Supplementary Material for PCCP
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Electronic Supplementary Information

Mg-25 Ultra-High Field Solid State NMR Spectroscopy and First Principles Calculations of Magnesium Compounds

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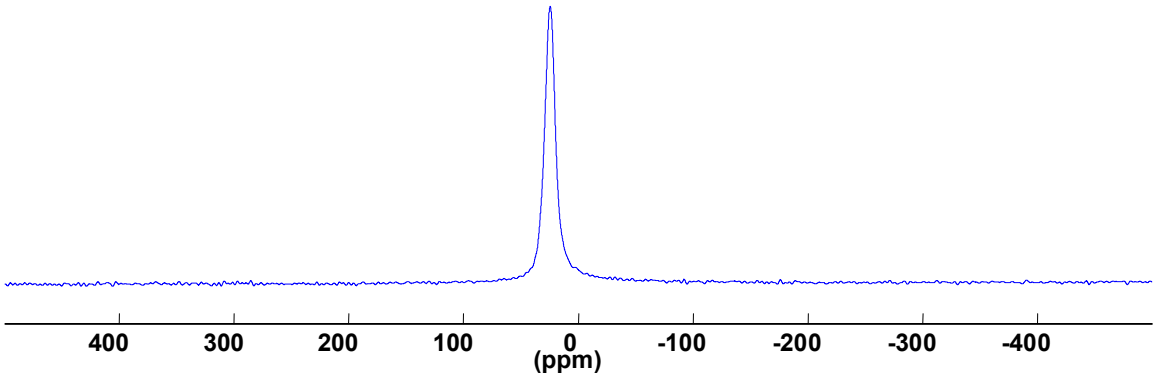

Figure S1 – Static Bloch Decay ^{25}Mg NMR spectrum of MgO.

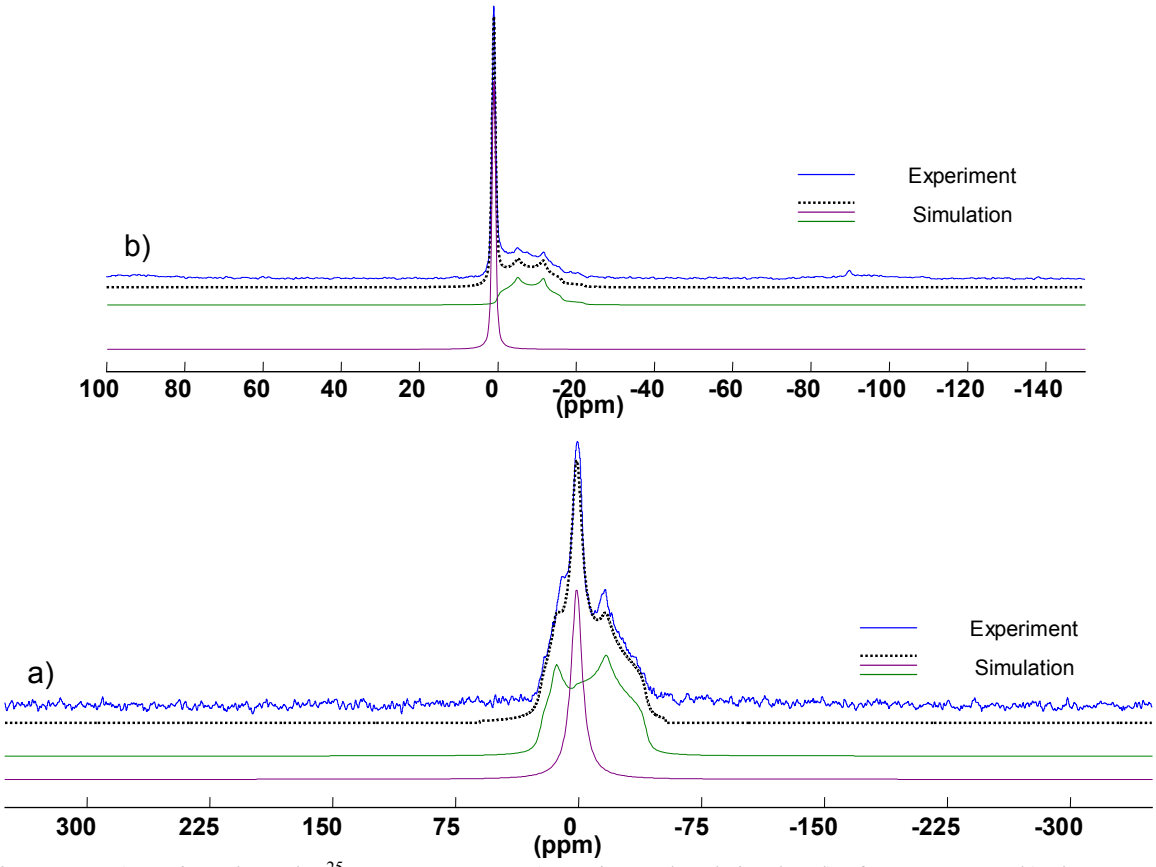

Figure S2 – a) Static Hahn Echo ^{25}Mg NMR spectra (experimental and simulated) of $MgSO_4 \cdot 6H_2O$ b) 5kHz MAS Bloch Decay spectra (experimental and simulated) of $MgSO_4 \cdot 6H_2O$.

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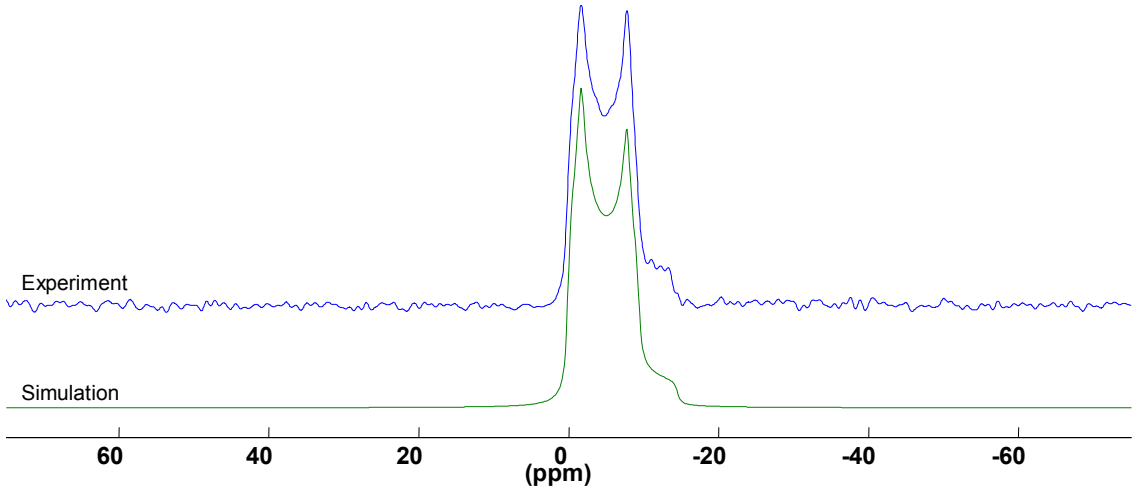

Figure S3 – 5kHz MAS Bloch Decay ^{25}Mg NMR spectra (experimental and simulated) of MgSO4·7H_2O.

