In-Silico Exploration of Noble Gas Dimer Enforced By Non-Covalent Interaction

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Abstract

Density functional calculations have been carried out to investigate the possibility of trapping of noble gas dimers by cyclo[18]carbon dimer. Parallel-displaced conformation of the cyclo[18]carbon dimer is found to be the minimum energy structure. Non-covalent interaction is found to hold the noble gas dimers. The lighter noble gases (He, Ne) posses repulsive interactions, the heavier one (Ar, Kr) are held by attractive interactions forming genuine bonds. Each of the noble gas atoms in turn forms non-covalent interaction with the cyclo[18]carbon monomers. The bond dissociation energy of the noble gas dimers dramatically increases inside the cyclo[18]carbon dimer. Energy decomposition analysis reveals that dispersion plays the major role towards the stabilization energy.

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