

ENERGIES OF SALT FORMATION FOR HETEROCYCLES

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Abstract: The combustion energies of 3,4,5-trinitropyrazole, 1-methyl-3,4,5-trinitropyrazole, and ammonium salts of 3,4,5-trinitropyrazole have been measured. Formation enthalpies of these compounds have been calculated and the energy loss by enthalpies of an anion and a cation at salt formation in a standard condition has been estimated. This value has been compared with similar values for 3,4-dinitropyrazole, 3,5-dinitropyrazole, 2,4-dinitroimidazole, and 4,5-dinitroimidazole. It has been shown that salt formation energy correlates with the acidity of the initial NH-pyrasoles.

Keywords: 3,4,5-trinitropyrazole; 1-methyl-3,4,5-trinitropyrazole; ammonium salts of 3,4,5-trinitropyrazole; combustion energy; formation enthalpy; energy of salt formation

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