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Synthesis, Crystal Structure and Properties of a Novel Energetic Material Dirubidium 5, 5'-Bis(tetrazole-1-oxide)

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Abstract: A new energetic material dirubidium 5,5'-bis(tetrazole-1-oxide) (BTORb) was synthesized by using 1*H*,1'*H*-5,5'-bistetrazole-1,1'-diolate (BTO) as the original material. The monocrystal of target salt was first cultivated by the method of gradual evaporation, and the single crystal structure was menstruated by single X-ray diffraction. It is found that the Rb^+ and BTO^{2-} formed a dissymmetrical structure. In different layers, they are alternately arranged and connected with each other, forming a three-dimensional reticular structure. Its thermal decomposition behavior was investigated through DSC and TG-DTG technologies, indicating a good thermal stability with a decomposition temperature beginning at 292 °C. Its kinetic parameters of non-isothermal reaction was calculated by Kissinger and Ozawa methods with the equation of Arrhenius is $\ln k = 13.51 - 186.3 \times 10^3 / RT$. Its standard heat of formation was calculated with the result of $274.91 \text{ kJ} \cdot \text{mol}^{-1}$. Its critical temperature of thermal explosion T_b is 356.7 °C, indicating that the salt has a good thermal stability. The impact sensitivity (H_{50}) of BTORb is 34.8 cm, with the drop hammer of 800 g. The friction sensitivity is 36%, under the condition of 70°, 1.23 MPa. The 50% fire energy of electrostatic spark sensitivity is 0.34 J.

Key words: energetic material; dirubidium 5, 5'-bis(tetrazole-1-oxide) (BTORb); synthesis; crystal structure; properties

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