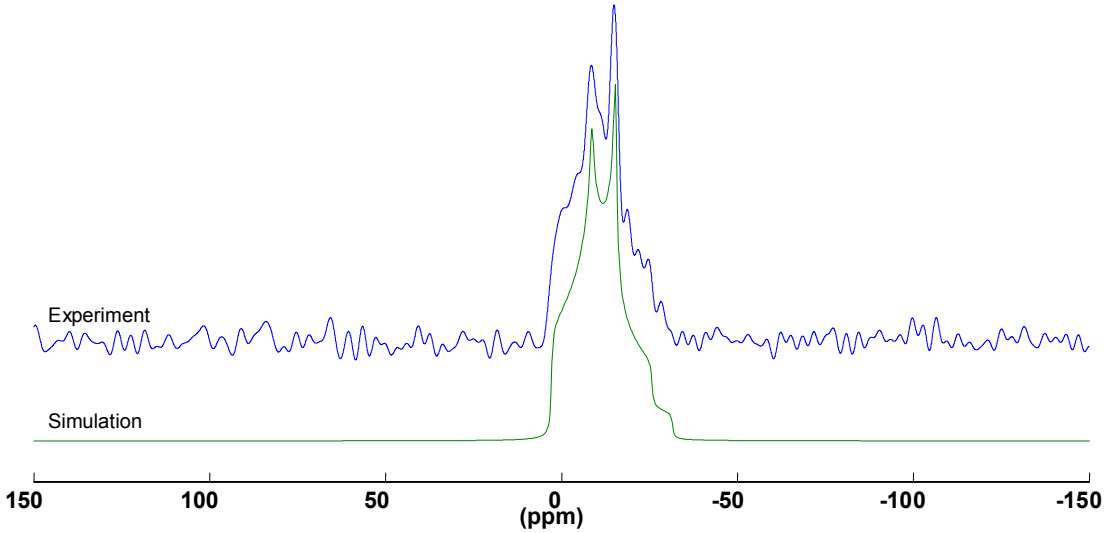

Figure S4 – 5kHz MAS Bloch Decay ^{25}Mg NMR spectra (experimental and simulated) of $Mg(NH_4)_2(SO_4)_2·6H_2O$.

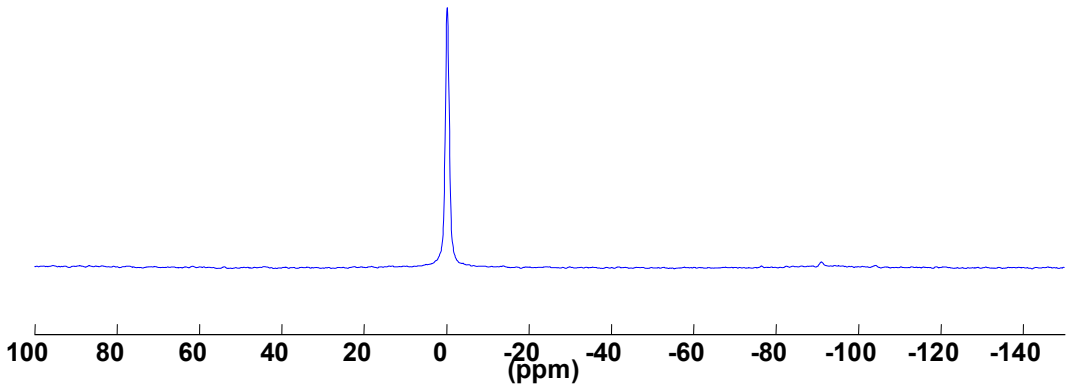

Figure S5 – 5kHz MAS Bloch Decay ^{25}Mg NMR spectrum of $MgCl_2·6H_2O$

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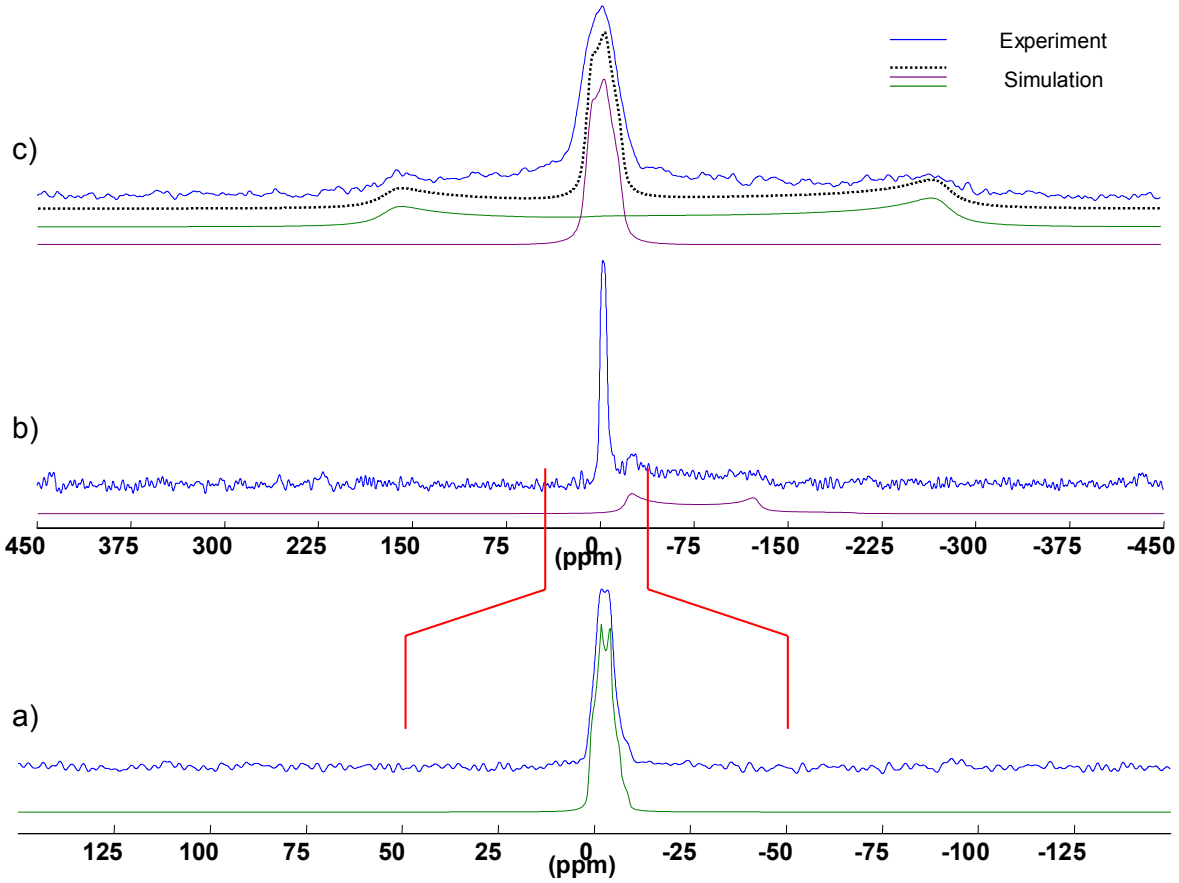

Figure S6 –. a) 5kHz MAS Bloch Decay ^{25}Mg NMR spectra (experimental and simulated) of one site in $MgPO_4 \cdot 8H_2O$. The second site (in b)) is too broad and weak to be seen at this spinning speed. b) 12kHz MAS full Hahn Echo ^{25}Mg NMR spectra (experimental and simulated) of the second site in $MgPO_4 \cdot 8H_2O$. Simulation of narrower signal shown in a). c) Static Hahn Echo ^{25}Mg NMR spectra (experimental and simulated) of $MgPO_4 \cdot 8H_2O$.

