Electronic Supplementary data

Extending motifs in lithiocuprate chemistry: unexpected structural diversity in thiocyanate complexes

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Infrared spectroscopy

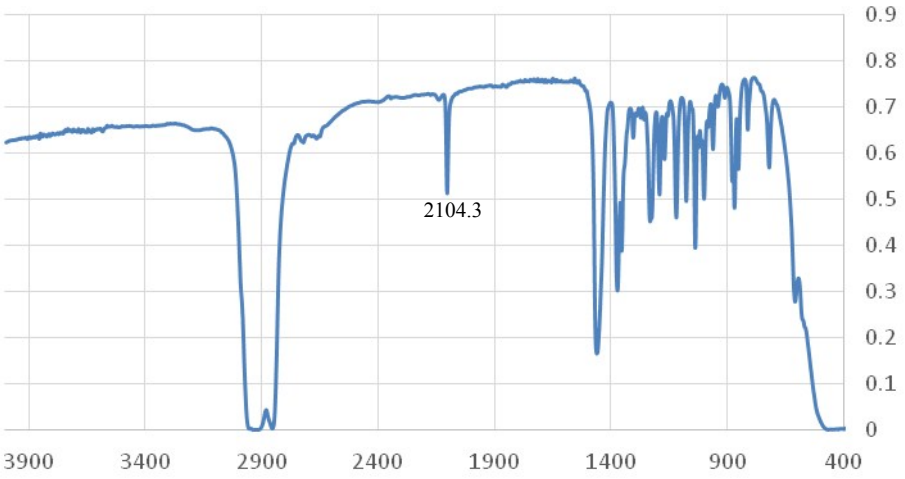

Figure S1a IR spectrum of $\mathbf{8}_2$.

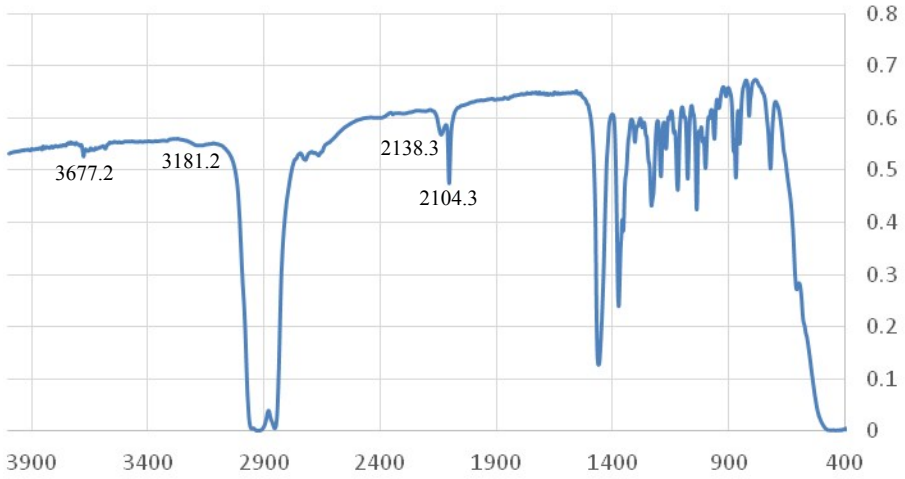

Figure S1b IR spectrum of $\mathbf{8}_2$ after air exposure.

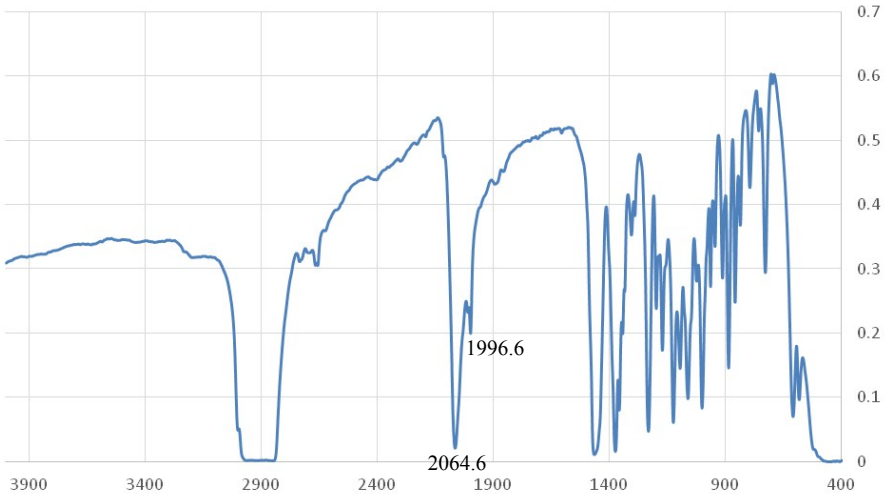

Figure S2a IR spectrum of $\mathbf{9}_2$.

