

MS30-P06 | PECULIARITIES OF SUPRAMOLECULAR ORGANIZATION IN CENTRIC, ACENTRIC AND CHIRAL KETONES WITH VINYLACETYLENE FRAGMENTS

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Crystal structures of a series of 1,5-diarylpentenones and cyclic ketones with vinylacetylene fragments were studied. These compounds are prospective for application in non-linear optics, and nearly half of them crystallize in acentric and chiral space groups. Full Interaction Maps were used to understand the features of their supramolecular organization [1,2]. Besides, topological features of isolated molecules and intermolecular contacts were studied by means of the theoretical charge density studies [1]. Studies have shown that molecular planarity does not affect crystal chirality, while electronic and steric factors govern the formation of chiral chains, and acentric crystals for all the homologues of (E)-1,5-diarylpent-1-en-4-in-3-ones. Energies of intermolecular interactions were found to correlate with melting temperatures of compounds. The charge density distribution in isolated molecules allows predicting the supramolecular organization of such compounds that can be useful in the development of new materials with nonlinear optical properties. Mutual disposition of olefin fragments in some ketones satisfy criteria needed to allow a photoinitiated cycloaddition reactions to occur. Thus, effect of irradiation on some compounds was studied using ^1H NMR technique.

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[1] E. D. Voronova, A. A. Golovanov, K. Yu. Suponitsky, I. V. Fedyanin, A. V. Vologzhanina, *Cryst. Growth Des.* **2016**, *16*, 3859–3868.

[2] E. D. Voronova, A. A. Golovanov, I. S. Odin, M. A. Anisimov, P. V. Dorovatovskii, Y. V. Zubavichus, A. V. Vologzhanina *Acta Cryst.* **2018**, *C74*, 1674–1683.