Theoretical study of intermolecular interactions in CB$_4$H$_8$–HOX (X = F, Cl, Br, I) complexes

Zohreh Derikvand$^{a,*}$, Abedien Zabardasti$^b$, Azadeh Azadbakht$^a$

$^a$Department of Chemistry, Faculty of Science, Khorramabad Branch, Islamic Azad University, Khorramabad, Iran
$^b$Department of Chemistry, Faculty of Science, Lorestan University, Khorramabad, Iran

**Highlights**

- Hypohalous acids show hydrogen bond and dihydrogen bond interactions with CB$_4$H$_8$ molecule.
- Non-classical B–B–H interactions are observed between HOX and CB$_4$H$_8$ molecules.
- Non-classical interactions are more stable than HB and DiHB interactions.
- The amount of charge transfers and $E^{(2)}$ depicted an increasing in stronger intermolecular complexes.

**Abstract**

The molecular aggregation based on intermolecular interactions between CB$_4$H$_8$ and HOX (X = F, Cl, Br and I) with particular emphasis on their bonding characteristics have been investigated using second order Moller–Plesset perturbation (MP2) method with aug-cc-pVDZ basis set. Different kinds of interactions including hydrogen bond (HB; H $\cdot$ O, XH; H $\cdot$ X), dihydrogen bond (DiHB; H–H) and non-classical B–B–H interactions were found between CB$_4$H$_8$ and HOX molecules. The structures of complexes have been analyzed using AIM and natural bond orbital methodologies. Good correlations have been found between the interaction energies (SE), the second-order perturbation energies $E^{(2)}$, and the charge transfer qCT in the studied systems.

**Introduction**

Intermolecular interactions play an important role in crystal engineering, molecular recognition as well as biomolecular systems [1,2]. The most research about intermolecular interactions has focused on the more frequent hydrogen-bonded interactions. According the traditional idea the hydrogen atoms involved in the HB should be electron-deficient (protic hydrogen). Another type of hydrogen bond is called dihydrogen bonding, in which interaction occurs between two hydrogen atoms, one positively charged and another negatively charged (hydridic hydrogen), this special kind of hydrogen bond has designated as dihydrogen bond [3–13].

The carboranes as an important class in inorganic chemistry are extensively used in coordination compounds [14–18], inorganic pharmaceuticals and biological systems, radiopharmaceuticals [19], polymers [20–22] as well as in neutron capture therapy [23]. CB$_4$H$_8$ is a carborane that has a square pyramidal structure, the carbon atom is located in the apex of pyramid and the boron...