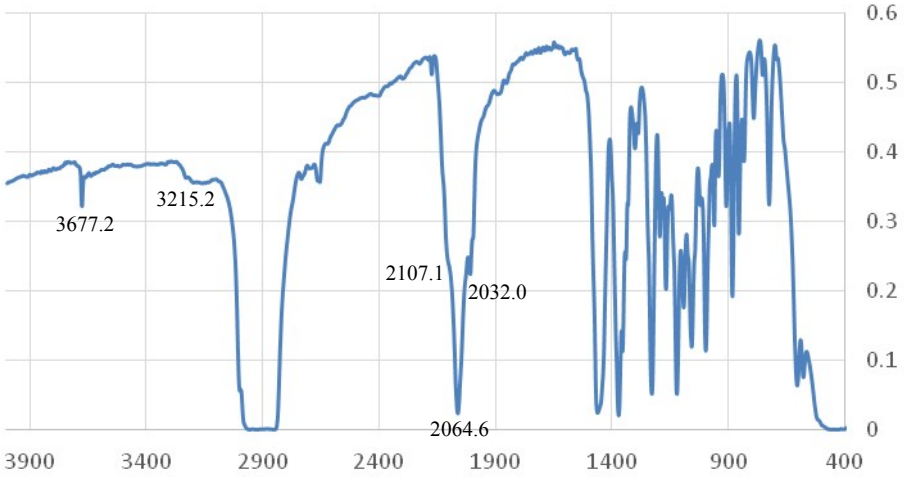

Figure S2b IR spectrum of $\mathbf{9}_2$ after air exposure.

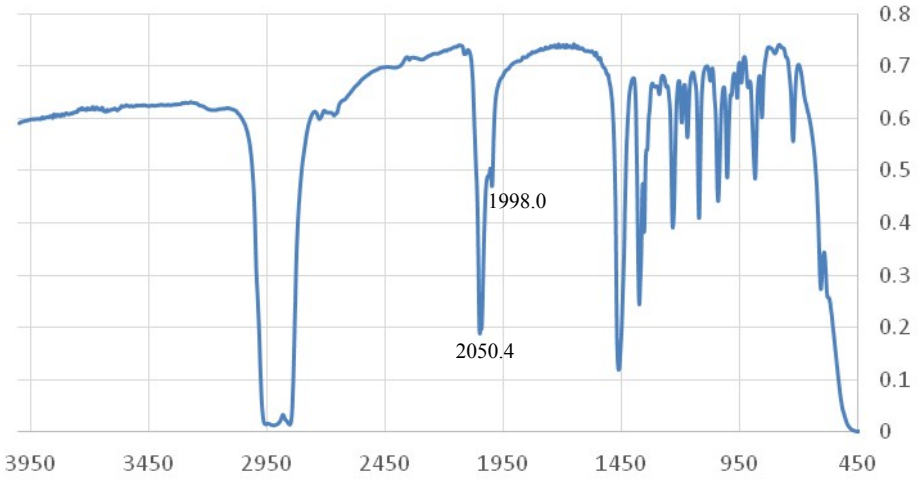

Figure S3a IR spectrum of $\mathbf{10}_2$.

