

s11.m1.p11 **Mineralogical and Structural Investigations of Volkonskoite from West Ural.** Y.S. Simakova, *Institute of Geology RAS, Syktyvkar, Russia.*
Keywords: volkonskoite, chromium, smectite.

Volkonskoite is unique mineral from smectite group containing dominant chromium in the octahedral position. Volkonskoites are differ not only in their chromium content but also in their basic structure, the species status of the mineral has been unclear. To resolve this uncertainty we examined about 15 samples of volkonskoites from permian deposits (West Ural) by several mineralogical techniques.

Chemical analysis shows great variations in chromium content (17-30 wt.%) in volkonskoites.

Calculated structural formulas show that mineral with 17-20 wt.% of Cr_2O_3 is dioctahedral smectite and volkonskoite with high chromium content is tri-dioctahedral one.

But IR and X-ray characteristics indicate dioctahedral type of structure of all the volkonskoites.

X-ray powder diffraction patterns of all samples have broad lines corresponding to minerals of the smectite group, and X-ray patterns of species with high chromium content indicate the presence of several smectites with different d_{001} value.

SEM investigations indicate the presence of different microstructures in volkonskoites: globular, acicular, tabular. The green and black varieties of volkonskoite has some differences in microstructures, IR-spectra and thermoanalytical characteristics.

SEM examinations suggest to exist a continuous solid solution series between volkonskoite and nontronite with Cr-Fe substitution in the octahedral position.

s11.m1.p12 **Electric-Field Gradients derived from CCD X-ray Diffraction Data in Silicates: the cases of ^{27}Al in Al_2SiO_5 Polymorphs and ^{25}Mg in Mg_2SiO_4 Forsterite.** N.E. Ghermani^a, S. Dahaoui^a, S. Ghose^b and J.A.K. Howard^c, ^a *Laboratoire de Cristallographie et Modélisation des Matériaux Minéraux et Biologiques, LCM^B, UPRES A CNRS 7036, Université Henri Poincaré, Nancy 1, Faculté des Sciences, Boulevard des Aiguillettes, BP 239, 54506 Vandoeuvre-lès-Nancy Cedex, France.* ^b *Mineral Physics group, Department of Geological Sciences, Box 351310, University of Washington, Seattle, Washington 98195, USA.* ^c *Crystallography Group, Department of Chemistry, University of Durham, South Road, Durham DH1 3LE, England.*
Keywords: EFG, CCD, silicates.

High-resolution single crystal X-ray diffraction intensities recorded with CCD (Charge-Coupled Device) detector at low temperature (100K) were used to derive the electron density distribution in three Al_2SiO_5 polymorphs [1] (andalusite, sillimanite and kyanite) and in Mg_2SiO_4 Forsterite. The goal of this study was twofold:(i) to estimate the nuclear quadrupole coupling tensors (QCT), at three types of ^{27}Al sites (octahedral, tetrahedral and trigonal-bipyramidal) in polymorphs and of ^{25}Mg in Forsterite, from the multipole refinements [2] using X-ray data and (ii) to show that the use of CCD detector for the accurate electron density determination can reproduce spectroscopic results. The ^{27}Al and ^{25}Mg nuclear quadrupole coupling tensors were estimated from both the internal polarization contribution of the aluminium and magnesium electron density and that of the lattice with electronic multipole parameters using MOLPROP93 program [3]. A new experimental estimation of ^{27}Al and of ^{25}Mg Sternheimer shielding/antishielding R and γ factors was made to achieve an agreement with ^{27}Al and ^{25}Mg NMR results [4, 5]. The quadrupole coupling tensors at the various Al-sites and Mg-sites determined by NMR were correctly reproduced from X-ray data for all three polymorphs of Al_2SiO_5 and for Forsterite compound.

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