A Quantum Mechanical Study of the Dative Bond in Metalloatranes

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Metalloatranes are a class of organometallic ring systems which contain a metal and an electron donating group. In the 1970s, some compounds in this class were synthesized which showed evidence of a dative bond between the metal and the electron donating group. Through our computational studies, we have examined the metals silicon, germanium, tin, and lead, and the donating groups nitrogen, phosphorus, and arsenic. We have found three conformations, boat-boat, boat-chair, and chair-chair, for the metals silicon(II), germanium(II), and lead(II) where the dative bond length was greater than the sum of the covalent radii but shorter than the sum of the van der Waals radii. For these same metals and conformations, it was found that the length of the dative bond increased as the size of the electron donating group increased moving down group 5A. Examination of molecular orbtials from HOMO-1 to HOMO-10 show a shared lobe of electron density between the metal and the donating group, further supporting the presence of a dative bond. Natural bond order analysis data also supports the existence of the dative bond in several of the systems studied.