ON ESTIMATING INTERSTELLAR POLYCYCLIC AROMATIC HYDROCARBON ABUNDANCES WITH CALCULATED OSCILLATOR STRENGTHS

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ABSTRACT

Vibronic bands of polycyclic aromatic hydrocarbons (PAHs) in the UV/visible range are often used to estimate the abundances of PAHs in the interstellar medium by comparing laboratory-measured spectra with astronomical observations. We investigate the errors introduced by associating theoretical electronic oscillator strengths with individual vibronic bands when estimating the abundances of interstellar PAHs. The vibronic oscillator strengths of the 0–0 bands of nine PAHs with two to seven benzene rings, spanning in the 2800–6700 Å spectral range, have been calculated using the Franck–Condon approximation and compared to their electronic oscillator strengths. It is found that the use of calculated electronic oscillator strengths rather than the more physically relevant vibronic oscillator strengths underestimates interstellar abundances of the nine PAHs under study, on average by a factor of about 2.4. It is recommended that vibronic oscillator strengths should be systematically used to analyze the vibronic spectra of specific PAHs and to estimate their abundances in the interstellar medium. An empirical correcting factor is suggested for the cases where the vibronic oscillator strengths are unknown for more realistic estimation of interstellar PAH abundances.

Key words: ISM: abundances – ISM: molecules

1. INTRODUCTION

The diffuse interstellar bands (DIBs) are a set of absorption bands commonly observed in the spectra of reddened stars whose carriers remain unidentified despite many decades of research (see, e.g., Herbig 1995; Sarre 2006, for reviews). Among the most promising candidates for the band carriers are polycyclic aromatic hydrocarbons (PAHs), whose presence in the interstellar medium is inferred from their strong and ubiquitous infrared emission features, and that represent about 10% of the cosmic carbon (see, e.g., Tielens 2008 for a review). Extensive studies have been conducted over the years to test the PAH–DIB proposal (Tielens & Snow 1995; van der Zwet & Allamandola 1985; Léger & d'Hendecourt 1985; Salama et al. 1996, 1999). Supporting laboratory experiments have resulted in a large body of PAH spectroscopic data in the UV/visible range, typically measured with matrix-isolation spectroscopy (MIS) in cryogenic rare-gas solid matrices (Salama & Allamandola 1991; Salama et al. 1994; Salama 1996; Ruiterkamp et al. 2002). The MIS spectra of PAHs are broadened and shifted due to the interaction of the trapped molecular PAHs with the neighboring atoms of the solid matrix. This interaction often renders the MIS spectra of PAH only partially vibronically resolved, in particular in the near UV spectral range. In recent years, cavity ring-down spectroscopy (CRDS; Herbelin et al. 1980; Anderson et al. 1984; O'Keefe & Deacon 1988; Berden et al. 2000)—a high sensitivity direct absorption technique—has made it possible to measure the UV/visible absorption spectra of jet-cooled PAHs in the gas phase (Romanini et al. 1999; Biennier et al. 2003, 2004; Sukhorukov et al. 2004; Staicu et al. 2004; Tan & Salama 2005a, 2005b, 2006; Rouillé et al. 2004, 2007). Unlike MIS spectra, CRDS spectra of jet-cooled PAHs in gas phase in the UV/visible range are fully vibronically resolved, and intrinsic band profiles can be derived (Tan & Salama 2005a, 2005b; Rouillé et al. 2007). This point is illustrated in Figure 1, which compares the vibronic spectra of perylene ($C_{20}H_{12}$) measured in an MIS experiment and in a jet-cooled CRDS experiment.

Experimental spectra (either MIS or CRDS) are regularly used to direct dedicated searches for specific PAH features in astronomical spectra, and to derive upper limits for the abundances of interstellar PAHs. This requires knowledge of the oscillator strengths of the relevant vibronic transitions. The experimental determination of the vibronic oscillator strengths of the PAH bands is difficult due to the problem of determining the column densities of the PAHs that are present in the absorption path in the MIS or in the CRDS experiments. A viable alternative to experiment is the use of quantum-chemical calculations to determine these vibronic oscillator strengths. Historically, calculations reported in the literature include only the electronic oscillator strengths rather than the more physically relevant vibronic oscillator strengths (e.g., Ruiterkamp et al. 2005; Kokkin et al. 2007, 2008; Iglesias-Groth et al. 2008; Tan 2009). The widespread use of electronic oscillator strength for abundance estimates stems from the fact that electronic oscillator strengths are readily calculated using widely available quantum-chemical calculation packages (e.g., *GAUSSIAN*, *NWCHEM*, *TURBOMOLE*, etc.). In contrast, theoretical determination of the vibronic oscillator strengths requires post-processing of various calculation data obtained from direct quantum-chemical calculations, as is discussed in this paper. Since several reports have used electronic rather than vibronic oscillator strengths to estimate the abundances of interstellar PAHs, we investigate in this paper the magnitude of the errors introduced by this approximation. This will help establish more accurate abundance constraints on the distributions of interstellar PAHs as potential carriers of the DIBs.

