

Supporting Information for 'Optimization of sol-gel formed ZnO:Al processing parameters by observation of dopant ion location using solid state ^{27}Al NMR'

Tim Kemmitt, Bridget Ingham and Rachael Linklater

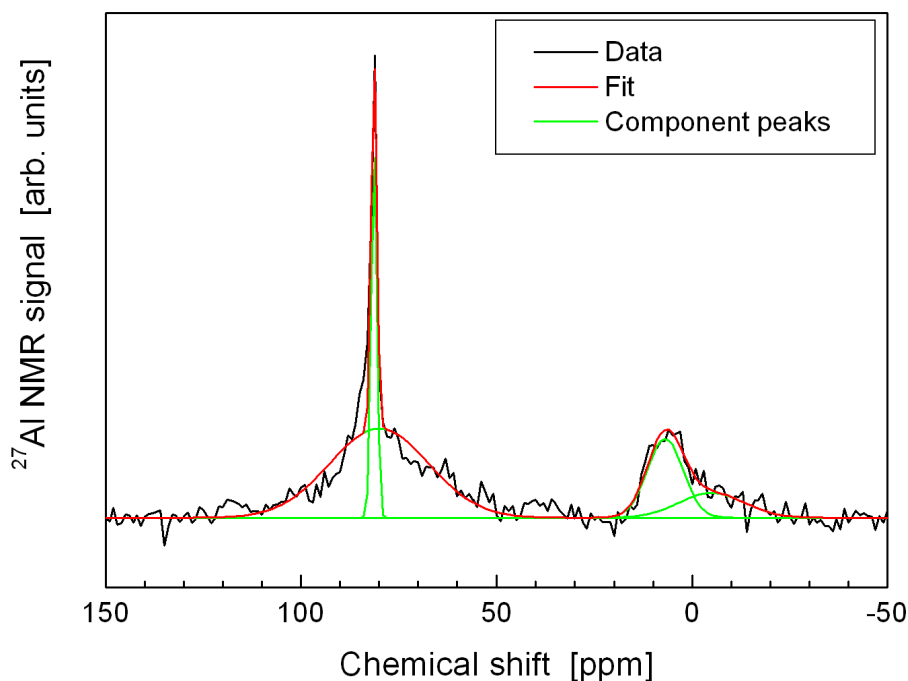


Figure S1. Example of deconvolution of ^{27}Al NMR spectrum for a 2 at% Al-doped ZnO samples prepared using ethanolamine, pre-heated at 90°C and calcined at 500°C for 1 hr.

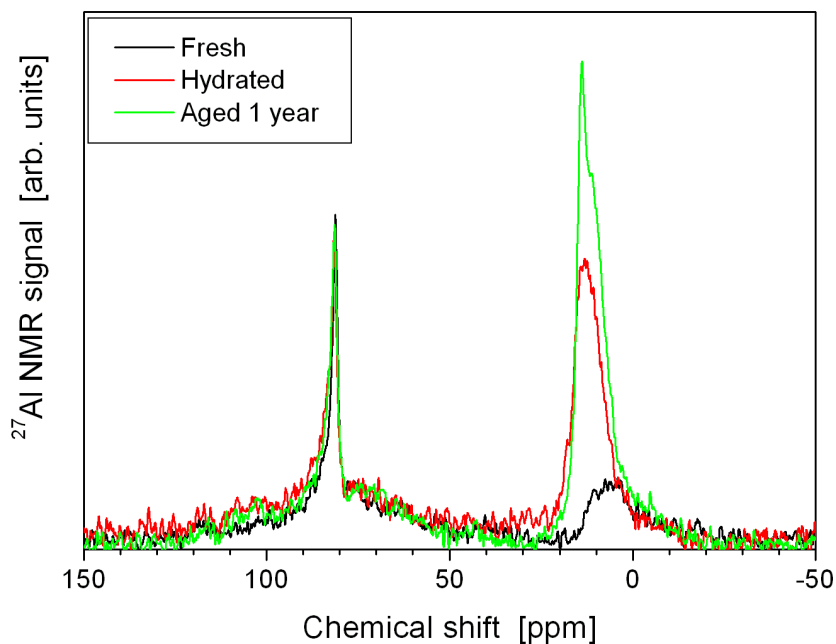


Figure S2. ^{27}Al NMR spectra for a sample prepared under 'standard' conditions (EA as aminoalcohol species, 2 at% Al) - freshly prepared (black), stored in 100% humid atmosphere for 3 days (red), stored in ambient conditions for 1 year (green).

