Binding of Fe and S atoms to corannulene: A Theoretical Study

ANIL KUMAR KANDALAM, Virginia Commonwealth University, BIJAN RAO[1], PURUSOTTAM JENA, Virginia Commonwealth University — The equilibrium geometries and binding energies of neutral and positively charged Fe –corannulene and S-corannulene complexes are calculated under the framework of density functional theory and generalized gradient approximation for exchange and correlation functional. The global geometries are obtained by carrying out geometry optimizations using 6-311G** basis and Gaussian98 code without any symmetry constraints. In the case of neutral Fe-corannulene, the convex-η^6 and convex-η^6 binding sites are found to be energetically degenerate, hence are equally preferred by the iron atom. In cationic Fe-corannulene complex, however, the convex-η^6 binding site is clearly preferred over the other binding sites. In the case of neutral and cationic S-corannulene complexes, the sulfur atom/ion prefers to occupy the edge η^2-site on the convex face of corannulene. Here, also the energy difference between the binding sites on convex and concave faces of corannulene is very small. The preferred binding sites, calculated magnetic moments, binding energies, and ionization potentials of Fe-corannulene and S-corannulene complexes will be compared.

[1]Deceased

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