DFT calculations of HRgX (Rg = rare gas; X = halogen) molecules.

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Streszczenie

The applicability of DFT calculations is tested on rare-gas-containing molecules. We examine the energetics, harmonic frequencies and electron density distributions for selected triatomic HRgX molecules, where Rg is He, Ne, Ar, Kr, Xe and X is a halogen atom. Our results indicate that the density functional theory is able to reproduce the structures and harmonic frequencies of studied molecules close to the MP2 theory. On the other hand, large discrepancies between DFT and high-level ab initio methods are occasionally found. The atoms-in-molecules method is used to analyse the electronic structure of the HRgX molecules and to distinguish the stable compounds from unstable ones. Generally it is found that the best performance is observed for the hybrid exchange-correlation functionals, i.e. those incorporating "exact" Hartree-Fock exchange. However, results obtained here indicate that DFT should not be used to predict the existence and properties of HRgX-type molecules on its own, but the results should be verified also with high-level ab initio calculations.

Adres publiczny

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