Nature of the bonding in the AuNgX (Ng = Ar, Kr, Xe; X = F, Cl, Br, I) molecules. Topological study on electron density and the electron localization function (ELF).

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Streszczenie

Topological analysis of the electron localization function (ELF) has been carried out for the AuNgX (Ng = Ar, Kr, Xe; X = F, Cl, Br, I) molecules using the wave function approximated by the CCSD, MP2, and DFT(B3LYP, M062X) methods including zero-order regular approximation (ZORA). In the Ng-F bond, the bonding disynaptic attractor V(Ng,F) is missing; therefore, there are no signs of the covalent binding. The nature of the Au-Ng bond depends on the computational method used. Analysis of the ELF carried out for the AuArF and AuXeF molecules, with the wave function approximated by the CCSD and MP2 methods, shows the V(Au,Ng) attractor possibly corresponding to a partially covalent binding between the gold and noble gas atom. However, its very small basin population (<1e) and a very large value of the variance of the basin population suggest that the Au-Ng bond has a very delocalized character. Such bond nature may be related to the charge shift concept with a resonance of the Au(-+)NgX, Au(+-)NgX hybrids. The weakest Au-Ng bond, in terms of the smallest amount of electron density for the V(Au,Ng) basin, is found for the AuKrF molecule with the CCSD method (0.13e). The MP2 method, however, does not yield any V(Au, Ng) population; hence, the covalent Au-Kr bond is not confirmed. Because the V(Au,Ng) attractor is also not observed with the DFT method, the proper characterization of the Au-Ng bond requires proper description of correlation effects. Additional studies on the Au2 and [AuXe](+) molecules, performed at the CCSD and B3LYP levels, exhibit no V(Au,Au) and V(Au,Xe) bonding basins either.

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