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交叉学科

密度泛函理论对Cu_6团簇异构的研究

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摘要

使用可视化图形用户界面程序GaussView给出了Cu_6团簇所有可能存在的结构， 用量化计算软件Gaussian03的B3LYP杂化密度泛函和SDD基组对所给结构进行优化， 最终得到了8种Cu_6团簇的异构体。 对所得异构体的结合能和结构进行了分析， 发现结合能和实验值以及理论值符合得很好， 在结构方面其最稳定的是平面三角形结构。 在8种异构中有正五边形等3种结构是首次模拟得到的， 所得结果为以后的理论和实验工作提供了参考。

The possible structure of Cu_6 cluster has been given with the GaussView that is a graphical user interface software. The structure optimization was performed on the B3LYP functional and SDD basic set of the quantum computational software of Gaussian03. And eight isomers of Cu_6 cluster were calculated. The binding energy and the structure of eight isomers have been investigated in detail. The result showed that the value of the binding energy was in reasonable agreement with available experimental data， as well as with other theoretical results， and the most stable structure was the triangle of plane. Three new isomers of the Cu6 cluster have been got in our work， which would be the valuable data for the further theoretical and experimental study.

关键词 Cu6团簇； 结合能； 结构； Gaussian03

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