

Alkali Salts of 1-Methyl-5-nitriminotetrazole – Structures and Properties

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Alkali salts of 1-methyl-5-nitriminotetrazole (**1**, 1-MeAtHNO₂) are common intermediates in the synthesis of alkylated nitriminotetrazoles and their derivatives and can be used as brilliant coloring agents in modern pyrotechnics, due to their cations in combination with the high nitrogen contents. The structures of the crystalline state of A⁺ 1-MeAtNO₂[−] · xH₂O (A = Li⁺, x = 1 (**2**), A = Na⁺ (**3**), A = K⁺ (**4**), A = Rb⁺ (**5**) and A = Cs⁺ (**6**), all x = 0) were determined using low temperature single crystal X-ray diffraction. In addition, the compounds were characterized using vibrational (IR and Raman) and multinuclear NMR spectroscopy (¹H, ⁷Li, ¹³C, ¹⁴N, ¹⁵N), elemental analysis and differential scanning calorimetry (DSC). Since tetrazoles are known to be promising energetic materials, the heats of formation were calculated using experimentally determined heats of combustion obtained by bomb calorimetry. The sensitivities of all compounds were tested using the BAM drophammer and friction tester showing them to have no sensitivity neither against friction (< 360 N) nor impact (< 50 J). Crystal data: **2**: monoclinic, P2₁, a = 3.5152(3), b = 12.3308(9), c = 7.3381(5) Å, β = 92.068(7)°, V = 317.86(4) Å³, Z = 2, δ = 1.756 g cm^{−3}; **3**: monoclinic, P2₁/n, a = 3.6071(2), b = 8.3254(5), c = 18.955(1) Å, β = 91.365(6)°, V = 569.07(6) Å³, Z = 4, δ = 1.939 g cm^{−3}; **4**: monoclinic, P2₁/c, a = 3.6310(1), b = 8.6487(2), c = 19.8598(5) Å, β = 94.945(2)°, V = 621.34(3) Å³, Z = 4, δ = 1.948 g cm^{−3}; **5**: monoclinic, P2₁/n, a = 8.7948(2), b = 10.1640(2), c = 15.0571(3) Å, β = 92.470(2)°, V = 1344.71(5) Å³, Z = 8, δ = 2.258 g cm^{−3}; **6**: monoclinic, P2₁/n, a = 6.3539(1), b = 13.4762(3), c = 8.2876(2) Å, β = 99.245(2)°, V = 700.42(3) Å³, Z = 4, δ = 2.618 g cm^{−3}.

Key words: 1-Methyl-5-nitriminotetrazole, Alkali Salts, Crystal Structures, DSC, Pyrotechnics, Calorimetry