PREDICTION OF THE CRYSTAL STRUCTURE AND ESTIMATION OF PHYSICOCHEMICAL CHARACTERISTICS OF COCRYSTALS OF BENZOTRIFUROXAN WITH NITROBENZENE

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Abstract: Based on the methods of quantum chemistry and atom-atom potentials, a structural search for the optimal crystal packings of cocrystals of benzotrifuroxan (BTF) with nitrobenzene (NB) at different ratios of components in the statistically most common space symmetry groups has been carried out. The possibilities of their cocrystallization are determined and the main interactions that form cocrystals are revealed. The physicochemical characteristics, including detonation properties, are calculated and the prospects for the use of cocrystalline forms as high-energy compositions are estimated. The theoretical predictions of cocrystallization of BTF with NB were partially confirmed by the experimental preparation of a cocrystal with the composition 1:1.

Keywords: method of atom-atom potentials; DFT method; B3LYP/6-31G (d,p) functional; crystal structure prediction; enthalpy of formation; molecular-crystalline density; detonation velocity; detonation pressure

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Figure Caption

Simulated (*a*) and experimental (*b*) packing of BTF-nitrobenzene cocrystal 1:1. Projection from the side [101]

Table Captions

Table 1 Space groups, lattice energies (E_{cocryst}), and cocrystallization energies (ΔE) corresponding to the global potential energy surface minima of BTF with NB cocrystals at various coformer ratios

Table 2 Comparison of unit cell parameters of model and experimental BTF-NB 1:1 cocrystals

Table 3 Calculated physicochemical characteristics of BTF and NB and their cocrystals with different ratios of components

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