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Carbon chain abundance in the diffuse interstellar medium

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Abstract. Thanks to the mid-IR sensitivities of the ISO and IRTS orbiting spectrometers it is now possible to search the diffuse interstellar medium for heretofore inaccessible molecular emission. In view of the recent strong case for the presence of C_7^- (Kirkwood et al. 1998, Tulej et al. 1998), and the fact that carbon chains possess prominent infrared active modes in a very clean portion of the interstellar spectrum, we have analyzed the IRTS spectrum of the diffuse interstellar medium for the infrared signatures of these species. Theoretical and experimental infrared band frequencies and absolute intensities of many different carbon chain species are presented. These include cyanopolyynes, neutral and anionic linear carbon molecules, and neutral and ionized, even-numbered, hydrogenated carbon chains. We show that – as a family – these species have abundances in the diffuse ISM on the order of 10^{-10} with respect to hydrogen, values consistent with their abundances in dense molecular clouds. Assuming an average length of 10 C atoms per C-chain implies that roughly a millionth of the cosmically available carbon is in the form of carbon chains and that carbon chains can account for a few percent of the visible to near-IR diffuse interstellar band (DIB) total equivalent width (not DIB number).

Key words: molecular data – molecular processes – ISM: abundances – ISM: general – ISM: molecules – infrared: ISM: lines and bands

1. Introduction

In two recent, very important papers Maier and co-workers report the gas-phase spectrum of the $A^2\Pi_u \leftarrow X^2\Pi_g$ electronic transition of C_7^- and show that this matches the positions and relative intensities of 6 diffuse interstellar bands (DIBs) (Kirkwood et al. 1998; Tulej et al. 1998). These impressive, elegant, experimental results make a strong case for the presence of carbon chains in the diffuse interstellar medium. They also represent a fundamental breakthrough in this field as they, for the first time, allow the direct test of DIB candidates using the gas phase spectra of highly reactive, complex, transient species.

At the low densities of the interstellar medium, molecular-sized species which have absorbed visible (or ultraviolet) photons can only relax via emission of infrared radiation at their fundamental vibrational frequencies. This fact provides an unprecedented opportunity to conduct an independent evaluation of the nature and abundance of carbon chain species since prominent infrared transitions of essentially all members of this chemical family fall in the 2300 to 1700 cm^{-1} (4.35 to 5.88 μm) region, a portion of the interstellar spectrum that is largely free of other molecular features. This rests on the intrinsic property of all molecular families, be they C-chains, aromatics, aliphatics etc., that they have characteristic, fundamental vibrational frequencies which are unique diagnostics of that family and that fall in the same spectral region. Thus IR spectroscopy of the interstellar medium generally allows one to assess the abundance of entire chemical families rather than individual family members, and in some favorable cases, make specific molecular identifications. Accepting the UV/Visible evidence in support of carbon chain molecules in the diffuse interstellar medium (ISM), we attempt to constrain the abundance of this chemical family by quantifying their expected infrared emission using measured and calculated infrared band strengths.

During the past decade, great progress has been made in the infrared spectroscopic studies of carbon clusters in the gas-phase. In a series of pioneering experiments, Saykally and his co-workers reported the vibrational spectra of neutral C_3, C_5, and C_7 (Heath et al. 1989, 1990; Schmuttenmaer et al. 1990). Further, Freivogel et al. (1997) present new results on mass-selected carbon chains in their neutral and anionic forms as well as compile previous work on the infrared spectroscopy of carbon clusters trapped in rare-gas matrices. This recent activity on carbon chains furthers the extensive matrix isolation studies of carbon chains and clusters pioneered at the University of Florida by W. Weltner and R. van Zee and their colleagues and most recently extended by Vala and his colleagues (Szczepanski et al. 1997a,b; 1998). All of this and important related work on carbon chains has been reviewed by van Orden & Saykally (1998). Furthermore, recent advances in computational methods have now made it possible to accurately determine harmonic frequencies and absolute infrared band intensities for these and other closely-related members of this chemical family in both their neutral and charged forms. This body of data, together with

