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29Si MAS-NMR spectroscopy of Phlogopite: simulated and observed Al-distribution in tetrahedral site.

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^{29}Si NMR spectroscopy is powerful method to know the chemical environment of target atoms. According to previous researchers, Si NMR peak positions of alluminosilicate minerals shift to positive region about 4ppm, that represent each neighboring tetrahedral Al numbers per Si is 0, 1, 2, 3, and 4. Many researchers studied the tetrahedral Al-Si distribution in the 2:1 type phyllosilicate minerals to clarify its regularity. In addition, they have studied the tetrahedral Al-Si distribution of phlogopite, a 2:1 type of phyllosilicate mineral with simple chemical formula of $KMg_3AlSi_3O_{10}(OH,F)_2$, by using Monte Carlo method and HDC (Homogeneous Dispersion of Charge) model, in which the hexagonal ring of tetrahedra were treated as a control-unit to minimize calculation. However, residual error and mismatch of chemical formula in partial structure have been known in these methods. In this study, we firstly simulated NMR spectra of phlogopite by using ab initio calculation method. In the calculation, GGA (Generalized Gradient Approximation) function characterized by PBE was selected in CASTEP (Cambridge Serial Total Energy Package) ab initio calculation program for the condition of simulation. In the next step, we used 'All possibility' method and unit cell possible model to avoid residual error and mismatch of chemical formula in partial structure. In the CASTEP ab initio calculation for the structure models of phlogopite, we constructed the Al-distribution models in the tetrahedral structure, consisting of 1×1, 1×2, and 2×2 unit cells, and selected 2, 6, 112 possible models, respectively, satisfying Lowenstein's rule and partial unit chemical formula. The simulated NMR spectra of the models have well matched peak with the reference NMR data from synthetic tri-octahedral mica and our natural samples.