

Single-crystal XRD and solid-state NMR structural resolution of a layered fluorinated gallium phosphate: $\text{RbGa}_4(\text{PO}_4)_3\text{F}_4 \cdot \text{C}_5\text{N}_2\text{H}_{14} \cdot 2\text{H}_2\text{O}$ (MIL-145)

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Electronic Supplementary Information

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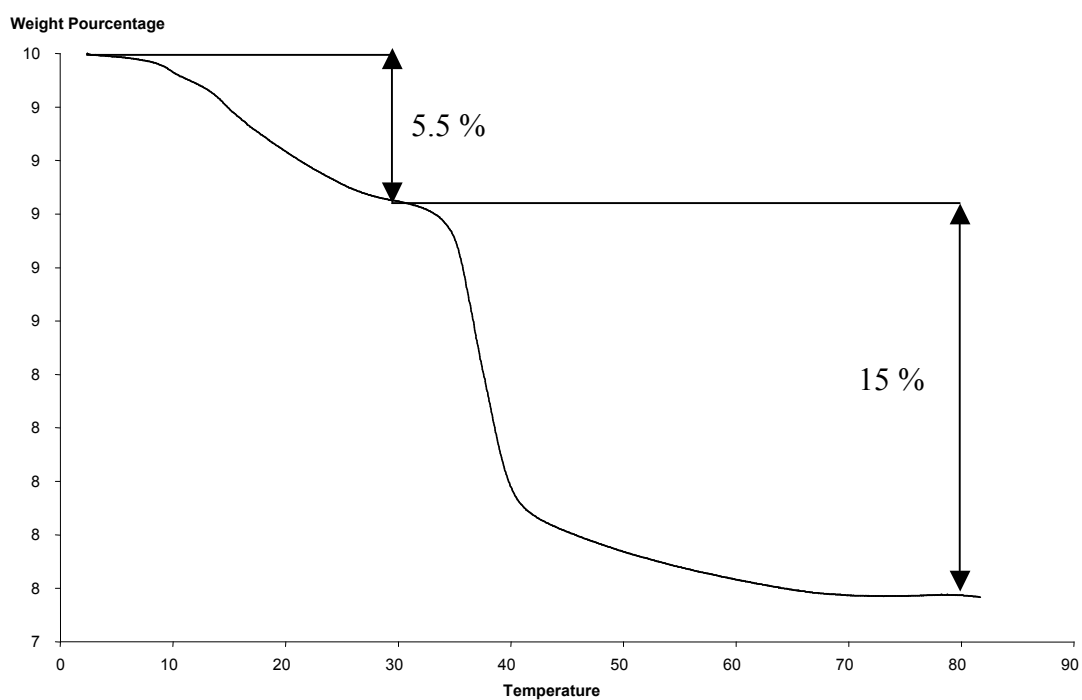


Fig. S1 Thermogravimetric curve of $\text{RbGa}_4(\text{PO}_4)_3\text{F}_4 \cdot \text{C}_5\text{N}_2\text{H}_{14} \cdot 2\text{H}_2\text{O}$ or MIL-145 (under O_2 , $2^\circ\text{C} \cdot \text{min}^{-1}$).

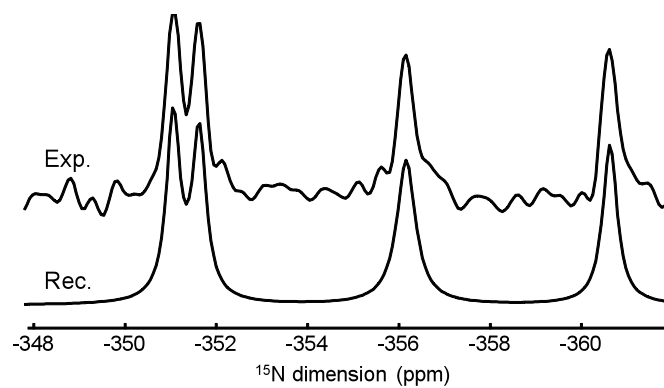


Fig S2 Experimental and reconstructed $^1\text{H}\rightarrow^{15}\text{N}$ CPMAS NMR spectra of $\text{RbGa}_4(\text{PO}_4)_3\text{F}_4\cdot\text{C}_5\text{N}_2\text{H}_{14}\cdot 2\text{H}_2\text{O}$ (MIL-145) showing the presence of four inequivalent nitrogen atoms.