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Send offprint requests to: L.J. Allamandola (lallamandola@mail.arc.nasa.gov) the mid-infrared spectra of the interstellar medium now available thanks to the ISO and IRTS spacecraft, makes it possible to search for these species as a class in the diffuse interstellar medium. Thus, for the first time, it is possible to concurrently observe both the pumping and relaxation channels of the interstellar UV-to-IR electromagnetic molecular energy conversion process. Moreover, knowledge of the infrared band strengths of these carbon chain species allows one to place strong limits on the column densities of these species in the diffuse ISM.

In this paper we summarize the previous spectroscopic studies as well as present new calculations on closely related carbon chain species and identify their characteristic IR signatures. Upper limits are then placed on the interstellar column densities of various carbon chain families by comparing their IR signatures with the spectrum of the diffuse interstellar medium. The theoretically calculated IR properties of the various species are summarized in Sect. 2 and astrophysical applications of both the theoretical and experimental spectra are presented in Sect. 3.

2. Theoretical calculations and the IR properties of carbon chains and related species

The geometries and harmonic frequencies for the carbon-chain species were computed using the B3LYP density functional (Becke 1993, Stephens et al. 1994) in conjunction with the 6-31G* basis (Frisch et al. 1984, and references therein). The B3LYP/6-31G* frequencies were scaled by the factor of 0.951. This factor resulted from a least squares fit of the 12 σ_u bands for C_3-C_{10} that fall in the frequency range between 1700 and 2200 cm^{-1}. This scale factor brings all of the theoretical frequencies to within 30 cm^{-1} of experiment. We should note that our theoretical approach is very similar to that employed by Szczepanski et al. (1997a,b), and thus their results are very similar to the values reported here for the smaller, odd-numbered cluster neutrals and anions.

Calibration calculations were carried out to assess the accuracy of the B3LYP/6-31G* intensities. We found that adding diffuse functions to the basis set (i.e. augmentation to 6-311+G*) had little affect on the intensities. However, augmenting the basis set with additional polarization functions (6-311+G(3df)) increased the σ_u intensity of C_3 from 718 to 876 km mol^{-1} (22%). We found a comparable percentage increase from basis set augmentation for the larger, odd-numbered, linear cluster neutrals that we examined up through C_{11}. However, while basis set saturation increases the intensity, higher levels of correlation apparently decrease it. We performed complete-active-space self-consistent-field (CASSCF) calculations on C_3 with the 2s and 2p electrons in the active space. In the 6-31G* basis, the CASSCF value was 556 km mol^{-1} compared to the B3LYP intensity of 718 km mol^{-1}, while in the larger 6-311+G(3df) basis the σ_u intensity was decreased from 876 to 674 km mol^{-1}. In both cases the decrease was about 23%. Thus the effects of basis set augmentation and improved treatments of non-dynamical correlation have opposite effects on the intensities. For such floppy molecules, anharmonic effects could have a large effect on the bending modes, but they should not significantly affect the intensities of the very strong σ_u C-C stretching modes. This leads to our contention that the B3LYP/6-31G* σ_u intensities reported in this work should be reliable.

Table 1. The most important infrared bands (intensity > 5 km mol^{-1}) of even numbered, neutral and anionic hydrogenated carbon chains, which fall in clear regions of the interstellar spectrum. These theoretical frequencies (in cm^{-1} and scaled by 0.951) and intensities (in km mol^{-1}) were obtained using the B3LYP functional and 6-31G* basis sets.