The paper is organized as follows. In Section 2, we briefly review the formulation of vibronic oscillator strength, its relation to electronic oscillator strength, and the Franck–Condon
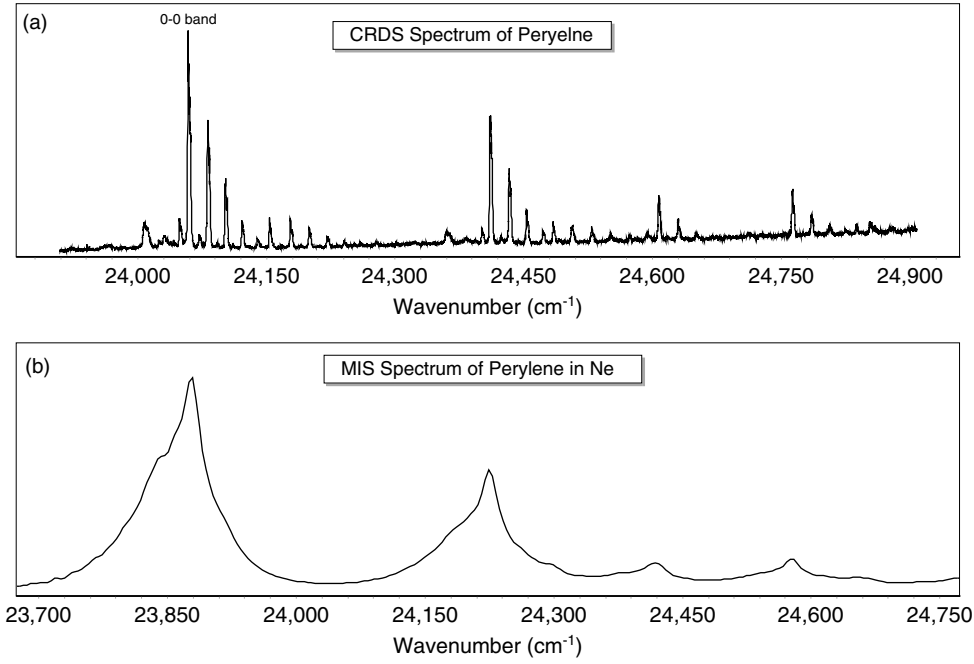
Figure 1. Major vibronic bands of the first electronic transition, $S_1(^1B_{3u}) \leftarrow S_0(^1A_g)$ of perylene taken in (a) a jet-cooled CRDS experiment and in (b) a solid-phase MIS experiment. For the purpose of comparison, the same vibronic features are aligned in the two spectra. A matrix-induced red shift of about 180 cm^{-1} can be observed in the MIS spectrum. Assignment of the bands can be found in Tan & Salama (2005a).

approximation (FCA) for calculating vibronic oscillator strengths of low-lying vibronic transitions of PAHs. In Section 3, we present the calculation results of the electronic and vibronic oscillator strengths of the 0–0 vibronic bands of nine PAHs comprised of two to seven benzene rings. General discussions and astrophysical implications are presented in Section 4.

2. FORMULATION OF VIBRONIC OSCILLATOR STRENGTH

The standard definition of the absorption oscillator strength of a dipole allowed vibronic transition is

$$f_{fi}^{ev} = (g'_f/g''_i)\frac{4\pi m_e \nu_{fi}}{3\hbar}\langle \chi'_f | \langle \Phi'_f | \vec{r} | \Phi''_i \rangle | \chi''_i \rangle^2$$

$$= (g'_f/g''_i)\frac{4\pi m_e \nu_{fi}}{3\hbar}\langle \chi'_f | \vec{M}^e_{fi} | \chi''_i \rangle^2, \qquad (1)$$

where m_e is the electron mass, $\vec{r}$ is the electric dipole operator, ν_{fi} is the frequency of the vibronic transition, g is the degeneracy of the vibronic state, and $\vec{M}^e_{fi} = \langle \Phi'_f | \vec{r} | \Phi''_i \rangle$ is the electronic transition dipole moment. The vibronic wavefunctions have been expressed in Equation (1) as the direct product of the normalized electronic wavefunction $|\Phi\rangle$ and the normalized vibrational wavefunction $|\chi\rangle$ on the basis of the Born–Oppenheimer approximation. The subscripts i and f denote the initial (lower) and final (upper) vibronic states in the absorption, respectively. The single and double primes denote quantities in the upper and lower electronic states, respectively.

