

Polarized FTIR spectroscopic examination on hydroxylation in the minerals of the wolframite group, (Fe,Mn,Mg)[W,(Nb,Ta)][O,(OH)]₄

DOMINIK TALLA^{1,2,*}, ANTON BERAN¹, RADEK ŠKODA², AND ZDENĚK LOSOS²

¹Institut für Mineralogie und Kristallographie, Universität Wien, Althanstrasse 14, 1090 Wien, Austria

²Department of Geological Sciences, Masaryk University, Kotlářská 2, 611 37 Brno, Czech Republic

ABSTRACT

Polarized FTIR spectroscopic measurements of 11 natural wolframite single crystals from different occurrences revealed the common presence of structurally bound OH groups in their crystal lattice, with potential influence on the properties of this geologically and technologically important group of compounds. Despite differences in the appearance of the OH absorption pattern, dependent among other on the end-member ratio, two types of “intrinsic” OH defects could be discerned from detailed studies of the pleochroic behavior of the absorption bands both at 80 K and room temperature. The accompanying chemical analyses by the electron microprobe helped to clearly identify the substitution trend $W^{6+} + O^{2-} \leftrightarrow (Nb,Ta)^{5+} + OH^-$ as the prevailing hydrogen incorporation mechanism into wolframite. The assignment of the observed IR absorption phenomena to hydrous defects was confirmed by the results of deuteration experiments and the negligible contribution of included impurities to the FTIR spectra in the OH absorption region. The results obtained in this study of natural wolframite crystals can be used to detect and analyze hydrous defects in synthetic technologically important tungstates.

Keywords: Wolframite, FTIR spectroscopy, OH defects, nominally anhydrous minerals, deuteration, flux synthesis