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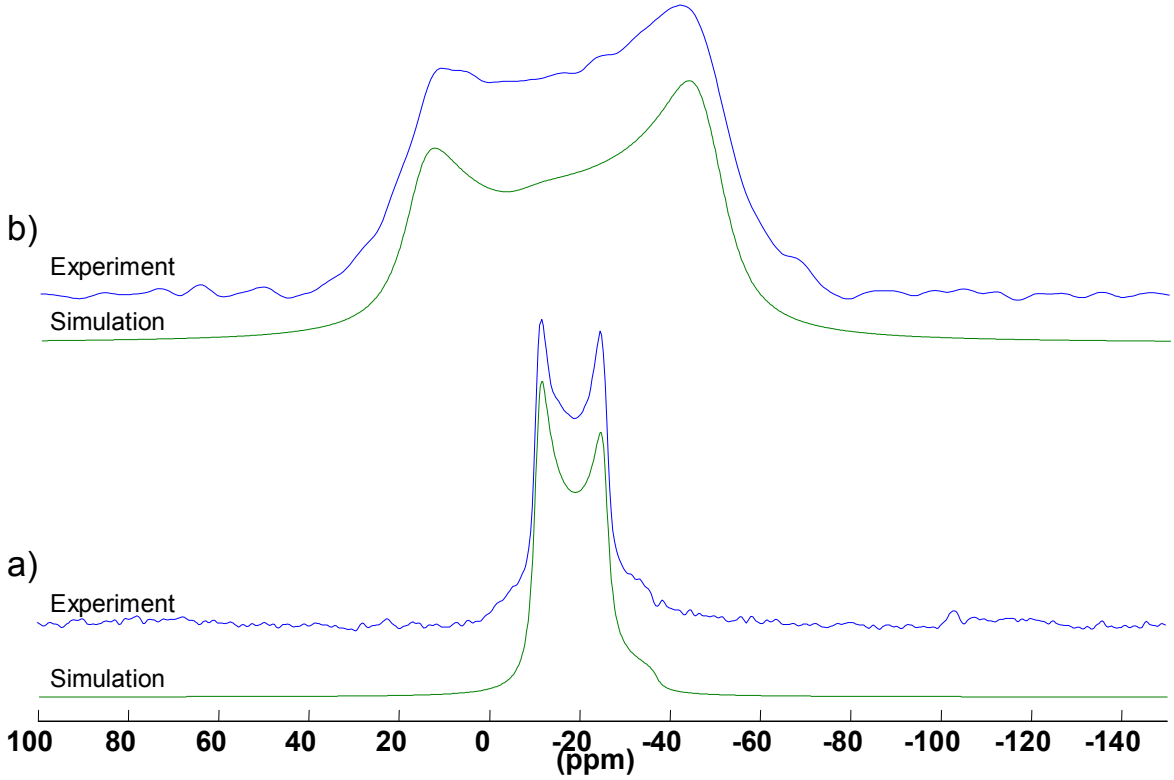

Figure S7 – a)5kHz MAS Bloch Decay ^{25}Mg NMR spectra (experimental and simulated) of $MgHPO_3 \cdot 3H_2O$. b) Static Hahn Echo ^{25}Mg NMR spectra (experimental and simulated) of $MgHPO_3 \cdot 3H_2O$.

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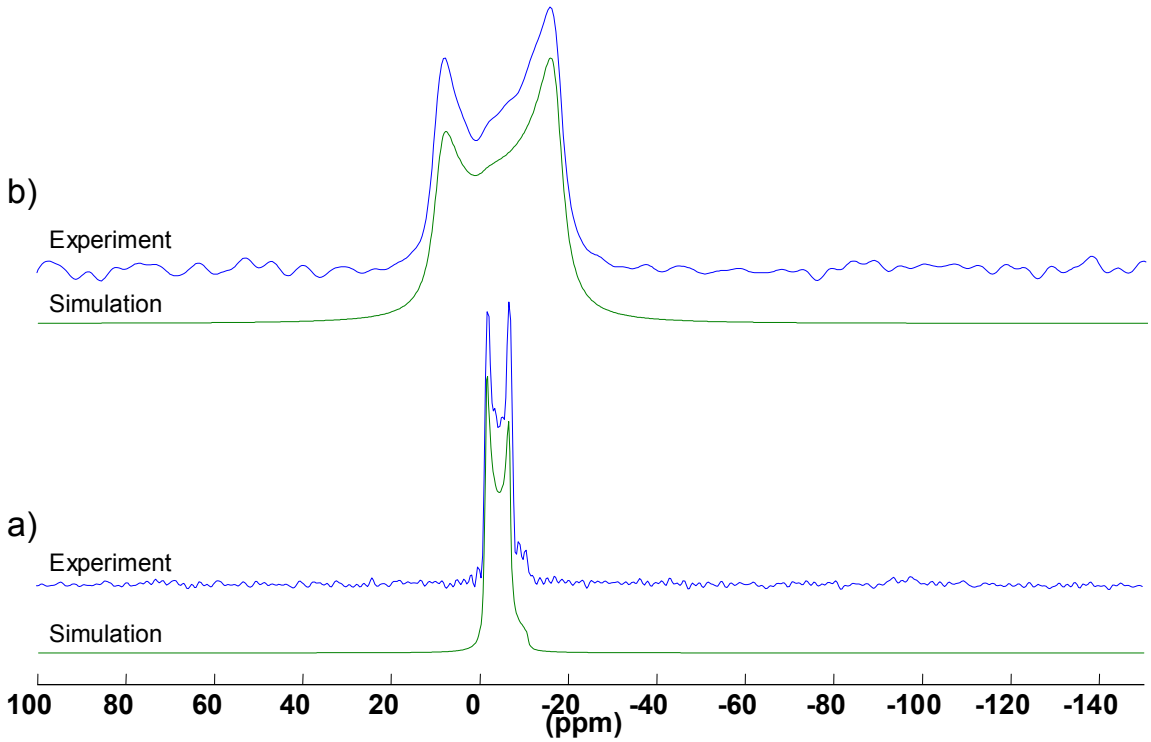

Figure S8 – a) 5kHz MAS Bloch Decay ^{25}Mg NMR spectra (experimental and simulated) of $Mg(NO_3)_2 \cdot 6H_2O$. b) Static Hahn Echo ^{25}Mg NMR spectra (experimental and simulated) of $Mg(NO_3)_2 \cdot 6H_2O$.

