AB INITIO POTENTIAL ENERGY SURFACE FOR THE Xe+OH INTERACTION

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Ab initio potential energy surface for the gorund and first excited states of the Xe+OH complex were calculated using the state-averaged complete active space MCSCF (CASSCF) and multi reference Cl methods as implemented in MOLPRO 2006 program. A large one-electron basis consisting of the augmented-correlation consistent polarized valence five zeta (aug-cc-pV5Z) set is used. Interaction energies were obtained as the difference between the energy of the complex and energies of the fragments. We computed the fragments in the same basis set as complex to avoid so called basis set superposition error. The Xenon atom has 54 electrons; the 28 inner shell electrons are described by a relativistic pseudopotential. The interaction energy derived for a T-shaped geometry in the ground state is about 250 cm^{-1}, which support the earlier reported value obtained by CCSD method.[a] Interestingly our calculation predicts that in the first excited state this interaction energy increases to 9321 cm^{-1} for the linear gemoetry of Xe+OH complex. Thus, however in the degenerate ground state interaction is weak, but in the first excited state this (Rare Gas-OH) Van der Waals interaction behaves just like a chemical bond. Comparison with other Rg-OH complexes has been carried out.

[a] J. A. Gilijamse et al. Science, 313, 1617 (2006).