

Testing the attribution of selected DIBs to dehydrogenated coronene cations

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Abstract. Dehydrogenated coronene molecules have been proposed as the source of the UV-bump in the interstellar extinction curve as well as of some of the diffuse interstellar bands (DIBs). To test this hypothesis we have recently undertaken a combined (a) modelling, and (b) observational work on the subject. (a) In the framework of a global approach to the photophysics of a PAH-like species in space, we used combined theoretical calculated properties, obtained with (time-dependent) density functional theory, and a Monte-Carlo model simulating the time evolution of the population of levels of a given molecule, to obtain the detailed ro-vibrational spectral structure of selected electronic transitions. (b) From the observational point of view, we compare our predictions with observations of the well-known $\lambda 6284$ and $\lambda 5780$ DIBs.

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1. Introduction

The carrier of the well-known bump at about 2175 Å in the interstellar extinction curve seems to require a free-flying form of carbon, either in the form of size-restricted graphite pieces (Draine 1985) or of single or stacked PAHs (Duley & Seahra 1998). Based on scattering calculations (Duley & Seahra 1998) in the discrete-dipole-approximation, Duley (2006a) suggested the possible assignment of this feature to a $\pi \rightarrow \pi^*$ plasmon resonance in dehydrogenated coronene molecules ($C_{24}H_n$, $n \leq 3$), and their corresponding cations. The same class of molecules has been proposed to explain some of the diffuse interstellar bands (DIBs, Duley 2006b).

2. Methods

To test the attribution of the $\lambda 6284$ and $\lambda 5780$ DIBs to the completely dehydrogenated coronene cation we have undertaken a combined modelling and observational work.

From the modelling side, we first computed the absorption cross-section, the complete vibrational spectrum (frequencies and intensities of the IR-active modes), and the rotational constants in the states involved of planar C_{24}^+ . We then used a Monte-Carlo model of the photophysics of isolated PAHs (Mulas 1998, Mallocci *et al.* 2003) to obtain the expected rotational band profiles under diffuse ISM conditions.

From the observational side we restricted ourselves to lines of sights characterized by very low color excess ($E_{B-V} < 0.15$ mag). These data, unpublished, have been obtained with the ESO 1.4 m CAT Telescope.

3. Results

We show in Figure 1 the comparison between the computed rotational profile of the “DIBs” of planar C_{24}^+ at 5780 and 6284 Å. According to the proposal by Duley (2006b) they should be the $0 \rightarrow 0$ and $0 \rightarrow 1$ bands in a vibronic progression of the $\pi_{-4} \rightarrow \pi_0^*$ electronic transition. Figure 2 shows the correlation plot for the equivalent widths of the 5780 and 6284 Å DIBs measured for selected lines of sight.

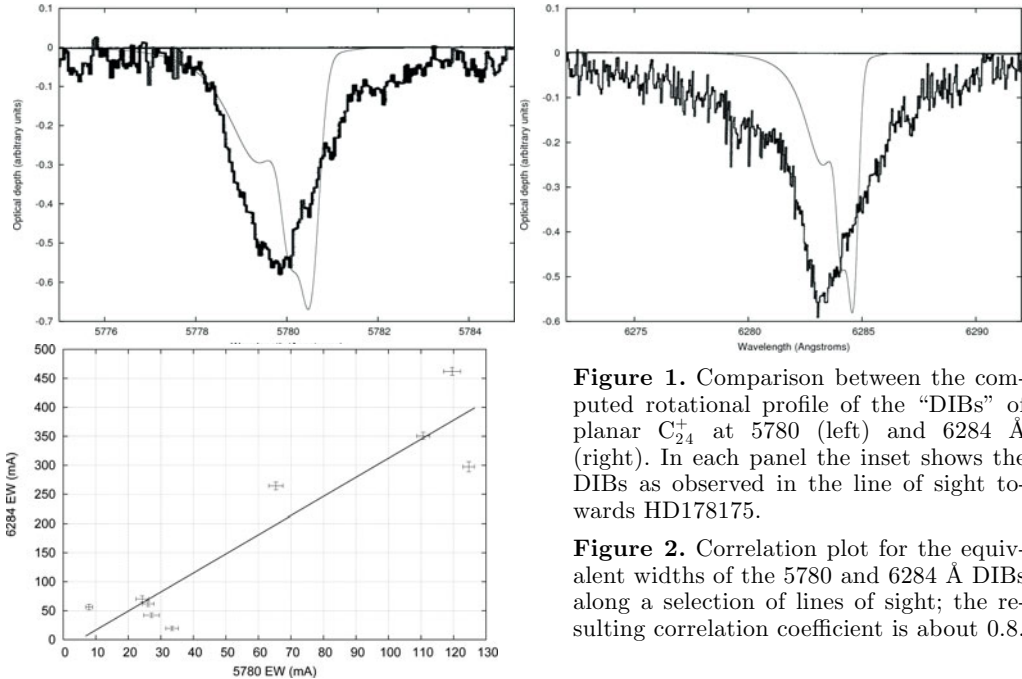


Figure 1. Comparison between the computed rotational profile of the “DIBs” of planar C_{24}^+ at 5780 (left) and 6284 Å (right). In each panel the inset shows the DIBs as observed in the line of sight towards HD178175.

Figure 2. Correlation plot for the equivalent widths of the 5780 and 6284 Å DIBs along a selection of lines of sight; the resulting correlation coefficient is about 0.8.

4. Discussion and future work

We find a relatively low correlation between the $\lambda 6284$ and $\lambda 5780$ DIBs. This is inconsistent with the hypothesis that they are due to different vibronic transitions from the same state of the same molecule, which would require a perfect correlation, with scatter only due to measurement errors. The higher correlation previously reported between these two bands on more reddened lines of sight (Moutou *et al.* 1999) may be due to statistical effects and/or from the two DIBs arising from different carriers that respond in a similar way to environmental conditions. Moreover, the specific transitions proposed in this hypothesis as tentative identifications of the two bands, are predicted to be blue-shaded, in stark contrast with the observed red-shaded profiles of the $\lambda 6284$ and $\lambda 5780$ DIBs. This excludes their common origin in C_{24}^+ , unless upon dehydrogenation this species relaxes to an isomer different from the planar, aromatic one we considered.

References

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