Infrared Emission From Interstellar PAHs, New Probes of the Interstellar Medium

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Tremendous strides have been made in the understanding of interstellar material over the past twenty years thanks to significant, parallel developments in two closely related areas: observational IR astronomy and laboratory astrophysics. Twenty years ago the composition of interstellar dust was largely unknown and the notion of abundant, gas phase, polycyclic aromatic hydrocarbons (PAHs) anywhere in the interstellar medium (ISM) considered impossible. Today the dust composition of the diffuse and dense ISM is reasonably well constrained and the spectroscopic case for interstellar PAHs, impossibly large molecules by early interstellar chemistry standards, is very strong. PAH spectral features are now being used as new probes of the ISM. PAH ionization states reflect the ionization balance of the medium while PAH size and structure reflect the energetic and chemical history of the medium. Aromatic carbon-rich materials ranging in size from PAHs and PAH nanoclusters, to sub-micron and micron-sized dust grains represent an important component of the ISM. These species: (1) dominate the heating and cooling of interstellar clouds via energetic photoelectron ejection and infrared (IR) emission; (2) moderate the ionization balance in photodissociation regions and molecular clouds; (3) moderate the composition of the gas phase and play an important role in determining the chemistry of the ISM; (4) contribute to the interstellar extinction in the near IR, visible, and UV spectral regions; and (5) convert UV, visible, and near-IR radiation to mid- and far-IR radiation in the ISM and, as such, are responsible for the well known, widespread family of mid-IR emission features with major components near 3.3, 6.2, 7.7, 8.6, and 11.3 μm.

Over the past two decades, PAH molecules have gained recognition as an important, ubiquitous component of interstellar dust (Duley and Williams 1981; Leger and Puget 1984; Allamandola, *et al.* 1985; Dwek *et al.* 1997; Draine and Li 2001, Li and Draine, 2001). Current estimates are that PAHs of 15-500 carbon atoms comprise 5 to 15% of all of carbon in the galaxy (Allamandola, *et al.* 1989; Dayal *et al.* 1998), implying that PAHs are more abundant than the other known interstellar, gaseous, polyatomic molecules. For comparison, the diaotmic CO comprises 10-20% of the elemental cosmic carbon. The proposed ubiquity and abundance of PAHs in the ISM explains their impact on so many interstellar processes. The fundamentals of the interstellar PAH model can be found in Allamandola *et al.* (1989) and Puget and Leger (1989). The power of the PAH model and the breadth and depth of the possible applications of combining laboratory data with astronomical observations and theory can be found in: Bakes *et al.* (2001a,b) and Pech, Joblin, Boissel (2002). Progress in the area of interstellar PAHs has been rapid in recent years. The launch of ISO in 1995 opened up the mid-IR window to systematic and coherent investigations of objects in the Solar neighborhood. These studies showed that the detailed profiles and relative strengths of the PAH emission features vary between sources, and these variations correlate with the characteristics of the astronomical sources. Clearly, the carriers are sensitive to the local physical conditions (Bakes *et al.* 2001a,b; Pech, Joblin, Boissel 2002). Extensive lab studies at NASA Ames and elsewhere (Piest *et al.* 1999a,b; and references therein), combined with quantum chemical calculations,

have pinpointed the origin of variations in the changing size, charge state, molecular structure, substitution, and clustering of the PAHs responsible. Table 1 lists the types of PAHs in the Ames IR spectral database.

There have been many comparisons between PAH spectra and the interstellar spectra over the years. As observational tools became more sensitive and lab techniques more appropriate to the interstellar case, the correlations have revealed more about PAH populations in different regions increasing insights into conditions in the emitting regions.

Figure 1 compares the spectrum produced by a mixture dominated by PAH cations and the 5-14 μm spectrum from the Orion ionization ridge. In objects with more benign radiation fields, neutral PAHs play a larger role (Allamandola et al. 1999). Analysis of the complete interstellar spectrum with laboratory and theoretical studies has shown that the 3.3 μm CH stretching band is dominated by neutral and negativley charged PAHs and the 6.2 and 7.7 μm CC stretching bands are dominated by PAH cations. Hence, the interstellar emission spectrum provides a measure of the degree of PAH ionization and this, in turn, is a measure of the flux, the exciting ionizing UV field, and the electron density (e.g., Hudgins and Allamandola, 1999b; Allamandola et al. 1999; Bakes et al. 2001 a,b; Draine and Li, 2001; Li and Draine, 2001).

