

s13.m35.p30 **Monitoring Photo-Induced Structural Changes in Crystals.** Ilona Turowska-Tyrk and Elzbieta Trzop, *Department of Chemistry, Wrocław University of Technology, Wybrzeże Wyspińskiego 27, 50-370 Wrocław, Poland.* E-mail: ilona.turowska-tyrk@pwr.wroc.pl

Keywords: Monitoring; Photochemical reaction; Structural changes

Photochemical reactions proceeding in crystals have been known for a very long time. During the last decade, interest in them increased significantly, which was connected with the development of modern technologies and selective chemical syntheses as well as with the appearance of new methods applied to studies of such reactions or with the improvement of the existing ones. In 80s and 90s the X-ray studies of the photochemical reaction course dealt with monitoring changes of cell constants or monitoring movements of an atom group inside a molecule. In this poster we will present the step-by-step X-ray structure analysis of movements of whole molecules during photodimerization reactions in crystals. The studies show that reactant and product molecules do not assume a fixed position in a crystal but move gradually along with the photoreaction progress. The product molecules move to the position assumed in the pure product crystal and the reactant molecules move from the position occupied in the pure reactant crystal. Moreover, as the photodimerization progresses the adjacent reactant molecules gradually come closer and change their mutual orientation to resemble the product [1] - [4]. For long irradiation time we observed changes of a reciprocal lattice after the irradiation [2]. The studies of initial structural changes in a crystal during photo-induced disappearance of its diffracting properties will be also presented [5].

- [1] Turowska-Tyrk I., *Chem. Eur. J.*, **7**, 3401-3405 (2001).
- [2] Turowska-Tyrk I., *Chem. Phys. Lett.*, **361**, 115-120 (2002).
- [3] Turowska-Tyrk I., *Acta Cryst.*, **B59**, 670-675 (2003).
- [4] Turowska-Tyrk I. and Trzop E., *Acta Cryst.*, **B59**, 779-786 (2003).
- [5] Turowska-Tyrk I., *Chem. Phys.*, **288**, 241-247 (2003).

s13.m35.p31 **Multi-Temperature Studies of Polymorphic Structures of p-nitrobenzoic Acid.** Grazyna Wojcik and Emilia Przybycien, *Institute of Physical & Theoretical Chemistry, Wrocław University of Technology, Wyb. Wyspińskiego 27, 50-370 Wrocław, Poland.* E-mail: g.wojcik@ch.pwr.wroc.pl

Keywords: Polymorphism; p-Nitrobenzoic acid ; TLS analysis

The polymorphic crystals of p-nitrobenzoic acid are built of hydrogen bonded molecular dimers. Molecular packing in the two crystals differs by the mutual orientation of the dimers [1], [2], [3]. They are arranged co-linearly in the low-temperature modification, while in the high-temperature form the mutual orientation of adjacent dimers is almost perpendicular. The objective of this work was: (a) to highlight the thermodynamic relationship between two forms through calorimetric (DSC) measurements; (b) to analyze multi-temperature anisotropic displacement parameters using the TLS formalism in order to get insight into the molecular motions and their thermal evolution. The low-temperature form undergoes a first-order, irreversible phase transition around 387 K. The rigid-body analysis with correlation of internal motions of large amplitudes [4], [5], [6] indicates a major role of nitro group torsional vibration in triggering the transition and a persistent metastability of the high-temperature form.

- [1] Tavale, S. S. & Pant, L. M. (1971). *Acta Cryst.* **B27**, 14790-1481.
- [2] Colapietro, M. & Domenicano, A. (1977). *Acta Cryst.* **B33**, 2240-2243.
- [3] Groth, P. (1980). *Acta Chem. Scand.* **A 34**, 229-233.
- [4] Cruickshank, D. W. (1956). *Acta Cryst.* **9**, 754-756.
- [5] Dunitz, J. D., Shomaker V., Trueblood K. N. (1988). *J. Phys. Chem.*, **92**, 856-867
- [6] Shomaker V., Trueblood K. N., (1998). *Acta Cryst.*, **B54**, 507-514.
- [7] Farrugia, L., (1987). *Appl. Cryst.* **30**, 565.