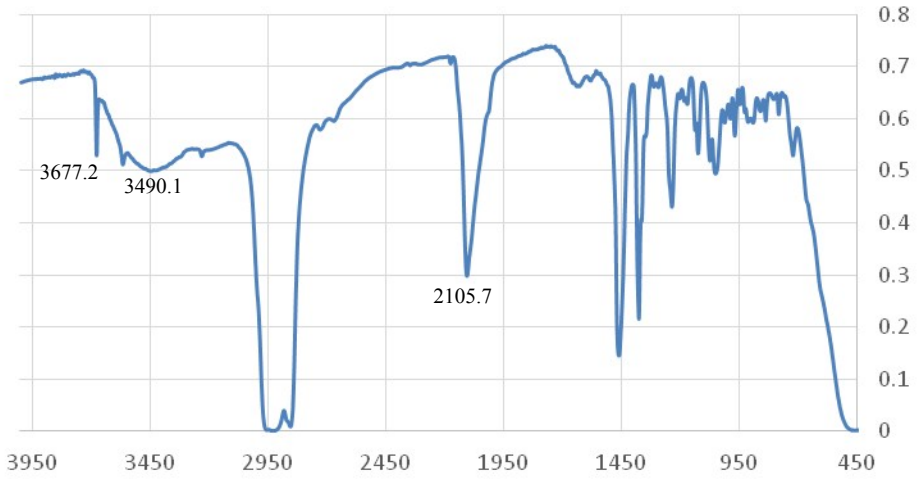

Figure S3b IR spectrum of $\mathbf{10}_2$ after air exposure.

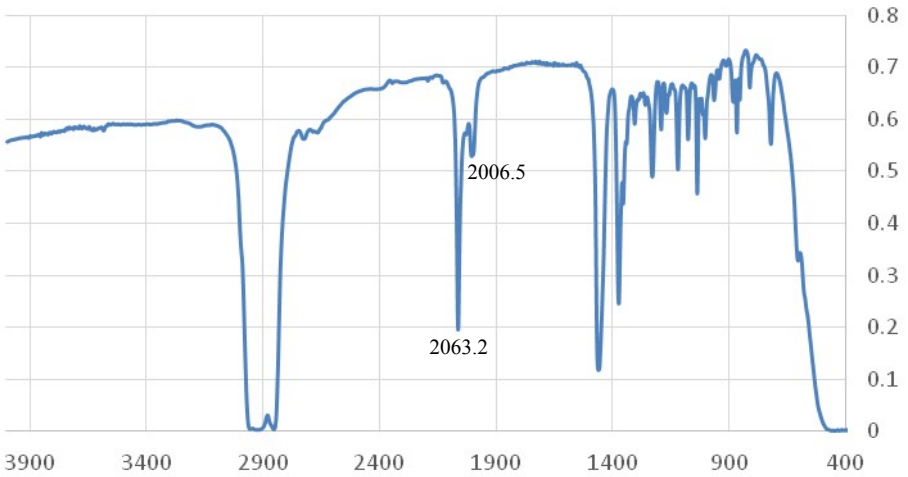

Figure S4a IR spectrum of $\mathbf{11}_2$.

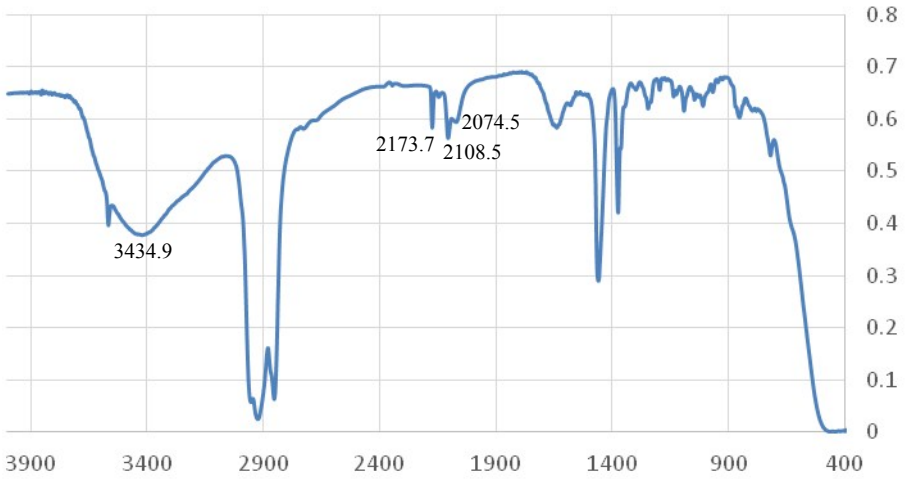

Figure S4b IR spectrum of $\mathbf{11}_2$ after air exposure.

