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Synthesis and properties of CL-20 cocrystals with some pyridine *N*-oxides

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Abstract

In the result of the work CL-20 cocrystals with pyridine-, 2-methylpyridine-, 4-methylpyridine-, and 4-nitropyridine *N*-oxides were synthesized for the first time. The effect of synthesis ways on thermal properties and impact sensitivity of cocrystals was studied.

General technique of synthesizing cocrystals was to solve components in stoichiometric ratio in acetone and then to remove solvent. In addition a technique to obtain the compounds out of melt was studieddue to low melting temperatures of pyridine *n*-oxide and its 2-methyl derivative. In the case reaction temperature exceeded melting point of the respective *N*-oxides by 5-7 °C. After adding equimolar amount of CL-20 with respect to *N*-oxide the reaction mass that is homogeneous visually hardens fast. In case of pyridine *N*-oxide and its 2-methylderivative a volume crystallization phenomenon was observed. According to IR spectroscopy the composition of cocrystals obtained in different ways coincided with each other. Unlike the other *N-oxides*, velocity of solvent removal effects particularly on co-crystallization of 4-nitropyridine *N*-oxide with CL-20. When acetone is removed slowly at rate of $5 \cdot 10^{-3}$ cm^3/h, recrystallization of initial *N*-oxide takes place instead of molecular complex formation.

Two-step decomposition is typical for all molecular complexes CL-20 with *N*-oxides. According to TGA data mass loss at the first stage is 20-23% of total sediment mass that agrees well with initial mass fractions of *N*-oxides.

To determine effect of *N*-oxides on explosive properties and impact sensitivity parameters of cocrystals with CL-20 comparative tests were performed. Co-crystallization CL-20 with inert compounds, as expected, leads to 2-3 times less sensitivity as compared with initial nitramine. Introduction of a nitric group into a pyridine cycle of *N*-oxide effects particularly on explosive properties of 4-NPNO/CL-20 cocrystals, impact sensitivity of which being at a level of CL-20.

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