Interstellar PAHs with five membered rings: TDDFT study

A. Pathak1, M. Buragohain1, M. Hammonds2, P.J. Sarre3, I. Sakon2, T. Onaka2

1. Physics Department, Tezpur University, Napaam, Tezpur – 784 028, INDIA
2. Department of Astronomy, Graduate School of Science, The University of Tokyo, Tokyo 113-0033, Japan
3. School of Chemistry, University of Nottingham, University Park, Nottingham – NG7 2RD, UK

The intriguing problem of the carriers of interstellar Diffuse Interstellar Bands (DIBs) remains unsolved despite of years of observational, theoretical and experimental effort [1]. Observational evidence has been found in support of molecular carriers [2] leading to experimental and theoretical investigations on polycyclic aromatic hydrocarbons (PAHs), carbon chains, fullerenes and other molecules. Intensive experimental and theoretical studies have shown that PAH molecules in various forms are the carriers of the unidentified infrared (UIR) bands. The stability of these molecules helps them to survive UV-rich interstellar conditions. The detection of ionized fullerene in the ISM [3] strongly supports the PAH proposal. Astronomers speculate that about 10% - 15% of the interstellar carbon budget is within PAHs.

We report the first *Time Dependent Density Functional Theory* (TDDFT) calculations on PAHs with five-membered rings. These PAHs are important as they are probably directly or indirectly related to the formation / dissociation of Fullerenes (C_{60}). The PAH molecules selected for investigation include Acenaphthylene ($C_{12}H_8$), Fluorene ($C_{13}H_9$), Fluoranthene ($C_{16}H_{10}$), Corannulene ($C_{20}H_{10}$) and Buckminsterfullerene (C_{60}). We report the TDDFT oscillator strengths for ionized as well as protonated versions of these PAHs. The results presented here assist in further narrowing down the carriers of DIBs. These results also act as pointers for laboratory studies.

References:

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