中南大学学报 自然科学版 英文版

教育部 主管
中南大学 主办

论文摘要

中南大学学报(自然科学版)

ZHONGNAN DAXUE XUEBAO(ZIRAN KEXUE BAN)

Vol.32 No.6 Dec.2001

[PDF全文下载] [全文在线阅读]

文章编号：1005-9792(2001)06-0591-04

四钼酸铵结构及稳定性的量子化学计算

吴争平, 尹周澜, 陈启元, 张平民, 李 洁

(中南大学化学化工学院,湖南长沙 410083)

摘 要：

关键字：四钼酸铵;结构;稳定性;量子化学

Theoretical calculation on the structure and stability of ammonium tetramolybdate

WUZheng-ping,YIN Zhou-lan,CHENQi-yuan,ZHANG Ping-min,LI Jie

（College of Chemistry and Chemical Engineering, Central South University, Changsha 410083, China）

Abstract: The total energy and atomic charges of ammoniumtetramolyb date with three possible structures were computed with RHF/3-21G, STO-3G, and their geometrical structures were optimized using the molecular mechanics optimization method. The algorithm of optimization used in this work is steepest descentmethod and the termination condition is RMS(Root-mean-square) gradient of 0.42 kJ·mol-1. The calculation modelswere protracted and optimized with CS Chem Office and HyperChemPro 6.0 programs. All calculation work was accomplished with Gaussian 98 program. The calculated results show that the structure of ammonium tetramolyb date with eight MoO6is relatively stable and its contortion is the smallest.

Key words:ammonium tetramolybdate; structure; stability; quantum chemistry

电 话： 0731-88879765 传真： 0731-88877727
电子邮箱： zngdxb@mail.csu.edu.cn 湘ICP备09001153号