Astronomy in Focus, Volume 1, Focus Meeting 12, E18
XXIXth IAU General Assembly, August 2015
Piero Benvenuti, ed.

doi:10.1017/S1743921317005087

Coronene and Pyrene (5,7)-member Ring Defects

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Abstract. Polycyclic aromatic hydrocarbons (PAHs) are one of the most interesting components of the interstellar medium (ISM). But different from laboratory - the isolation of a single species is not possible. The spectra contain a superposition of many different molecules. Therefore a sophisticated understanding of all possible subtypes is required. We present an investigation of the IR spectra of PAHs containing (5, 7)-member ring defects. Using density functional theory, the influence of those defects on the IR spectra of coronene ($C_{24}H_{12}$) and pyrene ($C_{16}H_{10}$) and their cations and anions were examined in detail. Additionally, the potential energy surface of the neutral species is explored and an alternative formation pathway is taken into account.

Keywords. astrochemistry, molecular processes, methods: numerical, ISM: molecules

Results

The addition of the pentagons and heptagons instead of some of the hexagons usually constituting PAHs result in a change of the IR spectra: coronene and pyrene lose both their typical spectroscopic signature. We find different additional features and shifts in the positions of the band; the intensities differ as well. The molecules are among the smallest PAHs that can exhibit such a ring defect. The minimum activation barriers for the transformation from ground to defected state can be found via investigating the minimum energy pathway. This leads to a result of 8.21 eV for pyrene and 8.41 eV for coronene. The formation of these (5, 7)-member ring defects in PAHs may be well supported in different astrophysical environments such as the ISM. The physical interactions of PAHs with stellar particle radiation will not necessarily destroy or fragment the molecules. If the particle has enough energy and exactly hits on a knot of the molecule, a change of the ring structure from 6-membered rings into pentagons and heptagons may occur (Huber *et al.* (2013)). Different environments strongly enable the transition from the ground to the defected state. Therefore, the knowledge of the IR spectra of coronene and pyrene including the defect will support future studies aiming for a thorough understanding of the unidentified infrared emission bands. The computational methods, additional spectra, the energetics and a detailed discussion of the formation of the defect is shown in detail in Öttl *et al.* (2014).

References

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