

FULL PAPERS

铁硫蛋白及其模型化合物中铁硫共价性研究

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摘要

铁硫团簇中金属和配体间强的共价性在决定其反应特性中具有重要作用。基于Phillips理论发展的一个半经验模型被应用于铁硫团簇共价性的定量计算。结果表明穆斯堡尔谱和吸收光谱对铁硫团簇的共价性能够提供直接的实验探测。

关键词 [穆斯堡尔谱](#), [铁硫团簇](#), [共价性](#)

分类号

**Studies of Iron-Sulfur Covalency in the Model System and Proteins**

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**Abstract** It was found that the highly covalent nature of the metal-ligand interactions in the Fe-S cluster clearly played an important role in determining the reactivity of the sites. A semi-empirical model, based on the Phillips theory of bonding was developed for quantitative explanation of covalency in Fe-S cluster, showing that Mossbauer spectroscopy and electronic absorption spectroscopy provided the direct experimental probe of covalency of Fe-S<sub>n</sub> clusters.

**Key words** [mossbauer spectroscopy](#), [iron-sulfur cluster](#), [covalency](#)

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