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Synthesis and Properties of 5-Methyl-4-nitro-1*H*-pyrazol-3-(2*H*)-one and its Energetic Ion Compounds

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Abstract: A new energetic compound 5-methyl-4-nitro-1*H*-pyrazol-3-(2*H*)-one (MNPO) was synthesized with total yield of 68%, using ethyl 3-oxobutanoate as raw material. Corresponding ion salts were prepared via metathesis reaction and neutralization reaction by the reactions of MNPO with a series of high nitrogen cation. Their structures were characterized by single-crystal X-ray diffraction, Fourier transform infrared(FT-IR) spectroscopy, nuclear magnetic resonance(¹H NMR, ¹³C NMR) spectrometry, elemental analyses and other means. Their thermal decomposition temperatures were measured by thermogravimetry(TG) and differential scanning calorimetry(DSC). Their detonation performances were calculated with Explo5 v6.02 software. Results show that the crystal of MNPO belongs to orthorhombic system, and its space group is *Pbca* with crystal parameters of $a=71495(18)$ nm, $b=1.1639(3)$ nm, $c=1.3834(3)$ nm, $V=1.1512(5)$ nm³ and $Z=8$. For energetic ion salts of MNPO with densities of 1.62–1.74 g·cm⁻³, their decomposition temperatures are in the range of 181–272 °C, theoretical detonation velocities are greater than 7000 m·s⁻¹ and detonation pressures are greater than 15 GPa. The measured impact and friction sensitivities are low, in which, the impact sensitivity of ammonium salt of MNPO is 28 J and the friction sensitivity 240 N.

Key words: synthesis; 5-methyl-4-nitro-1*H*-pyrazol-3-(2*H*)-one(MNPO); energetic ion compounds; single crystal structure

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