P-33 **Monday, 04.09., 16^{30} – 19^{00}**

High pressure studies on racemic and enantiopure 1-benzoyl-3-(1-phenylethyl)thiourea

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Most of the biologically active substances are chiral and enantiomers can interact differently with living organisms. Hence, enantiomer resolution and asymmetric synthesis are of great importance for the pharmaceutical, chemical, and food industries.

In 2013 we have reported our X-ray diffraction studies on racemic 1-benzoyl-3-(1-phenylethyl)thiourea (**1**) and its *S*-enantiomer (**2**) [1]. In next two years both *R* and *S*-enantiomers of this ligand were successfully used in synthesis of chiral ruthenium(II) catalysts for stereoselective reduction of ketones [2,3].

On the other hand, chiral resolution can be done chromatographically or, sometimes, by crystallization. According to Wallach's rule [4,5], racemates form denser, more stable crystals than enantiomers. However, the validity of the rule is often broken and many exceptions have been reported so far [6].

High pressure favours high density solids and therefore can be applied for enantiomeric resolution of the chiral compounds defying Wallach's rule [7]. It has been estimated by Jacques, Collet, and Wilen that the racemates less dense than the enantiomers should be spontaneously separated below 1 GPa [8].

Here we report our high pressure study of **1** (monoclinic crystals, space group *C*2/*c*) and **2** (orthorhombic crystals, space group $P2_12_12_1$) up to at least 3.45 GPa. A series of high-pressure single-crystal diffraction experiments have been performed at High Pressure ID09A Beamline at ESRF (Grenoble, France) using parallel monochromatic X-ray beam (E = 30 keV, λ = 0.413 Å) focused to 30 × 30 μm on the sample loaded into membrane Diamond Anvil Cell and topped by silicon oil.

Similarities and differences in **1** and **2**, as well as potential possibility of resolution under high-pressure will be discussed within the poster.

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[2] M. M. Sheeba, M. M. Tamizh, L. J. Farrugia, A. Endo, R. Karvembu: *Organometallics* **33** (2014) 540.
[3] M. M. Sheeba, S. Preethi, A. Nijamudheen, M. M. Tamizh, A. Datta, L. J. Farrugia, R. Karvembu: *Catal. Sci. Technol.* **5** (2015), 4790.
[4] O. Wallach, *Liebigs Ann. Chem.* **286** (1895) 90.
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[6] C. P. Brock, W. B. Schweizer, J. D. Dunitz, *J. Am. Chem. Soc.* **113** (1991) 9811.
[7] J. Marciniak, M. Andrzejewski, W. Cai, A. Katrusiak, *J. Phys. Chem. C* **118** (2014) 4309.
[8] J. Jacques, A. Collet, S. H. Wilen, *Enantiomers, Racemates and Resolutions*, Krieger Publishing Company: Malabar, FL, (1994).