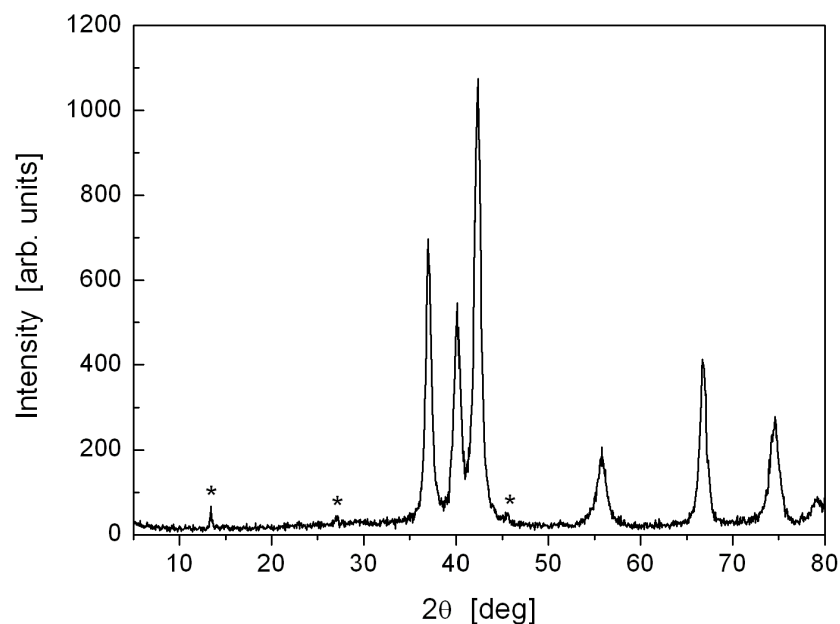


Figure S3. XRD pattern for the sample in Figure S1 stored in ambient conditions for 1 year, showing ZnO peaks and additional peaks (*) which can be assigned to a zinc aluminium carbonate hydroxide hydrate (ICDD pattern 48-1022).

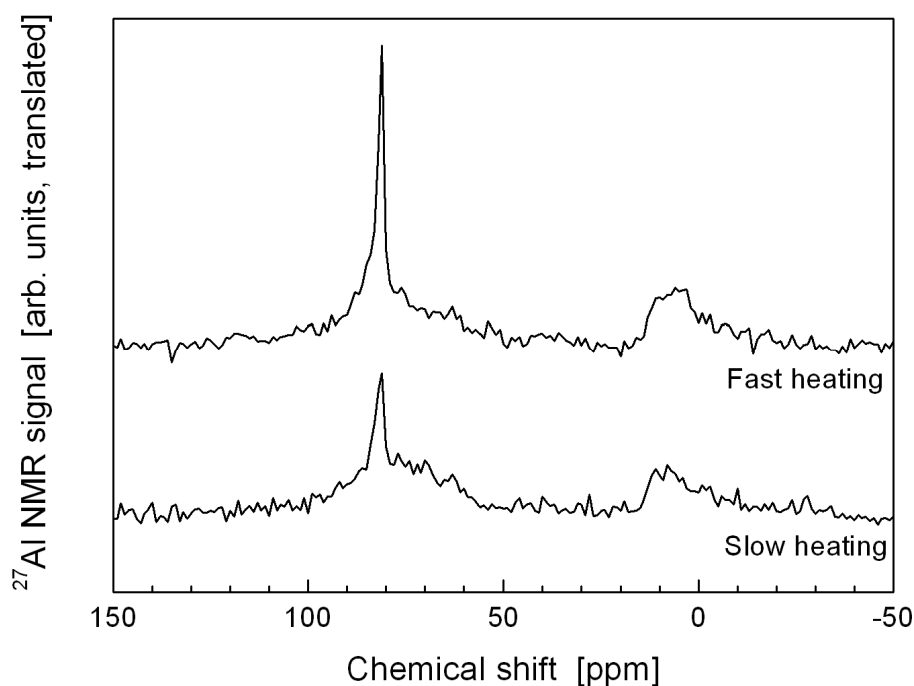


Figure S4. ^{27}Al NMR spectra of 2 at% Al-doped ZnO samples heated to 500°C for 1 h, in a preheated oven (top), and with a heating rate of 2° min⁻¹ (bottom).

