

Poster Presentation

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Chiroptical study on benzil crystal using G-HAUP

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There has been a great interest in understanding chiroptical properties such as optical rotatory power (ORP) and circular dichroism (CD) in anisotropic materials because these properties provide valuable information on molecular/crystal structure. In particular, generation of chiroptical properties in crystals composed of achiral compounds is considered as one of the most intriguing topics in the field of crystal optics. Benzil (C₆H₅COCOC₆H₅), which consists of two phenyl rings and two carbonyl groups, is achiral in solution, but exhibits chirality in the crystalline state. In the crystalline state, the molecules are arranged in a helical form and are put along three-fold left-handed screw axis or right-handed one. The benzil crystal belongs to trigonal crystal system with non-centrosymmetric space group P3121 or P3221. Hence, the crystal symmetry allows the benzil crystal to exhibit ORP and CD and indeed it is often used as a chiral reference crystal in visible/ultraviolet region (S. Chandrasekhar, 1954; N. K. Chaudhuri & M. A. El-Sayed, 1967) as well as α -quartz and nickel sulphate hexahydrate crystals. Meanwhile, ORP and CD reflect spatial dispersion of a second-rank permittivity tensor that depends on not only frequency but also wave vector of an electromagnetic wave. Furthermore, the magnitude of ORP and CD usually vary with the direction of an incident light. It is therefore much important in chiral science to discuss the relationship between ORP and CD along the principal axes and the molecular arrangements along them, respectively. In the case of benzil crystal, it is expected to show different ORP and CD along the a and c axes because of its trigonal crystal system, D₃. In this study, we attempt to measure the ORP and CD of benzil crystal in the direction of the c and a axes with the Generalized-High Accuracy Universal Polarimeter (G-HAUP)(M. Tanaka et al., 2012).

[1] S. Chandrasekhar, *Proceedings of the Indian Academy of Sciences – Section A*, 1954, 5, 243-253, [2] N. K. Chaudhuri, M. A. El-Sayed, *The Journal of Chemical Physics*, 1967, 47, 1133-1143, [3] M. Tanaka, N. Nakamura, H. Koshima, T. Asahi, *Journal of Physics D: Applied Physics*, 2012, 45, 175303-175310

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