A COMPUTATIONAL INVESTIGATION OF c-C_3H_2...HX(X = F, Cl, Br) H-BONDED COMPLEXES

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Cyclopropenylidene (c-C_3H_2) is of significant importance in interstellar chemistry and synthetic chemistry (e.g., transition metal and organic catalysis). Because of its peculiar structure, c-C_3H_2 can act as a hydrogen-bond donor or acceptor. In order to gain insight into this feature, the ground-state potential energy surfaces of singlet c-C_3H_2 complexed with hydrogen halides HX (X = F, Cl, Br) have been explored extensively by density-functional theory (B3LYP) and *ab initio* quantum chemistry (MP2) with a variety of basis sets, cc-pVxZ and aug-cc-pVxZ (x = D, T). The complexes characterized have the carbenic end of c-C_3H_2 H-bonded to HX, with some proton transfer occurring, the extent of which follows the order HF $<$ HCl $<$ HBr. Accompanying the complex formation are the dipole moment enhancement, the charge transfer, red shifts of the HX vibrational stretching frequencies together with the significant enhancement of band intensity and concomitant HX bond elongation. The nature of H-bonding in these complexes has been explored, based on energy decomposition schemes and the Baders quantum theory of atoms-in-molecules, with the conclusion that c-C_3H_2 is a strong H-bond acceptor with respect to the hydrogen halides.