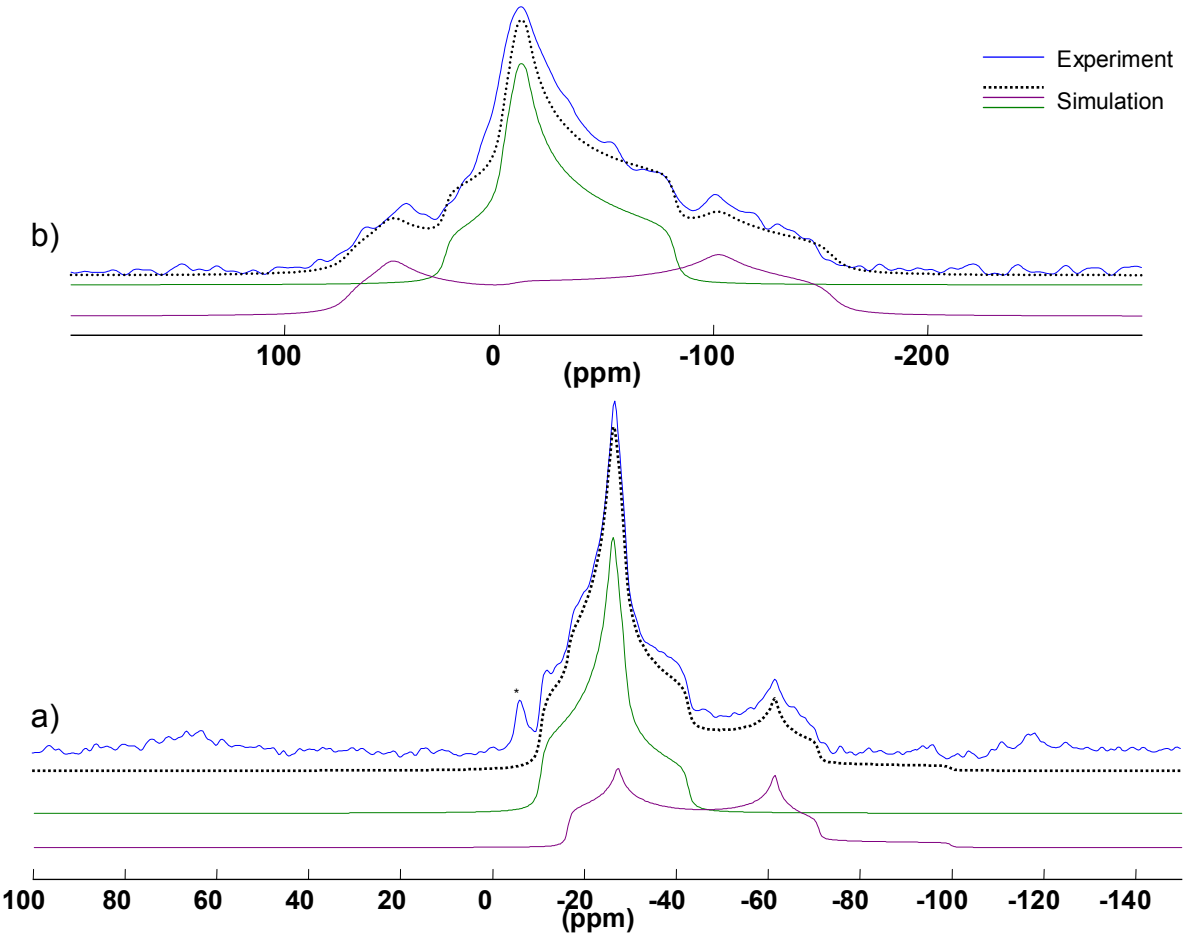

Figure S9 – a) 5kHz MAS Bloch Decay ^{25}Mg NMR spectra (experimental and simulated) of $MgMoO_4$. b) Static Hahn Echo ^{25}Mg NMR spectra (experimental and simulated) of $MgMoO_4$. *impurity.

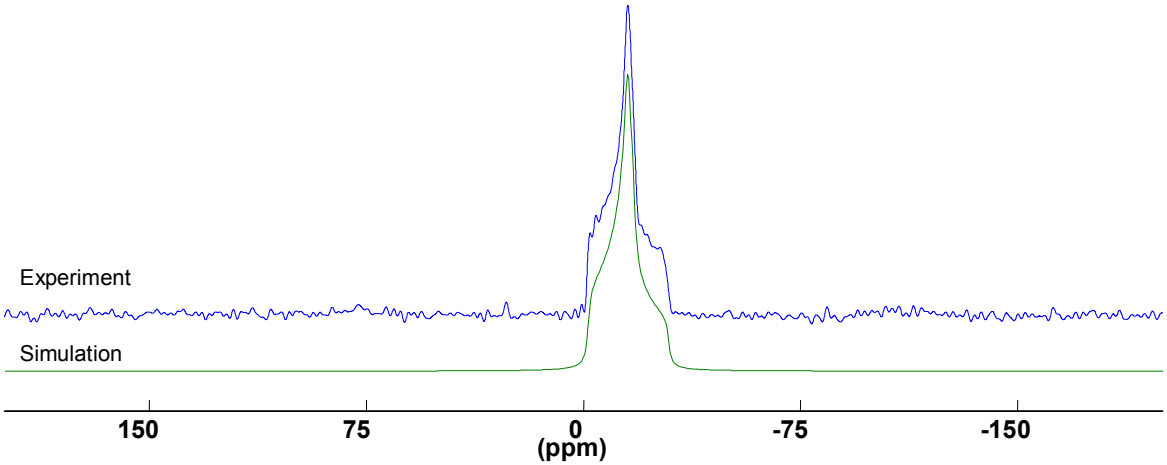

Figure S10 – 5kHz MAS Bloch Decay ^{25}Mg NMR spectra (experimental and simulated) of $MgWO_4$.

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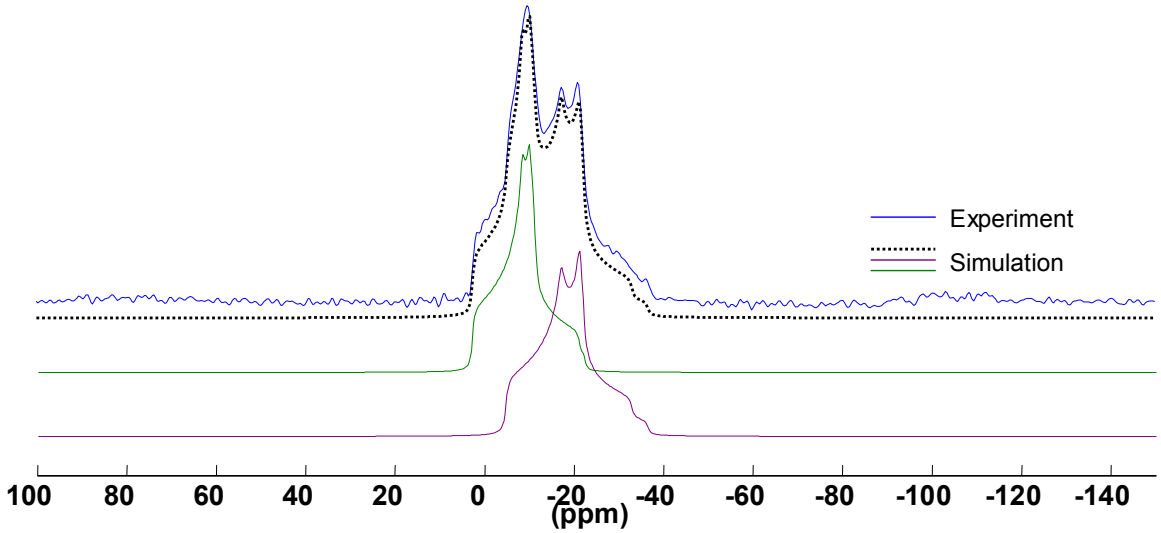

Figure S11 – 5kHz MAS Bloch Decay ^{25}Mg NMR spectra (experimental and simulated) of α-$Mg_2V_2O_7$.

