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**3,5-二羟基-2,4,6-三硝基苯酚氨基脒铵盐半水合物的合成、晶体结构和热分解特性**

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摘要 通过2,4,6-三硝基-1,3,5-苯三酚(TNPG)与氨基脒(SCZ)反应制备了新化合物3,5-二羟基-2,4,6-三硝基苯酚氨基脒铵盐半水合物(SCDHTNP·0.5H<sub>2</sub>O),用X-射线单晶衍射对其结构进行了测定,用元素分析、

FTIR、DSC、TG-DTG对其结构进行了表征.晶体结构分析表明,该化合物属单斜晶系, $P2_1/n$ 空间群,

化学计量式为: C<sub>7</sub>H<sub>9</sub>N<sub>6</sub>O<sub>10.50</sub>.晶体学参数为:  $a = 1.3791(3)$  nm,  $b = 0.9256(19)$  nm,  $c = 2.0468(4)$  nm,  $\beta = 106.93$

(3)°,  $V = 2.500(9)$  nm<sup>3</sup>,  $Z = 8$ ,  $D_c = 1.835$  g/cm<sup>3</sup>,  $M_r = 345.20$ ,  $F(000) = 1416$ ,  $s = 0.945$ ,  $\mu(\text{Mo } K\alpha) = 0.174$  mm<sup>-1</sup>.

最终偏离因子 $R = 0.0401$ ,  $wR = 0.0896$ .通过分析可知,SCDHTNP·0.5H<sub>2</sub>O的每个结构单元中有2

个氨基脒铵阳离子、2个3,5-二羟基-2,4,6-三硝基苯酚阴离子和1结晶水分子,分子中存在静电力和大量的氢键,形成稳定的层状结构.在线性升温条件下,SCDHTNP·0.5H<sub>2</sub>O的热分解过程为一个吸热脱水过程和178-241 °C之间有两个强烈分解放热过程,同时产生大量的气体产物.

关键词 [氨基脒,2,4,6-三硝基间苯三酚,制备,晶体结构,热分解](#)

分类号

### Synthesis, X-ray Crystal Structure and Thermal Decomposition Character of Semicarbazidium 3,5-Dihydroxy-2,4,6-trinitrophenolate Hemihydrate

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**Abstract** A new compound, semicarbazidium 3,5-dihydroxy-2,4,6-trinitrophenolate hemihydrate (SCDHTNP·0.5H<sub>2</sub>O), was synthesized by the reaction of the aqueous solutions of semicarbazide with trinitrophenol. Its structure was determined by single-crystal X-ray diffraction analysis and characterized by elemental analysis, FTIR, DSC and TG-DTG techniques. The crystal is monoclinic with space group  $P2_1/n$  and the empirical formula C<sub>7</sub>H<sub>9</sub>N<sub>6</sub>O<sub>10.50</sub>. The unit cell parameters are:  $a = 1.3791(3)$  nm,  $b = 0.9256(2)$  nm,  $c = 2.0468(4)$  nm,  $\beta = 106.93(3)^\circ$ ,  $V = 2.4995(9)$  nm<sup>3</sup>,  $Z = 8$ ,  $D_c = 1.835$  g/cm<sup>3</sup>,  $M_r = 345.20$ ,  $F(000) = 1416$ ,  $s = 0.945$ ,  $\mu(\text{Mo } K\alpha) = 0.174$  mm<sup>-1</sup>. The final  $R$  and  $wR$  are 0.0401 and 0.0896. Its structure consists of two semicarbazidium cations, two 3,5-dihydroxy-2,4,6-trinitrophenolate anions and one crystal water molecule, which are interconnected by electrostatic forces and hydrogen bonds into layer structure, making the title compound very stable. Under a linear heating rate, the thermal decomposition processes of SCDHTNP·0.5H<sub>2</sub>O have one endothermic dehydration stage and two intensive exothermic decomposition stages at 178—241 °C to evolve abundant gas products.

**Key words** [semicarbazide](#) [trinitrophenol](#) [synthesis](#) [crystal structure](#) [thermal analysis](#)

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