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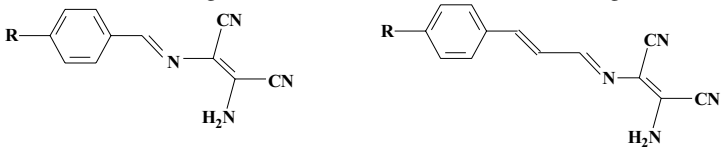
Crystal Engineering of Thermostable Acentric Crystals. Tatiana V. Timofeeva[1], Vladimir V. Nesterov[1], Volodymyr V. Nesterov[1], Mikhail Yu. Antipin[1,2,] [1]Dept. of Natural Sciences, New Mexico Highlands Univ., Las Vegas, NM, USA, [2]Inst. of Organoelement Compounds, Russian Academy of Sciences, Moscow, Russia.

In the course of a search for new thermostable acentric nonlinear optical crystalline materials, several imine derivatives with the general structure D-π-A(D') were designed.



R = HO (1), CH_3O (2), $(CH_3)_2N$ (3), $(C_2H_5)_2N$ (4) **R = $(CH_3)_2N$ (5), $(C_2H_5)_2N$ (6)**

Introduction of a donor amino group (D') into the acceptor moiety was expected to bring H-bonds into their crystal structures, and so to elevate their melting points and assist in an acentric molecular packing. Ten aromatic imines with structure shown above and six analogous heterocycle-containing compounds were prepared. For eleven of them single crystals were grown, and characterized by X-ray analysis. A significant melting temperature elevation was found for all of the synthesized compounds. Seven of these compounds were crystallized in acentric space groups. It was found that several acentric compounds have very similar molecular structures. In these structures molecules form one-dimensional H-bonded head-to-head supramolecular associates (chains) with significant gaps between molecules. In crystals gaps between molecules belonging to one chain are filled with molecule from the neighboring chain. The chains are non-parallel, angles between them are about 50-70 degrees, and they form vary unusual interpenetrating chain pattern that brings to acentric molecular packing. We were able to find certain similarities between molecular structures and behavior of the aromatic and heterocyclic imines, that brings to formation of thermostable acentric crystals, and that put us one step closer to the design of molecular packing in organic crystalline materials for nonlinear optical applications.