

The electronic structure of the xenon insertion compounds XXe-MX_2 ($\text{X} = \text{F}, \text{Cl}, \text{Br}, \text{I}$; $\text{M} = \text{B}, \text{Al}, \text{Ga}$).

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Nature of chemical bonding in the XXe-MX_2 ($\text{X} = \text{F}, \text{Cl}, \text{Br}, \text{I}$; $\text{M} = \text{B}, \text{Al}, \text{Ga}$) molecules have been investigated using topological analysis of Electron Localisation Function (ELF) and electron density. The wave function has been approximated by the DFT(B3LYP, M062X) and the CCSD methods using all-electron basis sets (TZVPPall, TZVall+) and the ecp-28 approximation for Xe, I with Def2-TZVPPD basis set. Electronic structure of the XXeMX_2 consists of the $[\text{Xe-MX}_2]$ fragment, bound non-covalently to the halogen atom, $\text{X}^{\delta-} \cdots [\text{Xe-MX}_2]^{\delta+}$ ($\delta = 0.4\text{--}0.7e$). The xenon-icosagen bond, Xe-M displays covalent nature in all studied molecules, confirmed by bonding disynaptic attractor $V(\text{Xe}, \text{M})$ for the ELF field with basin population ranging from 1.1 to 1.8e. The basin population of the Xe-M bond decreases together with the $r(\text{Xe-M})$ bond length increase and the increase of the polarisability of the respective halogen. The Xe-X bond always shows a non-covalent nature, confirmed by an absence of bonding attractor in the region between the core basins $C(\text{Xe})$ and $C(\text{X})$. M-X bonds can have either covalent or ionic nature depending on the type of icosagen and halogen involved in bonding. The Al-F and Ga-X ($\text{X} = \text{F}, \text{Cl}, \text{Br}$) bonds have ionic nature, except for the Ga-I bond, showing slightly covalent but highly delocalised character, confirmed by the presence of the bonding basin $V(\text{Ge}, \text{X})$ with the population of 0.64e. In addition to bonding population calculations, the analysis of the bond polarity, based on topological analysis of electron density combined with ELF fields, and delocalisation of electron density in bonding basins has been performed and discussed.

Słowa kluczowe

xenon, Electron localization function (ELF), electron density, bonding, Icosagen

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