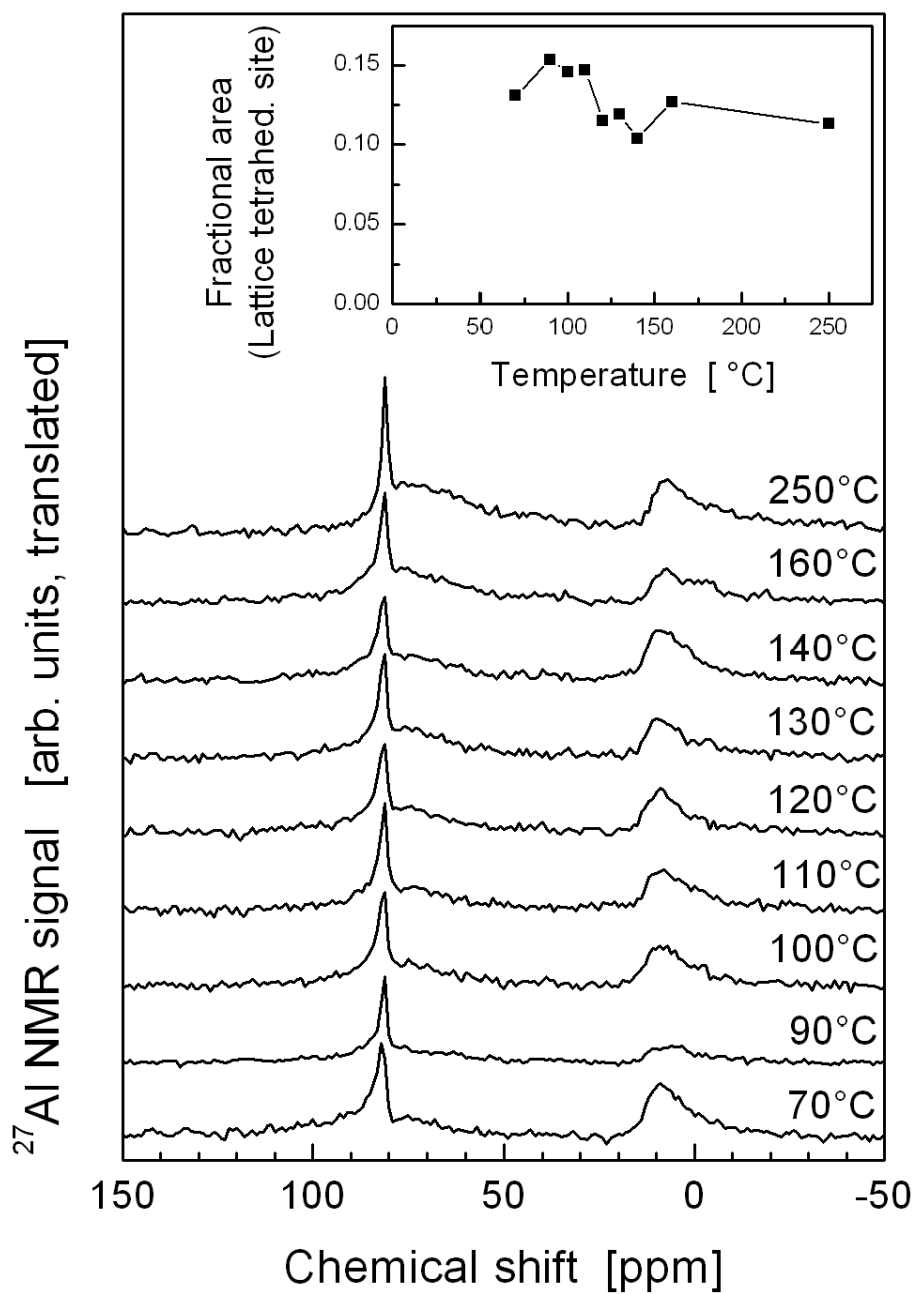


Figure S5. ^{27}Al NMR spectra of 2 at% Al-doped ZnO samples heated at various intermediate temperatures (as indicated) prior to calcination at 500°C for 1 hr.

