# $^{27}$Al MQMAS of the δ-$Al_{13}$-Keggin

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# *1. Fitting of the $^{23}Na$ spectrum*

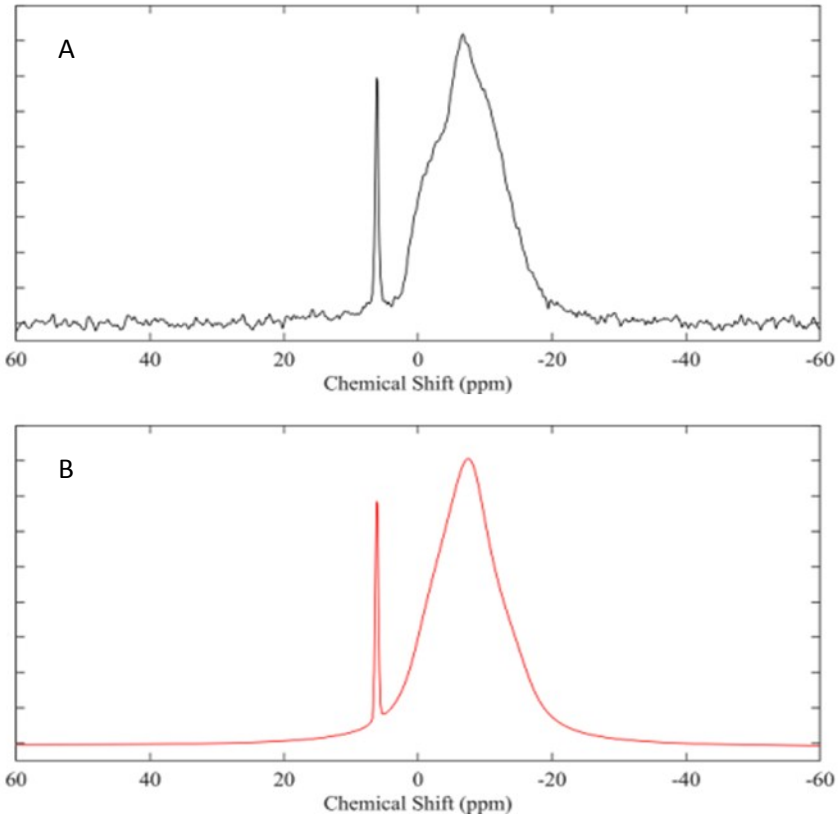


Figure S-1: One-dimensional $^{23}Na$ spectrum of the δ-$Al_{13}$ cluster, with A) the experimental data, and B) the fit of the data using Dmfit. The sharp peak at 6.2 ppm is from residual NaCl in the solid while the broad peak centered at -6.7 ppm is due to the $Na^+$ ion capping the δ-$Al_{13}$ ion.

| **$\delta_{iso}$ (ppm)** | **Peak Fitting Model** | **Amplitude (a.u.)** | **EM Parameter (a.u.)** | **$C_Q$ (MHz)** | **η** | **Width (ppm)** | **G/L Ratio** | **Integrated Intensity (%)** |
|---|---|---|---|---|---|---|---|---|
| 6.14 | Gaussian/Lorentzian | 133.12 | | | | 0.50 | 0.82 | 3.70 |
| 0.07 | Q MAS 1/2 | 751.38 | 986.76 | 2.36 | 1.00 | | | 96.30 |

Table S-1: Parameters for the fitting of the $^{23}Na$ spectrum using Dmfit. Two types of models were used, a quadrupolar lineshape model (Q MAS 1/2) to account for the quadrupolar shape of the central transition, and a Gaussian/Lorentzian model to account for the sharp peak seen at 6.14 ppm.

## *2. Compiled list of parameters for the fit of the $^{27}Al$ spectra*

| Peak Number | $\delta_{iso}$ (ppm) | Peak Fitting Model | Amplitude (a.u.) | EM Parameter (a.u.) | $C_Q$ (MHz) | η | Width (ppm) | G/L Ratio | Integrated Intensity (%) |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 4.53 | Q MAS 1/2 | 250.62 | 1407.52 | 4.55 | 0.04 | | | 21.41 |
| 2 | 6.17 | Q MAS 1/2 | 160.96 | 528.28 | 6.24 | 0.68 | | | 26.79 |
| 3 | 5.77 | Q MAS 1/2 | 91.68 | 255.66 | 10.57 | 0.20 | | | 44.20 |
| 4 | 67.75 | Q MAS 1/2 | 100.39 | 410.52 | 4.06 | 0.45 | | | 7.10 |
| 5 | 60.20 | Gaussian/Lorentzian | 7.75 | | | | 1.96 | 1.0 | 0.50 |

Table S-2: Parameters for the fitting of the 27Al spectrum using Dmfit. Two types of models were used, a quadrupolar lineshape model (Q MAS 1/2) to account for the quadrupolar shape of the central transition, and a Gaussian/Lorentzian model to account for the sharp peak seen at 60.20 ppm.