

system. The crystal structure was determined by single crystal X-ray diffraction (Xcalibur diffractometer, CCD detector, Mo $K\alpha$ radiation). The structure belongs to $TbFe_2$ structure type (space group $R-3m$, $a = 5.5900(8)$ Å, $c = 13.684(3)$ Å), which is deformed variant of $MgCu_2$ structure type.

[1] M.V. Dzvevenko *PhD thesis*, Ivan Franko National University of Lviv, 2006. [2] F. Weitzer, P. Rogl. *Journal of the Less-Common Metals*, 1990, 167, 135-142.

Keywords: intermetallic, crystal structure, rare-earth

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Preliminary neutron powder diffraction analysis of a meta-stable colored form in photochromic crystal using iMATERIA in J-PARC

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N-Salicylideneanilines, Schiff bases synthesized from salicylaldehydes and anilines, are well known to exhibit photochromism both in solution and in the solid state. The photochromic salicylideneanilines usually take “enol forms” with pale-yellow color in crystals, change to meta-stable photoproducts “trans-keto forms” with red color by irradiation of ultraviolet light (Fig 1). The red color erases by irradiation with visible light or by thermal fading in the dark. The structure of the photoinduced colored species, of *N*-3,5-di-*tert*-butylsalicylidene-3-nitroaniline (**1**), as shown in Fig. 2, was analyzed by X-ray using two-photon excitation, and showed pedal-like structural change around the $-C=N-$ bond during the reaction.^[1] This reaction begins with a hydrogen atom transfer from hydroxyl group to the nitrogen of the imine, and followed to the pedal motion. Previous X-ray study cannot find the hydrogen atom of the trans-keto form because the population of the photoproduct is only 10% in the single crystal. However, such a hydrogen atom or proton transfer is one of the important phenomena in chemical reactions and is a key role to make clear the whole reaction mechanism. To observe the hydrogen atom transfer clearly, we chose powdered sample with more surface area for light irradiation, and carried out the neutron diffraction measurement at iMATERIA (Ibaraki Materials Design Diffractometer), a time-of-flight neutron powder diffractometer, at BL20 in Materials and Life science Experimental Facility of J-PARC. We prepared a long-lifetime derivative, *N*-3,5-di-*tert*-butylsalicylidene-3-carboxyaniline (**2**) with irradiated using high pressure mercury lamp at -10 deg., and sealed into the vanadium cell. The neutron powder diffraction measurement conditions are as follow: the accelerator beam power is about 220 kW, the pulse repetition is 25 Hz, the range of wavelengths is about 0.2~7 Å, the measurement temperature is 173 K. We will present the detailed data statistics of the preliminary powder neutron diffraction analysis including the data processing and the structural refinement.

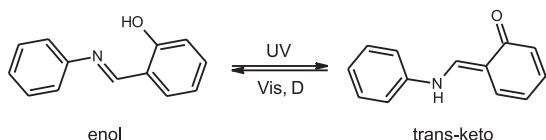


Fig. 1 Reaction mechanism of the photochromism of *N*-Salicylideneaniline

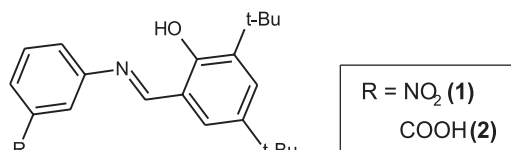


Fig. 2 Structures of *N*-Salicylideneaniline derivatives (**1**) and (**2**).

[1] J. Harada, H. Uekusa, Y. Ohashi, *J. Am. Chem. Soc.*, 1999, 121, 5809-5810.

[2] K. Johmoto, A. Sekine, H. Uekusa, Y. Ohashi, *Bull. Chem. Soc. Jpn.*, 2009, 82, 50-57.

Keywords: photochromism, neutron diffraction, J-PARC

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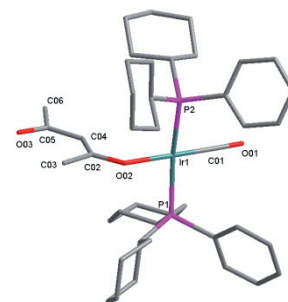
Model iridium phosphine compounds for use in olefin hydroformylation

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The functionalisation of olefins from petroleum sources to aldehydes through the process of Hydroformylation is of great industrial importance. High selectivity for the desired isomer of the aldehyde can be kinetically manipulated by variation of the ligands and process conditions. In rhodium systems, it is known that the presence of phosphine ligands give way to more active, highly selective catalysts reacting under milder reaction conditions [1].

Iridium compounds are often used as model complexes, since Ir(I) and Ir(III) complexes with similar ligand sets to those proposed in rhodium chemistry, tend to behave in the same way and are isolated more readily than the rhodium analogues. Ligand effects in model iridium systems containing tertiary phosphine and diphosphinoamine ligands are investigated to determine the importance of electronic factors and steric crowding from the phosphine based ligands for manipulating the reactivity of the Ir(I) centre [2].

In the present investigation, characterisation and structural evaluation of different complexes and intermediates [beta-diketonato ring opened example shown below], will be presented.



[1] J.A. Osborn, G. Wilkinson, J.F. Young, *Chem. Commun.* 1965, 17. [2] A. Roodt, G.J.J. Steyn, *Journal of Organomet. Chem.* 1997, 536-537, 197-205.

Keywords: iridium, hydroformylation, phosphine

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Structural studies of $SrTcO_3$, $CaTcO_3$ and $Pb_2Tc_2O_{7-d}$

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