

## Poster Presentation

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### Determination of Chirality of the Chiral Space Groups with Two-fold Screw Axis

K. Ishikawa<sup>1</sup>, M. Tanaka<sup>2</sup>, M. Shiro<sup>3</sup>, T. Asahi<sup>1,3</sup>

<sup>1</sup>Waseda University, Department of Life Science and Medical Bioscience, Tokyo, Japan, <sup>2</sup>National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan, <sup>3</sup>Waseda University, Consolidated Research Institute for Advanced Science and Medical Care, Tokyo, Japan

Crystals are classified according to their symmetry operations into 230 space groups. A two-fold screw axis,  $2_1$ , a symmetry operation, is frequently found in the crystal, especially non-centrosymmetric organic crystals. The two-fold screw axis shows a chiral character when molecules in the crystal tilt against the screw axis as shown in Figure. The crystals belonging to a chiral space group with two-fold screw axis such as a  $P2_1$  or  $P2_12_12_1$  exhibit two different types with opposite chirality. However, although the two crystals are not identical in a molecular arrangement, we cannot distinguish them with the present notation of space group. Recently, the idea of determining the handedness of two-fold screw axis have been successfully proposed using hierarchical interpretation of the crystals. (I. Hisaki, T. Sasaki et al., 2012) Nevertheless, the issue on a notation to distinguish chiral crystals with two-fold screw axis still remains unsettled as far as we know. Therefore, we attempt to propose a novel notation for the crystals belonging to chiral space groups with two-fold screw axis. We focus on the relationship between the absolute structure and optical activity of the crystals. We have selected alanine crystals, which belong to  $P2_12_12_1$ , as model crystals to discuss the notation. We have determined the absolute structure of the alanine crystals by X-ray diffraction and have measured their optical activity with Generalized High Accuracy Universal Polarimeter (G-HAUP). (M. Tanaka, N. Nakamura et al., 2012) G-HAUP is an apparatus that can measure simultaneously the linear birefringence, linear dichroism, circular birefringence, i.e., optical activity, and circular dichroism in any solid material. These experimental results have successfully correlated the absolute structure to the optical activity of the alanine crystals.

[1] I. Hisaki, T. Sasaki, K. Sakaguchi, et al., *Chem. Commun.*, 2012, 48, 2219-2221, [2] M. Tanaka, N. Nakamura, H. Koshima and T. Asahi, *Journal of Physics D*, 2012, 45, 175303-175311

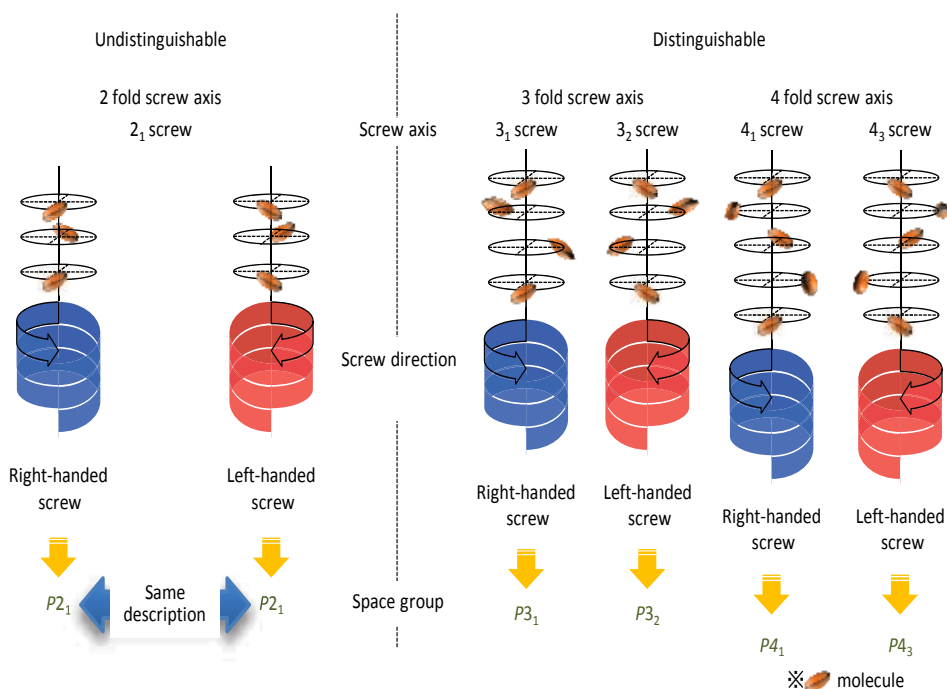


Fig. The relationship of screw axis to space group

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