“ Planar Hypercoordinate Carbon Atoms “

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Since the brave ideas of van’t Hoff and LeBel were made public in 1874, the tetrahedral geometry of tetracoordinate carbon has been axiomaticin organic chemistry.[1,2] Even though those ideas introduce chemistry into a three-dimensional world, the search for anti-vant’Hoff/LeBel compounds is extremely appealing. In 1970 Hoffmann, Alder and Wilcox suggested some rules on how to stabilize a planar tetracoordinate carbon (ptC) atom.[3] Each new ptC structure that is realized experimentally contradicts the classical structural theory of organic chemistry. Furthermore, it gives confidence in predictive theory as a discipline to establish the limits of such seemingly outlandish structures.

Recently, viable planar pentacoordinate carbon (ppC) atoms were predicted *in silico*.[4] Yet, there is increasing theoretical evidence that when metals surround carbon atoms it is possible for unusual coordinations to emerge that are more stable than alternative isomers with the familiar linear, trigonal, or tetrahedral geometry at the C center.

Here we report on the theoretical structure and bonding of the CE_4^{2-} and CBe_5E^- clusters (E = Al, Ga, In, Tl).[5,6] After a careful analysis of their corresponding potential energy surfaces, using a stochastic algorithm, we found that all these clusters have a ptC and a ppC structure, respectively. The bonding is analyzed in terms of the molecular orbitals and natural population analysis (NPA) charges. In the case of the CE_4^{2-} clusters, given that these doubly charged anions are not expected to be stable towards electron auto-detachments in its isolated state due to strong Coulomb repulsion, we explored also their parent alkali stabilized CE_4Li^- salt.

References

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