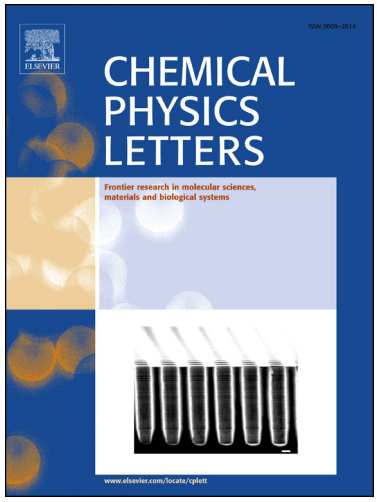

Single-electron aerogen bonds: Do they exist?

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Single-electron aerogen bonds: Do they exist?

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Abstract

A novel type of σ-hole interaction is characterized between some noble gas containing molecules ($KrOF_2$, KrO_3, $XeOF_2$ and XeO_3) and methyl (CH_3) or ethyl (C_2H_5) radical by means of ab initio calculations. This interaction is named as single-electron aerogen bond (SEAB), in view of the concepts of aerogen bond and single-electron bond interactions. The properties of SEABs are studied by molecular electrostatic potential, quantum theory of atom in molecules, natural bonding orbital and noncovalent interaction index analyses. The formation of an O···H interaction tends to increase the strength of the SEAB, when they coexist in a ternary complex.

Keywords: molecular electrostatic potential; ab initio; QTAIM; NBO; cooperativity.