COMPUTER SIMULATION OF THERMOCHEMICAL AND EXPLOSIVE CHARACTERISTICS FOR AMMONIUM SALTS OF TETRAZOL-FURAZANES AND TETRAZOL-FUROXANES DERIVATIVES

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Abstract: Quantum chemistry methods have been used to simulate the structure and to calculate the heat of formation for ammonium salts of tetrazol-furazane and tetrazol-furoxane derivatives. The molecular volume, enthalpy of sublimation, and density of molecular crystals for compounds were evaluated based on the original techniques. Some explosive characteristics of the substances were calculated.

Keywords: ammonium salts; tetrazolfurazanes; tetrazolfuroxanes; enthalpy of formation; enthalpy of sublimation; molecular volume; quantum-chemical methods; Glasser–Jenkins method

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