Theoretical investigation on structure and stability of some neutral rare gas molecules F-Rg-BR_2 (R = F, OH, CN, CCH)

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Abstract

Ab initio and DFT calculations were performed to investigate the structure, stability, and nature of chemical bonding of the F-Rg-BR_2 (R = F, OH, CN and CCH; Rg = Ar, Kr, Xe and Rn) molecules. The geometries are optimized for ground as well as transition states using the B3LYP-D3 and MP2 methods. It has been found that the F-Rg-B portion of F-Rg-BR_2 species is linear in the ground state but curved in the transition state. The NBO, AIM, ELF and EDA analyses suggest that the molecules can be expressed as $F^-(Rg\text{-}BR_2)^+$ due to the covalent Rg-B bond and the ionic interaction between F and Rg. Calculations assert the metastable behavior of the F-Rg-BR_2 molecules, thermodynamic data shows that F-Rg-BR_2 can spontaneously dissociates into BFR_2 + Rg, the considerable energy barrier of this two-body dissociation channel calculated by the B3LYP-D3, MP2 and CCSD(T) methods affirms the kinetic stability of the F-Rg-BR_2 molecules. Thus F-Rg-BR_2 molecules are kinetically protected against the decomposition reaction and may be identified under cryogenic conditions in solid rare gas matrices or in the gas phase.

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