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论文

含能配合物[Mn(DAT)₆](ClO₄)₂的合成、晶体结构、热行为及感度性质

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摘要:

合成了新型含能配合物[Mn(DAT)₆](ClO₄)₂(DAT=1,5-二氨基四唑), 用X射线单晶衍射法测定了其晶体结构. 该晶体属三方晶系, P3c1空间群, a=b=1.18435(17) nm, c=1.3081(3) nm, α=β=90°, γ=120°, V=1.5891(5) nm³, Z=2. 该配合物分子结构单元中有1个Mn²⁺离子、6个DAT分子和2个ClO₄⁻离子. 由6个DAT分子中的6个N原子与中心Mn²⁺离子配位形成六配位、非中心对称的畸变八面体结构. 利用元素分析、差示扫描量热分析(DSC)、热重-微分热重分析(TG-DTG)等方法进行了表征, 研究了其感度性能. 研究表明, 该配合物对外界刺激具有很高的响应性和危险性.

关键词: 锰含能配合物; 1,5-二氨基四唑; 合成

Synthesis, Crystal Structure, Thermal Behavior and Sensitivity Properties of New Energetic Compound [Mn(DAT)₆](ClO₄)₂

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Abstract:

A new energetic coordination compound [Mn(DAT)₆](ClO₄)₂(DAT=1,5-diaminotetrazole) was synthesized by DAT and manganese perchlorate and characterized by elemental analysis, differential scanning calorimetry, thermogravimetry-differential thermogravimetry, and X-ray single crystal diffraction method. The crystal belongs to trigonal system and its crystal structure data are as follows: a=b=1.18435(17) nm, c=1.3081(3) nm, α=β=90°, γ=120°, V=1589.1(5) nm³, Z=2. The molecule of the title compound contains one Mn²⁺ cation, six DAT molecules and two ClO₄⁻ anions. The central manganese(II) cation is coordinated by six N atoms from six DAT molecules to form a six-coordinated and distorted octahedral structure. In addition, the sensitivity properties of the title compound were studied. The result shows that the title compound has good sensitivity.

Keywords: Manganese(II) energetic compound; 1,5-Diaminotetrazole; Synthesis

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