Density Functional Theory Analysis of Borazyne Complexes of Ni, Ni(B\textsubscript{3}N\textsubscript{3}H\textsubscript{n}F\textsubscript{2-n})(CO)\textsubscript{2} (n=0-2)

Reza Ghiasi \textsuperscript{a}, Saeedeh Azmayesh \textsuperscript{b}

\textit{a) Department of Chemistry, Basic Science Faculty, East Tehran Branch, Qiam Dasht, Tehran, Islamic Azad University, Tehran, IRAN}
\textit{b) Department of Chemistry, Basic Science Faculty, Central Tehran Branch, Tehran, Islamic Azad University, Tehran, IRAN}
rezaghiasi1353@yahoo.com, rghyasi@qdiau.ac.ir

The structure and properties of benzyne have been studied theoretically and experimentally for many years\cite{1}. The replacement of CC by BN is known to lead to Borazyne that suggested as an intermediate in the formation of borazanaphthalene and diborazine, during the photolysis of borazine \cite{2}. Borazyne has not isolated and characterized. A few investigations have been reported about it \cite{3}.

The electronic structure and properties of Ni(B\textsubscript{3}N\textsubscript{3}H\textsubscript{n}F\textsubscript{2-n})(CO)\textsubscript{2} (n=0-2) complexes have been explored using hybrid density functional B3LYP theory. Calculations indicate B-fluorinated isomers are more stable, less polarizable, and harder than N-fluorinated isomers. The aromatic natures of the borazyne rings have been analyzed by nucleus independent chemical shift (NICS). The NICS values present the increasing of aromaticity in fluorinated rings. Furthermore, aromaticity of N-fluorinated rings is more than B-fluorinated ones.

The atoms in molecules (AIM) analysis indicates that Ni-C\textsubscript{carbonyl} bonds distance is well correlated with the electron density of critical point (\(\rho_{cp}\)) in all species. Additionally, the H(\(\rho\)) values are more negative for Ni–C\textsubscript{carbonyl} (trans to N) bonds, which is directly connected with relative greater predominance of \(IV(\rho)\) magnitude over the G(\(\rho\)) magnitude. This suggests a more covalent character of the Ni–C\textsubscript{carbonyl} (trans to N) bonds as compared with the trans to B ones. Generally, the greater value of H(\(\rho\)) (with negative sign), the more covalent character of the bond. It seems therefore that the covalent character of the Ni–CO bonds increases in bonds that are trans to N.

REFERENCES