NON-COVALENT INTERACTIONS IN COMPLEXES OF FLUORINATED AROMATIC RINGS INVESTIGATED BY ROTATIONAL SPECTROSCOPY

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Non-covalent inter- and intramolecular interactions involving aromatic rings are ubiquitous in chemical and biological processes. The presence of halogen atoms, fluorine in particular, can drastically change the binding properties of molecules and thus halogen or fluorine substitution are used to tune the properties of new materials, drugs or proteins. We report on a series of rotational spectroscopy studies performed with Molecular Beam Fourier Transform Microwave spectroscopy in which we have tested the binding abilities of fluorinated aromatic compounds, namely penta-fluoropyridine and hexafluorobenzene, with different ligands such as ammonia, carbon monoxide and halogenated methanes. The comparison to the analogous complexes formed by non-fluorinated aromatic moieties shows strickingly different structures. In the case of the fluorinated aromatic compounds the structures are dominated by π-hole interaction.