

Behavior of HF and (HF)₂ inside a fullerene cage: A benchmarking study using different density functionals

Arpita Poddar¹, Ramachandran CN², and Pratim Chattaraj³

¹Indian Institute of Technology Kharagpur

²Indian Institute of Technology Roorkee

³Indian Institute of Technology-Kharagpur

October 15, 2022

Abstract

A proper benchmarking on the properties of HF and its dimer inside C₆₀ using density functional theory (DFT) based approaches is presented. For this purpose, 10 different DFT functionals following Jacob's Ladder have been chosen. Geometrical parameters, viz., bond length, bond angle, etc., and dipole moment have been computed. Two types of orientations, viz., L-shaped and anti-parallel of (HF)₂ inside C₆₀ are considered, the latter with an extremely short hydrogen bond. HF bond lengths are elongated upon encapsulation in comparison to its free state analogue. The calculated stability of HF@C₆₀ is functional dependent whereas, (HF)₂@C₆₀ is thermodynamically unstable for all the functionals. The kinetic stability of (HF)₂@C₆₀ is observed through ADMP simulation at 300K temperature. The red shift in HF stretching frequencies is noticed in all cases. NCI analysis exhibits a non-covalent type interaction between HF dimer and the C₆₀ cage. The total interaction energy is found to be negative for HF@C₆₀. EDA analysis showed a high value of repulsive ΔE_{Pauli} which makes the (HF)₂@C₆₀ system unstable except for the functional BP86-D3 of GGA family. Furthermore, QTAIM analysis is performed and confirmed the presence of (3, -1) bond critical point along the hydrogen bond region for L-shaped (HF)₂@C₆₀.

Hosted file

MS.docx available at <https://authorea.com/users/514902/articles/590457-behavior-of-hf-and-hf-2-inside-a-fullerene-cage-a-benchmarking-study-using-different-density-functionals>

Hosted file

Images.docx available at <https://authorea.com/users/514902/articles/590457-behavior-of-hf-and-hf-2-inside-a-fullerene-cage-a-benchmarking-study-using-different-density-functionals>

Hosted file

tables.docx available at <https://authorea.com/users/514902/articles/590457-behavior-of-hf-and-hf-2-inside-a-fullerene-cage-a-benchmarking-study-using-different-density-functionals>