The Nature of the Fe-E (E= B-Tl) Bond in $Fe(CO)_4$-EAr* and $Fe(CO)_4$-ECp* complexes. *A theoretical study*

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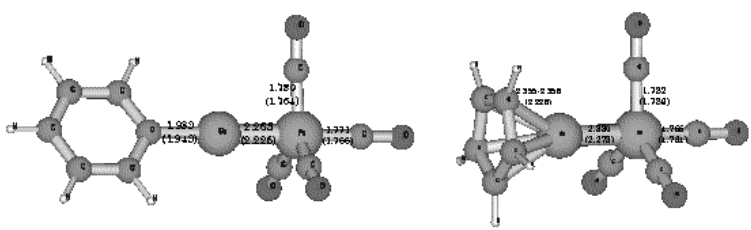
Gradient-corrected density functional (BP86) calculations have been done in order to settle the contradiction about Fe-Ga multiple bonding $Fe(CO)_4$-GaAr* and $Fe(CO)_4$-GaCp*. The stability and bonding analysis have also been done for other group-13 element complexes. Calculations are reported for model complexes $Fe(CO)_4$-EPh and $Fe(CO)_4$-ECp with (E=B-Tl).

The nature of bonding have been analyzed using NBO, CDA and ETS scheme. The analysis of bonding situation using the Charge Decomposition Analysis (CDA) and Natural Bond Orbital (NBO) partitioning scheme show that there is a substantially higher degree of Fe→E π-backbonding in PhE-$Fe(CO)_4$ than CpE-$Fe(CO)_4$ complexes, but it has revealed from NBO analysis that the nature of Fe-E bonding is mainly ionic and covalent contributions are less important. The covalent bond order is always < 1. The ETS scheme also supports the ionic nature of bonding.



The Fe-E bond dissociation energy in both complexes are quite high. Fe-E bond dissociation energies in $Fe(CO)_4$-EPh are significantly higher (roughly 15-25 kcal/mol.) than its $Fe(CO)_4$-ECp analogues. Ph→E poor π-donation indicates enhanced Fe-E(Ph) interaction. The trend for the Fe-E bond energies are fount to be B > Al > Ga ~ In > Tl.