CRYSTAL AND MOLECULAR STRUCTURES OF THE POTASSIUM SALT OF 2-METHOXY-4-DIMETHYLAMINO-6-DINITROMETHYL-1,3,5-TRIAZINE

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The X-ray diffraction study of the potassium salt of 2-methoxy-4-dimethylamino-6-dinitromethyl-1,3,5-triazine is carried out. The crystals are triclinic; $C_7H_9N_6O_5^-\cdot K^+\cdot 2H_2O$; $a = 7.645(7)$ Å, $b = 8.230(7)$ Å, $c = 12.435(9)$ Å; $\alpha = 99.99(8)°$, $\beta = 91.52(7)°$, $\gamma = 113.86(8)°$; $V = 701(1)$ Å^3, $\rho_{calc} = 1.58$ g/cm^3, $Z = 2$, space group P-1. The compound crystallizes as a crystalline hydrate with two water molecules. Two planar fragments of dinitromethyl and 2-methoxy-4-dimethylamino-1,3,5-triazine construct the anion. Their geometrical parameters are explored. The coordination of potassium cations and numerous hydrogen bonds are found which result in the development of a complex 3-D framework.

Keywords: organic chemistry, crystal structure, salt of 2-methoxy-4-dimethylamino-6-dinitromethyl-1,3,5-triazine.