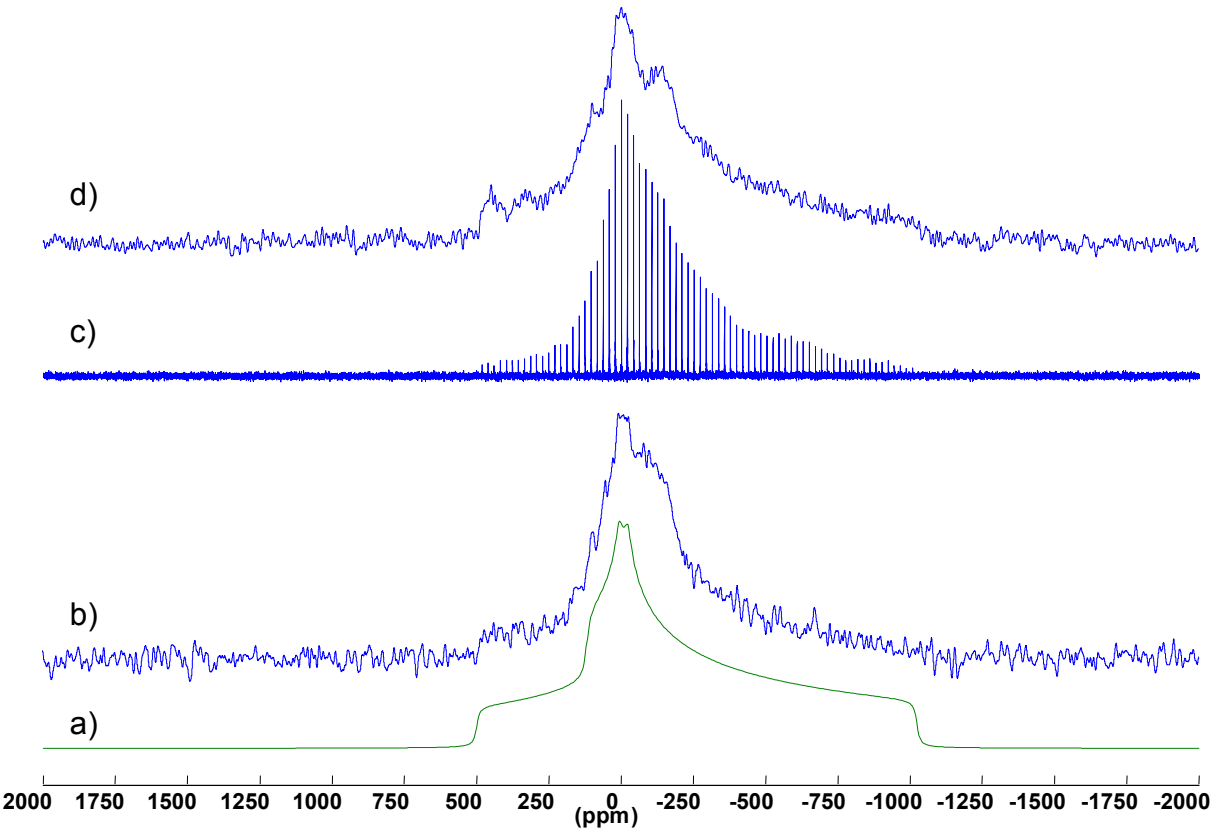

Figure S12 –a) Simulation of the one site in $Mg(VO_3)_2$. b) Static full Hahn Echo ^{25}Mg NMR spectrum of $Mg(VO_3)_2$. c) Static QCPMG ^{25}Mg NMR spectrum of $Mg(VO_3)_2$. d) Static full Hahn Echo ^{25}Mg NMR spectrum of $Mg(VO_3)_2$ obtained in 3 pieces using varying central excitation frequencies (O1) to observe edge singularities.

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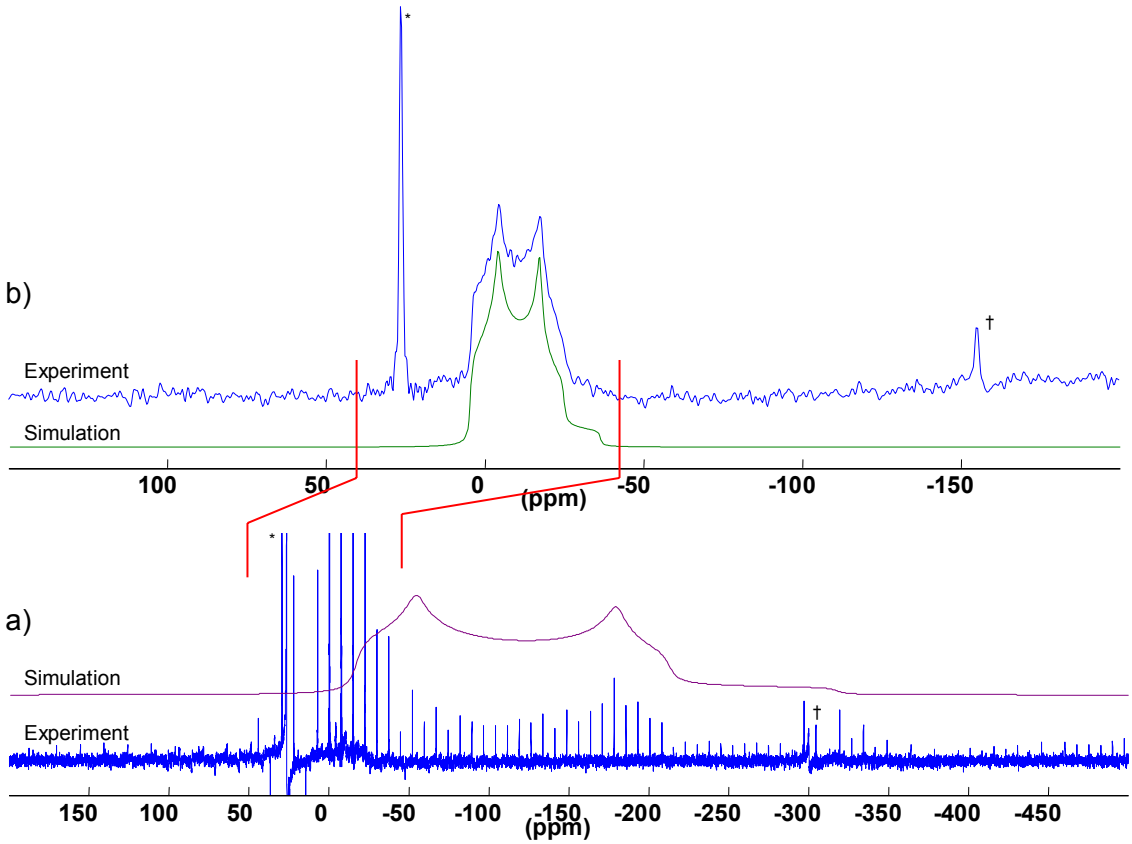

Figure S13 – $Mg_3(VO_4)_2$. a) 18kHz MAS QCPMG ^{25}Mg spectra (experimental and simulated) of $Mg_3(VO_4)_2$ zoomed in on the low intensity site with the larger C_Q. b) 10kHz MAS Bloch decay ^{25}Mg spectra (experimental and simulated) of $Mg_3(VO_4)_2$ showing the site with the smaller C_Q. The second site is too broad and weak to be seen at 10kHz MAS Bloch Decay. *MgO; †MgO spinning sideband.

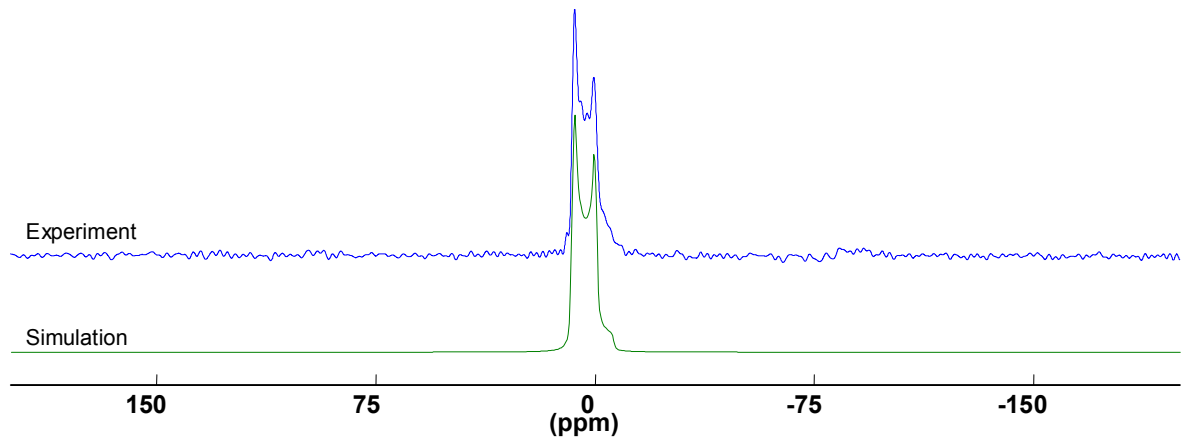

Figure S14 – 5kHz MAS Bloch Decay ^{25}Mg NMR spectra (experimental and simulated) of Perovskite, $MgTiO_3$.

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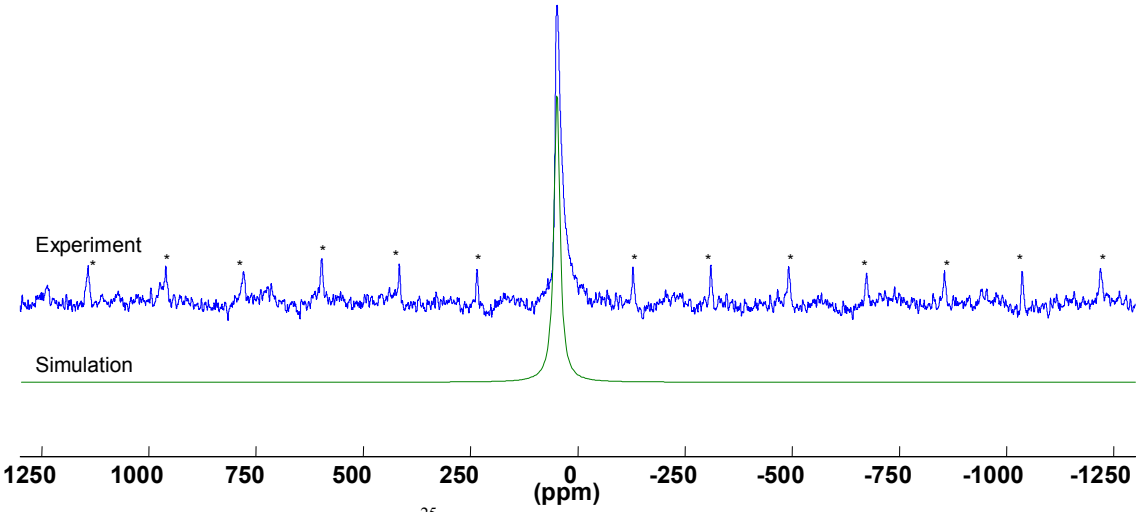

Figure S15 – 10kHz MAS Bloch Decay ^{25}Mg NMR spectra (experimental and simulated) of Spinel, $MgAl_2O_4$. *spinning sidebands.

