PAHs and PAH clusters in the far-IR

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Polycyclic aromatic hydrocarbon (PAH)–water complexes are an important link between molecular gas and condensed particles in both the earth's atmosphere and the interstellar medium[1]. We report on the experimental and theoretical investigations of the stepwise complexation of the PAH acenaphthene with itself and with water[2]. The far-IR region of the IR spectrum is especially interesting since it reveals spectral features that result from the complexation and/or microhydration and is therefore very sensitive for the molecular structure. Using mass- and conformer selective far-IR action spectroscopy, we show that the water clusters are locked with little perturbation on the PAH 'platform'[3]. Density functional theory (DFT) calculations to analyse our observed signatures are still challenging in predicting the far-IR frequency range, especially when hydrogen bond interactions are involved, although applying anharmonic corrections leads to improvements.

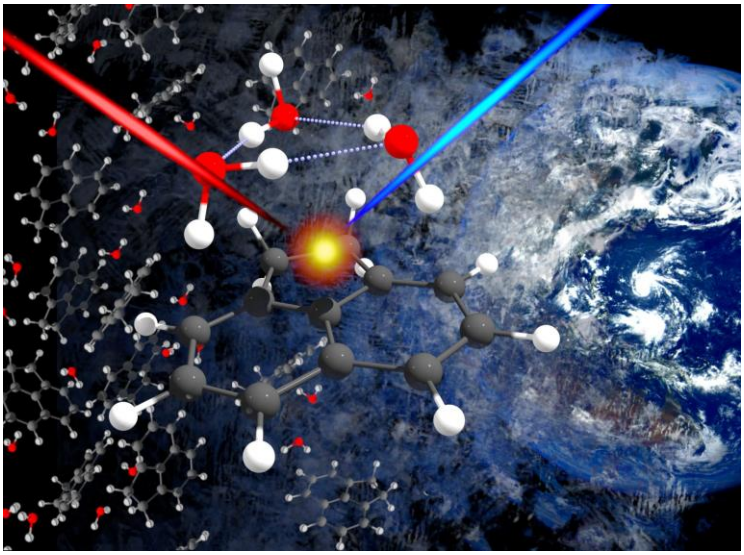

Figure 1: Impression of PAHs and PAH clusters studied in the far-IR, in both the earth's atmosphere and interstellar space

References

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