Synthesis, Crystal Structure and Properties of Potassium 7-Hydroxy-4, 6-dinitrobenzofuroxan Monohydrate (KDNP·H_2O)

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Abstract: The main disadvantages of lead 2, 4, 6-trinitroresorecinate (LTNR) are too high electrostatic sensitivity and the harm to the human body and the environment caused by lead. In search of a replacement for LTNR, potassium 4,6-dinitro-7-oxygen-benzofuroxan monohydrate(KDNP·H_2O) was synthesized by two-step method. The single crystal of the compoud was obtained by solvent evaporation method. Its structure was chracterized by elemental analysis, IR spectroscopy, ^{1}H NMR/^{13}C NMR spectroscopy and X-ray single-crystal diffraction. Its sensitivities were measured according to the Chinese military standard test method GJB-5891. The heat of detonation was calculated. The detonation parameters of the compoud were calculated by Kamlet-Jacobs equations. Results show that the crystal is triclinic, space group *P*-1 with one crystal water. For this primary explosives, the impact sensitivity (H_{50}) is 21.3 cm, the electrostatic sensitivity (E_{50}) is 0.69 J, the friction sensitivity is 56%, the flame sensitivity is 24.7 cm, the heat of detonation is 3.50 kJ·g^{-1}, the detonation velocity is 6.77 km·s^{-1} and detonation pressure is 21.25 GPa, revealing that KDNP·H_2O is a primary explosives with lead-free, safe and environmental protection.

Key words: potassium 4,6-dinitro-7-oxygen-benzofuroxan monohydrate (KDNP·H_2O); crystal structure; detonation performance; primary explosives

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