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Full Papers

聚合物$\{[Cu^{II}(Hpb)(mal)]H_2O\}_n$:单体的量子化学计算和磁性研究

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摘要 $\{[Cu^{II}(Hpb)(mal)]H_2O\}_n$(Hpb=2,2-联苯并咪唑，mal=顺丁烯二酸)是一个一维螺旋链状聚合物，为了研究其电子结构，截取该聚合物的单体并用不同的官能团对其进行封闭。应用混合的密度泛函B3LYP方法对所选的这些构型进行了量子化学的几何优化，结果表明用-OH_2封闭的构型与实验结果最为接近。该优化结构被用于后面的计算，如，前线分子轨道及自然电荷布居的分析。除此之外，实验研究发现该配合物的磁性特征为两个Cu(II)离子之间的弱的抗铁磁性交互作用。在破缺对称性方法的基础上，用密度泛函理论计算了该配合物的磁交换偶合常数，计算结果与实验数据符合良好。

关键词 聚合物,磁性,量子化学计算,自然键轨道

分类号

A Polymer $\{[Cu^{II}(Hpb)(mal)]H_2O\}_n$: Magnetic Studies and Quantum Chemical Calculation for Its Monomer

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Abstract $\{[Cu^{II}(Hpb)(mal)]H_2O\}_n$ (Hpb＝2-2'-pyridylbenzimidazole, mal＝maleic acid) is a helical chain-like polymer complex. In order to investigate the electronic structure of the complex, the monomer $Cu^{II}(Hpb)(mal)$ was obturated with different functional groups respectively. For these selective segments, the geometry optimizations were conducted by using hybrid DFT (B3LYP) methods to find that the structure obturated with H_2O was better consistent with the experiment, and then this model would be used to latter calculations, such as the frontier molecular orbital and the NBO charge population analysis. In addition the magnetic behaviors of this complex were analyzed by experiments and the weak antiferromagnetic couple between copper(II) ions was observed. The exchange coupling constant was calculated by DFT based on the spin broken symmetry formalism. The calculated coupling constants were in good agreement with the experimental data.

Key words polymer magnetic quantum chemical calculation natural bond orbital

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