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过渡金属异核原子簇化学键研究 **1:** Ⅷ-Ⅷ**,** ⅥB-Ⅷ族双金属原子簇电子结构研究

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摘要 本文对18个Ⅷ族双金属四面体簇和16个ⅥB-Ⅷ异金属四核簇进行了量子化学研究, 用DV-Xα方法讨论了它们的化学键、电荷转移、能级态密度。计算结果表明: Ⅷ族四面体簇需36个金属电子, 其中12个形成6个金属簇骼轨道, 24个与配体成键; ⅥB-Ⅷ异金属簇核中, 因两金属能带、电负性差异, ⅥB原子易向Ⅷ原子转移电荷, 环戊二烯基配体促进这一过程; 异金属簇能级总价带比单金属簇收缩, 而d能带比单金属簇展宽。

关键词 环戊二烯 P 化学键 电子结构 电荷转移 原子簇

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Quantum chemical research for heterometal four-nuclear cluster compounds of transition metal 1: Chemical bond of four-nuclear bimetal cluster formed from Ⅷ and ⅥB-Ⅷ elements

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Abstract In this paper 18 four-nuclear bimetal cluster compounds formed from Ⅷ group elements and 16 heteronuclear cluster formed from Ⅷ-ⅥB group elements have been studied using DV-Xα method of quantum chemistry. Their chemical bond, electron transfer and density of state in energy are discussed. The calculated results show: there are 6 metallic skeleton orbitals in Ⅷ group tetrahedral compounds and 36 metallic electrons, in which 12 electrons are used to forming cluster skeleton orbitals and 24 electrons to forming coordinate bond with carbonyl (if it is no enough to 24, may replenish by some hydrogen-bridge electrons). For metal core of Ⅷ-ⅥB cluster, electron transfer is clearer from ⅥB metal to Ⅷ metal, because d orbital energy of Ⅷ atom is lower than ⅥB atom and ⅥB atom coordinates with cyclopentadienyl, which pushes charges from ⅥB atom toward the cluster one. In general total valence band of energy in heterometal cluster is more constract than monometal cluster, but its d orbital energy is more extensive than later.

Key words CYCLOPENTADIENE P CHEMICAL BONDS ELECTRONIC STRUCTURE CHARGE TRANSFER

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