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四层过渡金属夹心化合物的电子构型

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摘要 本文利用共点稠合型硼烷的拓扑结构规则和EHMO量子化学计算方法,
讨论了四层过渡金属夹心化合物的电子构型, 以及它与几何结构之间的关系. 用于解释实际化合物的电子构型. 继而, 对四层、三层和双层夹心化合物的电子构型与几何结构之间的关系进行了比较和讨论.

关键词 量子化学 电子结构 过渡金属化合物 硼烷 硼杂环化合物 夹心化合物 休克尔分子轨道

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The electronic configurations of tetra-decker transition metal sandwich complexes

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Abstract A tetra-decker sandwich complex with normal geometry can be visualized as a common-vertices conjuncto-heteroborane and the no. of its valence bonding orbitals, 21, has been obtained by means of the structural rule of conjuncto-heteroboranes. By using EHMO quantum chem. calcns., the variations of MO energies with respect to the extent of stretch of the skeleton have been discussed to explain that the no. of valence bonding orbitals of the mol. changes from 21 to 23. Anal. of the results about the relationships between the electron configurations and geometries for actual tetra-decker sandwich complexes shows that the above discussion is correct. The comparison of tetra-decker with triple- and double-decker sandwich complexes indicates that the relationships are qual. the same, while varying rates increase with increasing no. of transition metal atoms.

Key words QUANTUM CHEMISTRY ELECTRONIC STRUCTURE TRANSITION METAL COMPOUND BORANE BORON HETEROCYCLIC COMPOUNDS SANDWICH COMPOUNDS HUCKEL MOLECULAR ORBITAL

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