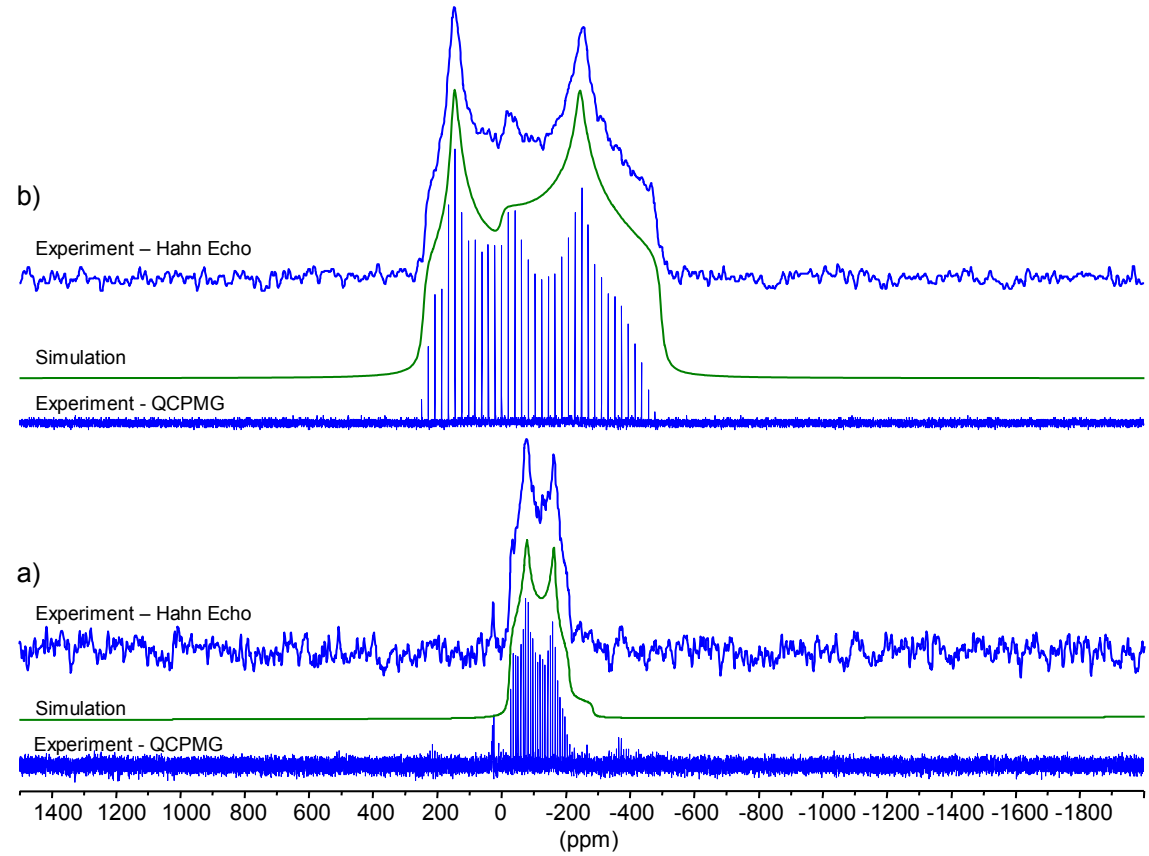

Figure S16 – α-$MgSO_4$. a) 16kHz MAS QCPMG, Hahn echo and simulated ^{25}Mg NMR spectra of α-$MgSO_4$. b) Static QCPMG, Hahn echo and simulated ^{25}Mg NMR spectra of α-$MgSO_4$.

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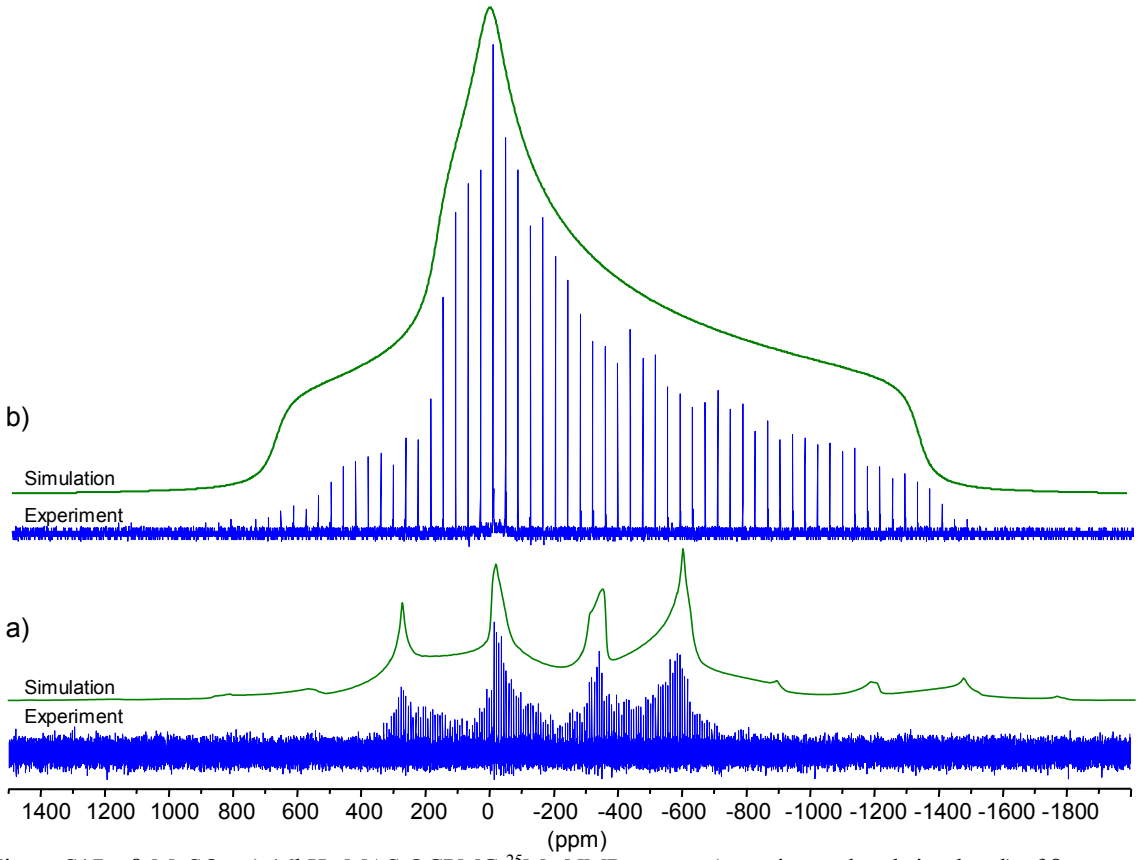

Figure S17 – β-$MgSO_4$. a) 16kHz MAS QCPMG ^{25}Mg NMR spectra (experimental and simulated) of β-$MgSO_4$. b) Static QCPMG ^{25}Mg NMR spectra (experimental and simulated) of β-$MgSO_4$.