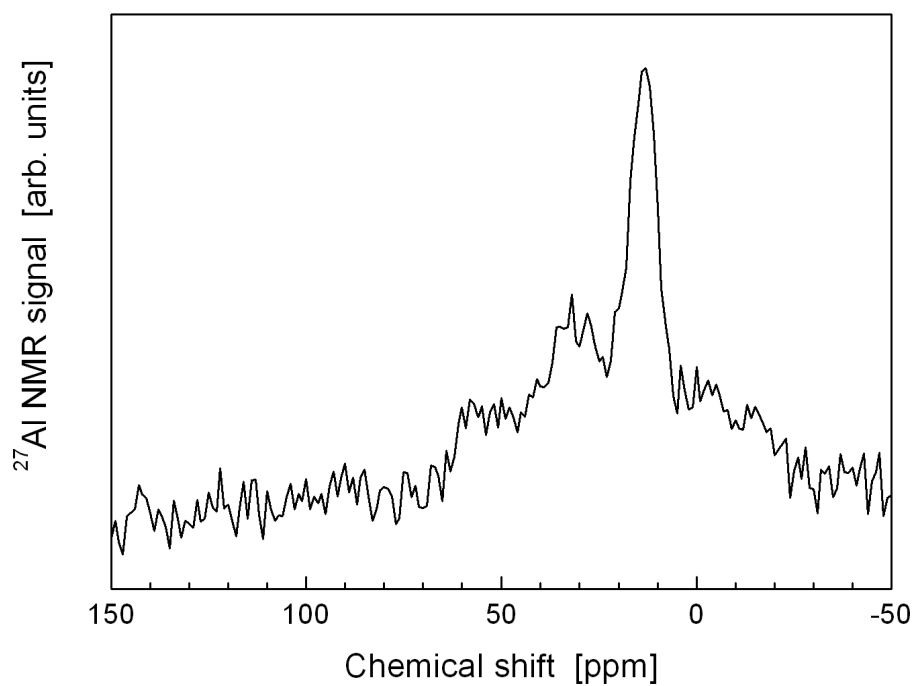


Figure S6. ^{27}Al NMR of 2 at % Al doped ZnO prepared using a precursor containing 40% v/v glycerol.

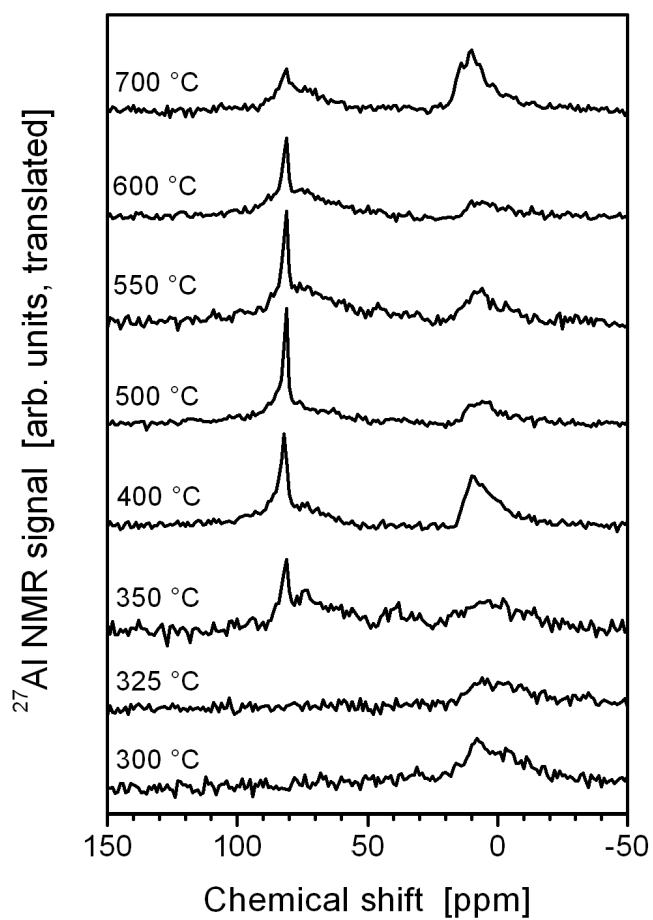


Figure S7. ^{27}Al NMR signals in 2 at % Al-doped samples heated for 1 h at various temperatures (as indicated).

