Chirality 2017
ISCD-29

29th International Symposium on Chirality

Full-page Abstracts

Waseda University International Conference Center
July 9 (Sun.)-12 (Wed.), 2017

©TCVB

©T.Satoh/©JNTO

Oral Presentations

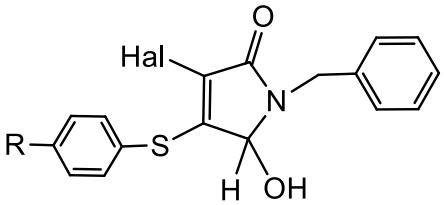
OL-3B10

"Doubly enantiophobic" crystallization of a series of 5-hydroxy-3-pyrrolin-2-one thioethers

O.A. Lodochnikova,[a,b] R.R. Fayzullin,[a] A.R. Zaripova,[a,b] A.I. Samigullina,[a] L.S. Kosolapova,[b]
I.I. Vandyukova,[a] I.S. Smirnov,[a,b] A.R. Kurbangalieva[b]

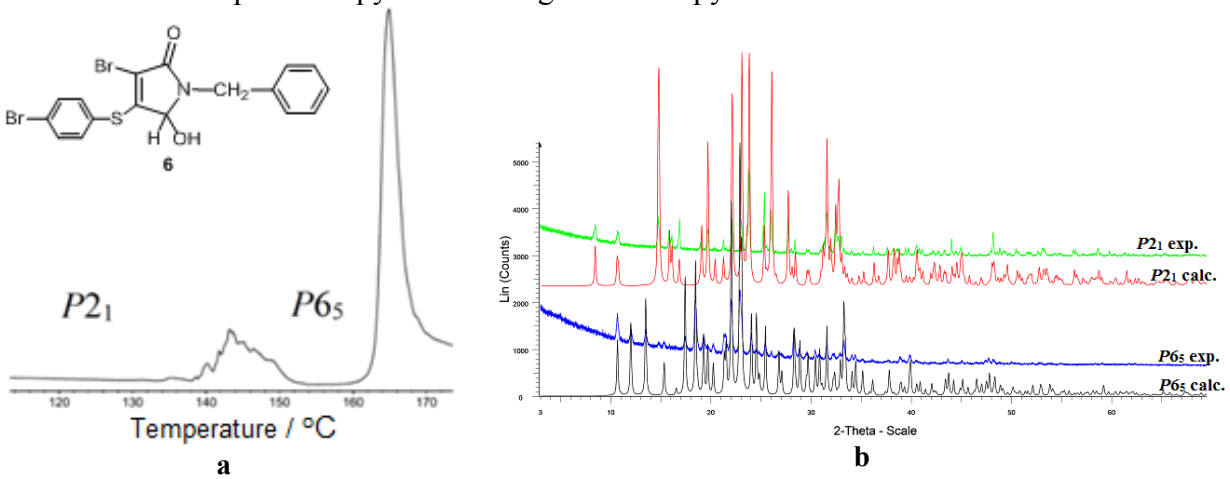
a) A.E. Arbuzov Institute of Organic and Physical Chemistry, Kazan Scientific Center of the Russian Academy of Sciences, Arbuzov St. 8, Kazan 420088, Russian Federation
b) Biofunctional Chemistry Laboratory, A. Butlerov Institute of Chemistry, Kazan Federal University, Kremlyovskaya St. 18, Kazan 420008, Russian Federation

The phenomenon of spontaneous resolution of enantiomers during crystallization is one of intriguing mysteries of crystallography and stereochemistry. In this work, we reported on crystallization, heterogeneous equilibria and phase transitions of a series of racemic *N*-substituted 4-arylsulfanyl-3-halogeno-5-hydroxy-3-pyrrolin-2-ones consisting an unsaturated γ-lactam ring that is an important pharmacophore group.



Scheme. Structural formula of the key compounds

All individual crystalline phases of compounds under investigation were studied by means of single crystal and powder X-ray diffractions. As a result, we found substances that demonstrate unusual "doubly enantiophobic" crystallization. Namely, these compounds form two polymorphic modifications, and both polymorphs appear to be conglomerates (the space groups $P2_1$ and $P6_5$, $P6_1$), which is an extremely rare phenomenon. Phase behavior of the substances was carefully analyzed by means of differential scanning calorimetry, temperature-resolved vibration spectroscopy and hot-stage microscopy.



Figures. The DSC data (a) and the XRPD patterns (b) of the individual polymorphs of one of the "doubly enantiophobic" compounds.

The financial support from the Russian Science Foundation (grant No 17-13-01209) and Russian Government Program of Competitive Growth of Kazan Federal University is gratefully acknowledged.