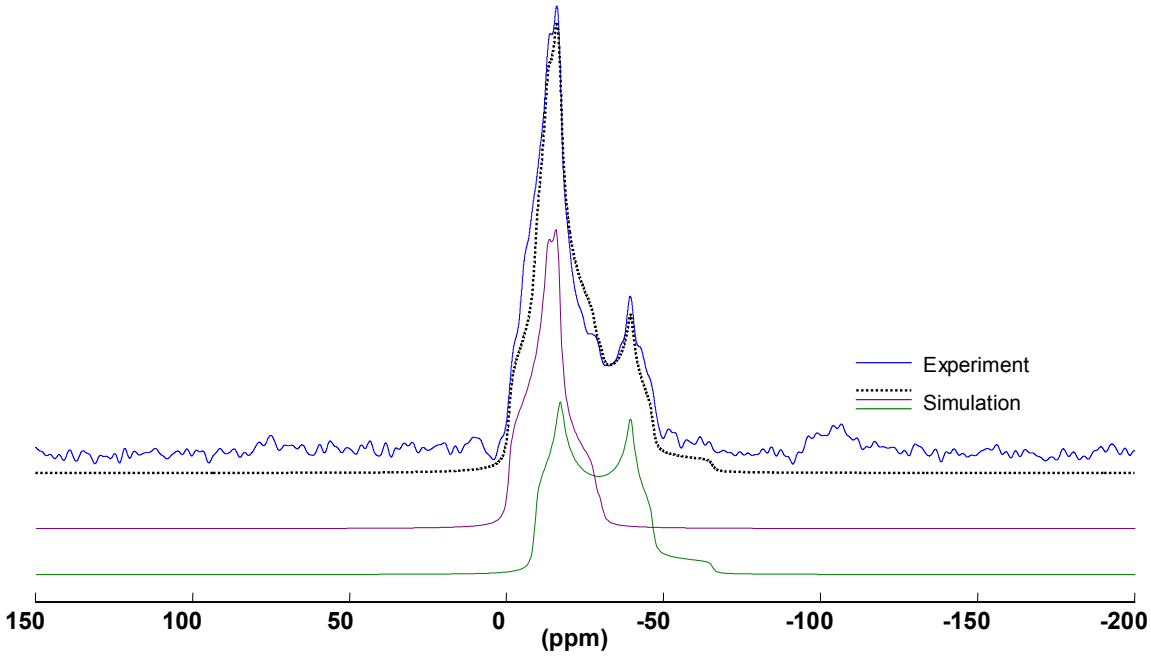

Figure S18 – 12kHz MAS Hahn echo ^{25}Mg NMR spectra (experimental and simulated) of $Mg(HCOO)_2{\cdot}2H_2O$.

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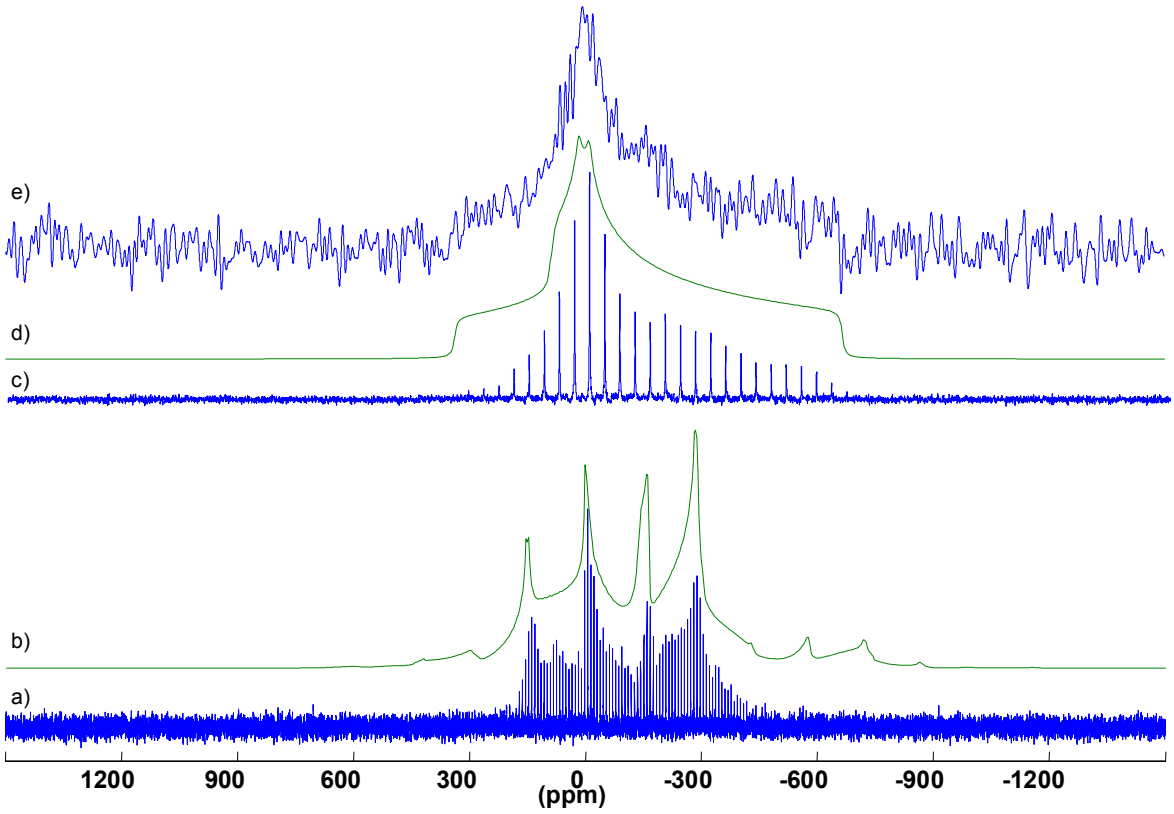

Figure S19 – a) 5kHz MAS QCPMG ^{25}Mg NMR spectrum of $Mg(Acac)_2{\cdot}2H_2O$. b) Simulation of a). c) Static QCPMG ^{25}Mg NMR spectrum of $Mg(Acac)_2{\cdot}2H_2O$. d) Simulated of c) and e). e) Static Hahn echo ^{25}Mg NMR spectrum of $Mg(Acac)_2{\cdot}2H_2O$ obtained in 3 pieces using varying central excitation frequencies (O1) to observe edge singularities.pieces.

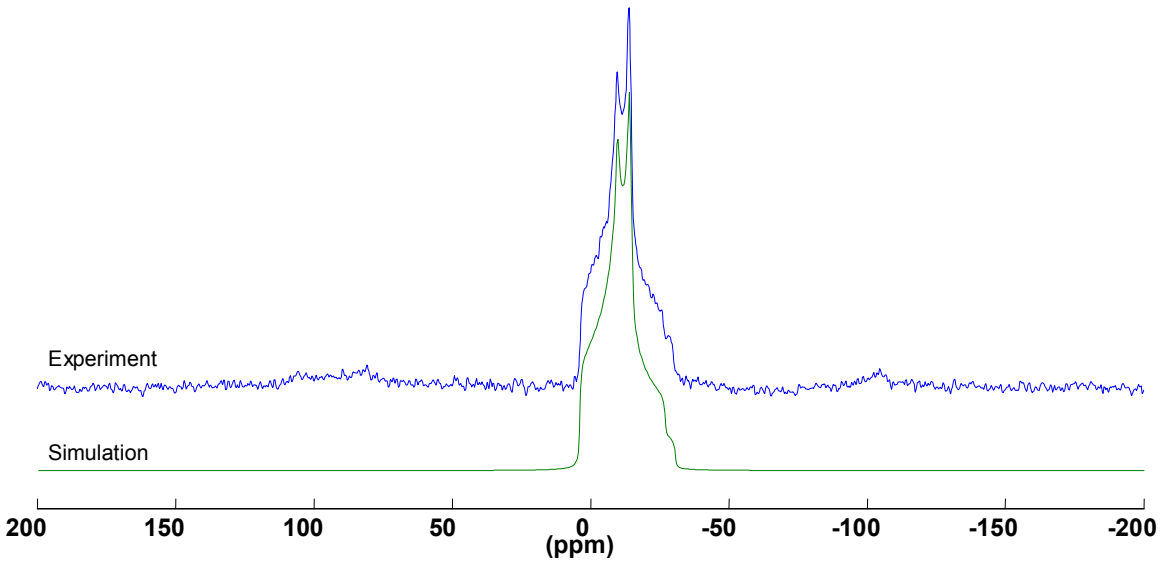

Figure S20 – 5kHz MAS Bloch Decay ^{25}Mg NMR spectra (experimental and simulated) of $Mg(OAc)_2{\cdot}4H_2O$.

