

## Supplementary Information for

### Multi-Technique Structural Analysis of Zinc Carboxylates (Soaps)

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Table S1: FTIR Bands for the series of zinc carboxylates

Compound	Frequency of bands cm <sup>-1</sup>								
	$\nu_s$ COO	$\nu_{as}$ COO	$\Delta\nu$	$\nu_{as}$ CH <sub>3</sub>	$\nu_s$ CH <sub>3</sub>	$\nu_s$ CH <sub>2</sub>	$\nu_{as}$ CH <sub>2</sub>	$\rho$ COO	$\rho$ CH <sub>2</sub>
ZnC8	1544, 1527 (s)	1408, 1396 (m, b)	136, 131	2956 (w, b)	2870 (w)	2923, 2913 (w, b)	2846 (w, b)	551 (w)	746, 723 (m)
ZnC9	1544, 1525 (vs)	1410, 1398 (m)	134, 127	2954 (m)	2868 (w)	2919, 2913 (m, b)	2846 (m, b)	551 (w)	752, 744, 721 (m)
ZnC10	1535 (vs)	1396 (m)	139	2958, 2950 (w)	2868 (w)	2916 (m)	2848 (m)	547 (w)	744, 723 (m)
ZnC11	1542, 1529 (vs)	1408, 1398 (m)	134, 131	2954 (m)	2869 (w)	2917 (s)	2848 (m)	553 (w)	746, 736, 721 (m)
ZnC12	1535 (vs)	1408, 1394 (m, b)	127, 141	2958, 2950 (m, b)	2867 (w)	2916 (s)	2848 (m)	549 (w)	742, 730, 723 (m)
ZnC16	1537 (s)	1396 (m, b)	141	2960, 2950 (w, b)	—	2916 (m)	2846 (m)	549 (w)	744, 723 (m)
ZnC18	1537 (vs)	1396 (m)	141	2958, 2950 (w, b)	—	2916 (m)	2846 (m)	549 (w)	744, 722 (m)
ZnZ-C18	1542, 1525 (s)	1408, 1398 (m, b)	134, 127	2954 (w, b)	2871 (w)	2918 (m)	2850 (m, b)	549 (w)	742, 723 (m)
ZnPiv	1550, 1521 (m)	1415 (m, b)	135, 106	2981, 2960 (w, b)	—	—	—	547 (w)	—
ZnAze	1544, 1529 (vs)	1405, 1392 (s)	139, 137	—	—	2923, 2906 (w)	2861, 2846 (w)	576 (w)	744, 723 (m)

(vs) Very Strong; (s) Strong; (m) Medium; (w) Weak; (b) Broad

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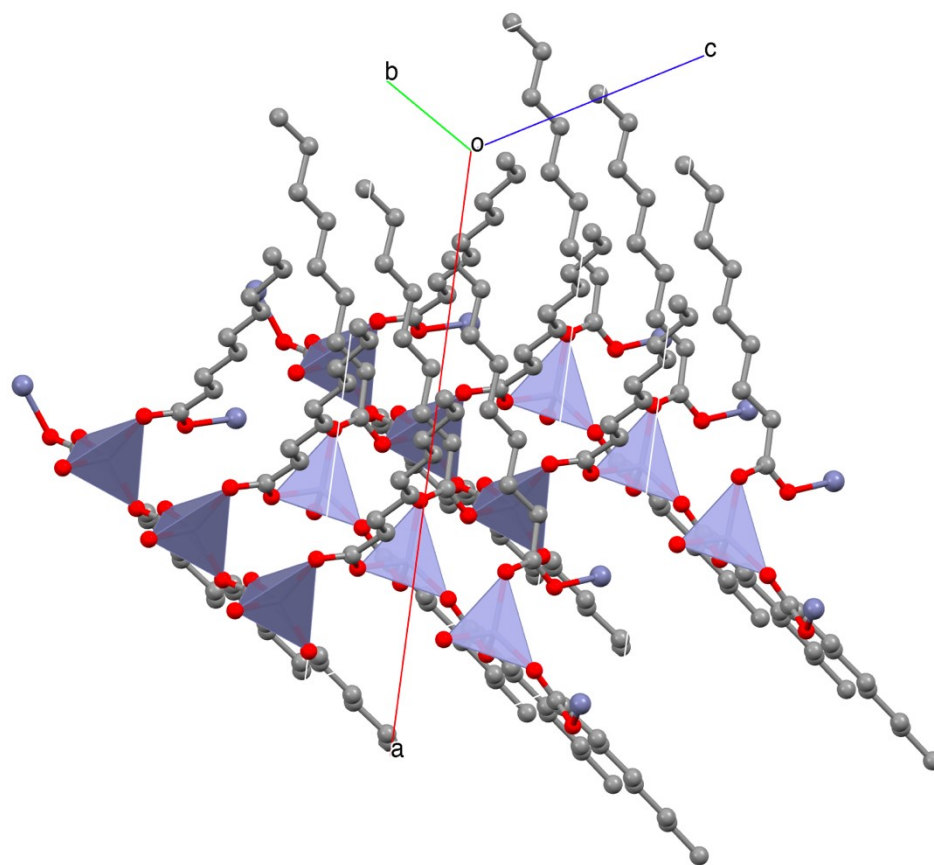
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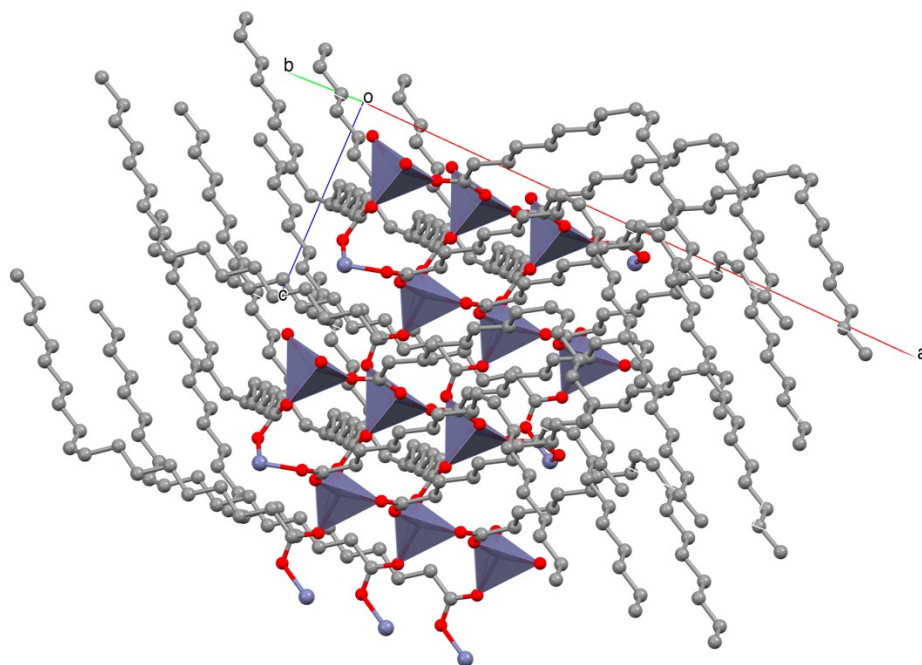
<sup>f</sup> Institute of Heritage Science, National Council of Research, Rome, Italy 00016

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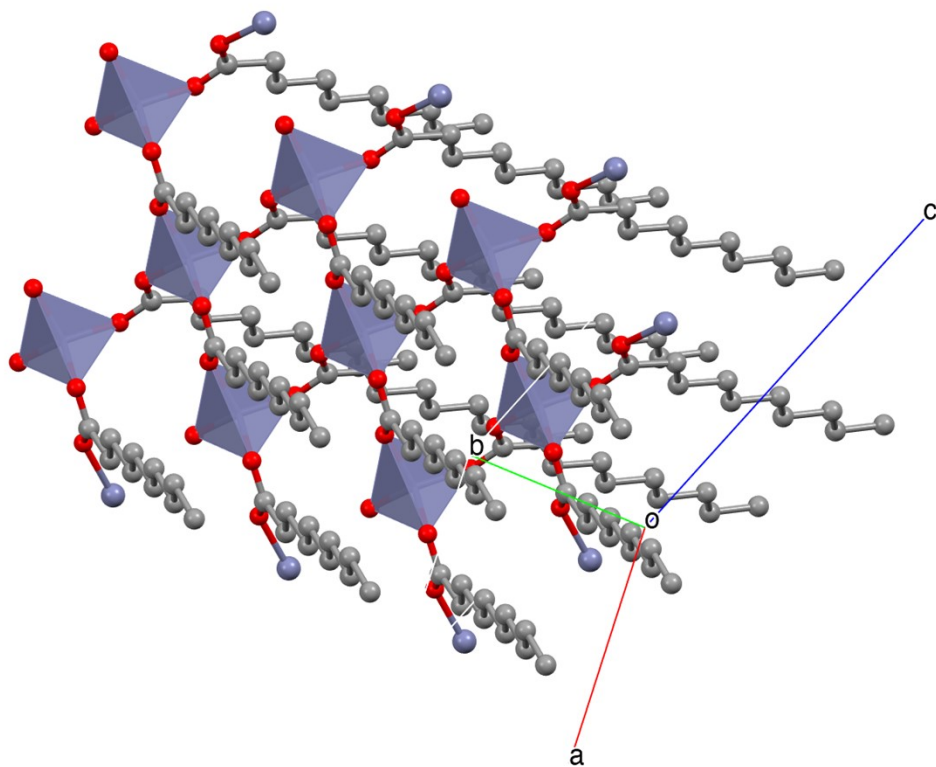
<sup>h</sup> National High Magnetic Field Laboratory, Tallahassee, Florida 32310



