Ab initio Study of the Interactions of imidazole-SF_6 and imidazole-CH_4 complexes

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Atmospheric pollution is one of several scientific researches that it affects human health and the environment. The search of new materials of low cost and high efficiency for the capture and storage of pollutants is the object of many studies focused to the development of new technologies. The interest is the capture and sequestration of pollutants by metal organic frameworks (MOFs) [1] and specially the Zeolitic Imidazolate Frameworks (ZIF's) [2,3]. Imidazole ($C_3H_4N_2$) has received a great deal of attention for pollutants capture applications.

For this reasons, we are interesting to study the interaction between imidazole and two greenhouse effect gases such as SF_6 and CH_4, by using high-accuracy ab initio methods. In this work, the electronic structure calculations were performed using second order Möller-Plesset theory (MP2) in combination with aug-cc-Pvtz bases set. We present the minimum energy geometries of the imidazole-SF_6 and imidazole-CH_4 complexes, as well as, the corresponding harmonic frequencies and binding energies have obtained. Our results demonstrated that the SF_6 presents very important binding energies compared to CH_4, and can be decomposed directly into SF_5.

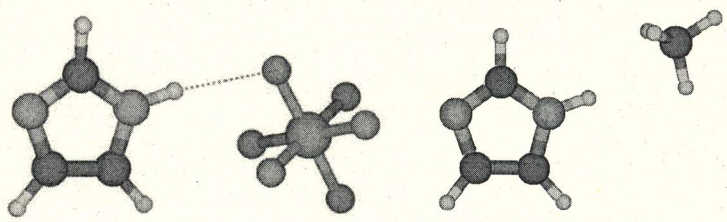

FIG. 1: Equilibrium structures of Imidazole-SF_6 and Imidazole-CH_4 complexes.

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