Development of a database of astrophysically relevant data, spurred efforts to construct comprehensive astrophysical models (Bakes et al. 2001 a,b; Li and Draine 2001; Draine and Li, 2001). Initial applications of the the Bakes et al. and Draine and Li models have already demonstrated their effectiveness in addressing such characteristics of the emitting PAH population as charge state, size distribution, molecular structure, degree of hydrogenation, and UV-Vis-Near IR absorption properties. Bakes et al. (2001) investigated the spectral variations of a PAH population at the surface of the Orion photodissociation region (PDR) and have found the IR spectrum of a PAH population varies dramatically as a function of depth (or radiation field) through the PDR. Figure 2 illustrates the modeled evolution of the PAH emission from the ionization ridge as a function of depth (radiation field) into the molecular cloud.

This revolution in our understanding of interstellar PAHs and the many roles they play in the ISM reflects a breakthrough in the IR spectral range. The Infrared Space Observatory (ISO) spectral archives are now publicly available, but are limited to the local Solar neighborhood. SIRTF will soon be launched and will provide observations in the mid- and far-IR with exceptional sensitivity allowing studies of the IR spectral characteristics of the whole local group of galaxies. Monitoring when the PAH features appear as a function of galactic metallicity is an important goal of the SIRTF mission. The laboratory data will aid in identifying the types, sizes, and charge states of PAHs present as a function of metallicity. Galactic spectra vary from one place to another. Our laboratory and theoretical program aims to understand the relationship between the conditions in galactic sources and the emitted spectra, and apply this understanding to other regions, galactic and extragalactic. Thus, measuring the differences in the PAH spectra between objects can be used as a new tool to probe the local environmental conditions. Lastly, all of these detailed spectral studies using template galaxies of the local universe, will facilitate the interpretation of the broad band data for the weaker, most distant galaxies.

Formula	Name	Ion State	Formula	Name	Ion State
C₉H₇N	quinoline	o	C₂₀H₁₂	benzo[j]fluoranthene	-,o,+
	isoquinoline	o		benzo[k]fluoranthene	o,+
C₁₀H₈	naphthalene	o,+		benzo[a]pyrene	o,+
C₁₂H₈	acenaphthylene	o		benzo[e]pyrene	o,+
C₁₃H₉N	acridine	o,+		perylene	o
	7,8-benzoquinoline	o,+	C₂₀H₁₄	7,8-dihydrobenzo[a]pyrene	o
	phenanthridine	o,+		9,10-dihydrobenzo[e]pyrene	o,+
C₁₄H₁₀	anthracene	o,+	C₂₁H₁₃N	dibenz[a,h]acridine	o,+
	phenanthrene	o,+		dibenz[a,j]acridine	o,+
C₁₄H₁₁N	2-aminoanthracene	o,+	C₂₂H₁₂	benzo[ghi]perylene	o,+
C₁₅H₉N	9-cyanoanthracene	o,+	C₂₂H₁₄	pentacene	-,o,+
C₁₅H₁₂	1-methylanthracene	o,+	C₂₂H₁₆	7,14-dihydrodibenz[a,h]anthracene	o
	9-methylanthracene	o,+	C₂₄H₁₂	coronene	o,+
C₁₆H₁₀	fluoranthene	o,+	C₂₄H₁₄	dibenz[a,e]pyrene	o,+
	pyrene	o,+		dibenz[a,l]pyrene	o,+
C₁₆H₁₂	4,5-dihydropyrene	o		naphtho[2,3;a]pyrene	o,+
C₁₆H₁₆	1,2,3,6,7,8-hexahydropyrene	o	C₃₆H₁₆	3,4;5,6;7,8;12,13-tetrabenzoperopyrene	o,+
C₁₈H₁₀	benzo[ghi]fluoranthene	o		3,4;5,6;10,11;12,13-tetrabenzoperopyrene	o,+
C₁₇H₁₁N	1-azabenz[a]anthracene	o,+	C₄₀H₁₈	dipyreno-(1',3';10,2),(1",3";5,7)-pyrene	o,+
	2-azabenz[a]anthracene	o,+	C₄₀H₂₂	dianthraceno-(2',3';3,4),(2",3";9,10)-pyrene	o,+
	1-azachrysene	o,+	C₄₂H₁₈	1,12;2,3;4,5;6,7;8,9;10,11-hexabenzocoronene	o,+
	2-azachrysene	o,+	C₄₂H₂₂	1,18;4,5;9,10;13,14-tetrabenzoheptacene	o,+
	4-azachrysene	o,+		2,3;12,13;15,16-tribenzoterrylene	o,+
C₁₈H₁₂	1,2-benzanthracene	o,+	C₄₄H₂₀	1,2;3,4;5,6;7,8;9,10;12,13-hexabenzoperopyrene	o,+
	chrysene	o,+	C₄₈H₂₀	dicoronylene	-,o,+
	tetracene	o,+			
	triphenylene	o			
C₁₉H₁₄	7,8-dihydro-9H-cyclopenta[a]pyrene	o			
C₂₀H₁₂	benzo[a]fluoranthene	-,o,+			
	benzo[b]fluoranthene	o,+			