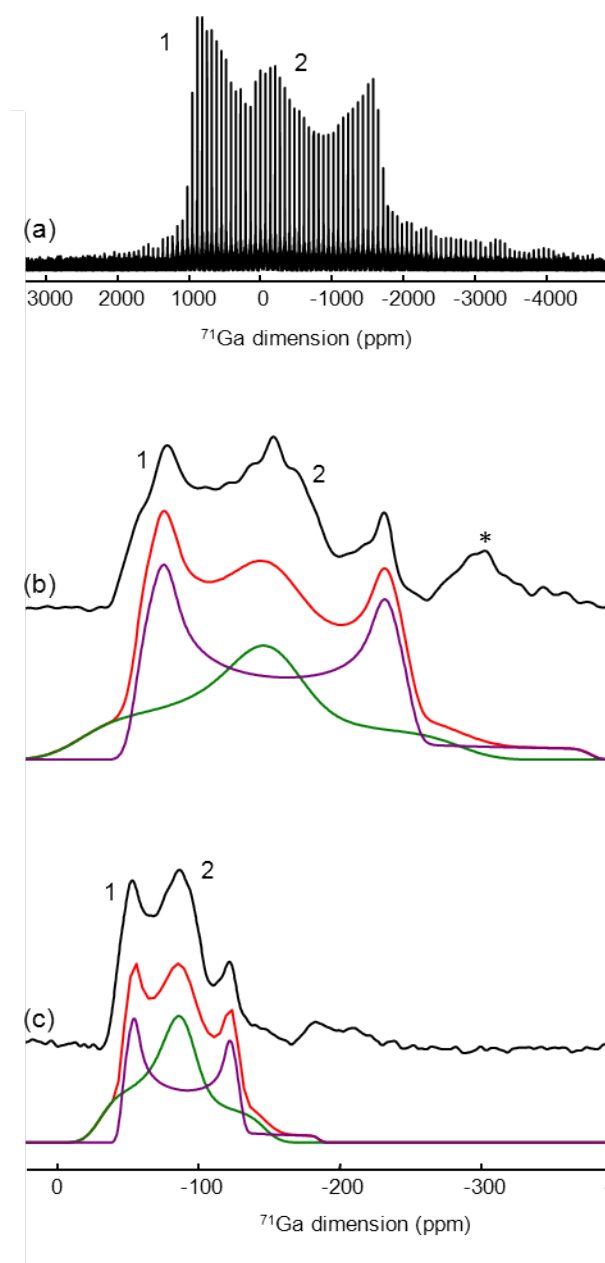


Fig. S3. ^{71}Ga NMR spectra of $\text{RbGa}_3(\text{PO}_4)_2(\text{HPO}_4)\text{F}_4 \cdot \text{C}_5\text{N}_2\text{H}_{16} \cdot 2\text{H}_2\text{O}$ (MIL-145). (a) Static WURST-QCPMG spikelet spectrum recorded at $B_0 = 4.7$ T. Single pulse NMR spectra recorded at (b) $B_0 = 11.7$ T and $\nu_{\text{MAS}} = 34$ kHz and (c) $B_0 = 17.6$ T and $\nu_{\text{MAS}} = 30$ kHz. The reconstructed MAS NMR spectra are shown below. The star represents an unidentified impurity.

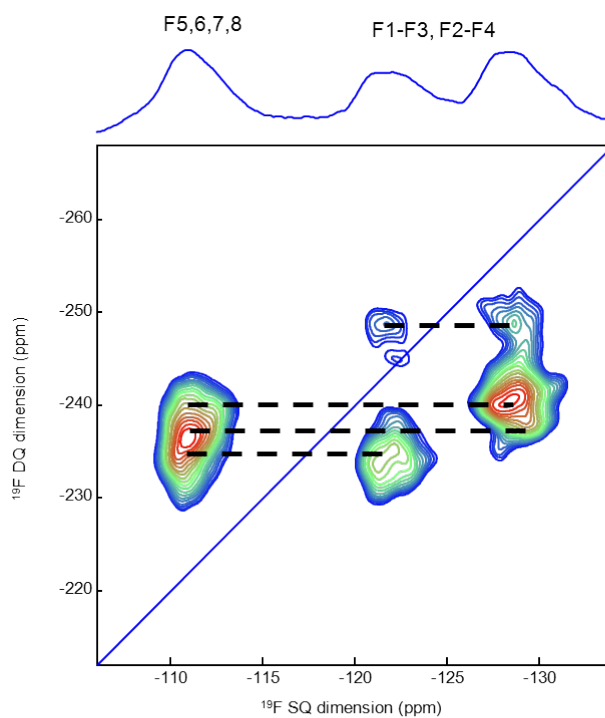


Fig. S4. 2D $^{19}\text{F} \rightarrow ^{19}\text{F}$ DQ-SQ NMR spectrum of $\text{RbGa}_4(\text{PO}_4)_3\text{F}_4 \cdot \text{C}_5\text{N}_2\text{H}_{14} \cdot 2\text{H}_2\text{O}$ (MIL-145). The top spectrum, on which lines are labeled, is the full projection on the horizontal dimension. The thick line indicates the diagonal of slope 2. Dash lines indicate F-F cross-correlations.

Some additional comments on the data collection:

The completeness is reported as 0.913 is quite low but if one slightly reduces the theta range, the completeness is greater than 0.99 for the coverage up to 28.0° for instance.