Boron-noble gas covalent bonds in borenium and boronium compounds

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Abstract
The capability of the BH_2^+parent cation to bind noble gases (Ng) has been evaluated. The results show its potential to form borenium (BH_2Ng^+) and boronium ($BH_2Ng_2^+$) cations. Conformational search using the recently developed AUTOMATON program andCoalescence Kickmethod, in addition to thermochemical and Born-Oppenheimer molecular dynamics (BOMD) calculations, were performed. Results show that compounds containing Ng = Ar-Rn are thermodynamically and kinetically stable. Furthermore, it was found that the B-Ng bond has high dissociation energy values at both DFT and CCSD(T) levels suggesting a strong interaction. The nature of the chemical bond has been assessed according to the Quantum Theory of Atoms in Molecules (QTAIM), Natural Bond Orbital Theory (NBO) and Energy decomposition Analysis (EDA). Negative values of local energy densityH(r_c) and high values of the Wiberg bond Index (WBI) reveal its covalent nature that is confirmed by localized natural bond orbitals with 2.0 |e| occupations. Additionally, it could be observed that the orbital term (ΔE^{orb}) is the most important component (84.6-90.1%) of the interaction energy between the parent $BH_2^+$and Ng atoms, supporting the polar covalent nature of the B-Ng bond.

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