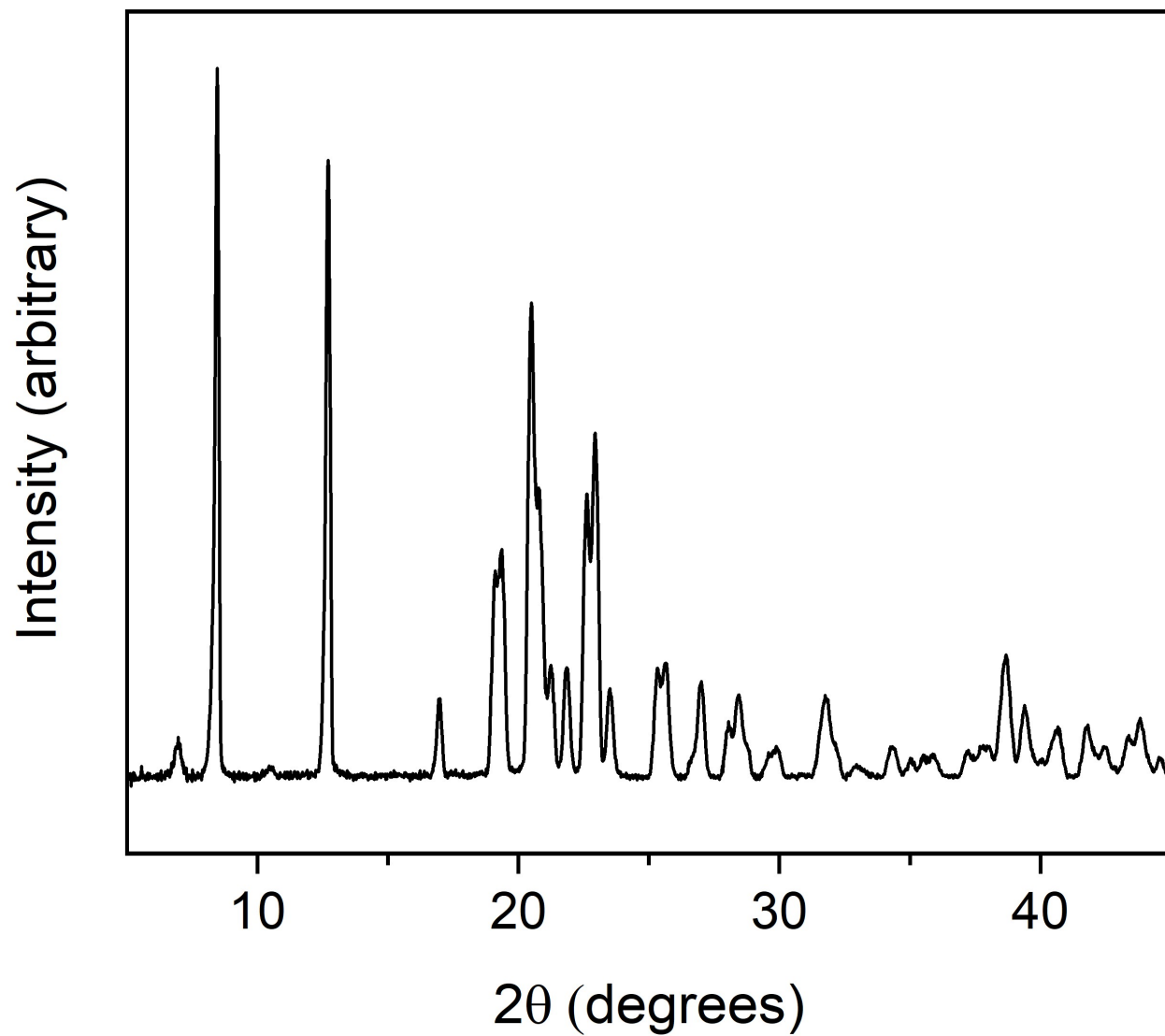
*Figure S1: Expanded packing diagram for ZnC9 indicating AB packing between layers of alternating Zn tetrahedra.*



*Figure S2: Expanded packing diagram for ZnZ-C18 indicating AB packing between layers of alternating Zn tetrahedra.*



*Figure S3: Expanded packing diagram for ZnC10 indicating AB packing between layers of non-alternating tetrahedra.*



*Figure S4: Experimental PXRD pattern for ZnC8. Cu-K $\alpha$  radiation.*

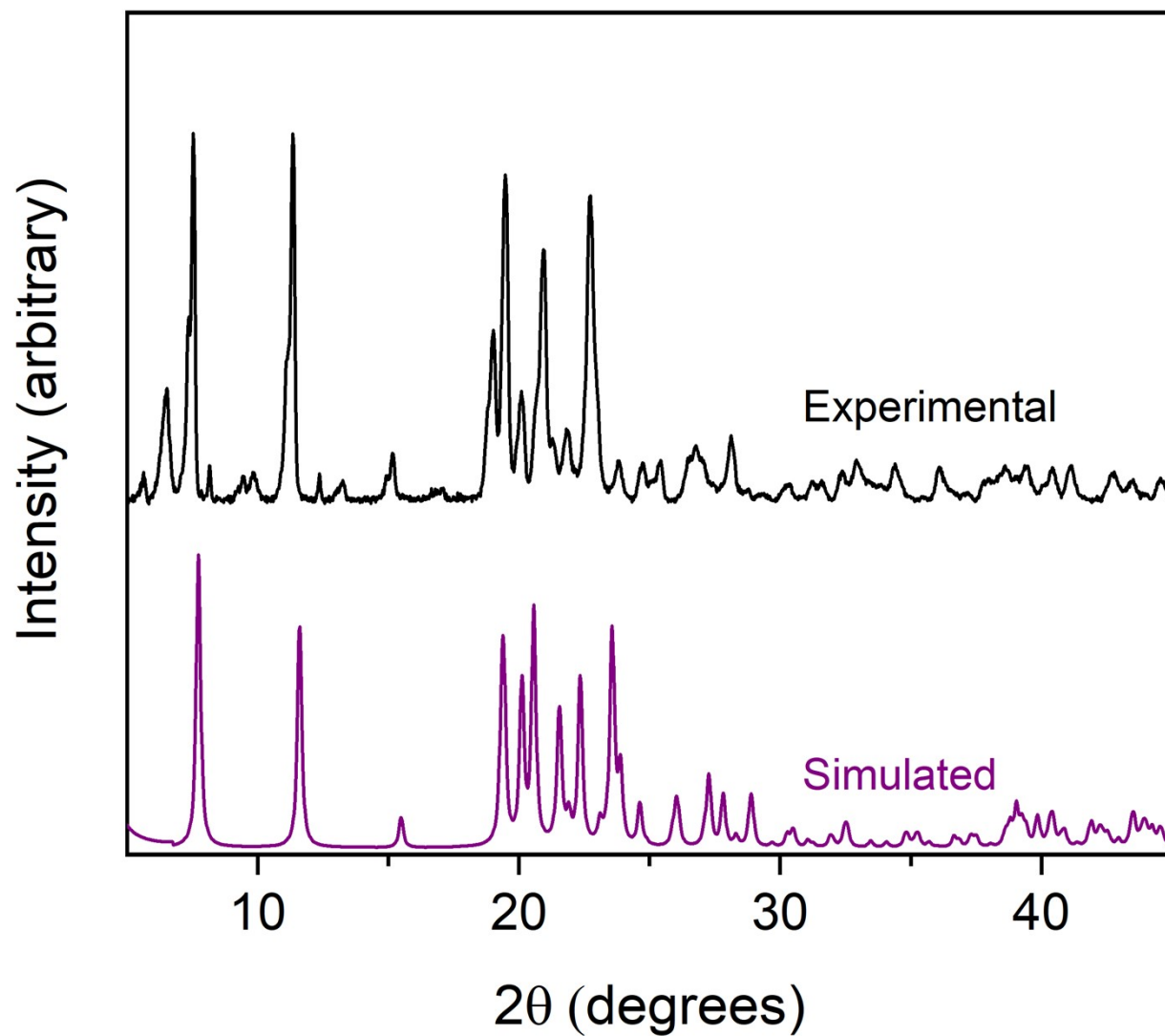


Figure S5: Experimental PXRD pattern for ZnC9 bulk (black, top) and simulated PXRD pattern from the ZnC9 single-crystal (purple, bottom.) Cu-K $\alpha$  radiation.