Numeric evaluation of Equation (1) is computationally expensive for molecules with multiple atoms since it involves the evaluation of the electronic transition dipole moment as a function of the nuclear coordinates, which are $3N - 6$ or $3N - 5$ dimensional for a nonlinear or linear molecule with N atoms, respectively. The FCA can be used to greatly simplify the evalu-

ation of Equation (1). In FCA, $\vec{M}^e_{fi}$ is assumed to be independent of the nuclear coordinates and thus Equation (1) can be rewritten as

$$f_{fi}^{ev} = (g'_f/g''_i)\frac{4\pi m_e \nu_{fi}}{3\hbar}\langle \chi'_f | \chi''_i \rangle^2 M_{\mathrm{equ}}^2, \qquad (2)$$

where M_{equ} is the electronic transition dipole moment at the equilibrium geometry of the lower vibronic state. The term $\langle \chi'_f | \chi''_i \rangle^2$ in Equation (2) is the well-known Franck–Condon factor between the two vibrational states. Under the FCA, the electronic oscillator strength simplifies to

$$f_{fi}^{e} = (g'_f/g''_i)\frac{4\pi m_e \nu_{fi}}{3\hbar} M_{\mathrm{equ}}^2. \qquad (3)$$

This leads to the final expression for the vibronic oscillator strength,

$$f_{fi}^{ev} = f_{fi}^{e} \cdot \langle \chi'_f | \chi''_i \rangle^2. \qquad (4)$$

It is shown from Equation (4) that if one uses the electronic oscillator strength to estimate the absorption coefficient of a vibronic feature of the PAH molecule, one will overestimate the absorption coefficient of the PAH by a factor of $1/\langle \chi'_f | \chi''_i \rangle^2$.

3. CALCULATION RESULTS OF NINE PAHs

Using Equation (4), we have calculated the vibronic oscillator strengths of 11 0–0 vibronic bands of 9 PAHs (8 neutral molecules and 1 cation as shown in Figure 2) spanning the 2800–6700 Å spectral range. Eight of these PAHs (except coronene) have been studied in our CRDS experiments: the naphthalene cation ($C_{10}H_8^+$; Biennier et al. 2003), benzo[ghi]perylene ($C_{22}H_{12}$; Tan & Salama 2005b), perylene ($C_{20}H_{12}$; Tan & Salama 2005a), pentacene ($C_{22}H_{14}$), pyrene ($C_{16}H_{10}$), phenanthrene ($C_{14}H_{10}$), acenaphthene ($C_{12}H_{10}$), and 2-methylnaphthalene ($C_{11}H_{10}$; L. Biennier & F. Salama 2009, private communication). We chose the 0–0 vibronic bands because they are normally the strongest absorption bands within
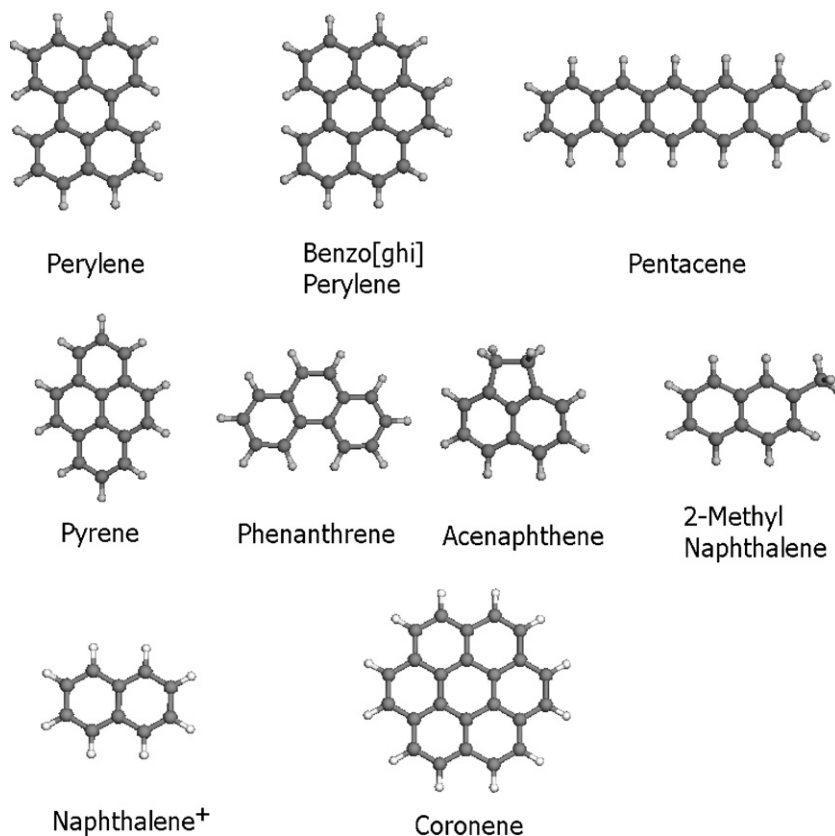
Figure 2. Nine PAHs (eight neutral molecules and one cation) calculated in this paper.

