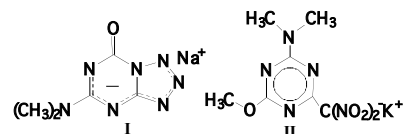


W0011

The X-ray Structure of Novel Tetrazolo[1,5-a]-1,3,5-triazine and 1,3,5-triazine Derivatives. E.V. Mironova¹, D.B. Krivolapov¹, I.A. Litvinov¹, V.V. Baharev², A.A. Gidasov², A.E. Arbutov Institute of Organic and Physical Chemistry¹, Russian Academy of Sciences, Arbuzov Str. 8, Kazan, 420088 Russia, Samara State Technical Univ.², Samara, Russia.

Tetrazolo[1,5-a]-1,3,5-triazine derivatives are the 5,8-diazaanalogues of guanine, which is the one of important building blocks of nucleic acid. The crystal and molecular structures of 5-aminotetrazolo[1,5-a]-1,3,5-triazin-7-one sodium salt (I) and 2-methoxy-4-dimethylamino-6-dinitromethyl-1,3,5-triazine potassium salt (II), which are used as precursors in the synthesis of the biologically active 1,3,5-triazine derivatives, are reported. In structure I two independent sodium cations have the special positions in the center of symmetry. The sodium cations have practically undistorted octahedral configuration. The polymer chains containing of the four-membered non-planar Na_2O_2 cycles are formed in crystal owing to the coordination of sodium cations with water molecules and with anions. The molecules I and II form the solvates with water. The anion of II is non-planar. The potassium cation is in general position and has nine coordination bonds. The potassium cations, anions and water molecules form the polymer chains similarly to I.



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