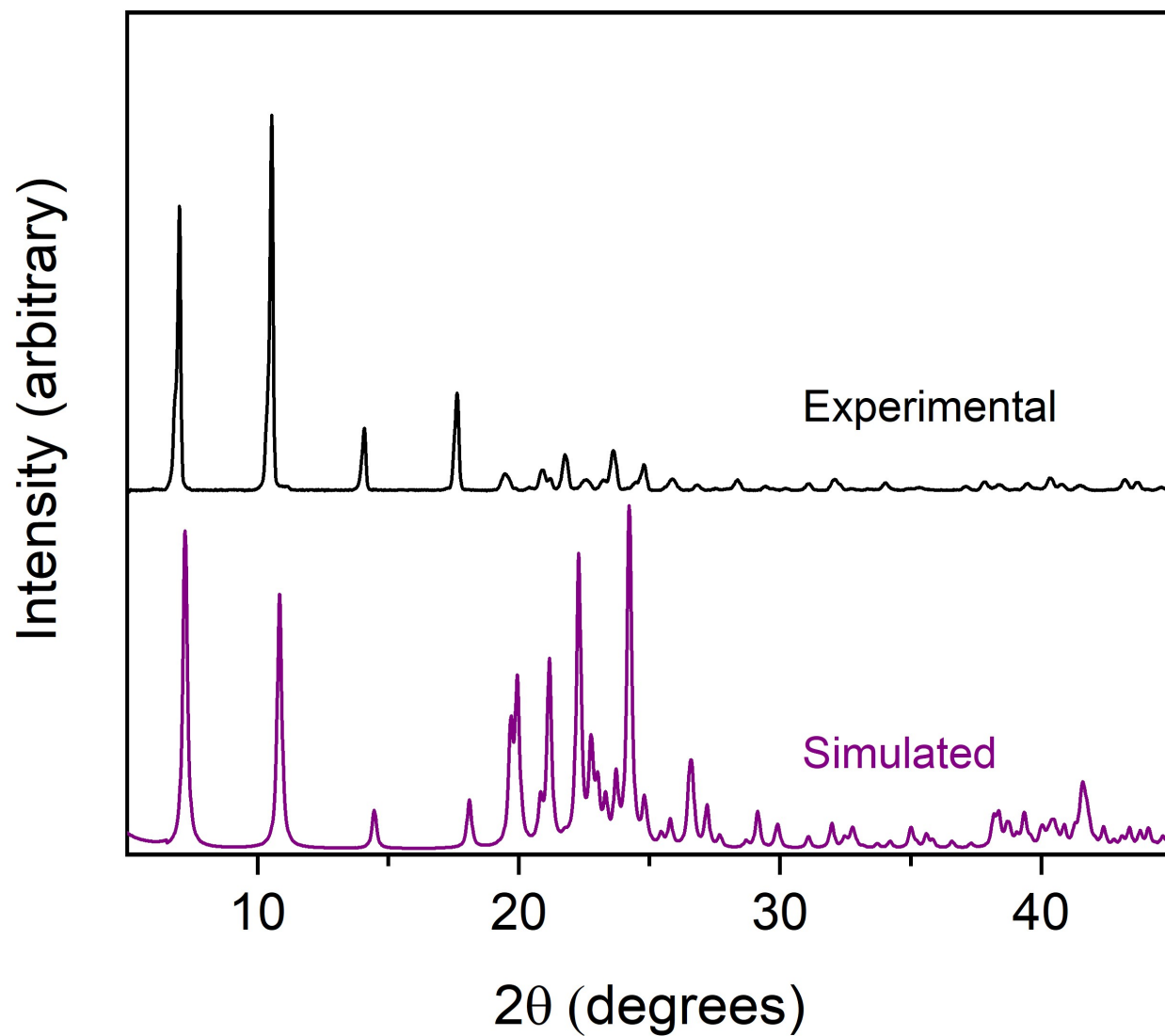
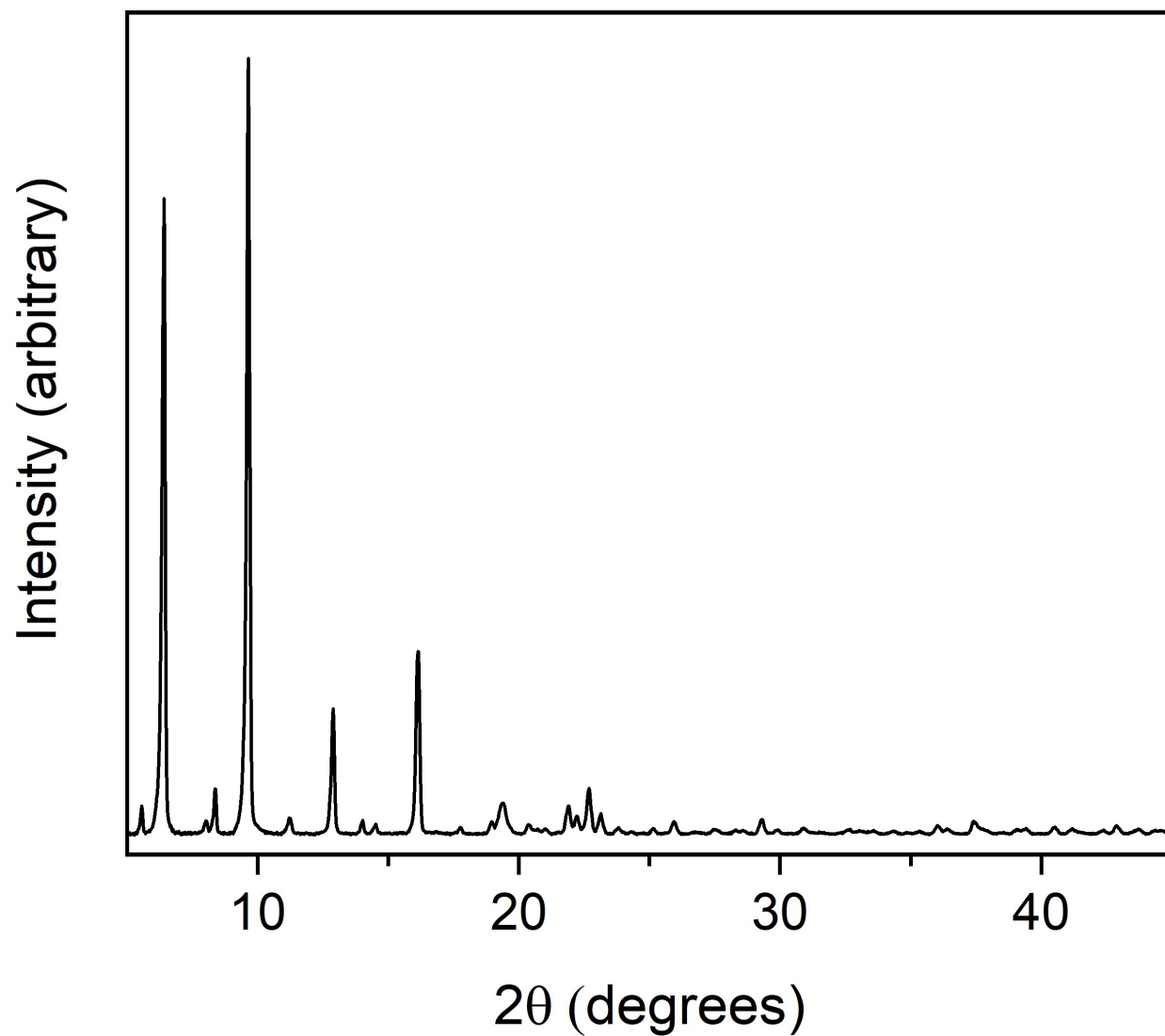
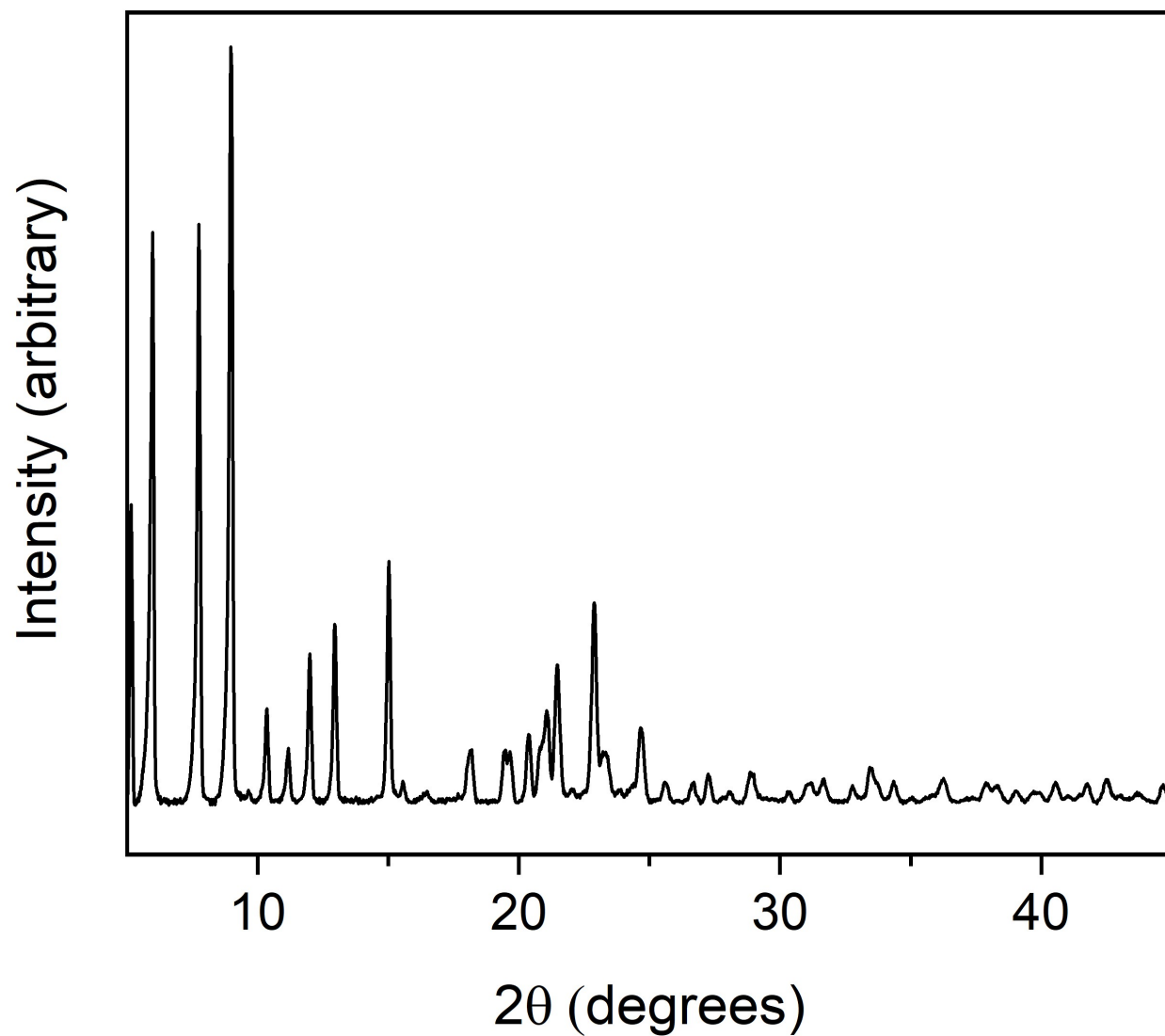