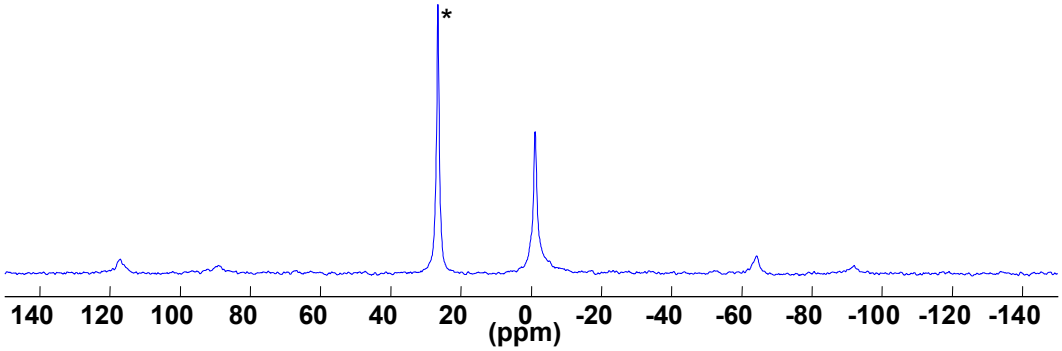

Figure S21 – 5kHz MAS Bloch Decay ^{25}Mg NMR spectrum of MgS. *MgO.

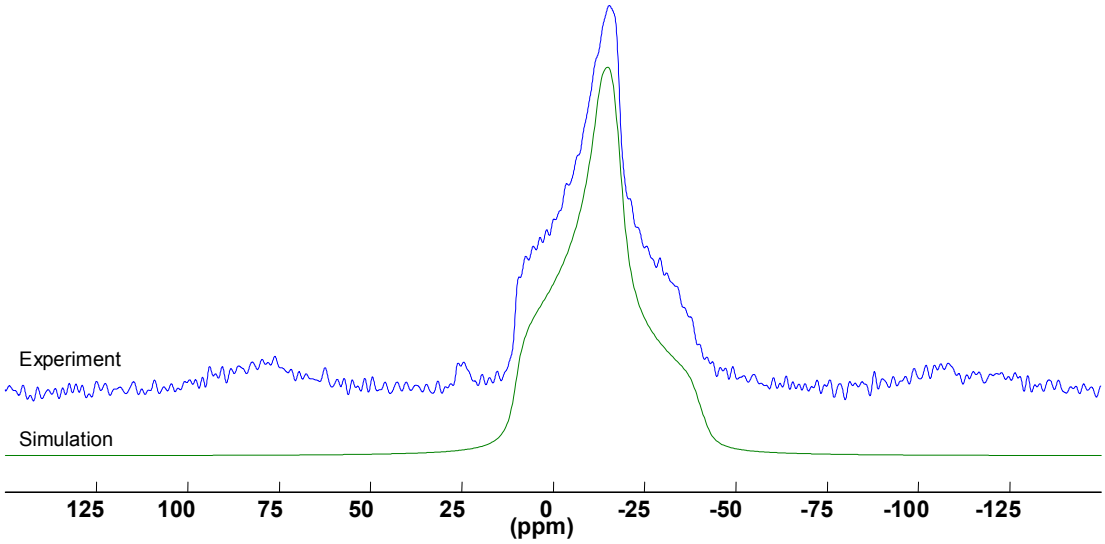

Figure S22 – 5kHz MAS Bloch Decay ^{25}Mg NMR spectra (experimental and simulated) of MgH_2.

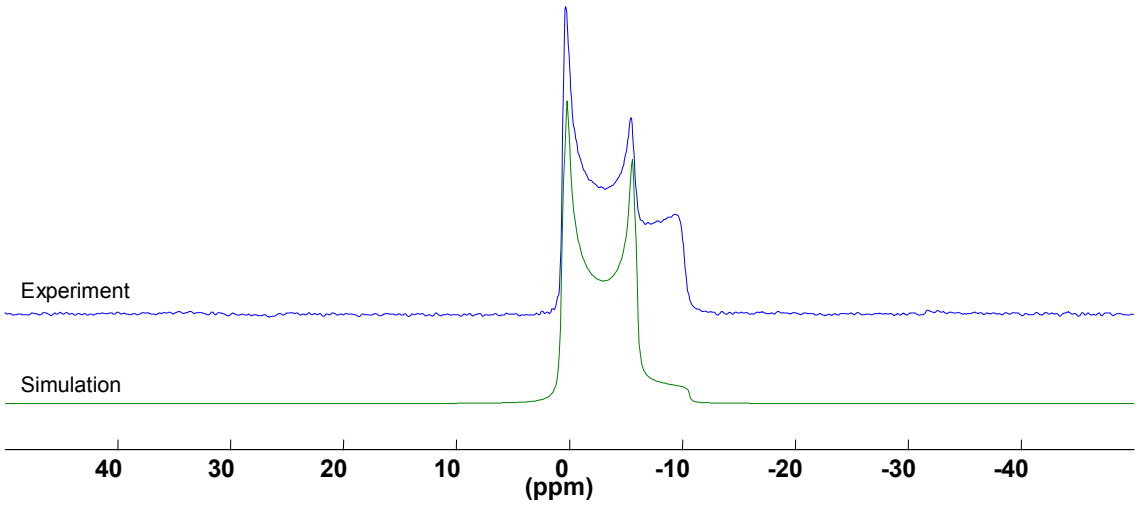

Figure S23 – 5kHz MAS Bloch Decay ^{25}Mg NMR spectra (experimental and simulated) of $MgCl_2$.

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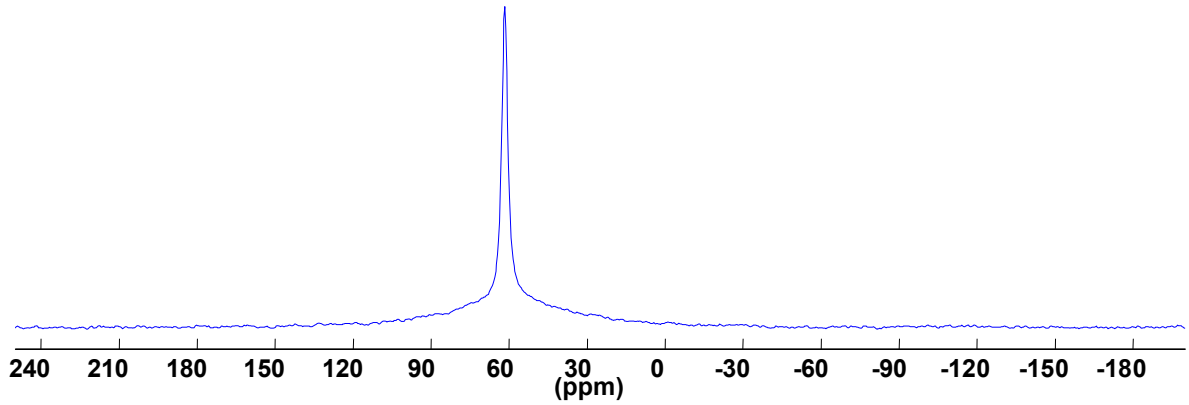

Figure S24 – Static Bloch Decay ^{25}Mg NMR spectrum of Mg_2Si.