MS37-P03 | {1H/19F} -> 29Si/27Al CPMAS and HETCOR spectroscopy of synthetic lepidolites: Connectivities between F/OH and Si/Al in the octahedral and tetrahedral sheets

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The lithian muscovite-lepidolite composition series involves the minerals muscovite ($K(Al_2)(AlSi_3O_{10})(OH)_2$), trilithionite ($K(Li_{1.5}Al_{1.5})(AlSi_3O_{10})(F,OH)_2$) and polylithionite ($K(Li_2Al)(Si_4O_{10})F_2$). The main interest of our work focuses on the spectroscopic investigation of the order / disorder of Si and Al in the tetrahedral sheets and of Al, Li, F, and OH in the octahedral sheets of lepidolites.

Direct neighbourhoods of F/OH- to Si/Al can be checked by application of cross polarization (CP) experiments. The polarisation transfer is strongly dependent on the spatial distance between fluorine/proton and Si/Al. By variation of contact time the distance between the two nuclei could be estimated (cross polarization time t_{CP}) and additional information about the bonding behaviour of these nuclei is given by the longitudinal relaxation time of the ^{19}F or ^{1}H nucleus in the rotating frame ($T_1\rho$).

HETCOR (heteronuclear correlation) experiments are also useful for determination of site connectivities between different nuclei. The two-dimensional correlation is achieved by cross-polarization. Similar as in previous studies[1], $\{^{1}H/^{19}F\} \rightarrow {}^{29}Si$ HETCOR NMR- experiments should show that the tetrahedral sheets containing a high Al content are in direct neighbourhood of Al-rich clusters of the octahedral sheets. In addition, CPMAS-experiments could clarify if even OH and F are ordered in clusters.

[1] Langner, R., Fechtelkord, M., Garcia, A., Palin, E.J., Lopez-Solano, J. (2012) American Mineralogist, 97, 341–352.