On the nature of interactions in the $F_2OXe\cdots NCCH_3$ complex : is there the Xe(IV)—N bond?

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Streszczenie

Nature of the bonding in isolated XeOF2 molecule and (F2OXeNCCH3)-N-... complexes have been studied in the gas phase (0 K) using Quantum Chemical Topology methods. The wave functions have been approximated at the MP2 and DFT levels of calculations, using the APFD, B3LYP, M062X, and B2PLYP functionals with the GD3 dispersion correction. The nature of the formal XeO bond in the XeOF2 monomer depends on the basis set used (all-electron vs. the ecp-28 approximation for Xe). Within the all-electron basis set approach the bond is represented by two bonding attractors, V-i (= 1,2)(Xe,O), with total population of about 1.06e and highly delocalized electron density in both bonding basins. No bonding basins are observed using the ecp-28 approximation. These results shows that the nature of xenon-oxygen is complicated and may be described with mesomeric equilibrium of the Lewis representations: Xe(+)O(-) and Xe(-)O(+). For both the xenon-oxygen and xenon-fluorine interactions the charge-shift model can be applied. The (F2OXeNCCH3)-N-... complex exists in two structures: parallel, stabilized by non-covalent (CO)-O-... and (XeN)-N-... interactions and linear stabilized by the (XeN)-N-... interaction. Topological analysis of ELF shows that the (F2OXeNCCH3)-N-... molecule appears as a weakly bound intermolecular complex. Intermolecular interaction energy components have also been studied using Symmetry Adapted Perturbation Theory.

Słowa kluczowe

Electron localization function (ELF), SAPT, noble gas, Complex, Bond

Adres publiczny

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