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Crystallographic clearance of the product of CL-20

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Abstract

This article presents the results of development of methods of crystallization of the product of CL-20 (ε-polymorphic modification hexanitrohexaazaisowurtzitane. The purpose of this research is the synthesis of CL-20 with the optimal crystallographic clearance: 100% polymorphic purity and the desired shape of the crystal.

Was developed a convenient method for qualitative and quantitative analysis of polymorphs composition of CL-20 – based methods IR-Raman-spectroscopy. This was synthesized reference samples stable polymorphic modifications hexanitrohexaazaisowurtzitane (α-; β-; γ- and ε-), methods of synthesis are given in the experimental part of this article.

It was found that the contamination of CL-20 α-polymorphic impurity caused by the presence of water in the crystallization system. The presence of γ-polymorphic impurity in the product – the result of the increase in temperature of crystallization of the system above +85 °C. β-Impurity – a sign of a significant dilution of the crystallization system. Thus, the process of formation of polymorphic pure ε-CL-20 stabilizes the humidity control of all components of the crystallization of the system; a pre-filtration solution from agorastoudis hexanitrohexaazaisowurtzitane particles; depositing into a crystallization system the seed crystals of the desired ε-polymorphs, as well as compliance with the mass ratios of the components and the recommended temperature regimes.

For the production of modern fuel compositions preferred rounded, ideally spherical, the shape of the crystals of CL-20 with no surface defects. This was achieved through the study of the processes of precipitation and evaporation crystallization of CL-20 from three-component blends hexanitrohexaazaisowurtzitane – solvent – precipitator. The solvent was investigated ethyl acetate, acetonitrile, acetone, and as a precipitator of aliphatic and aromatic hydrocarbons (hexane, dean, toluene, xylene), alcohols (benzyl alcohol, ethanol), halogenoalkane (chloroform, carbon tetrachloride). Studies have shown that the most stable and technologically advanced a product with a spherical form crystal can be achieved in the systems of acetonitrile – toluene and acetone – *o*-xylene. The optimal conditions for carrying out these processes. The developed methods presented in the experimental part of the article.

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