Synthesis, Structure and Properties of an Energetic Coordination Polymer [Pb(BTO)(H$_2$O)]$_n$

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Abstract: An energetic coordination polymer, [Pb(BTO)(H$_2$O)]$_n$(BTO=1*H*,1′*H*-5,5′-bistetrazole-1,1′-diolate) was synthesized by a simple one-step solvothermal method using Pb(NO$_3$)$_2$ and H$_2$BTO·2H$_2$O as raw materials. The target compound was characterized by single-crystal X-ray diffraction, Fourier transform infrared (FT-IR) spectra and elemental analysis. The thermal decomposition process of the energetic coordination polymer was studied by differential thermal analysis (DTA), differential scanning calorimetry (DSC) and thermogravimetry-derivative thermogravimetry (TG-DTG). Its kinetic parameters of thermal decomposition (activation energy E_K、E_O and pre-exponential factor A) were calculated by Kissinger's method and Ozawa's method. Its characteristic drop height of impact sensitivity (H_{50}) was determined by WL-1 type impact sensitivity test instrument. The compound was explored as additive to promote thermal decomposition of ammonium perchlorate (AP) by DTA. Results show that the crystal belongs to monoclinic, its space group is *C*2/*c* with crysta parameters of *a*=14.342(3) Å, *b*=6.5757(12) Å, *c*=8.4715(16) Å, *V*=683.3(2) Å^3, D_c=3.823 g·cm^{-3}, *Z*=4. Its thermal decomposition temperature on DSC curve at 5 K·min^{-1} is 582.2 K, there are three mass loss stages on TG curve with a main mass loss between 543.9 K and 599.5 K, the mass of the final residue is 44.60%. E_K=211.67 kJ·mol^{-1}, E_O=210.64 kJ·mol^{-1}, ln(A/s^{-1})=18.594, H_{50}=7.6 cm, revealing that it has better thermal stability and appropriate sennsitivity. When the addition amount of the coordination polymer is 10 wt%, the high temperature decomposition peak of AP is decreased by 40.1 K, the intense degree of the thermal decomposition reaction is also greatly improved, showing that it has good catalytic performance to AP.

Key words: energetic coordination polymer; 1*H*,1′*H*-5,5′-bistetrazole-1,1′-diolate (BTO); single crystal structure; thermal behavior; [Pb(BTO)(H$_2$O)]$_n$

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更 正

《含能材料》2017 年第 1 期《混合炸药设计研究进展》一文中,第 4 页,图 1 的序号应为图 2,英文 Fig.1 应为 Fig.2。特此更正。

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