Crystal Structure of KLiSO₄ at High Temperatures

Hyun Min Park, Yang Koo Cho, Su Jin Chung, New Materials Evaluation Center, Korea Research Institute of Standards and Science, P.O. Box 102, Taejon, 305-600 Korea. E-mail: hmpark@kriss.re.kr

Above room temperature there are three modifications of KLiSO₄ ; i.e. phase I, II and III. Phase transitions temperatures between them are 435°C and 668°C respectively. The x-ray diffraction intensities of phase I at about 700°C and of phase II at about 600°C were collected on the CAD4 single crystal diffractometer equipped a self-made furnace. During collection of intensities data, a prominent decay of intensities was observed. The crystal structure of phase I is the tridymite derivatives with ordered arrangement of SO₄- and LiO₄tetrahedra similar to that of phase III. The statistical data of the structure refinement for phase I with polar space group of P63mc was R = 0.057, Rw = 0.056 and S (goodness-of-fit) = 1.859. The crystals of phase II usually exhibit misleading hexagonal twinned cell which is composed of three orthorhombic twin domains in the temperature range between 435°C and 668°C. An almost twin-free single crystal of Phase II was observed at the elevated temperature. The crystal structure of phase II was refined with this crystal is orthorhombic with the polar space group $Pc2_1n$. The final statistical data was R = 0.077, Rw = 0.073 and the S = 1.028 with ordered arrangement of atoms. This data was compared with that of the twinned crystal corrected with twin ratio and further discussed previously reported disordered model with the space group of Pmcn.

Keywords: KLiSO4, structure analysis, high temperature