Neutral	Freq.	Int.	Anion	Freq.	Int.
HC_2^a	—	—	HC_2^-	1818	31
HC_4^a	—	—	HC_4^-	2091	436
HC_6^b	1813	213	HC_6^-	1895	204
	2014	57		2058	14
	2042	187		2140	1340
HC_8	1820	307	HC_8^-	1894	169
	1962	45		2017	956
	2019	135		2116	2370
	2097	475		2139	16
HC_{10}	1824	399	HC_{10}^-	1886	615
	1884	15		2008	82
	2005	345		2055	5561
	2084	652		2115	103
	2111	294		2156	89
HC_{12}	1802	164	HC_{12}^-	1881	793
	1835	368		1983	3940
	1993	194		2027	5365
	2061	1508		2078	14
	2086	417		2142	398
	2131	22			

[a] The theoretical results for these systems are unreliable due to symmetry breaking problems.

[b] HC_6 breaks symmetry for some basis sets and thus the results reported here may be less reliable than for other systems.

Table 1 lists the important (intensity > 5 km mol^{-1}) bands of even-numbered neutral (HC_n, n=6-12) and anionic (HC_n^-, n=2–12) hydrogenated carbon chains. The values for HC_2 and HC_4 are not reported due to symmetry breaking problems at the B3LYP/6-31G* level of treatment. A number of these bands in the clear region of the interstellar spectrum between 1800–2200 cm^{-1} are quite intense, especially for the longer carbon chains and the anions.

Table 2 lists the prominent hydrogenated cyanopolyyne ($HC_{2n+1}N$, n=0-5) bands between about 2100–2250 cm^{-1}. The intensities are comparable to those for the neutral hydrogenated carbon chains and an order of magnitude less than that for the comparable length anionic hydrogenated carbon chain species.

Tables 3 and 4 list the prominent vibrational frequencies for the linear carbon chain anions (C_n^-, n=4–19) and the linear carbon molecules (C_n, n= 3–13, 15), respectively, which fall in the astrophysically clear spectral region. The scaled theoretical frequencies for the linear carbon molecule vibrational bands are in excellent agreement with experiment, except for

Table 2. The prominent calculated cyanopolyyne bands and intensities in the clear region of the interstellar spectrum.

Neutral Species	B3LYP/6-31G* Frequency[a] (cm^{-1})	Intensity km mol^{-1}
HCN	2105	2
HC_3N	2268	29
HC_5N	2185	6
	2249	95
HC_7N	2138	9
	2177	145
	2236	71
HC_9N	2105	22
	2126	286
	2231	93
$HC_{11}N$	2071	372
	2086	109
	2181	13
	2227	137

[a] Scaled by 0.951.

Table 3. Theoretically predicted positions (cm^{-1}) and intensities (km mol^{-1}) of the prominent bands of linear carbon chain anions C_n^- (n=4–19) between 2100 cm^{-1} and 1700 cm^{-1} compared with available experimental data (n=5–10,12).

Species	Experimental[a] Frequency	Theory Frequency[b]	Theory Intensity
C_4^-		1695	87
	2047[c]	2007	0
C_5^-	1822.3	1809	856
C_6^-	1938.5	1938	727
C_7^-	1736.4	1744	2325
		1893	164
C_8^-	1796.0	1789	515
	2067.8[d]	2068	1560
C_9^-	1692.6	1726	4211
		1982	258
C_{10}^-	2094.5	1900	1621
		2095	2638
C_{11}^-		2053	1096
C_{12}^-	1819.3	1812	1138
	2012.6	2020	3454
		2089	2900
C_{13}^-		1942	623
		2080	2043
C_{14}^-		1875	2860
		2049	8751
		2092	91
C_{15}^-		1840	358
		2022	1706
		2081	2828
C_{16}^-		1819	2137
		1977	6837
		2027	6420
C_{17}^-		1909	1329
		2061	6400
		2076	107
C_{18}^-		1861	4943
		1983	14992
		2051	783
C_{19}^-		1831	878
		1983	3252
		2047	5968
		2095	1616

[a] Neon matrix-isolated values reported in Freivogel et al. (1997).
[b] The theoretical frequencies are scaled by 0.951.
[c] Matrix-induced infrared inactive mode.
[d] Neon matrix results at 12 K, Szczepanski et al. (1998).

