

# 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.

**Keywords.** Astrochemistry, ISM: lines and bands, line: profiles, molecular processes

## 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

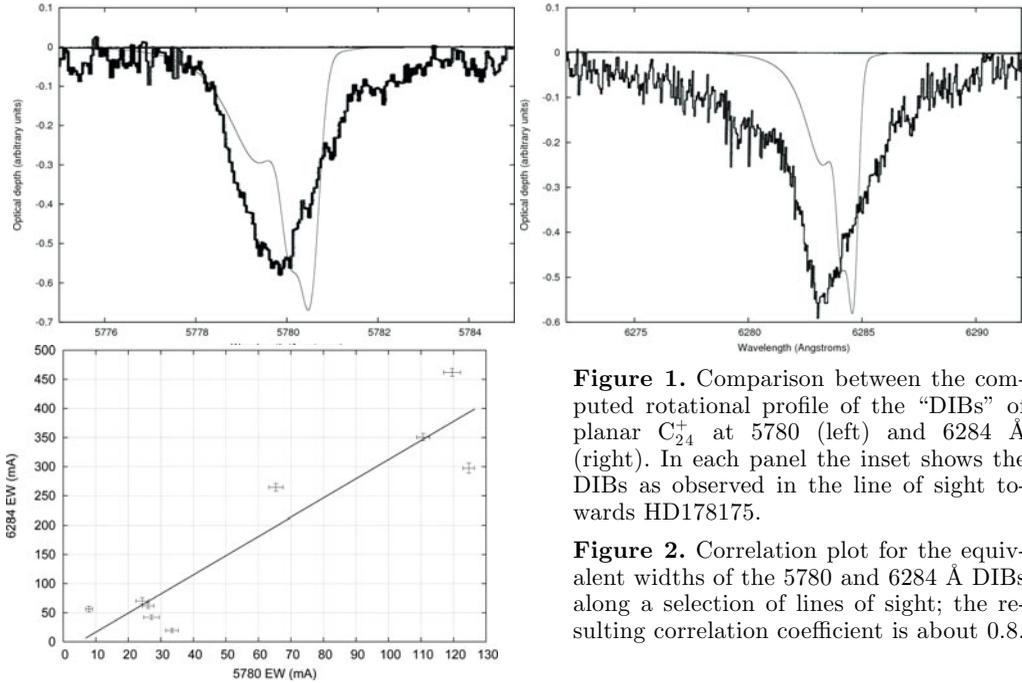
To test the attribution of the  $\lambda 6284$  and  $\lambda 5780$  DIBs to the completely dehydrogenated coronene cation we have undertaken a combined modelling and observational work.

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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