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Research Project:

Synthesis and Physical-Chemical Studies of Molecular Complexes of Donor-Acceptor Type

Abstract:

The project is aimed on the synthesis and throughout physical-chemical characteristics of an organic molecular complex of bromanilic acid and a substituted heterocyclic amine. The system under interest belongs to the family of molecular crystals of donor-acceptor type, which are potentially attractive as building blocks for crystal engineering and supramolecular chemistry. This project is oriented toward principal investigations, looking for a link between the structure and the spectral response.

This practicum consists of the following steps:

1. The synthesis of the title compound
2. Studying the crystal structure with powder X-Ray diffraction
3. Raman spectroscopy measurements
4. Introduction to inelastic neutron scattering at NERA spectrometer, analysis of the experimental data for the system under interest
5. Modeling of the vibrational response by means of quantum-chemical calculations
6. Preparing the oral presentation

Requirements:

The program is well-suited for the students of chemistry and for a candidate with a strong interest in chemistry. General knowledge of molecular spectroscopy techniques is an advantage. The student is requested to use his own personal computer.

The training is dedicated to one student

References:

1. K. Łuczyńska, K.Druźbicki, K.Łyczko, W.Starosta, "Complementary Optical and Neutron Vibrational Spectroscopy Study of Bromanilic Acid: 2,3,5,6-Tetramethylpyrazine (1:1) Cocrystal", *Vibrational Spectroscopy* 75 (2014) 26.
2. K. Łuczyńska, K.Druźbicki, K. Lyczko. J. Cz. Dobrowolski, "Experimental (X-ray, ¹³C CP/MAS NMR, IR, RS, INS, THz) and Solid-State DFT Study on (1:1) Co-Crystal of Bromanilic Acid and 2,6-Dimethylpyrazine", *J. Phys. Chem. B* 119 (2015) 6852.
3. K. Łuczyńska, K. Druźbicki, K. Lyczko, J.Cz. Dobrowolski, „Structure-Spectra Correlations in Anilate Complexes with Picolines”, *Crystal Growth & Design*, 2016, 16(10), 6069.