The tensors of thermal deformation cyclotrimethylene trinitramine and hexanitrostilbene at atmospheric pressure

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Anisotropic thermal deformation of α-cyclotrimethylene trinitramine (RDX) and hexanitrostilbene (JD-X) in the range from 150 to 470 K for RDX and from 150 to 570 K was studied by powder x-ray diffraction. The points of structural changes of energetic materials was by increments of 10 K. Calculations of x-ray diffraction data were performed using full-profile analysis integrated into the algorithm by loop quantum modeling of molecular structures [1]. As reference methods used a full-profile analysis method Pawley [2], Le Bail [3], Rietveld [4] (WPPD) and WPPM [5]. The main crystallographic axes and the characteristic surface of the tensors of thermal expansion are determined. The tensor of thermal expansion and the temperature dependence are presented numerically, algebraically and graphically. The obtained results can be used to construct equations of state of condensed α-RDX and JD-X.

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[4] Young R (ed) 1996 *The Rietveld Method* (Oxford Univ. Press)
[5] Scardi P and Leoni M 2002 *Acta Cryst.* **58** 190–200