the 1938.6 cm^{-1} band of C_{11} observed in a neon matrix and the 1808.96 cm^{-1} gas-phase vibrational band reported for C_{13}. There are several possible explanations for this disagreement: 1) The computational model has begun to fail for the larger chains; however the agreement between experiment and theory for C_{12}, suggests that this is unlikely. 2) The experimental spectra are not linear C_{11} and C_{13} as believed. Perhaps some of the more stable ring structures have formed, and/or some C_{13} has been produced in the C_{11} experiment and/or the spectrum of C_{13} is misassigned and it is actually C_{15}. Given the experimental evidence for the current assignment, this seems unlikely. 3) As suggested by Martin et al. (1996), there are Fermi resonances, such that the observed fundamentals differ from the computed harmonic frequencies.

3. Carbon chain abundances in the diffuse interstellar medium

Perusal of Tables 1 through 4 shows that strong transitions for most of the pure carbon chain molecules lie between about 2100 and 1700 cm^{-1} (4.76 and 5.88 μm) and that the strongest bands for the hydrogenated carbon chains and cyanopolyynes fall between 2300 and 2000 cm^{-1} (4.35 and 5.00 μm).

Fig. 1 shows the mid-infrared spectrum of the diffuse galactic light from 4.6 to 11.8 μm (2170 to 847 cm^{-1}) measured with the IRTS satellite (Onaka et al. 1996). Similar spectra, but covering a narrower range, have been measured by ISO (Mattila et al. 1996). Fig. 1 shows that there is indeed some weak substructure in the carbon-chain region, particularly at about 1890 and 1730 cm^{-1} (5.3 and 5.8 μm). While a weak, broad feature near 1890 cm^{-1} is expected within the framework of the PAH model (Allamandola et al. 1989a), for the purposes of this analysis it will be assumed that all of the emission in this spectral region originates from carbon chain carriers. In terms of flux, Fig. 1 shows that the substructure represents, at best, a few percent of the total IR emission from the well-known members of the IR emission band family at 6.2, 7.7, and 11.2 μm. These features, which reflect the fundamental vibrational frequencies of

Table 4. Astronomically accessible linear carbon molecule vibrational bands listed by Freivogel et al. (1997) compared to their theoretical counterparts and calculated intensities.

Species	Experiment	Theory			
		Present Work B3LYP/6-31G*		Kurtz and Adamowicz MBPT(2)/6-31G*	
	Frequency[a]	Frequency[b]	Intensity	Frequency[c]	Intensity
C_3	2040.02^{gp}	2058	718	2184	390
C_4	2032^{gp}	2027	0[d]	2150	0
C_5	2169.44^{gp}	2163	2387	2358	1243
C_6	1959.86^{gp}	1938	992	2009	1456
C_7	1898.38^{gp}	1894	1184	1962	464
	2138.32^{gp}	2138	4444	2405	2053
C_8	1707.4^{Ne}	1685	652	1786	562
	2067.8^{Ne}	2061	1881	2119	1478
C_9	2014.28^{gp}	2030	6085	2133	824
	2079.67^{gp}	2108	3984	2426	2628
C_{10}	1915.4^{Ne}	1900	1840		
	2074.5^{Ne}	2087	2721		
C_{11}^{e}	1853.4^{Ne}	1853	2161		
	1938.6^{Ne}	2022	14556		
C_{12}	2003.9^{Ne}	2009	4486		
		2079	2367		
C_{13}^{f}	1808.96^{gp}	1941	20562		
		1996	3050		
		2147	1522		
C_{15}		1831	6742		
		1902	26771		
		2060	579		
		2147	2670		

[a] The superscripts refer to the gas-phase and Ne matrix results, respectively.

[b] The frequencies are scaled by the factor of 0.951.

[c] The frequencies are unscaled by Kurtz & Adamowicz (1991).

[d] This is a symmetric mode that carries no intensity.

