MS35-03 | Crystallization of Chiral 2,4-Dinitrophenyl Pyridoxine Derivatives in «no Zonk» Groups: Regularity or Randomness?

Samigullina, Aida (A.E. Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russian Academy of Sciences, Kazan, RUS); Garipov, Marsel (Kazan Federal University, Kazan, RUS); Lodochnikova, Olga (A.E. Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russian Academy of Sciences, Kazan, RUS); Gubaidullin, Aidar (A.E. Arbuzov Institute of Organic and Physical Chemistry, FRC Kazan Scientific Center, Russian Academy of Sciences, Kazan, RUS)

Materials with nonlinear optical properties are widely used in medicine, computer and laser technology, photonics and optoelectronics. At present more attention is paid to researching the new classes of compounds and establishing the features of their molecular and crystalline structure for designing the NLO-materials.

Recently we have demonstrated that the 2,4-dinitrophenyl pyridoxine with achiral center crystallizes in the noncentrosymmetric space group $Pca2_1$ regardless of the used solvent and its crystals exhibit nonlinear optical properties. In this work, we report the investigating of the structural analogs of this compound, the chirality of which were varied by changing the type of substituents. It was found, that even in the presence of the chiral center in the molecules of 2,4-dinitrophenyl pyridoxine derivatives, there is a tendency for their crystallization not in the Zonk group, but in the centrosymmetric space groups. And even in the case of isopropyl substituted derivative crystallization in P212121 space group, in the independent part of the unit cell is an enantiomeric pair, so that the compound crystallizes as a pseudo-racemate. At the same time, compounds of this series with an achiral center in molecules tend to form crystals in non-centrosymmetric groups, and this is one of the requirements for obtaining crystals with potential nonlinear-optical properties. The geometry of the molecules, the peculiarities of intermolecular interactions and their relationship with the crystallographic parameters of the crystals are discussed.

This work was financially supported by the Russian Science Foundation (grant No 17-13-01209)