Intermolecular complexes between nitric oxide (NO) and closed shell molecules: A theoretical study.

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The interactions between nitric oxide (NO) and a set of small closed shell molecules were considered using *ab initio* and DFT methods. The closed molecules were: CH_4, H_2O (and the ions: H_3O^+ and OH^-) and imidazole (neutral and charged forms). According to the stabilization energies, the studied complexes are from very weak complexes to moderately strong. The features of the interactions were analyzed employing Atoms in Molecules Theory and the analysis based on Natural Bond Orbitals (NBO). The weakest complexes (CH_4…NO) were studied at corrected and non corrected counterpoise Potential Energy Surfaces (PES). The analysis of PES shows that CH_4…NO system is affected by dynamical Jahn Teller Effect as it was suggested by experimental results. The analysis of NO...H_2O complexes shows that the unpaired electron has an important role in the stabilization of complexes. According the criteria of Koch and Popelier, the *C-H…N-O*, *C-H…O-N*, *O-H…N-O*, *O-H…O-N* interactions found in NO...H_2O, NO... H_3O^+, imidazole…NO and imidazoleH^+…NO complexes can be classified as hydrogen bonds. The most stable complexes can be stabilized by charge transfer, which can be from NO to the closed shell partner or from the NO molecule to the closed shell ones depending on the nature of the interaction.