

The Electric Field Gradient In Natural Chrysoberyl And Sinhalite

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This work reports on the evaluation of the electric field gradient EFG in two olivine-type minerals with low iron content, viz. a natural chrysoberyl (ideal formula $\text{Al}_2\text{BeO}_4:\text{Fe}$, 0.03 Fe ions pfu, space group Pnma, $a = 9.4203(9)\text{Å}$, $b = 5.4871(5)\text{Å}$, $c = 4.4331(4)\text{Å}$, $Z=4$) and sinhalite (ideal formula $\text{MgAlBO}_4:\text{Fe}$, 0.04 Fe ions pfu, space group Pnma $a = 9.906(1)\text{Å}$, $b = 5.691(1)\text{Å}$, $c = 4.337(1)\text{Å}$, $Z=4$). Iron in the olivine structure may be located on the two non-equivalent crystallographic sites M1 (point symmetry -1) and M2 (point symmetry m), respectively. Unlike in the isostructural alexandrite (Weber et al. 2007), there is no indication for Fe^{2+} in the chrysoberyl lattice, but the temperature-dependent Mössbauer spectra can all be reproduced by three subspectra with hyperfine parameters typical for Fe^{3+} located. In accordance with the results on alexandrite powder samples (Weber et al. 2007), Fe^{3+} in chrysoberyl has strong preference for the M2 site with a minor tendency to occupy M1. Whereas the angle parameters can unequivocally be assigned to Fe^{3+} on M1, on M2 they cannot due to the large linewidth. However, the calculated angles are not contradictory to ascribing this subspectrum to M2. In addition, the calculated quadrupole splittings and asymmetry parameters are in quantitative agreement with the experimental values. Experiments for explaining the large linewidth mentioned above are on course.

In the Mössbauer spectra of sinhalite the doublets exhibit distinct asymmetries with regard to the direction of the incident γ -rays. Nevertheless, the spectra have been fitted with a single doublet without any restrictions using starting parameters for the quadrupole splitting and the angles between the EFG and the crystallographic axes as obtained by the electronic structure calculations for Fe^{2+} at the M2 position. Unlike in our earlier investigations (Weber et al. 2009) there is no indication for a second doublet associated with Fe^{2+} on the M1 position. The detected asymmetry in the powder spectrum has therefore to be attributed to texture. This conclusion is confirmed by the single crystal Mössbauer spectrum recorded under magic angle that yields a completely symmetric doublet. Hence, the whole iron content of sinhalite is divalent and can be located on the M2 position exclusively. This is in accordance with other experimental results, as well as the electronic structure calculations. Summarizing, even small amounts of Fe in minerals can be used as “nanoprobe” in order to derive reasonable EFG tensors leading to distinct site attributions.

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References:

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