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Disorder in a natural ixiolite: high resolution studies at 293 K and 120 K.

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Grice, Ferguson and Hawthorne [1] describes the ixiolite of Bernic Lake, Manitoba, Canada. According to these authors, the ixiolite is part of the Ixiolite-Tantalite-Wodgnite system and crystallizes in space group Pbcn, with general formula MO_2 , in a α - PbO_2 structure type. The structure of the mineral ixiolite from Volta Grande pegmatite, in Brazil, is herein described from high resolution (0.5 Å) X-ray diffraction data using MoK α radiation. This mineral has formula MO_2 , with M = Fe, Mn, Nb or Ta. Data were collected at 293 K and at 120 K from a well formed crystal (0.6 x 0.4 x 0.3 mm). 49868 and 32294 reflections were collected at 293 K and at 120 K, respectively. The structure of the ixiolite was well solved in both temperatures: at 293 K the mineral crystalizes in the space group Cmcn, and the structure was refined to $R(F^2)=0.0476$, from 728 independent reflections. At 120 K, the mineral crystalizes in space group Pbcn, and the structure was refined to $R(F^2)= 0.0537$ from 1357 independent observations. It is interesting to notice that the different space groups of the herein described ixiolite at 120 K (Pbcn) and at 293 K (Cmcn) is related to the different occupations of oxygen sites, as expected from the high mobility of oxygen atoms.

[1] *Canadian Mineralogist*, 14, 540-549, 1976

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