

# Mid-Infrared vibrational study of substituted PAHs : implications to Aromatic Infrared Bands

Mridusmita Buragohain<sup>1</sup>, Amit Pathak<sup>1</sup>, Peter Sarre<sup>2</sup>,  
Takashi Onaka<sup>3</sup>, Itsuki Sakon<sup>3</sup>

<sup>1</sup>*Department of Physics, Tezpur University, Assam, PIN 784028*

<sup>2</sup>*School of Chemistry, The University of Nottingham, University Park, Nottingham, NG7 2RD, UK*

<sup>3</sup>*Department of Astronomy, Graduate School of Science, The University of Tokyo, 7-3-1, Hongo,  
Bunkyo-ku, Tokyo 113-0033, Japan*

Polycyclic Aromatic Hydrocarbon (PAH) molecules have been long proposed to be a major source of the mid-infrared bands observed in the interstellar medium (ISM). Vibrational relaxation of PAHs on absorption of a UV photon produces distinct features at 3.3, 6.2, 7.7, 8.6, 11.2 and 12.7  $\mu\text{m}$  popularly known as ‘Aromatic Infrared Bands’ (AIBs). Apart from these, several other weak features are distributed in an emission plateau of 3 – 20  $\mu\text{m}$ . Despite the fact that PAHs are ubiquitous in the ISM, the exact form of PAHs responsible for producing these features are not yet known. Several substituted PAHs have been studied both experimentally and theoretically to correlate with interstellar AIBs. Owing to the presence of deuterium in the ISM, deuterium containing PAHs are highly preferred among the substituted PAHs.

Density Functional Theory (DFT) calculation has been carried out on a variety of PAHs with a deuterium to study the infrared properties of these molecules. These include deuterated PAHs (PADs and  $\text{D}_n\text{-PAHs}$ ), cationic PADs, deuterated PAHs ( $\text{DPAH}^+\text{s}$ ) and deuterated-deuterated PAHs ( $\text{DPAD}^+\text{s}$ ). A comparison has been made to see the size effect of PAHs and impact of deuteration. We present a D/H ratio calculated from our theoretical study to compare with the observationally proposed D/H ratio.