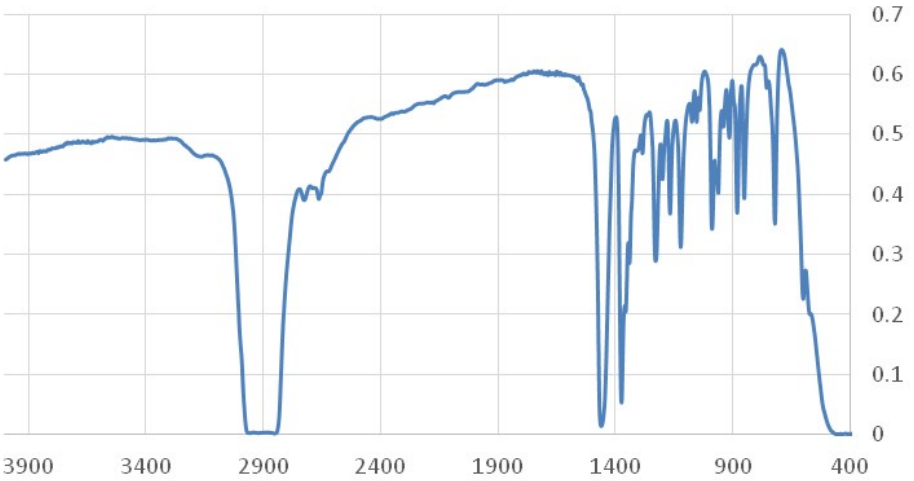

Figure S5 IR spectrum of $\mathbf{12}_2$.

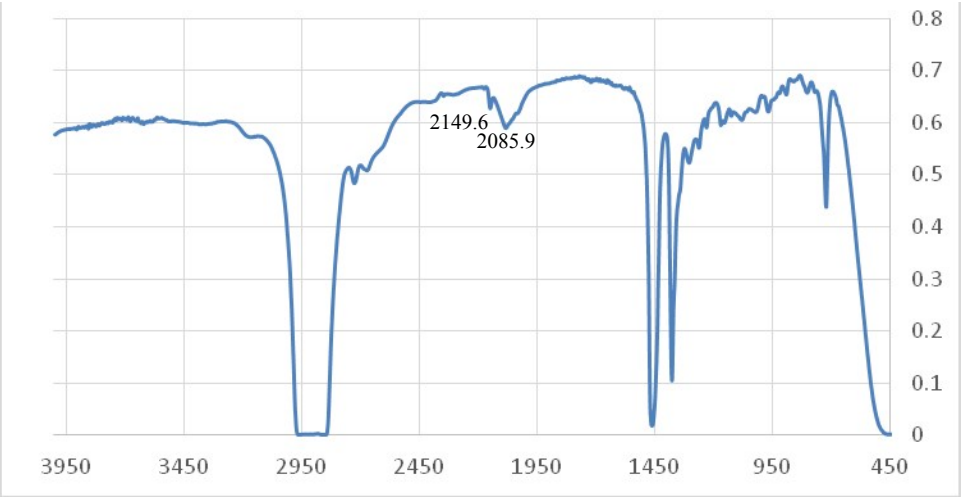

Figure S6a IR spectrum of precipitate obtained after dissolving $\mathbf{10}_2$ in benzene, showing a thiocyanate signal.

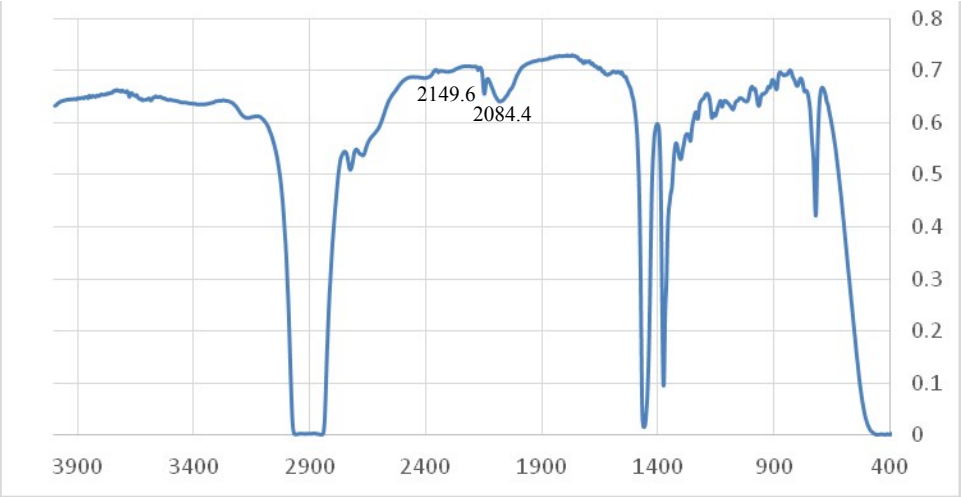

Figure S6b IR spectrum of precipitate obtained after dissolving $\mathbf{10}_2$ in benzene after subsequent air exposure.

