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Keywords: diffuse scattering, molecular crystals, rotational disorder

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Photo induced isomerization reaction and phase transition of an organo-dirhodium dithionite complex

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An organo-dirhodium dithionite complex [$\{\text{Rh}(\eta^5\text{-C}_5\text{Me}_5)\}_2(\mu\text{-CH}_2)_2(\mu\text{-O}_2\text{SSO}_2)$] (**1**) shows fully reversible photochromism in which one of four terminal oxygen atoms in the side-on type dithionite $\mu\text{-O}_2\text{SSO}_2$ moiety is converted to a bridged one to produce geometrical isomer form $\mu\text{-OSOSO}_2$ by visible light irradiation in crystalline-state [1]. An analogous dirhodium complex [$\{\text{Rh}(\eta^5\text{-C}_5\text{Me}_4\text{Et})\}_2(\mu\text{-CH}_2)_2(\mu\text{-O}_2\text{SSO}_2)$] (**2**) that contains $\eta^5\text{-C}_5\text{Me}_4\text{Et}$ instead of $\eta^5\text{-C}_5\text{Me}_5$ has similar crystal structure with (**1**). We have tried to analyze the photo-isomerization process of the dirhodium complex (**2**) in single crystals by X-ray structure analyses [2]. The photo-irradiation wavelength, intensity and time dependencies of the photo-generated isomer ratio were measured for (**2**). By using Xeon light passing through band pass filters, it was revealed that the light not on absorption peaks but on absorption tail produced photo-generated isomers. This should be owing to that the light on the absorption peak could not pass through the crystal. At the initial stage of the photo-isomerization process, it was revealed that the cell volume becomes half by the light irradiation. Structure analyses were made for the crystals before and after the photo induced phase transition, indicating that $\eta^5\text{-C}_5\text{Me}_4\text{Et}$ rings are positionally disordered for the original crystals but is ordered for the photo irradiated crystals which is isostructure to (**1**) with space group $P2_1/n$.

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Keywords: solid state reaction, photo chemical reaction, phase transition

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Atomic displacement parameters and specific heat of α -glycine polymorph between 10 and 298 K

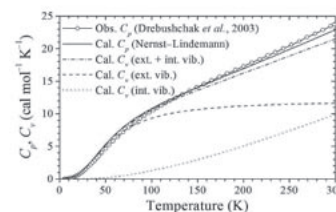
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Synchrotron data to 0.5 Å resolution of the α -polymorph of glycine were collected between 10 and 298 K at the two synchrotron sources in Japan, KEK Photon Factory (PF) and SPring-8. Data from KEK-PF and SPring-8 were processed with RAPID AUTO and DENZO/SCALEPACK and refined with SHELXL-97, yielding comparable data quality. Simultaneous analysis of the multi-temperature atomic displacement parameters (ADPs) were performed to obtain the

libration and translation frequencies [1]. The six external vibration frequencies from normal mode analysis and the intramolecular vibration frequencies from *ab initio* calculations were used together with the molecular Einstein, Debye, and Nernst – Lindemann models to estimate heat capacities C_v , C_p and found to be in fair agreement with C_p from calorimetric measurements [2]. Figure below shows the results obtained from SPring-8.

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Keywords: atomic displacement parameters, specific heat, polymorphs

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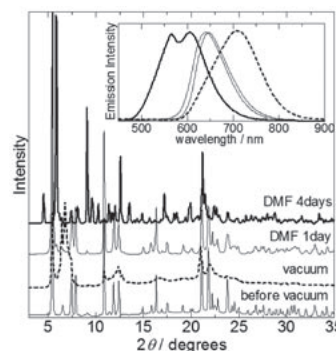
A structural study on a nano-porous vapochromic Pt complex

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One-dimensional stacking Pt-diimine complexes have attracted much attention because of their characteristic luminescence based on the Pt-Pt interaction and potential for a chemical sensors [1,2]. Our attention have been focused on the properties of $\text{Pt}(\text{CN})_2(\text{dc bpy})$ (dc bpy = 4,4'-dicarboxy-2,2'-bipyridine) which has nano-size pores and exhibits interesting vapochromism [3]. In this paper, we discuss the vapochromism on the basis of powder X-ray diffraction (PXRD). Fig. 1 shows the PXRD patterns in vacuum and DMF (*N,N*-dimethylformamide) vapor. Observed PXRD patterns indicate that the porous structure could be broke down by removal of crystal water in vacuum and then regenerated on exposure to DMF vapor. The emission peak also shifted from 647 nm to 710 nm and returned to 640 nm. Further exposure to DMF vapor induced the structural phase transition and a new emission peak appeared at 560 nm. These results suggest that the vapochromism of this complex originates from the structural flexibility and nano-sized pore which can absorb various organic vapors.

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Keywords: coordination chemistry compounds, luminescence, crystal synthesis and phase transitions