Figure S6: Experimental PXRD pattern for ZnC10 bulk (black, top) and simulated PXRD pattern from the ZnC10 single-crystal (purple, bottom.) Cu-K $\alpha$  radiation.

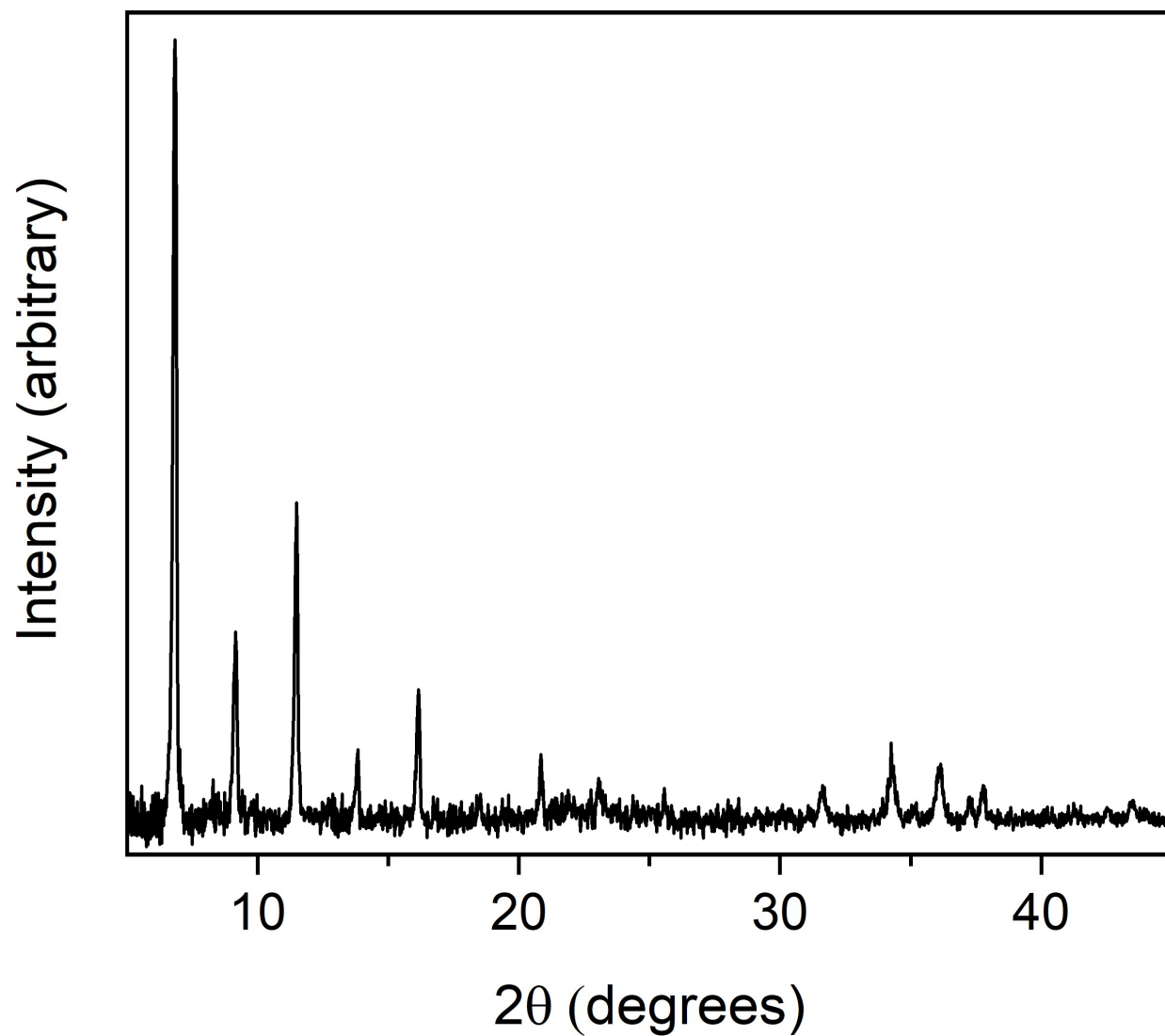


*Figure S7: Experimental PXRD pattern for ZnCl<sub>2</sub>. Cu-K $\alpha$  radiation.*

