ROTATIONAL SIGNATURES OF DISPERSIVE STACKING IN THE FORMATION OF AROMATIC DIMERS

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Non-covalent molecular aggregate formation is dictated by inter- and intramolecular forces. The role of these interactions in stabilizing biological molecules is of great interest to many scientific communities. Characterizing these forces has also gained a lot of importance for understanding grain formation in the interstellar medium, especially for aromatic systems such as polycyclic aromatic hydrocarbons (PAHs).[a] Broadband rotational spectroscopy studies of weakly bound complexes are able to accurately reveal the structures and internal dynamics of molecular clusters isolated in the gas phase. To understand the weak interactions in biological and astrochemical relevant molecules, we report here our studies on the homodimers of fluorene ($C_{13}H_{10}$), dibenzofuran ($(C_6H_4)_2O$), and diphenylether ($(C_6H_5)_2O$). While their structures show overall similarities, they differ in structural flexibility, planarity, and dipole moment. In order to determine the structure of the corresponding homodimers, we targeted transitions in the 2-8 GHz range using broadband rotational spectroscopy. Our experimental results show that all the observed homodimers are dominated by dispersion interactions such as CH-π or π-π, but the dibenzofuran dimer is also influenced by repulsion between the free electron pairs of the oxygen atoms and the π clouds.[b]

[a] A. L. Steber, et al., J. Phys. Chem. Lett., 8 (2017), 5744-5750.

[b] M. Fatima et al., Angew. Chem. Int. Edit., 131 (2019), 3140.