Towards a complete database of polycyclic aromatic hydrocarbons and the identification of some resolved diffuse interstellar bands

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Abstract

Polycyclic aromatic hydrocarbons (PAHs) have been suggested as important organic molecules in space. They are commonly believed to be responsible for the infrared emission bands and to be one class of molecular carriers of the diffuse interstellar bands (DIBs) that were first discovered in 1919. Recent high resolution astronomical spectra have shown resolved band profiles of several strong DIBs (e.g. the λ6614, λ5797, and λ6196 DIBs). If these DIBs were really absorption features of some PAH species, a complete database that contains the spectroscopic properties (e.g. vibronic energies and rotational constants) of all relevant PAHs would be needed to identify possible PAH carriers. Unfortunately, up to date only very limited PAHs have been studied either experimentally or theoretically (e.g. $\sim 0.1\%$ PAHs out of all possible PAHs containing up to 10 fused benzene rings). A big question to ask therefore is: "what PAHs out of infinite number of PAHs should we study?" In an attempt to answer this question and to identify possible PAH carriers of the aforementioned resolved DIBs, we introduce a novel approach to generate a complete database of PAHs. In the first phase of this approach, a computer algorithm is invented to generate all possible unique shapes, or T shapes, that contain n fused benzene rings (where n is an integer). Each T shape corresponds to the carbon skeleton of a PAH species. In the second phase, a ultrafast force-field and PPP computer code is used to generate the vibronic energies and rotational constants of all the PAHs generated in phase one. Possible PAH carriers are then pre-selected according to their vibronic transition wavelengths and the simulated vibronic band profiles. In the last phase, high level time-dependent density functional theory (TDDFT) calculations are performed to further narrow down the candidate list. With this approach, we have generate all T shapes that contain up to 10 fused benzene rings (38,959 T shapes in total). T shapes containing 11 rings are currently being generating. Several possible candidates for the λ6614 DIB have been selected and are currently being tested by TDDFT calculations and band profile simulations. This approach holds great power in understanding the spectroscopic properties of PAHs and in solving the PAH–DIB problem.