the corresponding electronic transitions of a PAH molecule at the low temperatures found in typical jet-cooled CRDS and MIS experiments, and also in the interstellar medium.

Density functional theory (DFT; Hohenberg & Kohn 1964; Kohn & Sham 1965; Parr & Yang 1989) and time-dependent density functional theory (TDDFT; Gross et al. 1996; Bauernschmitt & Ahlrichs 1996) calculations were performed to calculate the electronic transition dipole moments for the electronic transitions and the normal coordinates for both the lower and upper electronic states. Except for benzo[ghi]perylene and coronene, all the calculations of the normal coordinates were performed with the B3LYP functional (B3LYP; Lee et al. 1988; Miehlich et al. 1989; Becke 1993; Stephens et al. 1994). The normal coordinates of benzo[ghi]perylene and coronene were calculated with the BP86 functional (Perdew 1986; Becke 1988) and the resolution of identity (RI) approximation (Eichkorn et al. 1995, 1997) to reduce computational cost. The RI approximation allows for efficient computation of the electronic Coulomb interaction and leads to more than a 10-fold speedup compared to the conventional method. In all cases, the split valence polarization (SVP; Schäfer et al. 1992) basis set $\{(7s4p1d)/[3s2p1d]\}$ was used. The calculations of the excited states of the neutral PAHs were performed within the Tamm–Dancoff approximation (TDA; Hirata & Head-Gordon 1999), which has been shown (Tan & Salama 2005b) to give better excitation energies for benzo[ghi]perylene than the random phase approximation (RPA; Bouman & Hansen 1989; Hansen et al 1983). The RPA was used to calculate the excited state of the naphthalene cation. For all the DFT and TDDFT calculations the *TURBOMOLE* 5.7 code (Ahlrichs et al. 1989) was used. The Franck–Condon factors were evaluated using the *MOLFC* computer code developed by Borrelli & Peluso (2003).

Table 1 presents the electronic transitions, transition frequencies in wavenumbers, electronic oscillator strengths, Franck–Condon factors, and vibronic oscillator strengths of the 11 0–0 vibronic bands of the aforementioned nine PAHs. The vibronic oscillator strengths are calculated using the FCA as described in Section 2. For transition frequencies, the zero-point energy-corrected electronic term energies E_{00} are reported, except for benzo[ghi]perylene and coroene, for which the vertical transition energy calculated at the B3LYP/SVP level of theory is reported. The calculated Franck–Condon factors $\langle \chi'_0 | \chi''_0 \rangle^2$ of the 11 0−0 vibronic transition of the nine PAHs are found to be in the range from 0.19 to 0.59 with an average of 0.42 and a standard deviation of 0.11.

