Structural Diversity and Fluxionality in Half Sandwich Phenalenyl Complexes

Jason Andresen
University of Richmond

Organometallic sandwich and half sandwich complexes are used in the treatment of gasoline and are also being used in organic chemistry as potential catalysts. As advances in nanochemistry and new potential roles for organometallic complexes in electronics are developed, the information gained through theoretical analyses of these complexes will become increasingly important. We examine the structural possibilities of M*P* half sandwich complexes of group 1 and 11 metals as well as a selection of transition metals (M=Groups 1, 5-8, and11) for which such complexes are known to be or may be stable. We looked at the group 1 and 11 metals as metal-only complexes and the transition metals are studied traditional "piano-stool" complexes. Of particular interest for us is the distinction between interactions of the 5-electron and 6-electron systems within the ring structure. The structural preferences of the group 1 and 11 half sandwich complexes are markedly different from one another. Optimizations are completed for the transition metal half sandwich complexes; the thermodynamic and binding properties of these complexes are currently under investigation.