

MS37. Molecular crystalline processes at ambient and non-ambient conditions

Chairs: Elena Boldyreva, Gareth Lloyd

MS37-O1 Structural changes induced in crystals by photochemical reactions at ambient and high pressure

Julia Bąkowicz¹, Krzysztof Konieczny¹, Ilona Turowska-Tyrk¹

1. Faculty of Chemistry, Wrocław University of Technology, Wybrzeże Wyspińskiego 27, 50-370 Wrocław, Poland

email: julia.bakowicz@pwr.edu.pl

The main subject of our interest is monitoring the paths of photo-induced structural transformations in single crystals by means of X-ray structure analysis (for instance [1-6]). In particular, we analyze structural changes brought about by photochemical reactions in ambient and extreme conditions. The studies facilitate gaining the knowledge of influence of pressure on the course of photochemical processes in crystals.

Studies of this type require data collection and structure determination for many partly reacted crystals, *i.e.* containing reactant and product molecules in different proportions. In the case of high-pressure experiments this is a big challenge for researchers.

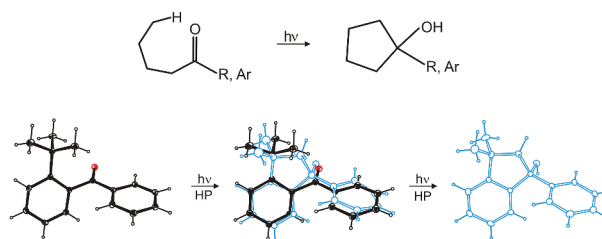
The results on monitoring the structural changes in crystals of 2-*tert*-butylphenylphenylmethanone (I) [6] and benzylammonium 4-(2,4,6-triisopropylbenzoyl)benzoate (II) brought about by the photocyclization reactions at different pressures will be presented (Figure 1).

Variations in the unit cell parameters, molecular geometry and molecular orientation brought about by the photochemical reactions at various pressures will be shown. Additionally, changes in a reaction rate and crystal structure caused by only high pressure, *i.e.* without photo-induction, will be discussed.

References

- [1] I. Turowska-Tyrk, J. Bąkowicz, J.R. Scheffer, *Acta Cryst.*, 2007, B63, 933-940.
- [2] E. Trzop, I. Turowska-Tyrk, *Acta Cryst.*, 2008, B64, 375-382.
- [3] J. Bąkowicz, J. Skarzewski, I. Turowska-Tyrk, *CrystEngComm*, 2011, 13, 4332-4338.
- [4] J. Bąkowicz, I. Turowska-Tyrk, *J. Photochem. Photobiol. A*, 2012, 232, 41-43.
- [5] J. Bąkowicz, J. Olejarz, I. Turowska-Tyrk, *J. Photochem. Photobiol. A*, 2014, 273, 34-42.
- [6] J. Bąkowicz, I. Turowska-Tyrk, *CrystEngComm*, 2014, 16, 6039-6048.

compound (I):



compound (II):

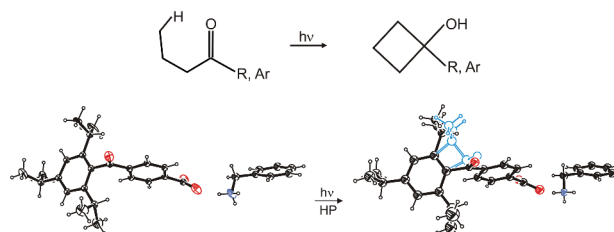


Figure 1. The equations of the studied photochemical reactions and the molecular structures in pure reactant, partly reacted and pure product crystals.

Keywords: single-crystal X-ray structure analysis, photochemical reactions, high pressure