[e] The ring structure is more stable than the linear chain. The strong bands of the ring form lie at 1836 cm^{-1} (212 km mol^{-1}) and 1959 cm^{-1} (120 km/mol^{-1}).

[f] The ring structure is more stable than the linear chain. The strong bands of the ring form lie at 1852 cm^{-1} (122 km mol^{-1}), 1990 cm^{-1} (253 km mol^{-1}), and 1991 cm^{-1} (226 km mol^{-1}).

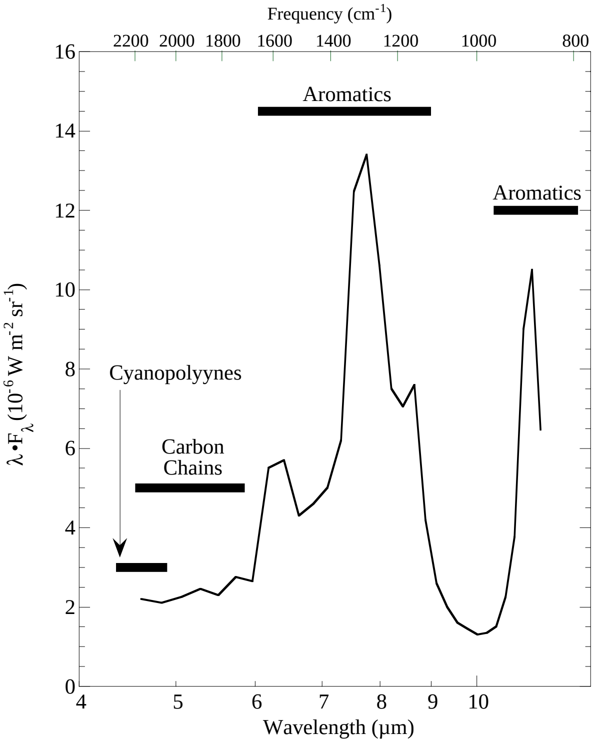

Fig. 1. Spectrum of the diffuse galactic radiation measured with the Mid-Infrared Spectrometer on the Infrared Telescope from Space (IRTS) adapted from Onaka et al. (1996). Galactic longitude approximately 50°, galactic latitude $-0°40' < b < 0°$. The infrared spectral regions diagnostic of the carbon bearing interstellar species including carbon chains and aromatics are also indicated.

their carriers, are generally attributed to the relaxation of highly vibrationally excited aromatic species (polycyclic aromatic hydrocarbons, PAHs) which have been pumped by the absorption of UV and visible interstellar radiation (e.g. Duley & Williams 1981, Allamandola et al. 1989b; Puget & Leger 1989; Allamandola et al. 1999). Sigma- and conjugated π-orbitals which are responsible for the UV/visible absorption in aromatic systems, are also intrinsic to unsaturated carbon chains such as those considered here. The smallest carbon chains are very strong absorbers in the ultraviolet, with the long-wavelength limit increasing well into the visible range as chain length increases (e.g. Silverstein & Bassler 1967; Forney et al. 1996, Forney et al. 1997). This behavior is very similar to that exhibited by PAHs and other aromatic systems (e.g. Salama et al. 1996). Given that the absolute infrared band intensities for these carbon chain species are at least comparable to, and often an order-of-magnitude larger than those of aromatics [several thousand km mol^{-1} versus several hundred km mol^{-1} for the PAH cation modes (Langhoff 1996) which produce the strongest features near 1600 and 1300 cm^{-1} (6.2 and 7.7 μm)], and that a similar UV-Vis vibrational pumping mechanism must hold for the carbon chains, one would conclude that the relative abundances of the carbon chain family to the canonical IR emission feature carriers is, at the very most, a few tenths of a percent.