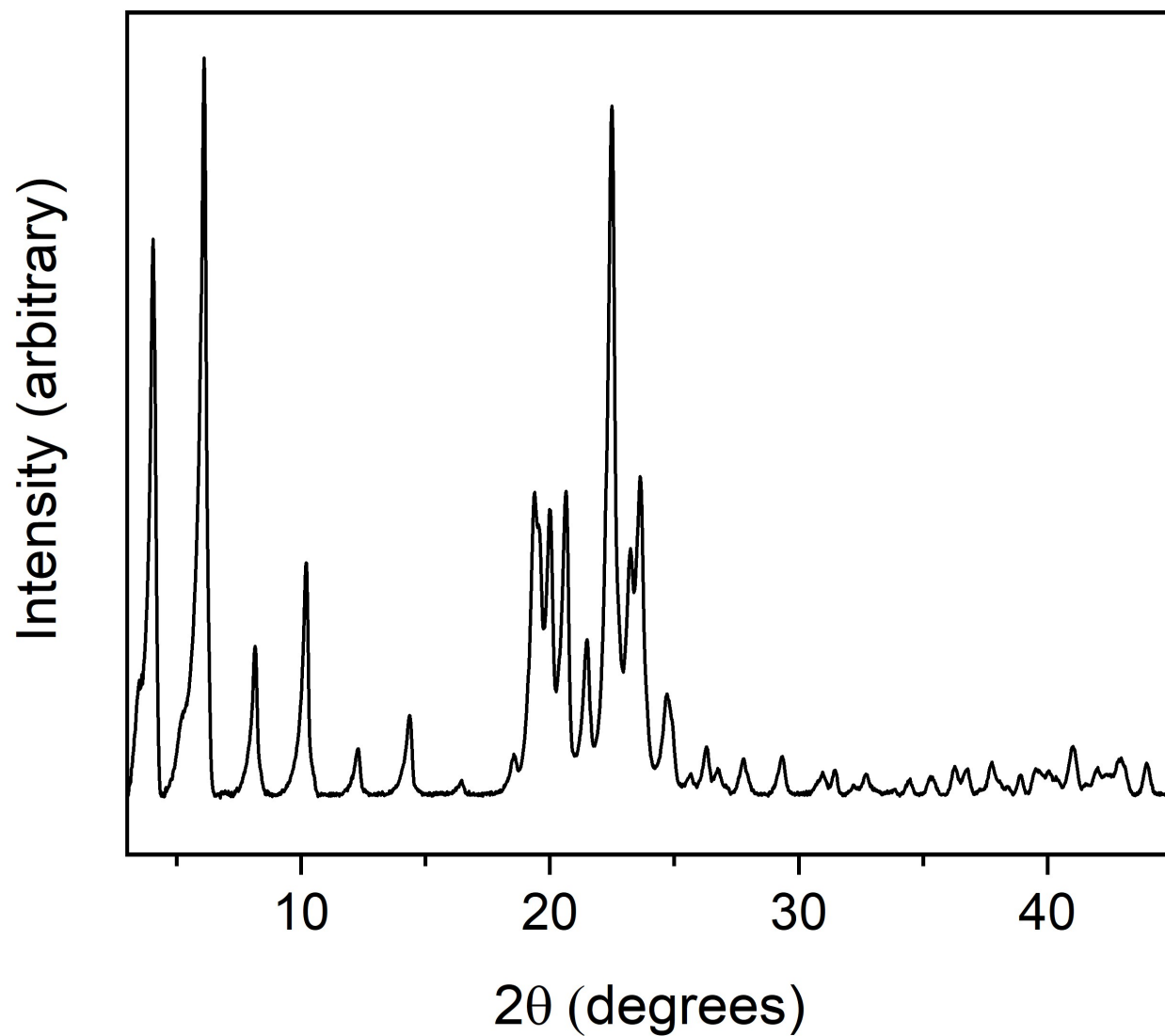




*Figure S8: Experimental PXRD pattern for ZnCl<sub>2</sub>. Cu-Kα radiation.*



*Figure S9: Experimental PXRD pattern for ZnCl<sub>6</sub>. Cu-K $\alpha$  radiation.*



*Figure S10: Experimental PXRD pattern for ZnCl<sub>8</sub>. Cu-K $\alpha$  radiation.*

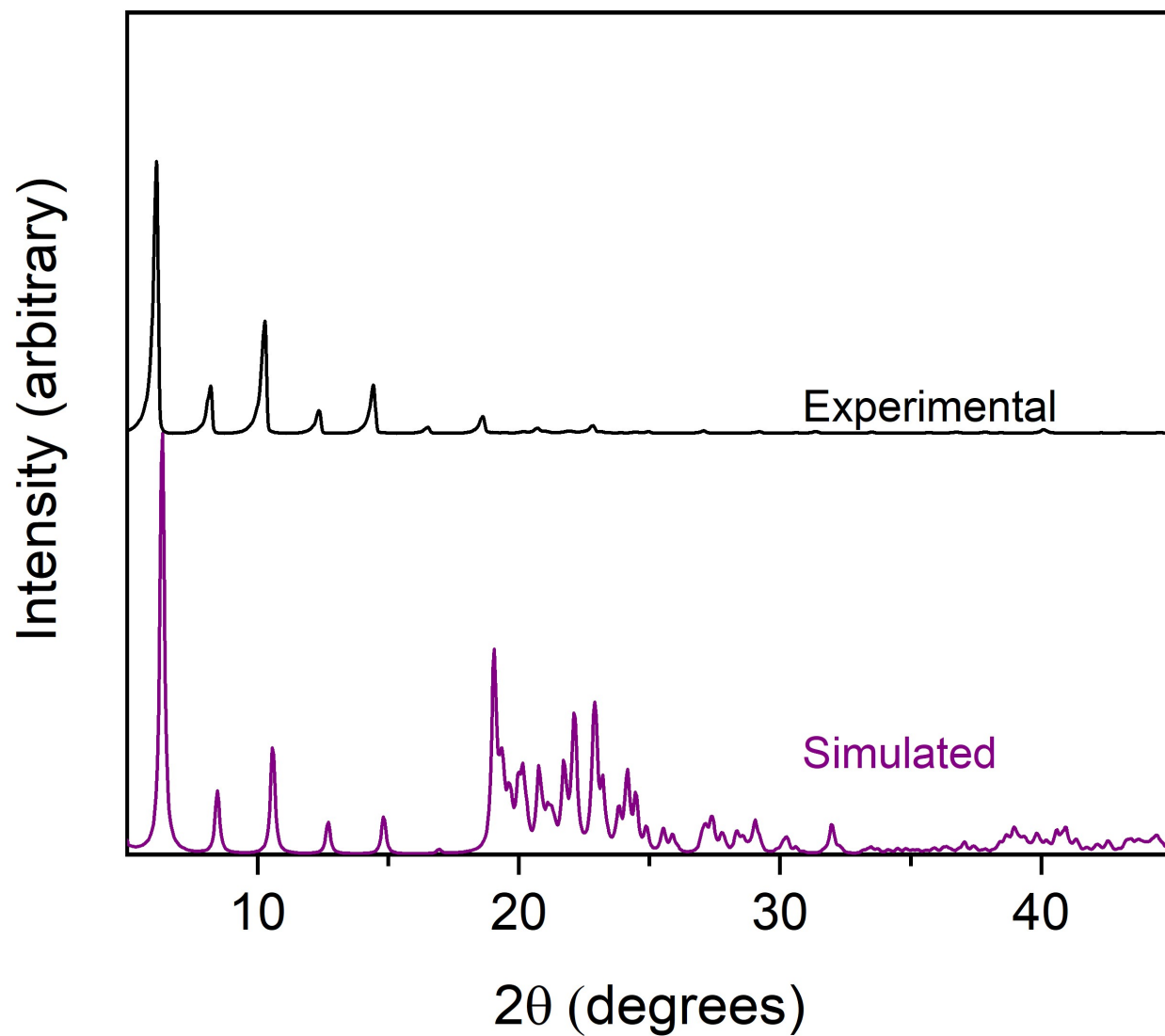


Figure S11: Experimental PXRD pattern for ZnZC18 bulk (black, top) and simulated PXRD pattern from the ZnZC18 single-crystal (purple, bottom.) Cu-K $\alpha$  radiation.

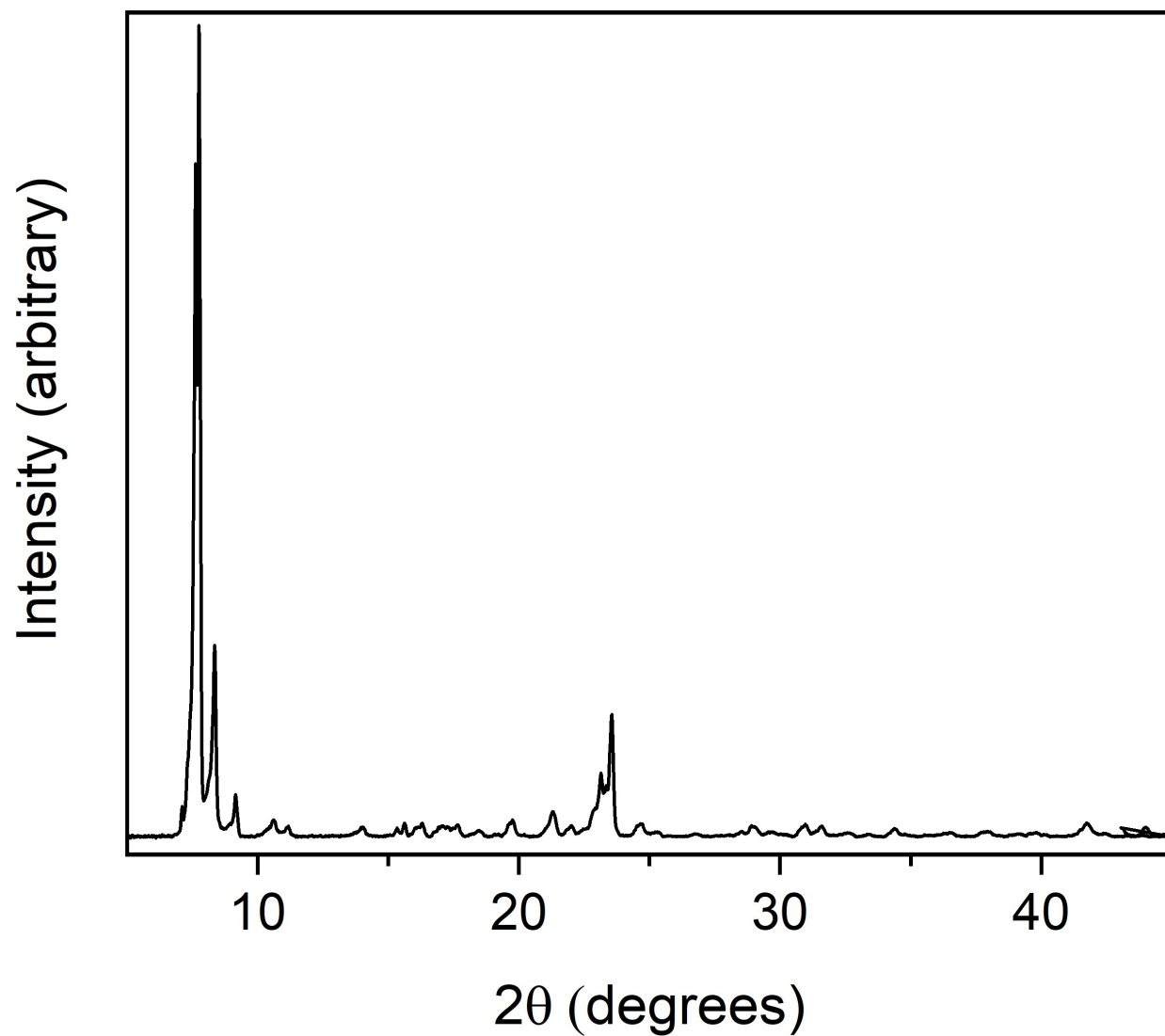


Figure S12: Experimental PXRD pattern for ZnPIV. Cu-K $\alpha$  radiation.

