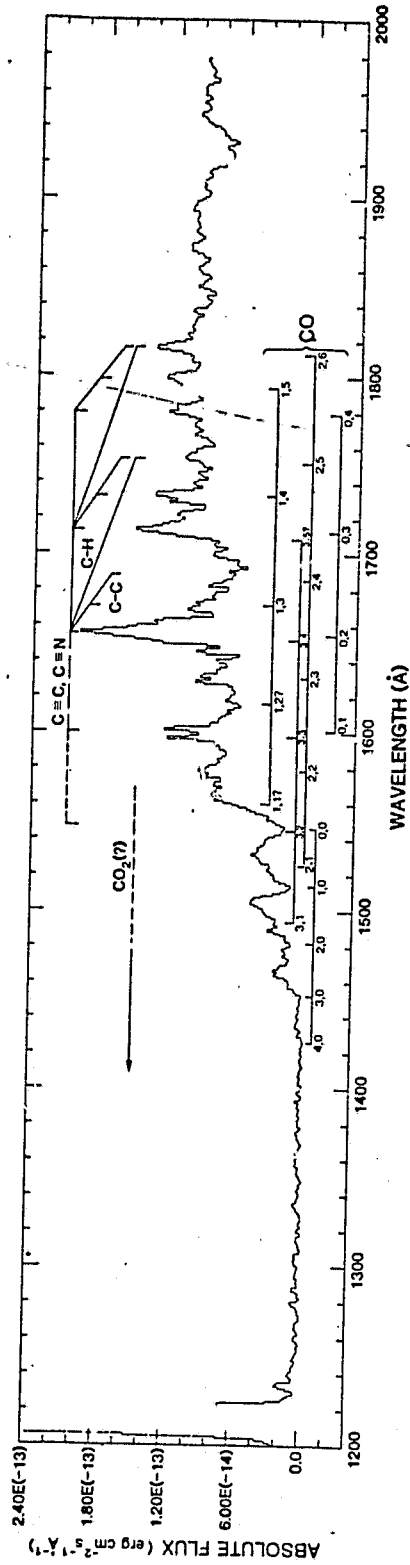


Fig 1

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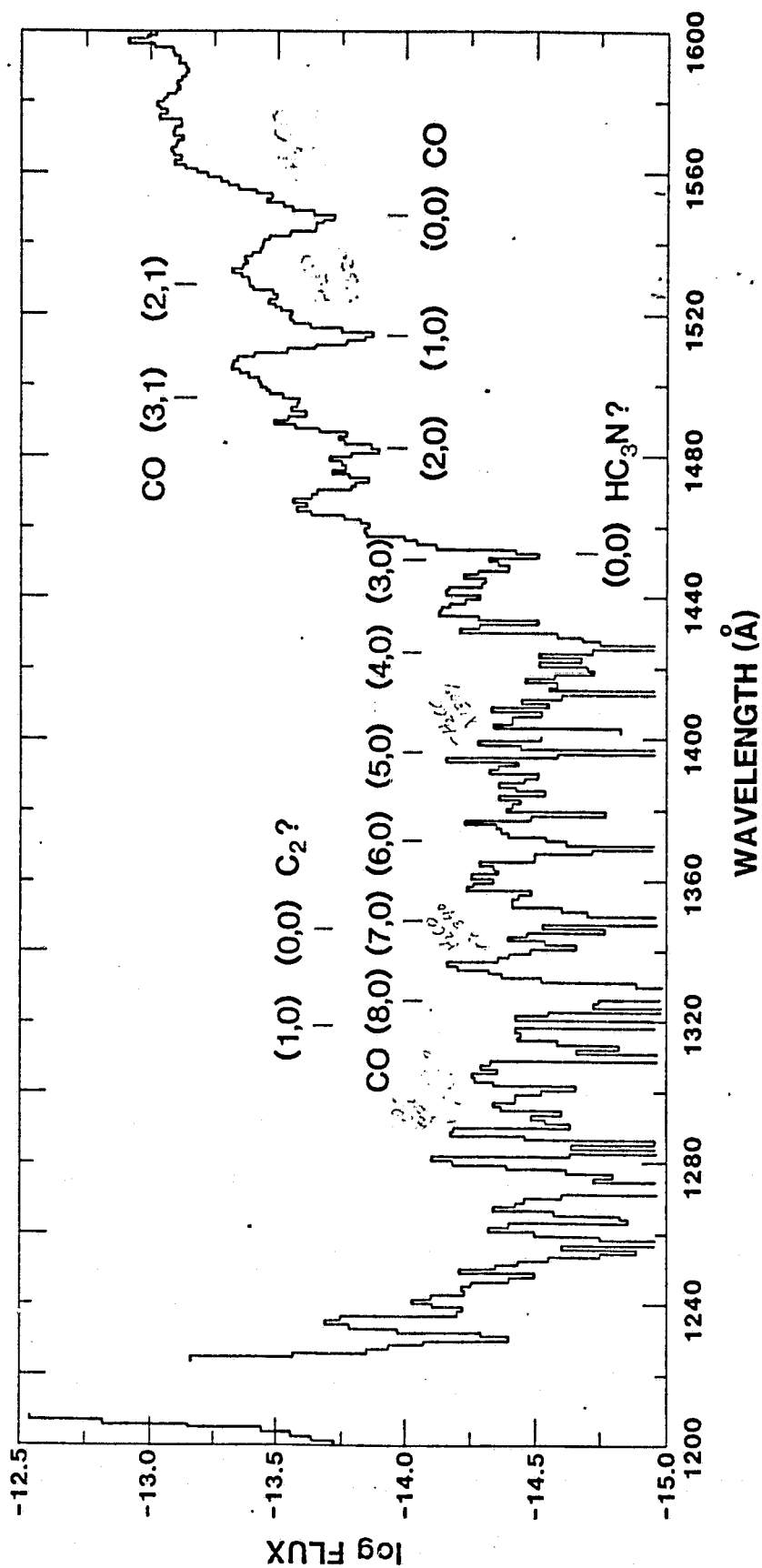


Fig 2