The shape of molecules and molecular complexes: flexibility and non-covalent interactions at play, a rotational spectroscopy view

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The flexibility of molecular systems related to the presence of multiple torsional degrees of freedom and different non-covalent interactions occurring within the molecule or with the surroundings give rise to complex conformational surfaces.

Accurate data on the structures, conformational energies and dynamics of complex organic molecules and their molecular complexes can be obtained by rotational spectroscopy performed in the cold isolated conditions of a free jet expansion and these properties can be directly compared to the outcome of accurate quantum mechanical calculations obtained in the same isolated conditions.

Through chosen results on flexible organic molecules, bioactive molecules (drugs and their halogen substituted analogs), astrophysical targets and molecular complexes formed in supersonic expansions and characterized by rotational spectroscopy, we will show how non-covalent interactions (hydrogen bonds, weak hydrogen bonds, halogen bonds, pnicogen bonds and lp-p-hole interactions) compete to shape the conformational potential energy surface of the complexes, determine their shapes, their dynamics and even influence molecular reactivity. We will also show how these interactions can be drastically changed through substitution (in particular with halogen atoms) or complexation with solvent molecules.