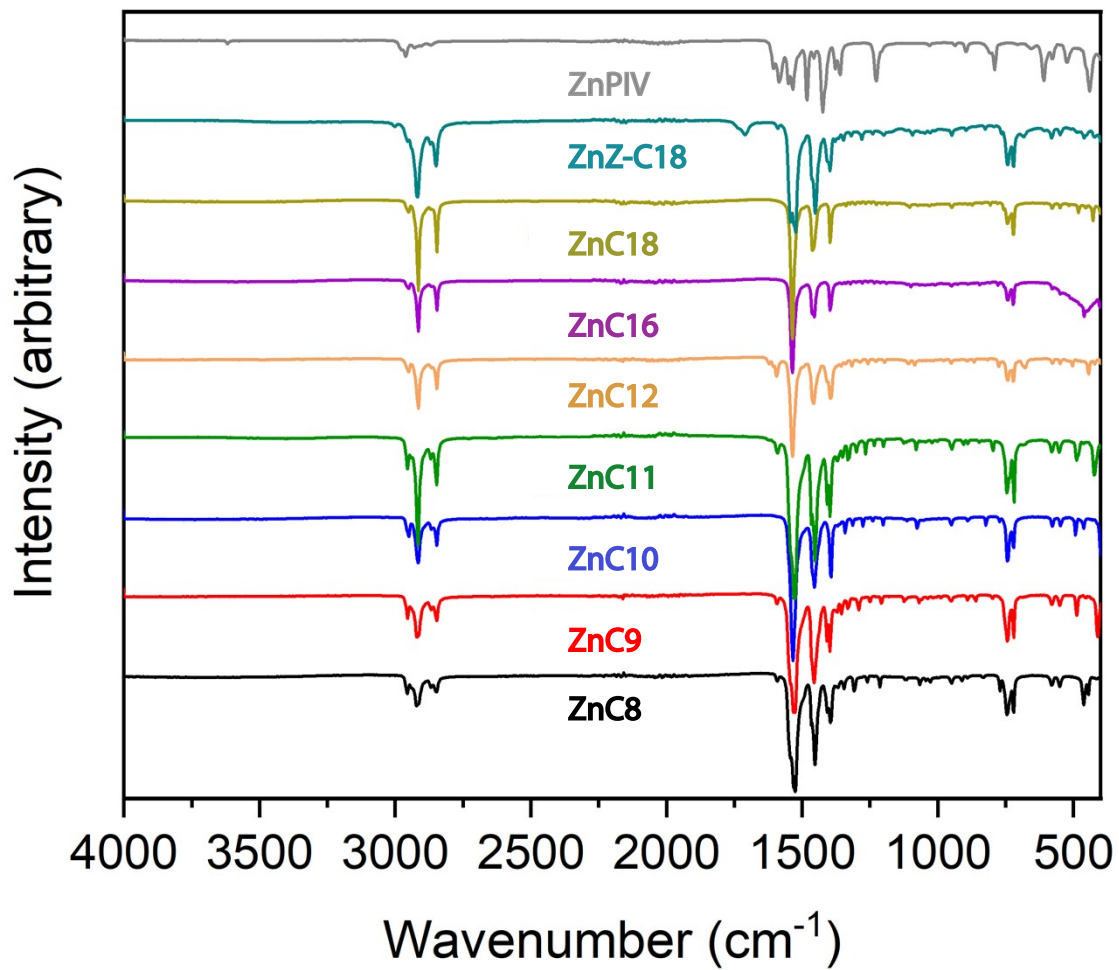


Figure S13: Full FTIR spectra for the carboxylate series.

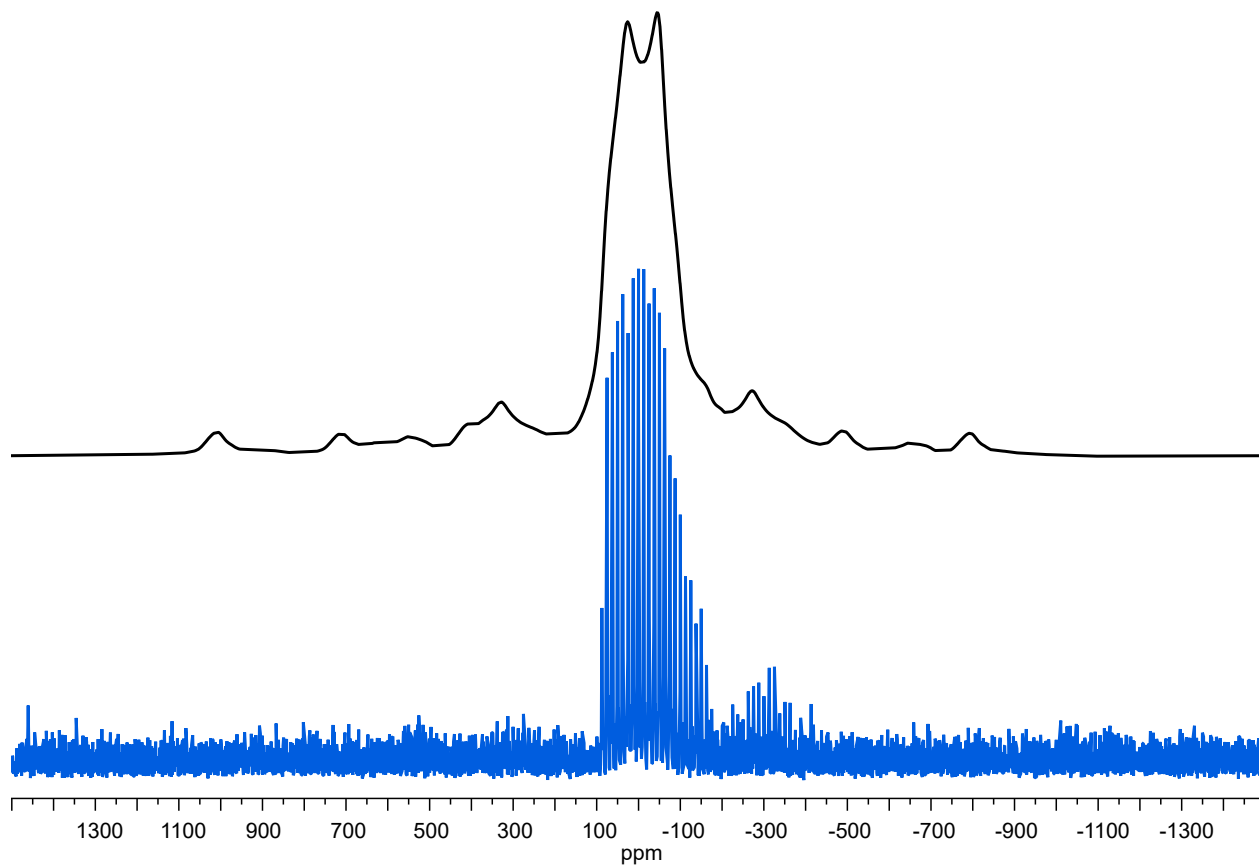


Figure S14:  $^{67}\text{Zn}$  spectra for ZnAZE. (Top, Black) Ssnake fitting parameters visualized in TopSpin; (Bottom, Blue) WURST-QCPMG spectrum at 15625 Hz MAS.  $B_0$  19.6 T

