Electron localization function studies of the nature of binding in neutral rare-gas containing hydrides: HKrCN, HKrNC, HXeCN, HXeNC, HXeOH, and HXeSH.

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Streszczenie

Neutral rare-gas containing molecules HRgCN (Rg=Kr, Xe), HXeSH and HXeOH are investigated by means of topological analysis of the electron localization function (ELF). This analysis explains the type of bonding and delocalization of electron density in chemical systems based on the indirect probability of finding two electrons with the opposite spins. The calculations reveals that all studied species are charge-transfer systems with the approximate formulas: [HKr]+0.65[CN]−0.65, [HXe]+0.66[CN]−0.66, [HXe]+0.45[SH]−0.45, and [HXe]+0.57[OH]−0.57. The isomerization process from HRgCN to HRgNC increases the charge separation to 0.72e for Kr and 0.74e for Xe containing molecules. It is shown that the Rg–C, Rg–N, Xe–S, and Xe–O bonds belong to the unshared electron type and are mainly of the electrostatic origin. The minimum of ELF in the Kr–C and Kr–N linkage, studied at the B3LYP/6-311++G(2d,2p) computational level, yields relatively high values of about 0.4 and 0.3, respectively. There is a correlation between larger stability of HRgCN isomers and an increased exchange of the electron density between the lone electron pair of carbon and the nonbonding electron density of xenon: V(C)↔V(Xe) as compared to smaller V(N)↔V(Xe) delocalization in less stable HRgNC isomers. The analysis of the CN group reveals the covalent character of the carbon–nitrogen bond, which is confirmed on the basis of presence of the disynaptic valence V(C,N) attractor positioned near to nitrogen. The HRgCN→HRgNC isomerization results in depletion of the carbon–nitrogen bond V(C,N) and a large saturation of the valence nitrogen basin V(N).REFERENCES

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