



[Rh(DIPHOS)(MAC)]⁺结构优化的量子化学方法研究

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The geometry optimizations of [Rh(DIPHOS)(MAC)]⁺ complex with quantum chemistry

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摘要 采用相对论赝势abinitio从头算及密度泛函B3LYP方法,对[Rh(DIPHOS)(MAC)]⁺络合物的结构进行了优化,并将采用不同方法和基组的优化结果与X射线衍射实验数据对照.结果表明用量子化学方法,优化含金属重原子的较大体系中间态的结构是方便可行的.B3LYP方法能改善与Rh有关的结构参数,对P原子加极化d函数还能改善P-Rh键长.

关键词: B3LYP [Rh(DIPHOS)(MAC)]⁺ 结构优化 中间态

Abstract: The relativistic pseudopotential ab initio calculation and the density functional theory(B3LYP)were separately used to perform the geometry optimizations for the cationic [Rh(DIPHOS)(MAC)]⁺ complex.The geometry optimized conformed perfectly to the data of x-ray diffraction in the different basis sets and methods.The results show these calculation methods can be used in the optimization of the larger intermediates including heavy metal.The B3LYP method can improve the geometry parameters in relationship with Rh.P-Rh bond lengths also are improved when increasing a d-polarization function to the basis set of P atoms.

Key words: B3LYP [Rh(DIPHOS)(MAC)]⁺ geometry optimization intermediate

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