Taking the specific case for C_7^-, for which there is now strong evidence supporting its assignment to several DIBs (Tulej et al. 1998), one would anticipate emission near 1736 cm^{-1} (5.78 μm), precisely where the interstellar spectrum shows a weak feature. However, the expected IR emission from carbon chain anions may represent a special case in UV-Vis excitation mechanism for the carbon chain family. In the anion case, electron photodetachment may be an important competing process. For C_7^-, electron detachment onset occurs near 370 nm (Forney et al. 1997). However, it has also been shown that there are transitions above and below the photodetachment threshold (Forney et al. 1997). Furthermore, neutral carbon chains have very high electron affinities, on the order of several eV. Thus, counterbalancing each photodetachment event, electron recombination will produce a product carbon chain anion in a highly vibrationally excited state. Thus, the overall analysis presented above for the UV-Vis pumping of highly vibrationally excited carbon chains, both ion and neutral, which leads to the conclusion that that the relative abundances of the entire carbon chain family to the canonical IR emission feature carriers is, at the very most, a few tenths of a percent, should apply to the anions as well.

This abundance is, indeed, qualitatively consistent with the relative abundances of these different species deduced in quite disparate interstellar regions using other techniques. Based on the IR emission feature intensities normalized to the total far IR emission, interstellar aromatic species are thought to have abundances of very roughly 10^{-7} with respect to hydrogen (Allamandola et al. 1989b; Puget & Leger 1989; Leger & Puget 1984; Allamandola et al. 1985). The interstellar carbon chains HC_7N, HC_9N, and $HC_{11}N$ have column densities of $330x10^{11}$, $19x10^{11}$ and $2.8\,x10^{11}$ cm^{-2}, respectively, in TMC-1 (Bell et al. 1997). These correspond to abundances with respect to hydrogen (Irvine et al. 1987) of $3.3x10^{-9}$, $2x10^{-10}$, and $2.8x10^{-11}$ respectively. Given the revised cosmic carbon abundance of 225 ppm with respect to hydrogen (Witt & Snow 1995) and assuming an average of 10 carbon atoms per carbon chain species, these results imply that on the order of one part in 10^6 (1 ppm) of the cosmically available carbon is tied up in interstellar carbon chains. For comparison, $\approx$10% of the cosmic carbon is in interstellar aromatics (Allamandola et al. 1989b; Puget & Leger 1989; Leger & Puget 1984; Allamandola et al. 1985).

This result also sheds some light on the relative abundances of DIB carriers. Under the optically thin conditions of the diffuse ISM, for materials such as the carbon chains and PAHs which both have conjugated π-electron systems and thus are expected to have comparable absorption cross sections and spectral properties in the ultraviolet and visible/near IR spectral regions, the fraction of UV/visible/near IR light absorbed is directly proportional to the relative concentrations. Thus, the conclusion that the carbon-chain family-as a whole-is on the order of a tenth of a percent as abundant as the aromatic hydrocarbons carries with it the direct implication that carbon chains can account for, at most, on the order of a few percent of the total integrated DIB absorption (not DIB number) even if the average PAH UV/visible cross section is an order of magnitude greater than that for the carbon-chain molecules.

4. Conclusions

Thanks to the mid-IR sensitivities of the IRTS and ISO orbiting spectrometers, coupled with the inherent advantage of IR spectroscopy as a uniquely suited probe of entire chemical families, it is now possible to search the diffuse interstellar medium for heretofore inaccessible molecular emission. The recent, excellent spectral match between several diffuse interstellar bands with the spectrum of C_7^- implies that carbon chains are present in the diffuse interstellar medium. Since carbon-chains possess prominent infrared active modes in a very clean portion of the interstellar spectrum, we have an unprecedented opportunity to search for the entire carbon-chain family and determine their abundance. In order to conduct this analysis, theoretical infrared band frequencies and absolute intensities of many different carbon chain species were calculated. The species considered include cyanopolyynes, neutral and anionic linear carbon molecules, and neutral and ionized, even-numbered, hydrogenated carbon chains. These theoretical results are compared to and combined with experimental data reported in the literature and used to analyze the IRTS spectrum of the diffuse interstellar medium. We show that – as a family – these species have abundances on the order of 10^{-10} with respect to hydrogen, values consistent with their abundances in dense molecular clouds. Assuming an average length of 10 C atoms per C-chain implies that roughly a millionth of the cosmically available carbon is in the form of carbon chains. This is to compare with the approximately 10% of the cosmic carbon tied up in the carriers of the prominent infrared emission features attributed to aromatic compounds (PAHs). This also implies that carbon chains can account for a few percent of the DIB total integrated absorption (not DIB number).

