
Nucleophilic or electrophilic character of C2 interacting with HX systems (X = F, Cl, Br)

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Résumé

Highly correlated ab-initio wavefunctions within the MRCI approaches are used in a comparative study of the interactions between C2 and the three hydrogen halides HX (X = F, Cl, Br). Some test results are also presented within the UCCSD(T)-F12 approach. The asymptotic regions are investigated for different relative orientations of the two moieties. It is shown that the three systems C2 + HX are bound, for intermolecular distances close to 3 Å, through nucleophilic interactions between C2 and HX for approaches perpendicular to the C-C axis, with decreasing interaction energies from HF to HBr. For HX approaching C2 along its axis, the interactions are governed by the electrophilic character of C2 and the interaction energies are decreasing from HBr to HF. Activation barriers towards the molecular systems HCCX or CCHX (0.58 eV and more) are calculated at short distances, making difficult the reactions towards the corresponding tetra-atomic systems.

Mots-Clés: electrophilic, nucleophilic, ab, initio, reactivity, dissociation, activation barriers.

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