Assessing the Potential of Natural Abundance ^{67}Zn solid-state NMR at 35.1 T, for the Characterization of Zn- Complexes with Organic Ligands

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Introduction

^{67}Zn SSNMR spectroscopy was previously used to characterize Zn-amino acid complexes [1] and MOFs [2]. Our research is motivated by the need to characterize zinc-based pigments in paints. ^{67}Zn is a low gamma, low natural abundance quadrupolar nucleus, which requires the use of ultra-high magnetic fields.

Experimental

The ^{67}Zn SSNMR spectra of three zinc carboxylates (Table I, Fig. 1) were recorded at 35.1T and 19.5T using the QCPMG pulse sequence.

Sample	C_q / MHz	η	δ / ppm
Zn palmitate	2.74	0.48±0.05	113±1 ppm
Zn nonanoate	6.98	0.66±0.05	83±1 ppm
Zn octanoate	6.80	0.64±0.05	81±1 ppm

Table I NMR parameters obtained from simulations of the 35.1 T 67Zn NMR spectra of the zinc carboxylates studied in the present work.

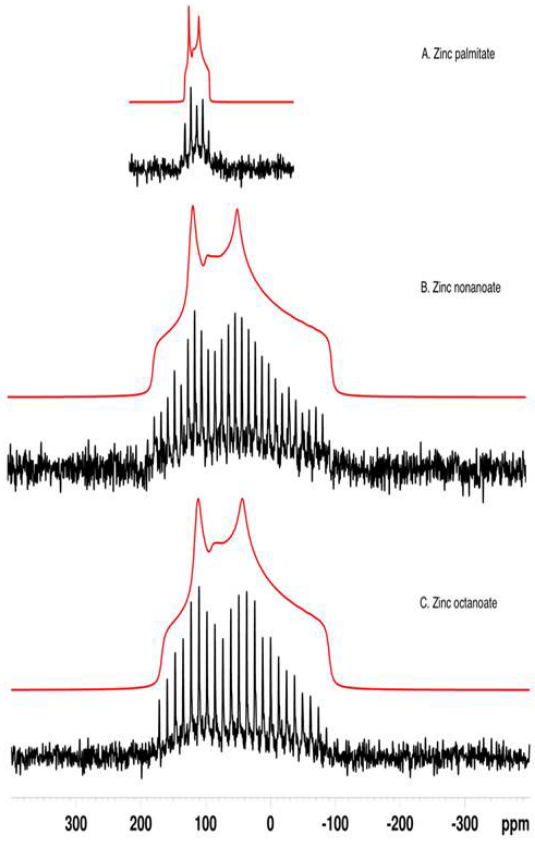

Fig.1 35.1 T 67Zn NMR spectra and simulated powder patterns for (A) Zn palmitate, (B) Zn nonanoate, and (C) Zn octanoate. The NMR parameters are given in Table 1.

Results and Discussion

Higher polarization and a reduced second order quadrupole effect at 35.1T enable the detection of natural-abundance ^{67}Zn SSNMR in higher molecular weight compounds, despite lower Zn molarity. The ^{67}Zn NMR parameters are sensitive to hydrocarbon chain length and packing effects.

Conclusions

Our results lay the groundwork for further experiments that will provide detailed answers to questions about the geometry, morphology, and miscibility of Zn carboxylates using natural-abundance ^{67}Zn NMR spectroscopy.

Acknowledgements

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References

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