

担载四核羰基簇:FeCo~3(CO)~11PPh 在聚苯乙烯表面簇畸变的EXAFS研究

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**摘要** 通过配体取人工将四核羰基簇FeCo~3(CO) 锚联在磷化的聚苯乙烯表面,获得担载簇FeCO~3(CO)~11PPh/poly,目的在于使簇结构偏离较高对称性,以考察锚联过程对簇结构的影响.本文以EXAFS(Extended x-ray Absorption Fine Structure)方法研究了担载样品的结构.结果显示担载簇与FeCO~3(CO)~11PPh 晶体具有相同的结构模式,尤其是磷配体确实与一Co原子相连接.EXAFS结果表明:(1)与FeCO~3(CO) (其簇具有三重对称结构)比较,锚联使Co-Fe键增长0.005nm;金属-金属及金属-桥联碳壳层Debye-Waller因子均增大一倍而金属一端碳壳层的值变化很小.说明金属-金属间实际键长值具有一较宽分布,因而其簇已偏离了三重对称结构;(2)与FeCO~3(CO)~11PPh 晶体的结构比较,Co-Fe键长长0.003nm而Co-Co键长则短约0.002nm.考虑到EXAFS分析只能给出平均键长值,因此认为,存在于FeCO~3(CO)~11PPh 晶体中的由于一个羰基被磷配体取代而引起的簇畸变,在锚联后被加剧.

**关键词** [聚苯乙烯](#) [铁络合物](#) [羰基化合物](#) [三苯基膦](#) [钴络合物](#) [EXAFS](#)

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## Immobilized detranuclear carbonyl cluster:EXAFS investigation on the framework distortion of FeCoo~3(CO)~11PPh on the surface of polystyrene

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**Abstract** The aim of anchoring the cobalt-iron tetranuclear carbonyl cluster FeCo<sub>3</sub>(CO)<sub>12</sub>- on the phosphinated surface of the polystyrene through ligand substitution was to obtain the cluster FeCo<sub>3</sub>(CO)<sub>11</sub>PPh<sub>3</sub>-/poly. The structural model of the mol. studied was the same as in the FeCo<sub>3</sub>(CO)<sub>11</sub>PPh<sub>3</sub>- crystal: the phosphine ligand was indeed bonded to one Co atom. In comparison with those of FeCo<sub>3</sub>(CO)<sub>12</sub>-, the structure has a three-fold symmetry. The bond length Co-Fe was longer by 0.005 nm. The Debye-Waller factors of the M-M and M-C(b) (M = metal; C(b) = bridging carbon) shells were about two times greater, but that of C(t) (C(t) = terminal carbon) shell, remained almost the same. In comparison with the FeCo<sub>3</sub>(CO)<sub>11</sub>PPh<sub>3</sub>- structure, the Co-Fe bond length was 0.003 nm longer, and the Co-Co bond length was 0.0 (2 nm shorter. The distortion of FeCo<sub>3</sub>(CO)<sub>11</sub>PPh<sub>3</sub>- is caused by substituting one CO by PPh<sub>3</sub>.

**Key words** [POLYSTYRENE](#) [IRON COMPLEX](#) [CARBONYL COMPOUNDS](#) [TRIPHENYLPHOSPHINE](#) [COBALT COMPLEX](#)

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