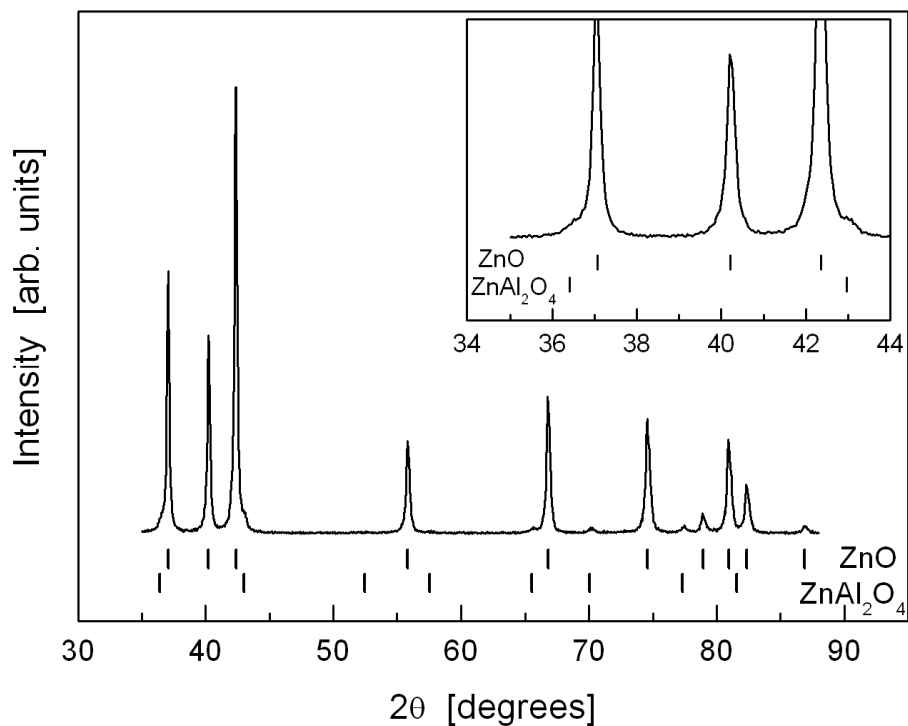


Figure S8. XRD of sol-gel formed ZnO containing 8 at% Al dopant calcined at 800°C, showing the presence of the gahnite (ZnAl_2O_4) phase.

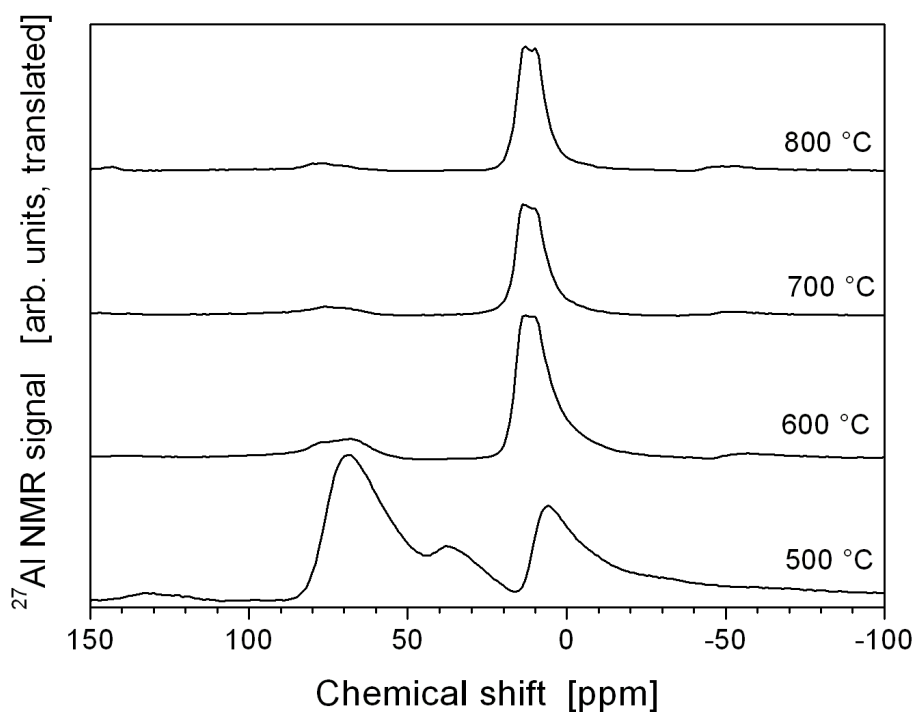


Figure S9. Evolution of ^{27}Al NMR spectra with temperature, of gahnite formation from ZnAl_2O_4 gel calcined at various temperatures (as indicated).