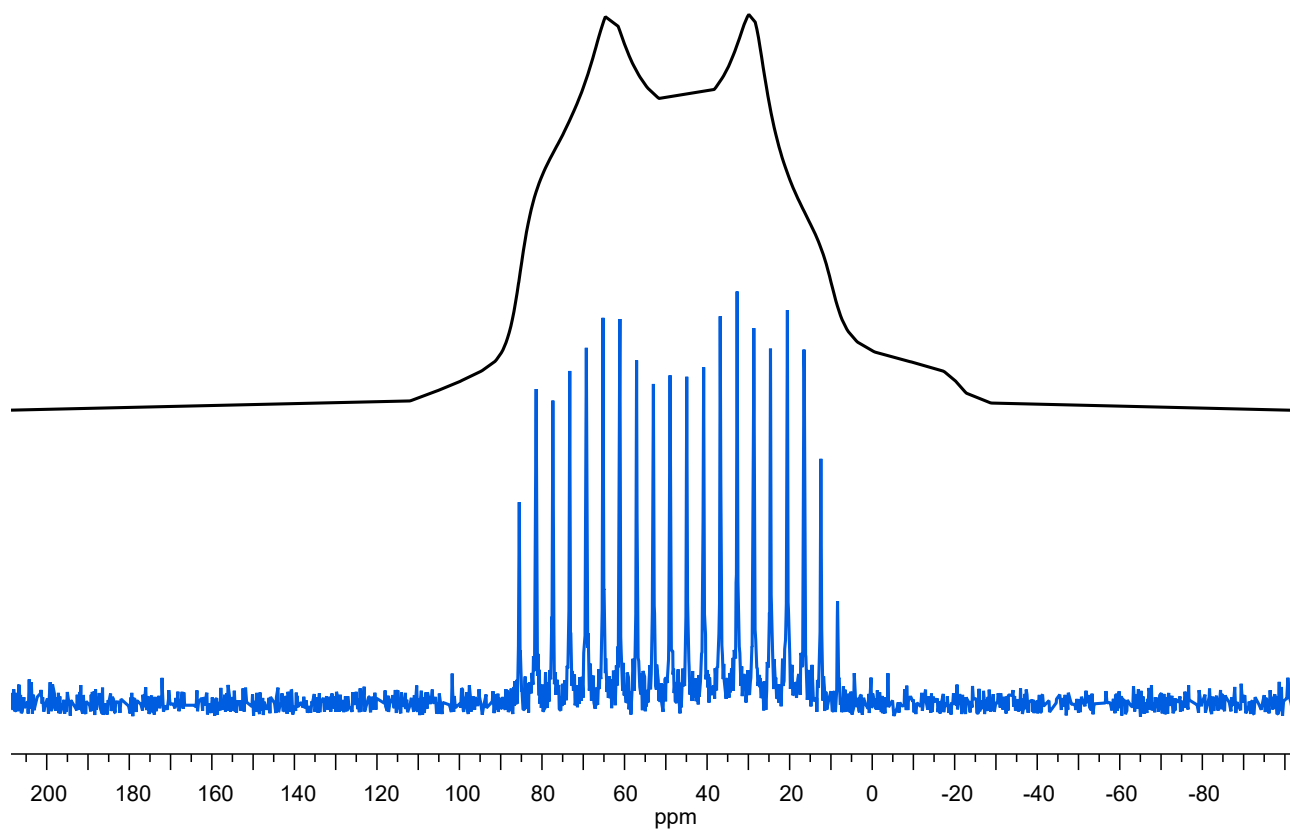


Figure S15:  $^{67}\text{Zn}$  spectra for ZnC9. (Top, Black) Ssnake fitting parameters visualized in TopSpin; (Bottom, Blue) WURST-QCPMG spectrum at 15625 Hz MAS.  $B_0$  35.2 T



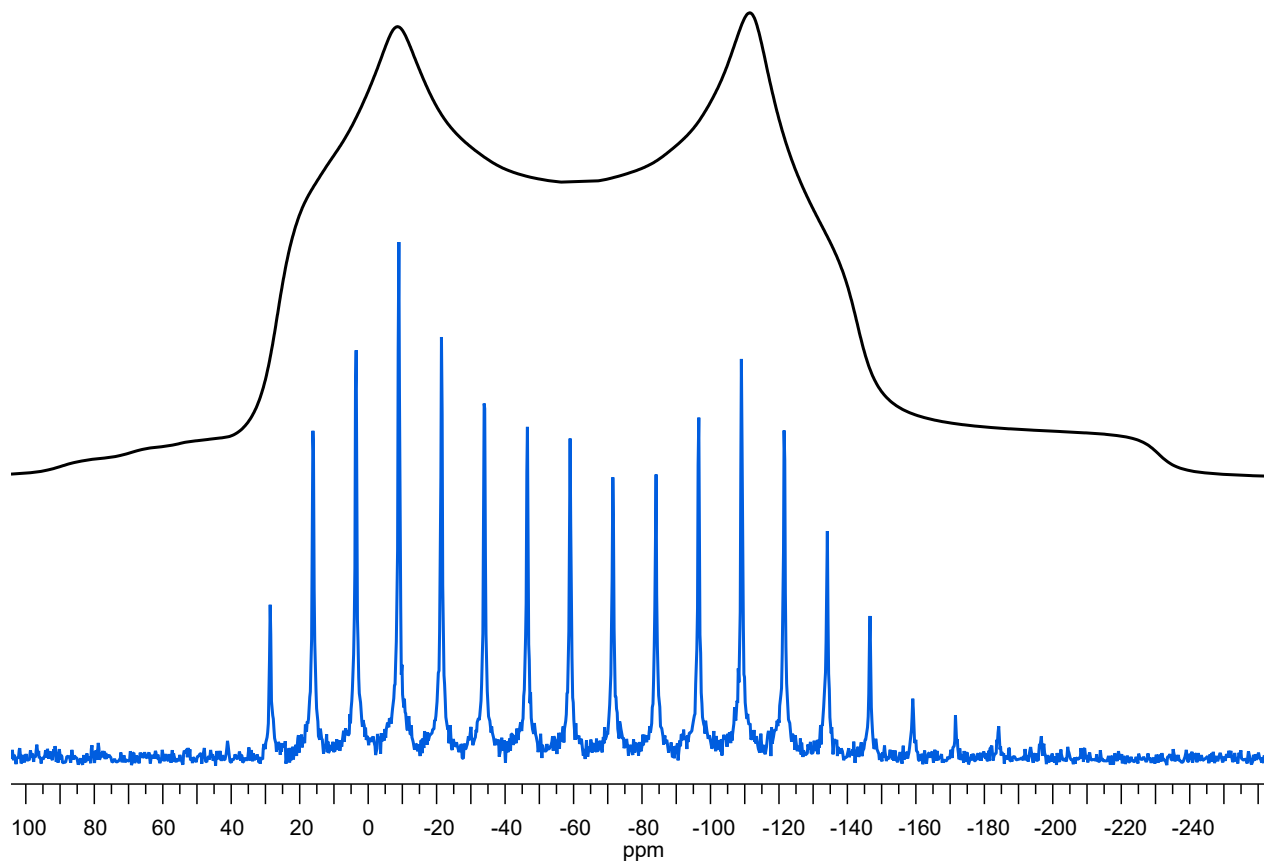
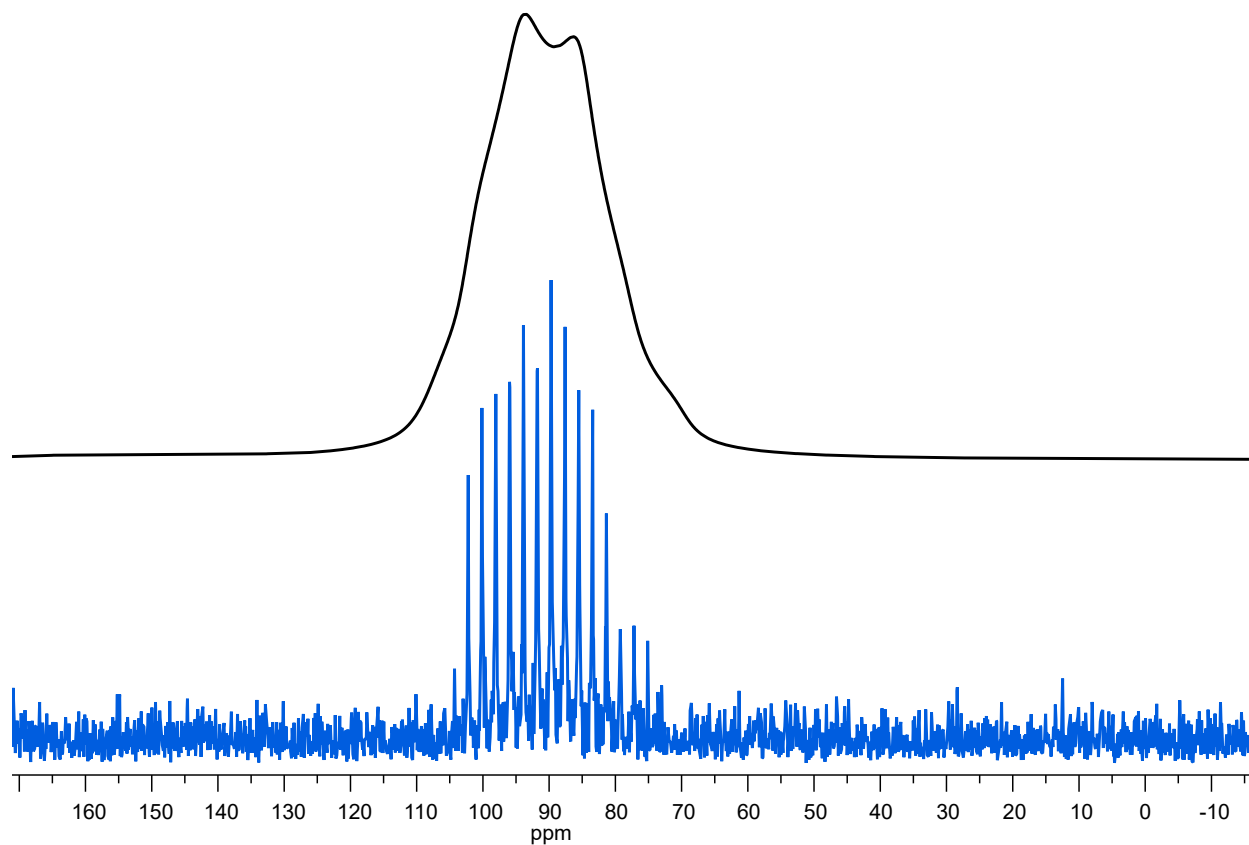


