

ON THE NATURE OF THE INTERACTION OF CO WITH PERFLURINATED AROMATICS: NEW INSIGHTS FROM THE EXPERIMENTAL DATA AND THEORETICAL STUDY

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The rotational spectra of pentafluoropyridine-CO and hexafluorobenzene-CO have shown unambiguously that substitution by fluorine atoms on the ring strongly influences the binding abilities of the aromatic ligand. Differently from their non-substituted counterparts, both molecules interact with CO forming a perpendicular $lp \cdots \pi$ interaction between the carbon and the ring. We report earlier the rotational spectroscopy studies performed with a Molecular Beam Fourier Transform Microwave spectrometer in which we have tested the binding abilities of the fluorine substituted aromatics molecules with CO. Now local energy decomposition analysis of the relative conformational energies shows the interplay between the non-covalent interactions which led to the final configuration preference of CO with respect to the aromatic rings in the supersonic expansion. Although the relative complexity of the non-covalent interactions made these molecular systems challenging to study, the progress in theoretical modelling have shown to physical explain the origin of the molecular binding.