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Crystal Lattice Free Volume in a Study of Initiation Reactivity of Nitramines: Friction Sensitivity.

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Abstract

The relationship between friction sensitivity (FS) and the crystal lattice free space per molecule, ΔV, of thirteen nitramines is described by a linear equation, divided into a number of the partial relationships with strong limitations by their molecular structure characteristics. Increasing FS due to raising of the ΔV values is not clearly confirmed. The influence of the ΔV values on friction sensitivity of nitramines is similar to that of their aza atoms which influence the mutual orientations of nitro groups in neighboring molecules. The dipole-dipole interaction of the oxygen and nitrogen atoms of nitro groups in neighboring nitramine molecules has a major effect on their own FS. In accordance with this interaction, a directly proportional relationship was derived between FS and the intrinsic gas phase molecular volume, V_{int}, of the nitramines mentioned, which is divided also into several straight lines according to relatively tight molecular structure similarity. The relationships found again confirm a level of disorder in the distribution of the forces in the crystal lattice of the "common" quality of ε–2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane, in comparison with its reduced sensitivity (RS) or chemically pure analogue.

Keywords: Crystal lattice; Friction; Initiation reactivity; Nitramines;

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