ARE CARBON CLUSTERS THE CAUSE OF INTERSTELLAR DIFFUSE BANDS?

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ABSTRACT: Theoretically determined vertical excitation energies of C_5 and C_7 molecules have been shown to agree with the strongest diffuse interstellar band at 4430Å. Several other weak diffuse bands can be identified with vibrational transitions, if 4430Å band is taken as 0-3 transition and vibrational constant have a value of $2190cm^{-1}$. The vertical excitation energy of a second electronic transition of C_7 molecule agrees with diffuse band at 6177Å. This electronic band system may account for diffuse bands at 5778Å, 6660Å and other bands near them.

1. INTRODUCTION

Since the discovery by Merril (1936), advancement in observations lead to the identification of a large number (about 50) of interstellar diffuse bands, a comprehensive study of which are given by Herbig (1975, 1988). The bands, however, still elude identification. Here we compare the wavelengths of theoretically determined vertical transitions of C_5 and C_7 molecules with the interstellar diffuse bands.

2. CALCULATION OF EXCITATION ENERGIES

The calculation was done in two steps. Firstly, geometrical information regarding equilibrium bond lengths was obtained in all-electron ab initio molecular orbital calculations using unrestricted self-consistent-field Hartree-Fock techniques and optimizing by means of Murtagh-Sargent algorithm (Murtagh and Sargent 1970). The excitation energies and oscillator strengths to low-lying electronic states from ground level were carried out in the second step by means of the semi-empirical HAM/3 (cf. Lindholm and Asbrink 1985) method using the sum of the kinetic energy, electron-electron potential energy, exchange energy and correlation energy as electronic energy. The transition energies and oscillator strengths for C_3, C_5 and C_7 are given in Table 1. For each transition energies of C_5 and C_7 two values

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– one for the determined geometry with different inner and outer bond lengths and the other for the assumed equal bond lengths – are given. The fare agreement between theoretical and experimental (2.992ev) transition energies for C_3 suggests that transition energies of C_5 and C_7 may be reasonably accurate. However, the same confidence cannot be put on the oscillator strengths which should, therefore, be used for relative comparison.

TABLE 1. Transition Energies and relative oscillator strengths of lowest transitions for C_3, C_5 and C_7. Two entries for C_5 and C_7 are for two different geometrics.

C_3		C_5		C_7	
Trans En(ev)	Rel Osc St	Trans En(ev)	Rel Osc St	Trans En(ev)	Rel Osc St
2.992	0.026	2.793-2.764	0.032-0.029	1.962-1.994	0.010-0.008
–	–	–	–	2.799-2.816	0.002-0.013
7.395	2.018	7.008-6.981	5.99-6.09	6.386-6.357	8.539-9.151
9.836	0.054	7.677-7563	0.051-0.003	6.720-6.678	2.231-1.001

3. COMPARISON OF THEORETICAL WAVELENGTHS WITH INTERSTELLAR DIFFUSE BANDS

Table 1 shows that both C_5 and C_7 have electronic transition near 2.8ev. The wavelengths corresponding to these transitions match well with strongest interstellar diffuse bands at 4428Å. Our calculation does now allow the determination of upper (v') and lower (v'') vibrational levels of transition nor the vibrational constants w'_e and $w'_e x'_e$. However, if we assume $v'' = 0, v' = 3, w'_e = 2190cm^{-1}$ and $w'_e x'_e = 15cm^{-1}$, we can determine the wavelengths for different vibrational transitions and compare them with the observed diffuse bands (Table 2). The observed band wavelengths are put in two columns - one column giving diffuse band wavelengths falling within the theoretical range defined by the geometry and the other outside the theoretical range. Table 2 shows that a large number of diffuse bands fall in the theoretical wavelength range for C_5 and C_7. The diffuse bands falling outside but near the theoretical range could arise from other vibrational mode of transition together with the vibrational modes given in the table and if the vibrational constants of the new mode are in the range of $300 - 500cm^{-1}$ Such values of w'_e are plausible (cf. Herzberg 1966). Besides the transition near 2.8ev, C_7 has a strong transition near 2.0 ev. The corresponding wavelength range overlaps a number of diffuse bands (Table 2). The wavelengths of theoretical vibrational transitions are determined assuming 2.0 ev transition to be 0-1 transition, $w'_e = 1170cm^{-1}$ and $w'_e x'_e = 25cm^{-1}$. Table 2 shows that almost all observed interstellar diffuse bands can arise from C_7 molecule. The observed strengths of 6177Å and 4428Å bands are also consistent with their relative theoretical oscillator strengths. Table 1 shows that C_5 has transitions in the range $1615 - 1639Å$ and $1769 - 1776Å$ and C_7 in the ranges $1941 - 1946Å$ and $1847 - 1851Å$ besides those discussed above. The IUE

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TABLE 2. Comparison of diffuse bands with transition wavelengths of C_5 and C_7 arising from transition near 2.8 ev and of C_7 from that near 2ev (2nd rows).

Vib trans $v'' - v'$	C_5-trans	C_7-trans	Observed diffuse bands	
			Within*	Outside*
0–3	4439-4485	4403-4429	4428	4501
0–2	4895-4952	4851-4883	4882	4726,4754,4763
0–2†		5789-5829	5778,5780,5797	5705,5844,5849
0–1	5465-5536	5410-5450	5420,5449,5487	5361,5404,5544
0–1†		6171-6217	6177,6195,6203	6314,6353,6362
0–0	6196-6287	6126-6178	6234,6264,6283	6010,6042,6113
0–0†		6621-6682	6613,6660,6666	6507,6742,6770

*Within and outside the theoretical range of wavelengths.
† From C_7 transition near 2.0ev.

spectra shows that there are no diffuse bands in above wavelength ranges. It is, however, possible, that these bands in UV have disappeared as a result of merger of upper electronic levels of these bands with the continuum in the event of C_5 and C_7 residing on a grain surface or in the form small solids. Note that the C_5 and C_7 molecules have to reside on a grain surface or in the small solid form for their survival in interstellar diffuse clouds.

4. REFERENCES

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