Study of NO^+…X (X = CO, Ne, H_2S, N_2) Complexes. Analysis of the Interaction Energy

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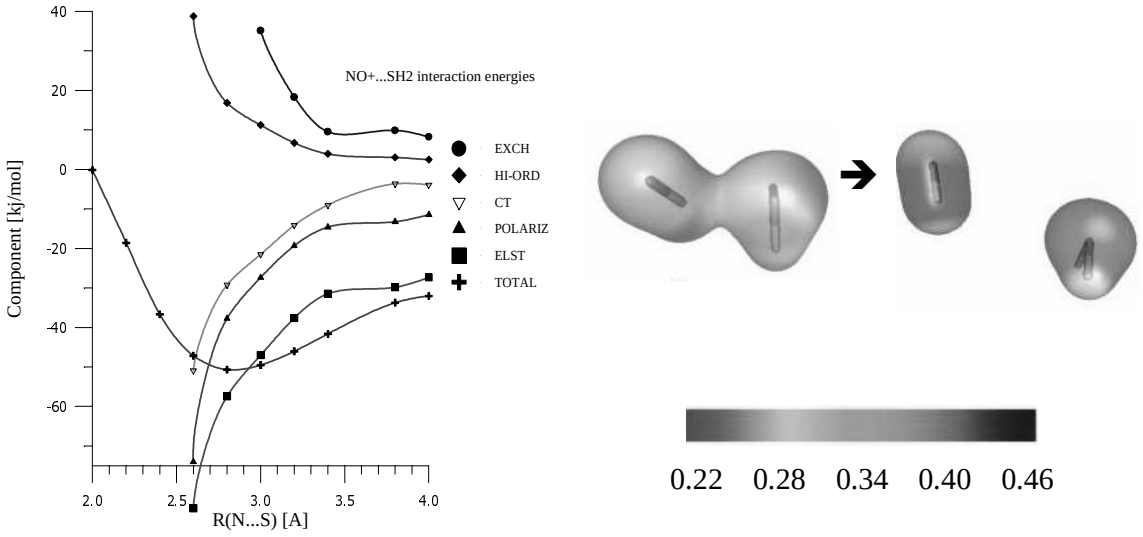
Ion molecular reactions are playing important role in the chemistry of Earth's atmosphere, in particular, in the *D layer* (from 60 to 90 km). Among the most abundant pollutants in the *D layer* is NO^+, one of the major contributors to acid rains. Complexes with NO^+ have received considerable experimental and theoretical attention recently. They represent wide variety of bonding situations, e.g., weakly bound, charge-transfer ones or complexes leading to chemical reactions.

In the first part of this study we have analyzed the components of the SCF/cc-pVTZ interaction energy of the NO^+…X complexes using Kitaura and Morokuma scheme. The resulting potential energy curves show interplay of various components of the interaction energy between ion and pertinent molecule. In the second part we present the results of MBPT[2] and CCSD[T] calculations of correlation contribution to the total interaction energy. Thermodynamic stability of the complexes in the low pressure/low temperature conditions is discussed.



NO^+...SH_2: SCF/cc-pvtz interaction energy components and electrostatic potential painted electron density transient surface of complex and monomers.