CONTRIBUTION OF THE AZIDE ANION TO THE ENTHALPY OF FORMATION OF ENERGETIC SALT COMPOUNDS

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Abstract: A new method of ions and cocrystals contribution mixing for estimating the enthalpies of formation of salt compounds has been applied to hydrazoic acid salts. The method is based on the simulation of two types of crystal packings: a "true" salt in the ionic form and a quasi-salt in the form of a cocrystal followed by calculations of the average value of the enthalpies of formation of these two forms. The effectiveness of the method is confirmed by comparing the calculation results with experimental data obtained by combustion calorimetry.

Keywords: method of atom-atom potentials; quantum chemical methods; crystal structure modeling; enthalpy of sublimation; enthalpy of formation; azides

DOI: 10.30826/CE23160211 **EDN:** OMNWHF

Table Captions

Table 1 Contributions of ionic components (K_{an} and K_{cat}, kcal/mol) to the enthalpy of formation of the considered hydrazoic acid salts

Table 2 Calculated and experimental enthalpies of formation of hydrazoic acid salts 1–6 (kcal/mol)

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Received March 28, 2023

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