NON COVALENT INTERACTIONS AND INTERNAL DYNAMICS IN ADDUCTS OF FREONS

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The complexation of chlorofluorocarbons (CFCs) with atmospheric water and pollutants of the atmosphere affects their reactivity and it seems to accelerate, for example, the decomposition rate of freons in the atmosphere [1]. For this reason we characterized shapes, stabilities, nature of the non-covalent interactions, structures and internal dynamics of a number of complexes of CFCs with water and of their dimers or oligomers by rotational spectroscopy. It has been found that hydrogenated CFCs form adducts with other molecules through weak hydrogen bonds (WHBs). Their C-H groups can act as proton donors, enhanced by the electron withdrawing of the halogen atoms, interacting with the electron rich regions of the partner molecules [2]. Also in adducts or oligomers of hydrogenated CFCs the monomer units are held together by nets of WHBs [3]. When CFCs are perhalogenated, the positive electrostatic region ("σ-hole") can interact electrostatically with negative sites of another, or of the same molecular entity, giving rise, according to IUPAC, to the so called halogen bond (HaB). However, it has been observed that when the perhalogenated CFCs has a Π electron system, a lone pair$\bullet\bullet\bullet\Pi$ interaction (Bürgi-Dunitz) is favoured [4]. We describe here the HaBs that CF_4 and CF_3Cl form with a variety of partner molecules such as water, ammonia, dimethyl ether, etc. Important spectroscopic features outline strong dynamics effects taking place in this kind of complex.

References

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