4. DISCUSSIONS

In this study, we report the errors that are introduced by the approximation of associating calculated electronic oscillator strengths to the vibronic spectra of PAHs in the UV/visible range when estimating the abundances of the PAHs in the interstellar medium. It was shown earlier that this approximation results in the abundance of the interstellar PAH being underestimated by a factor of $\langle \chi'_f | \chi''_i \rangle^2$, the Franck–Condon factor between the two involved vibrational states. For the nine PAHs with two to seven benzene rings that we have calculated, the Franck–Condon factors of the 0–0 vibronic bands range from 0.19 to 0.59. We conclude that if experimental vibronic spectra and astronomical observations are used to estimate the abundances of specific interstellar PAHs, the vibronic oscillator strengths should be calculated and used instead of the electronic oscillator strengths; otherwise, the abundances of the PAHs in the interstellar medium may be underestimated by a factor

Table 1
Electronic Transitions, Transition Wavenumbers, Electronic Oscillator Strengths, Franck–Condon Factors, and Vibronic Oscillator Strengths of the 0–0 Vibronic Bands of Nine PAHs (Eight Neutral Molecules and One Cation)

Molecule	Transition	Wavenumber[a]	$f^{e\,\mathrm{b}}$	$\langle \chi_0' \mid \chi_0'' \rangle^{2\mathrm{c}}$	f_{00}^{ev}
Perylene	$S_1(^1B_{3u}) \leftarrow S_0(^1A_g)$	24112 (24060[d])	5.6 E−01	0.42	2.4 E−01
Benzo[ghi]perylene	$S_2(^1B_1) \leftarrow S_0(^1A_1)$	27401 (27132[e])	2.7 E−01	0.50	1.4 E−01
Pentacene	$S_1(^1B_{2u}) \leftarrow S_0(^1A_g)$	16755 (18649[f])	8.3 E−01	0.49	4.1 E−01
Pyrene	$S_2(^1B_{3u}) \leftarrow S_0(^1A_g)$	30672 (30970[g])	3.0 E−01	0.54	1.6 E−01
Phenanthrene	$S_1(^1A_1) \leftarrow S_0(^1A_1)$	31206 (29328[h])	1.1 E−03	0.42	4.6E−04
	$S_2(^1B_1) \leftarrow S_0(^1A_1)$	34030 (35375[h])	6.3 E−02	0.36	2.3 E−02
Naphthalene$^+$	$D_2(^2B_{3g}) \leftarrow D_0(^2A_u)$	16234 (14906[i])	5.2 E−02	0.33	1.7 E−02
Acenaphthene	$S_1(^1A_1) \leftarrow S_0(^1A_1)$	34428	1.2 E−01	0.19	2.3 E−02
	$S_2(^1B_2) \leftarrow S_0(^1A_1)$	34847	5.1 E−03	0.43	2.2 E−03
2-MethylNaphthalene	$S_1(A') \leftarrow S_0(A')$	34811	5.8 E−03	0.39	2.3 E−03
Coroene	$S_5(E_{1u}) \leftarrow S_0(A_{1g})$	35307	1.7 E00	0.59	1.0 E00

Notes.

[a] For benzo[ghi]perylene and coronene, the vertical transition energy calculated at the B3LYP/SVP level of theory with TDA is reported; for others, the reported values are E_{00} calculated at the B3LYP/SVP level of theory with RPA (naphthalene$^+$) or TDA (others); Experimental values are listed in the parentheses.

[b] Calculated at the B3LYP/SVP level of theory with the TDA.

[c] For benzo[ghi]perylene and coronene, the normal coordinates are calculated at the BP86/SVP level of theory with the TDA and the RI approximations; for others, the normal coordinates are calculated at the B3LYP/SVP level of theory with the TDA approximation.

[d] Tan & Salama (2005a).

[e] Tan & Salama (2005b).

[f] Hoheisel et al. (2003).

[g] Ohta & Baba (1987).

[h] Warren et al. (1986).

[i] Biennier et al. (2003).

ranging from 2 to 5. For example, recent studies (Iglesias-Groth et al. 2008) have reported the observation of three weak broad DIBs in the 6000–6800 Å range where vibronic transitions associated with the naphthalene cation $C_{10}H_8^+$ fall. Using the calculated electronic oscillator strength of 0.05 for the strongest 0–0 vibronic band at 6707 Å, these authors estimated a probable $C_{10}H_8^+$ column density of 1×10^{13} cm^{-2} and a fraction of 0.008% of total carbon being in the form of $C_{10}H_8^+$ in the intervening cloud. Using our calculation results as shown in Table 1, we improve the estimation of $C_{10}H_8^+$ column density to 3×10^{13} cm^{-2} and carbon fraction to 0.02%.