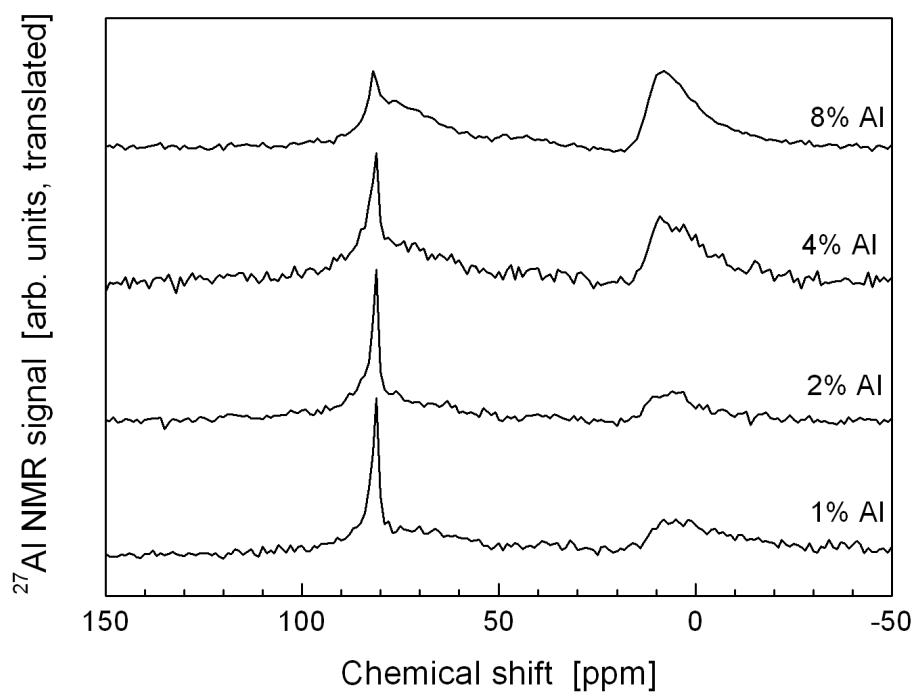


Figure S10. ^{27}Al NMR spectra of ZnO samples containing various levels of Al dopant (as indicated). Gels were pre-heated at 90°C and calcined at 500°C .

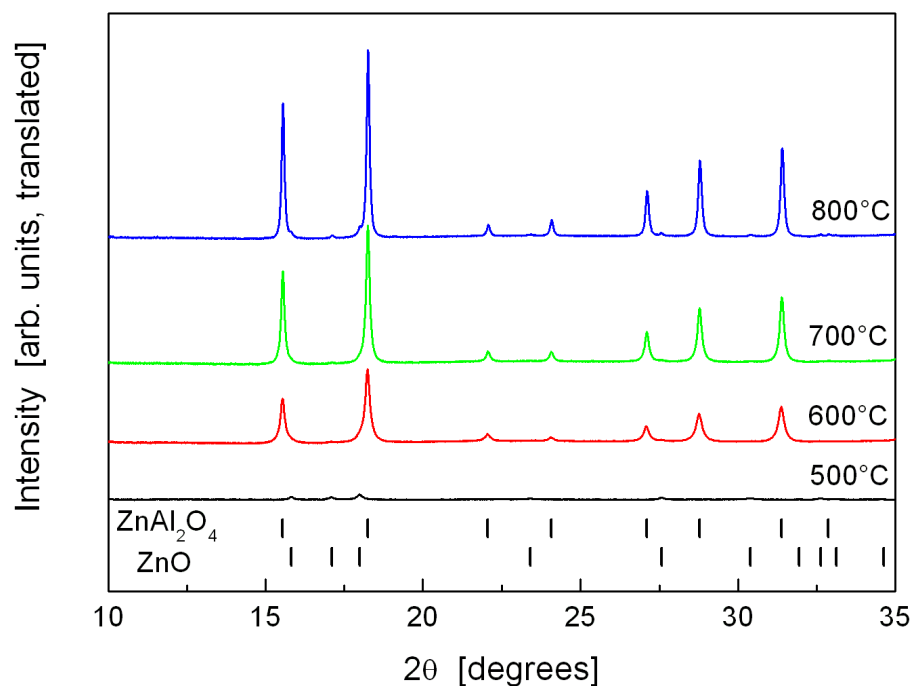


Figure S11. Synchrotron powder XRD patterns of ZnAl_2O_4 gel calcined at various temperatures (as indicated).