

## ELECTRONIC SPECTRA OF *PERI*-HEXABENZOCORONENE AND OVALENE ISOLATED IN SOLID *PARA*-HYDROGEN

ISABELLE WEBER, JOHANNA LANGNER, HENRYK A. WITEK, *Department of Applied Chemistry, National Yang Ming Chiao Tung University, Hsinchu, Taiwan*; YUAN-PERN LEE, *Department of Applied Chemistry, Institute of Molecular Science, and Centre for Emergent Functional Matter Science, National Yang Ming Chiao Tung University, Hsinchu, Taiwan*.

Diffuse interstellar bands (DIB), narrow absorption features observed from the near IR to the UV, have drawn a lot of interest since their first discovery in 1922. Polycyclic aromatic hydrocarbons (PAH) and their cationic, protonated and hydrogenated derivatives are considered particularly promising candidates for the DIB carriers, but laboratory spectra of these unstable species suitable for comparison to astronomical observations are scarce.

*para*-Hydrogen (*para*-H<sub>2</sub>) matrix isolation spectroscopy has frequently been employed to record the IR spectra of PAH derivatives. The obtained spectra exhibit only small shifts in line positions due to small interactions with the matrix host, in line with the ‘softness’ of the quantum solid *para*-H<sub>2</sub>. However, electronic spectra of PAH isolated in solid *para*-H<sub>2</sub> have rarely been reported.

Ovalene (C<sub>32</sub>H<sub>14</sub>) and *peri*-hexabenzocoronene (HBC, C<sub>42</sub>H<sub>18</sub>) have both been discussed as potential DIB carriers and, therefore, their electronic absorption spectra have been studied in the gas-phase and in rare gas matrices. To assess the properties of *para*-H<sub>2</sub> as a matrix host for electronic spectroscopy, we present the fluorescence excitation and dispersed fluorescence spectra of these two large PAH isolated in solid *para*-H<sub>2</sub>. We located the 0<sub>0</sub><sup>0</sup> bands of the S<sub>1</sub>–S<sub>0</sub> transitions at 21049 cm<sup>-1</sup> and about 22075 cm<sup>-1</sup> for ovalene and HBC, respectively. The recorded excitation spectra in general show a good agreement with previously reported absorption spectra indicating a matrix shift below 100 cm<sup>-1</sup> due to the *para*-H<sub>2</sub> matrix host, consistent with our earlier experiments on several smaller PAH. We complemented our experimental work with Franck-Condon Herzberg-Teller simulations on the basis of optimized geometries and vibrational frequencies obtained from (TD-)DFT calculations to derive a first assignment of individual vibrational modes to the observed absorption and emission bands associated with the electronic S<sub>1</sub>–S<sub>0</sub> transition. For ovalene, we find that a consideration of the closely lying S<sub>2</sub> state is required to reproduce the complexity of the experimental excitation spectrum by the simulation.