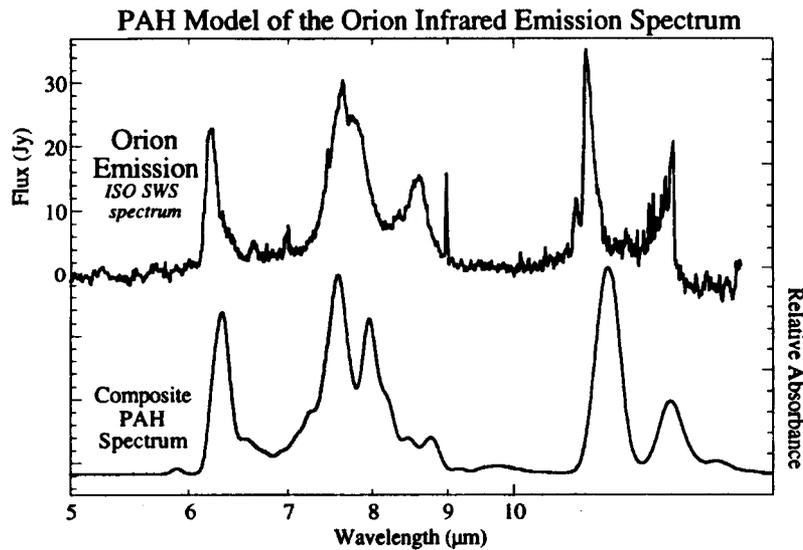Table 1 The Ames-Astrochemistry Lab PAH IR Spectral Database (Hudgins et al. 1994 - 1999.)

Figure 1. The 5 - 14 μm ISO SWS spectrum (top) from the Orion ionization ridge compared with (bottom) the composite absorption of a mixture of PAHs produced by coadding laboratory spectra of 11 different PAH cations (Peeters et al. 2002, in press).
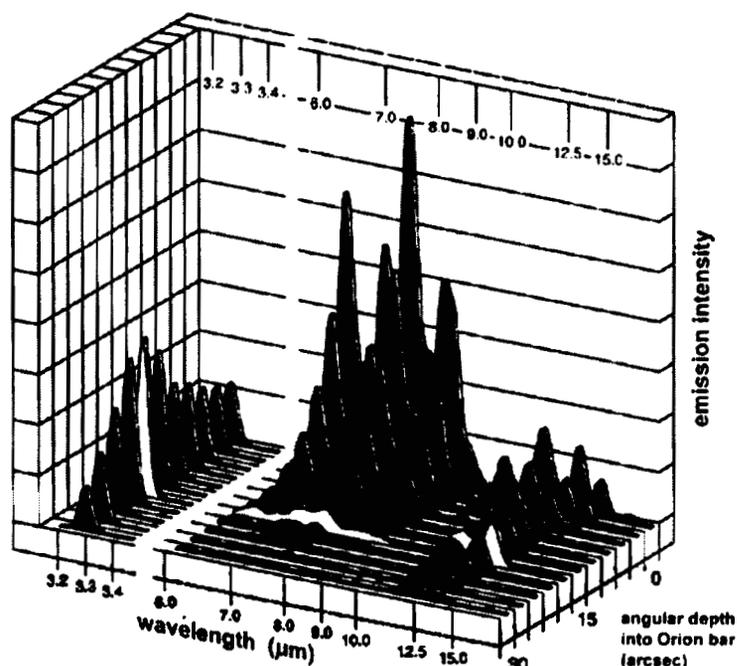
Figure 2. PAH emission spectral evolution predicted from the Orion ionization bar into the Orion molecular cloud utilyzing the model of Bakes, Tielens and Bauschlicher (2001a).

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