
DISORDER IN NATURAL IXIOLITE: HIGH RESOLUTION STUDIES AT 293 K AND 120 K

Leandro Almeida^{1,*}; Bernardo Rodrigues²

¹ PANalytical Brasil, São Paulo, SP

² Departamento de Química da UFMG, Belo Horizonte, MG

*leandro.almeida@panalytical.com

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 $\alpha\text{-PbO}_2$ structure type. The structure of the mineral ixiolite from Volta Grande pegmatite, in Brazil, is herein described from high resolution (0.5\AA) X-ray diffraction data using $\text{MoK}\alpha$ radiation. This mineral has formula MO_2 , with $\text{M} = \text{Fe, Mn, Nb or Ta}$. Data were collected at 293 K and at 120 K from a well formed crystal ($0.6 \times 0.4 \times 0.3 \text{ mm}$). 49868 reflections were collected at 293 K and 32294 reflections at 120 K. The structure of the ixiolite was well solved in both temperatures: at 293 K the mineral crystalized 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 (same as reference), 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 [1]