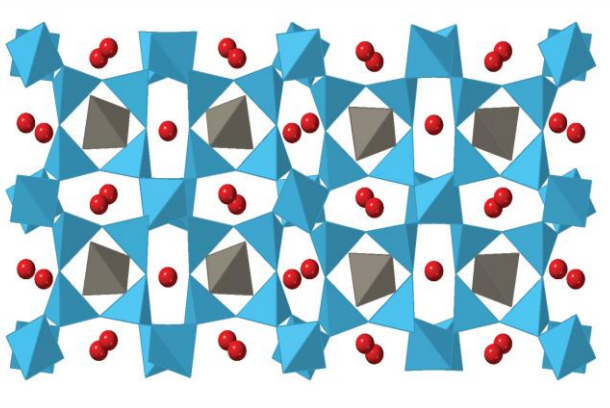
Using Solid-State NMR Spectroscopy and DFT Calculations to Study Disorder in Aluminate Sodalites

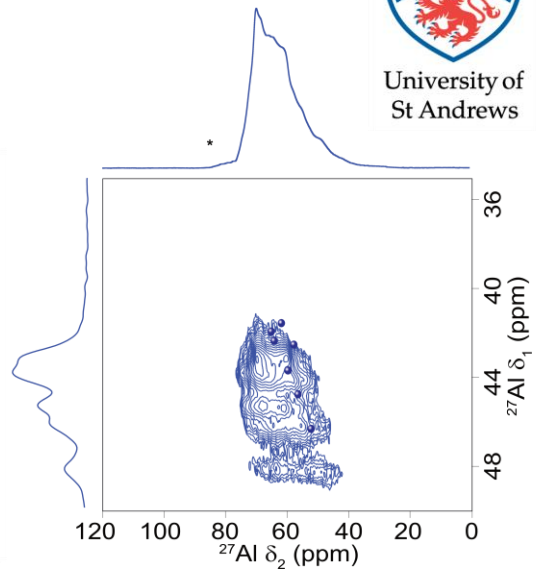
Sharminaz. C. S.,[1] Toby A. H. Fairs,[1] Daniel M. Dawson,[1] Finlay D. Morrison[1] and Sharon E. Ashbrook[1]
[1]School of Chemistry, EaStCHEM and Centre of Magnetic Resonance, University of St Andrews

University of St Andrews

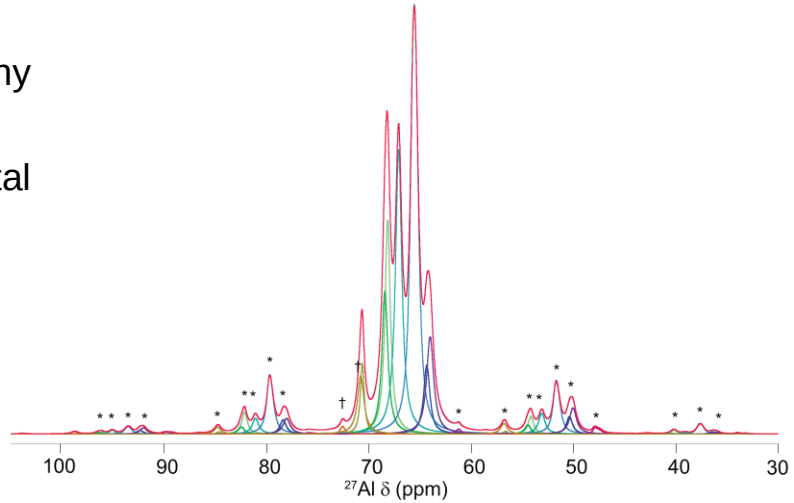
- Ferroelectrics offer a wide range of applications in energy storage devices, sensors, tunnel junctions and field effect transistors.
- Aluminate sodalites $M_8[Al_{12}O_{24}]X_2$ have ferroelectric properties.
- Materials under study have M = Ca or Sr and X = W or S, (giving CAW, SAS, and SAW end members and a solid solution of SAS and SAW).
- Solid-state NMR spectroscopy aids in understanding the local structure and disorder, with initial focus on ^{27}Al (I = 5/2).
- MAS is used to remove the anisotropic interactions and MQMAS/DOR are performed to remove the second-order quadrupolar broadening.
- VT NMR experiments help to identify any anion dynamics and any phase transitions.
- DFT NMR calculations are used to help interpret the experimental data.



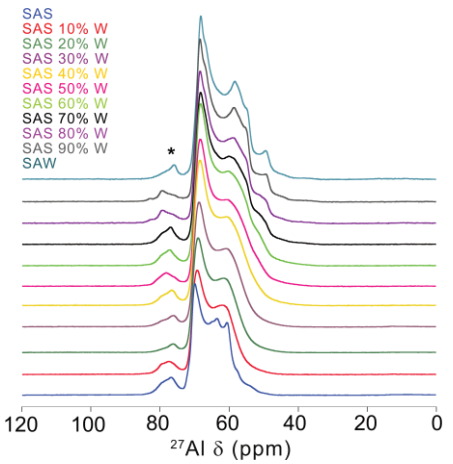
Schematic structure of CAW with corner-sharing tetrahedral Al (cyan), WO_4 (grey) and Ca (red).[5]



^{27}Al (14.1 T) MAS and MQMAS NMR spectra of CAW, with an overlay of DFT predictions.



^{27}Al DOR NMR spectrum of CAW.



^{27}Al MAS NMR spectra of solid solution of SAS and SAW.

Future Work

DOR NMR | ^{183}W NMR | VT NMR | ^{17}O NMR | ^{17}O - ^{27}Al NMR