Figure S16:  $^{67}\text{Zn}$  spectra for ZnZ-C18. (Top, Black) Ssnake fitting parameters visualized in TopSpin; (Bottom, Blue) WURST-QCPMG spectrum at 15625 Hz MAS.  $B_0$  19.6 T



*Figure S17:  $^{67}\text{Zn}$  spectra for  $\text{ZnCl}_2$ . (Top, Black) Ssnake fitting parameters visualized in TopSpin; (Bottom, Blue) WURST-QCPMG spectrum at 15625 Hz MAS.  $B_0$  19.6 T*

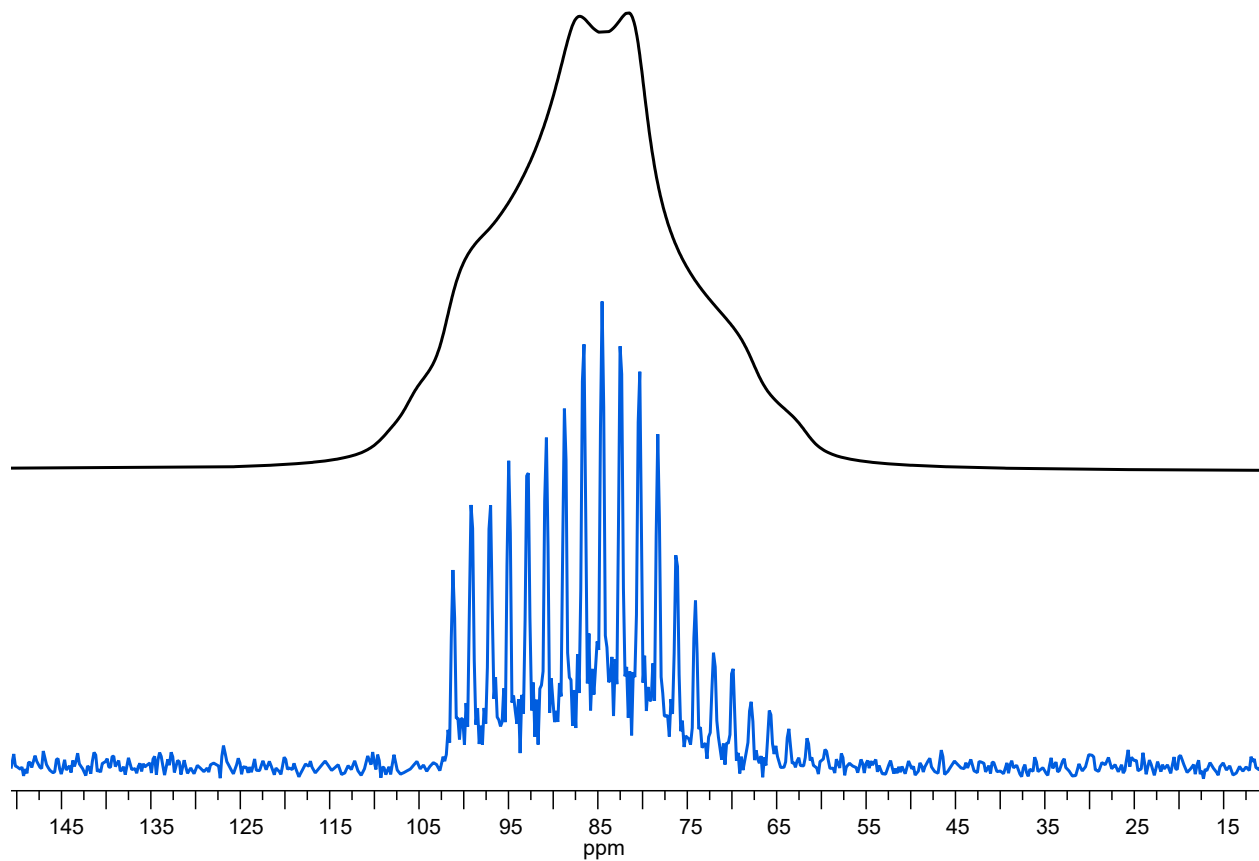
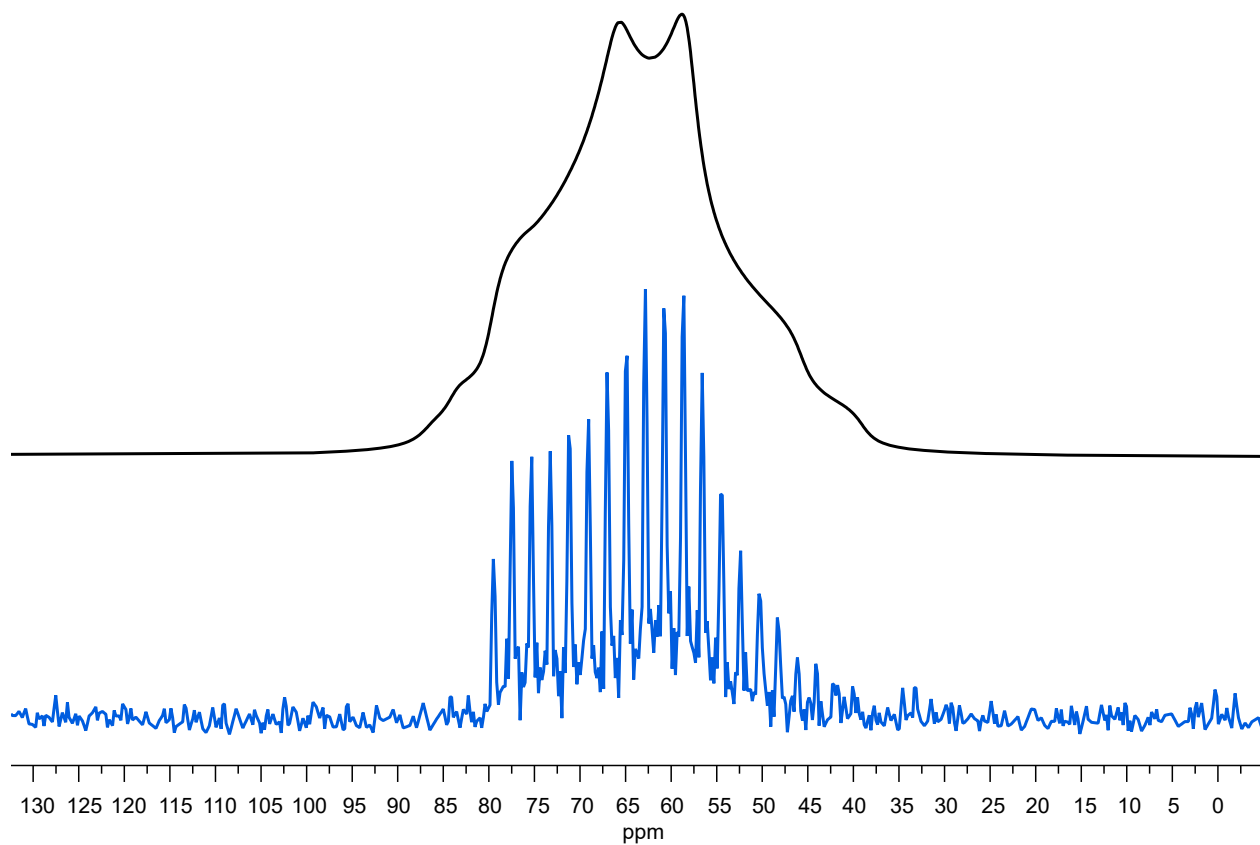


Figure S18:  $^{67}\text{Zn}$  spectra for  $\text{ZnC16}$ . (Top, Black) Ssnake fitting parameters visualized in TopSpin; (Bottom, Blue) WURST-QCPMG spectrum at 15625 Hz MAS.  $B_0$  19.6 T



*Figure S19:  $^{67}\text{Zn}$  spectra for  $\text{ZnCl}_8$ . (Top, Black) Ssnake fitting parameters visualized in TopSpin; (Bottom, Blue) WURST-QCPMG spectrum at 15625 Hz MAS.  $B_0$  19.6 T*