SIMULATION OF THE CRYSTAL STRUCTURE AND DENSITY OF AMMONIUM SALT OF AZIDOTETRAZOLFUROXANE

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Abstract: The crystal structure of the ammonium salt of 5-(4-azido-2-oxido-1,2,5-oxadiazol-3-yl)-1H-tetrazole (I) was simulated. The three-dimensional distributions of molecular electrostatic potential from *ab initio* calculation of the components of the model were approximated by point charges (PC) with varying both the magnitude and location of charges. The best PC-model was used to calculate the crystal packing of the molecules in the framework of AAP (atom-atom potential) method by optimization of parameters and localization of the corresponding potential energy minimum with the specified parameters of Lennard–Jones (6-12) for the nitrogen–nitrogen interactions. Simulated crystal structure I and the corresponding molecular crystal density are in agreement with the experimental data.

Keywords: ammonium salts; tetrazolfuroxanes; enthalpy of formation; molecular volume; intermolecular interaction; crystal structure energy; molecular electrostatic potential; crystal structure prediction

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