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References

Allamandola L.J., Tielens A.G.G.M., Barker J.R., 1985, ApJ 290, L 25
Allamandola L.J., Bregman J.D., Sandford S.A., et al., 1989a, ApJ 345, L59
Allamandola L.J., Tielens A.G.G.M., Barker J.R., 1989b, ApJS 71, 733
Allamandola L.J., Hudgins D.M., Sandford S.A., 1999, ApJ 511, L115
Becke A.D., 1993, J. Chem. Phys. 98, 5648
Bell M.B., Feldman P.A., Travers M.J., et al. 1997, ApJ 483, L61
Duley W.W., Williams D.A., 1981, MNRAS 196, 269
Forney D., Freivogel P., Grutter M., Maier J.P., 1996, J. Chem. Phys. 104, 4954
Forney D., Grutter M., Freivogel P., Maier J.P., 1997, J. Phys. Chem. A 101, 5292
Freivogel P., Grutter M., Forney D., Maier J.P., 1997, Chem. Phys. 216, 401
Frisch M.J., Pople J.A., Binkley J.S., 1984, Chem. Phys. 80, 3265
Heath J.R., Cooksey A.L., Gruebele M.H.W., Schmuttenmaer C.A., Saykally R.J., 1989, Science 244, 564
Heath J.R., Sheeks R.A., Cooksey A.L. Saykally R.J., 1990, Science 249, 895
Irvine W.M., Goldsmith P.F., Hjalmarson A.,1987, in Interstellar Processes, D.J. Hollenbach, H.A.Thronson, Jr. eds. (D. Reidel, Dordrecht) p. 561
Kirkwood D.A., Linnartz H., Grutter M.,et al., 1998, Faraday Discuss. 109, 109
Kurtz J., Adamowicz L., 1991, ApJ 370, 784
Langhoff S.R., 1996, J. Phys. Chem. 100, 2819

Leger A., Puget J.L., 1984, A&A 137, L5

Martin J.M.L., El-Yazal J., Francois J.-P., 1996, Chem. Phys. Lett. 252, 9

Mattila K., Lemke D., Haikala L. K., et al., 1996, A&A 315, L353

Onaka T., Yamamura I., Tanabe T., Roellig T.L., Yuen L., 1996, Publ. Astron. Soc. Japan 48, L59

Puget J.L., Leger A., 1989, ARA&A 27, 161

Salama F., Bakes E.L.O., Allamandola L.J., Tielens A.G.G.M., 1996, ApJ 458, 621

Schmuttenmaer C.A., Cohen R.C., Pugliano N., et al., 1990, Science 249, 897

Silverstein R. M., Bassler G. C. 1967, Spectrometric Identification of Organic Compounds, (Wiley and Sons, New York) p. 401

Stephens P.J., Devlin F.J., Chabalowski C.F., Frisch M.J., 1994, J. Phys. Chem. 98, 11623

Szczepanski J., Auerbach E., Vala M., 1997a, J. Phys. Chem. 101, 9296

Szczepanski J., Ekern S., Vala M., 1997b, J. Phys. Chem. 101, 1841

Szczepanski J., Hodyss R., Vala M., 1998, J. Phys. Chem. 102, 8300

Tulej M., Kirkwood D.A., Pachkov M., Maier J.P., 1998, ApJ 506, L69

Van Orden A., Saykally R.J., 1998, Chem. Rev. 97, 2313

Witt A.N., Snow T.P., 1995, Science 270, 1455