Theoretical Studies on Structure and Properties of Bis-(5-nitro-tetrazolato) Tetraammine Cobalt (Ⅲ) Perchlorate Molecule and Crystal

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Abstract: The density functional theory(DFT) was used to study molecule and crystal of bis-(5-nitro-tetrazolato) tetraammine cobalt (Ⅲ) perchlorate (BNCP). DFT calculations of BNCP were performed using four different spin-restricted functionals (SVWN5, PBE, TPSS and B3LYP) with the 6-31G** as the basis set. The results show that the TPSS (Tao, Perdew, Staroverov and Scuseria) functional best reproduce the experimental geometries. At the same time, the crystalline of BNCP was studied by PW91 of DMOL^3. Then, the electronic structure of molecule and density of state, lattice energy, thermodynamic parameters of BNCP crystal were explored. The results show that the metal-ligand interaction in the title complex is covalent. And the frontier band consisted in the main of perchlorate ion, so it is the most active part of the compound. Meanwhile, the relationship between the temperature and thermodynamic parameters was obtained.

Key words: physical chemistry; density functional theory(DFT); periodical calculation; density of state; thermodynamic parameter; bis-(5-nitro-tetrazolato) tetraammine cobalt (Ⅲ) perchlorate (BNCP)

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西北工业大学航天学院汪亮教授编著的普通高等教育“十一五”国家级规划教材《燃烧实验诊断学》第2版由国防工业出版社于2011年7月出版。

该书较系统地介绍了有代表性的燃烧实验诊断技术，并以光谱法为重点，包括一阶弹性与非弹性散射法、三阶非线性散射法以及光学发射与吸收法，着重讲述了每种诊断技术的工作原理、测量方法、实验装置和应用举例，为读者了解与应用这些诊断技术提供了必需的基本知识。

与第1版相比，该书一方面新增了3章：分子光谱学、平面流场的二维测速仪和内燃机的燃烧实验诊断法。另一方面该书对第1版各章进行了不同程度的充实与完善，主要涉及：增加了散射横截面、光与粒子的相互作用等基本概念的描述；补充了光纤耦合红外吸收法，新增了燃速测量用X射线吸收法和密闭燃烧器法；充实了拉曼散射法、激光诱导荧光法和简并四波混频法等章节的内容。

全书共12章，内容涉及分子光谱学、拉曼散射法、激光诱导荧光法、相干反斯托克斯拉曼散射法、简并四波混频法、红外吸收法、原子谐振吸收光谱法、固体推进剂燃速测量用X射线法、超声波法和密闭燃烧器法。本书还介绍了激光多普勒测速仪、相位多普勒粒子分析仪、粒子成像测速仪、平面多普勒测速仪、分子示踪测速仪、激波管技术、燃烧声导纳测量以及内燃机汽缸内的流场与燃烧测量等。

该书可作为工程热物理、热能动力、汽车内燃机、航空宇航推进理论与工程等学科专业的本科生与研究生教材或参考书，亦可供相关专业的科研和技术人员参考。

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