Although it is always a good practice to calculate the relevant vibronic oscillator strengths while analyzing vibronic transitions of PAHs, it is may be useful to have an empirical multiplier that can be readily applied to the electronic oscillator strengths to estimate the corresponding 0–0 vibronic oscillator strengths of PAHs. Based on the average of the 11 0–0 vibronic oscillator strengths calculated in this work, we suggest a multiplier of 0.42. This multiplier is useful in the cases where the evaluations of the vibronic oscillator strength are too expensive to afford. In using this multiplier, one should note that it pertains to PAHs with a few (less than 10) benzene rings.

To explain the variation of this multiplier with the size of the PAH, we write the Franck–Condon factor f_{00}^{ev} of the 0–0 vibronic band of a PAH molecule in the following form, based on the harmonic approximation:

$$f_{00}^{ev} = \prod_{i=1}^{3N-6} f_{00}^{ev}(\nu_i), \qquad (5)$$

where $f_{00}^{ev}(\nu_i)$ is the 0–0 Franck–Condon factor of the ith normal mode ν_i, and N is the number of atoms in the PAH. If we further assume that $f_{00}^{ev}(\nu_i)$ is independent of the vibrational mode, we

can reduce Equation (5) to the following form:

$$F_{00} = \prod_{i=1}^{3N-6} f_{00}^{ev}(\nu_i) = (1-\delta)^{3N-6}, \qquad (6)$$

where δ is the average "deviation" for all modes in the molecule. It is a measure of the similarity of the two vibrational wavefunctions of the same normal mode in the two involved electronic states: the smaller the δ is, the more similar the two vibrational wavefuctions are. Taking the typical values of $f_{00}^{ev}(\nu_i) \approx 0.99$ (or $\delta \approx 0.01$) and $N = 25$, one ends up with $f_{00}^{ev} \approx 0.5$, which is close to the multiplier reported in this work. Based on Equation (6), we have derived the δ values for all the 11 vibronic transitions studied in this work. These δ values are listed in Table 2. It is shown from Table 2 that in general the δ value decreases as the size of the PAH molecule increases. This is mainly due to the fact that a low-lying electronic excitation causes a less significant electronic reconfiguration in a large PAH than in a small PAH since there are more electrons in the larger PAH. The final 0–0 Franck–Condon value is a result of two opposing factors: the $3N$–6 exponent in Equation (6) that is proportional to the size of the molecule and the δ value in Equation (6) that tends to decrease as the size of the molecule increases. For the nine PAHs with two to seven benzene rings studied in this work, the resulting Franck–Condon values span a relative small range of 0.19–0.59. How these two factors interact in larger PAH molecules is yet to be determined in future work when more calculation data are available. Though it is clear that quantitative astronomical work should aim toward using the vibronic rather than the electronic oscillator strengths when addressing abundances of PAH molecules.

With the availability of the vibronic oscillator strengths of the PAH electronic transitions in Table 1, one can now quantitatively

Table 2
The δ Values of the 11 Vibronic Bands Reported in Table 1

Molecule	Number of Atoms	Transition	δ
Naphthalene$^+$	18	$D_2(^2B_{3g}) \leftarrow D_0(^2A_u)$	2.3 E−02
2-MethylNaphthalene	21	$S_1(A') \leftarrow S_0(A')$	1.6 E−02
Acenaphthene	22	$S_1(^1A_1) \leftarrow S_0(^1A_1)$	2.7 E−02
		$S_2(^1B_2) \leftarrow S_0(^1A_1)$	1.4 E−02
Phenanthrene	24	$S_1(^1A_1) \leftarrow S_0(^1A_1)$	1.3 E−02
		$S_2(^1B_1) \leftarrow S_0(^1A_1)$	1.5 E−02
Pyrene	26	$S_2(^1B_{3u}) \leftarrow S_0(^1A_g)$	8.5 E−03
Perylene	32	$S_1(^1B_{3u}) \leftarrow S_0(^1A_g)$	9.6 E−03
Benzo[ghi]perylene	34	$S_2(^1B_1) \leftarrow S_0(^1A_1)$	7.2 E−03
Pentacene	36	$S_1(^1B_{2u}) \leftarrow S_0(^1A_g)$	7.0 E−03
Coroene	36	$S_5(E_{1u}) \leftarrow S_0(A_{1g})$	5.2 E−03

compare the spectra of these PAHs measured in our recent CRDS experiments with astronomical observations and derive the abundances of these specific PAHs in the regions of the interstellar medium that are probed by the observations. Such a work is currently in progress and will be published separately.

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