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Computer modeling of the structure and spectral characteristics of rondorfite series minerals

M. Dulski (1), R. Wrzalik (1), and E. V. Galuskin (2)

(1) University of Silesia, Katowice, Poland (mdulski@us.edu.pl), (2) University of Silesia, Sosnowiec, Poland

Our researches are focused on the study of crystal structure and spectral characteristic of rondorfite with empirical formula Ca8Mg(SiO4)4Cl2 and a new phases possessing the similar structure. Rondorfite was first described from the Belleberg volcano in Germany. Rondorfite analyzed by us comes from the Upper Chegem volcanic structure, Northern Caucasus, Russia. Rondorfite forms isometric, rounded grains up to 0.3mm in size, it crystallizes in a cubic system (Fd-3 space group). The main structural unit is magnesiosilicate Si4MgO16, pentamer, in which the atomic arrangement is characterized by four isolated SiO4 tetrahedra combined by four-coordinated Mg2+ cation and sometimes by Al3+ and Fe2+/3+ cations. The structural configuration, where Mg2+ is in tetrahedral position, is very atypical for silica-minerals due to the geometry restrictions. The magnesiosilicate Si4MgO16 pentamers is complemented by 12 CaO6 octahedra. To balance the charge, big structural ceges are occupied by Cl or OHgroups. Wide isomorphism between Mg and Al3+ or Fe2+/3+ and also substitution of Cl by OH and H_2O allow us to expect a finding new mineral species in the rondorfite group. Theoretical calculation of structures supposed new mineral phases based on rondorfite structure and checking a stability of these phases make easier the procedure of new mineral species definition.

The structural data obtained for rondorfite crystal using powder and single crystal X-ray analyses were the starting data of our calculations. Modeling of the new phases in the rondorfite group using the isomorphic substitutions (Ca2+ + Mg2+→ Al3+ + Na+, Mg2+→Fe2+ or Ca2+ + Mg2+→ Fe3+ + Li+, Cl-→OH-), checking a stability of these crystal structures and determination of its spectral parameters were performed. Molecular dynamics calculation shows how different type of atoms affects to the reconstruction of the crystal structure of initial minerals. Molecular dynamics allows us also to carry out the calculation under various temperatures and pressures. This calculation allows to predict spectral parameters, i.e infrared (IR), Raman (RS), X-ray photoelectron spectra (XPS) or K- and L1-edge X-ray Absorption Spectra (XAS). These results will be helpful to recognize the new mineral species, processes and conditions, in which these minerals could be formed.

The calculations has been performing by QUANTUM ESPRESSO software using primitive unit cell. This program is based on density-functional theory, plane waves, and pseudopotentials (norm-conserving, ultrasoft, and projector-augmented wave).