

“Endless” Multidecker Sandwich Compounds

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Abstract: Donald and Bober recently investigated the bonding and stability in a series of sandwich complexes where three ansa fragments (see Figure) were bound to a common central (benzene) ring. The focus in that work was the stability of novel organometallic sandwich systems and an assessment of the Mills-Nixon effect. The latter effect persisted as an essentially unconfirmed hypothesis that strain imposed by substitutes around a benzene ring will stabilize a distorted form of the ring where the electrons are largely localized. The work uncovered no such localization, but demonstrated the significant stability of the tris-sandwich structure. One intriguing category of sandwich complex is the group of multidecker sandwich systems where the ring-metal-ring- sequence is extended to two, three, or more repeating units. In this work, we examined the structure, bonding, and stability of end-linked multidecker chain building on the motif examined by Donald and Bober. The stability of the complexes relative to the isolated hexaphenyl benzene and the six metal atoms is assessed and the relative energies are reported along with the geometrical information for the systems considered. Our work is ongoing; the entropy contributions to the free energy of the complex and the potential utility of novel ansa-ring structures for polymer catalysis, which is one of the prominent applications of ansa-complexes, are two aspects for future consideration.