[1]H NMR spectroscopy

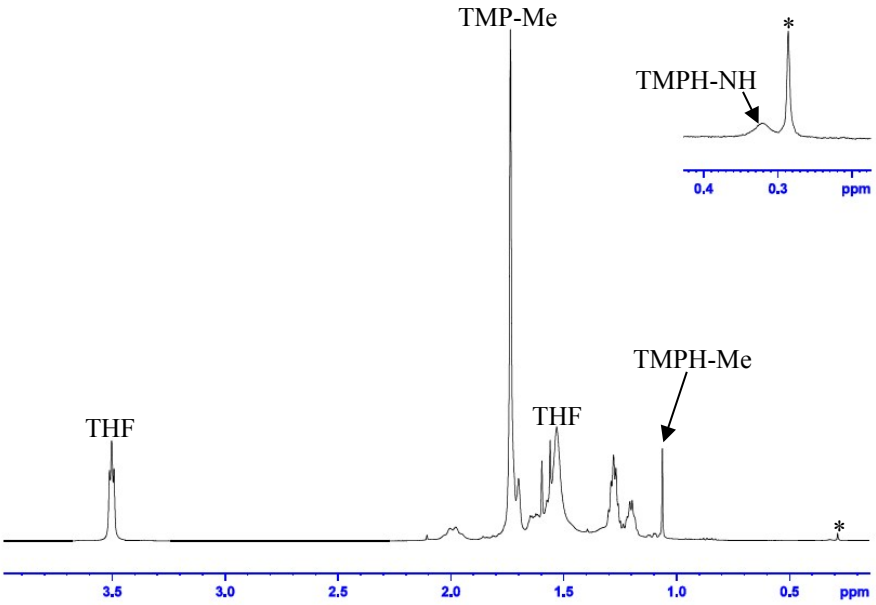

Figure S7 ^{1}H NMR spectrum of $\mathbf{8}_2$. Inset: NH peak attributable to trace TMPH and vacuum grease (*).

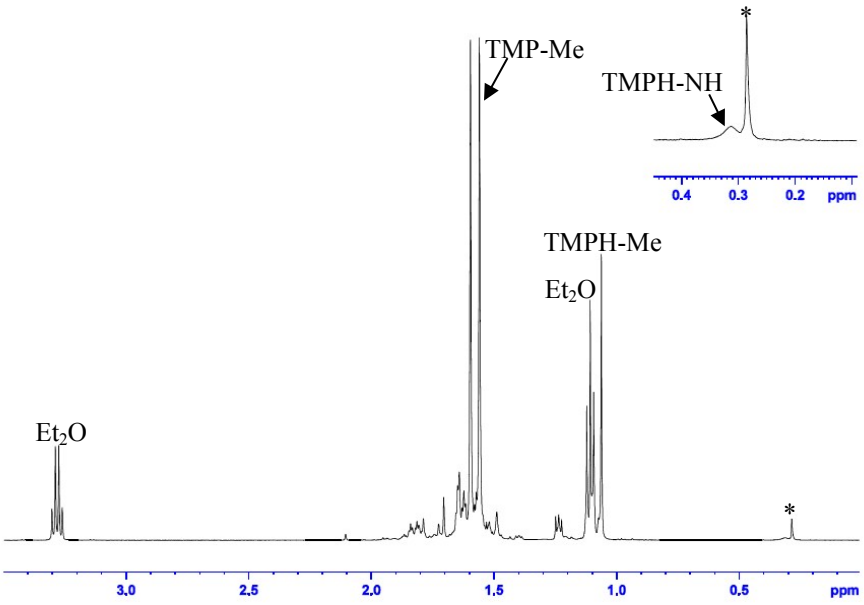

Figure S8 ^{1}H NMR spectrum of $\mathbf{9}_2$. Inset: NH peak attributable to trace TMPH and vacuum grease (*).

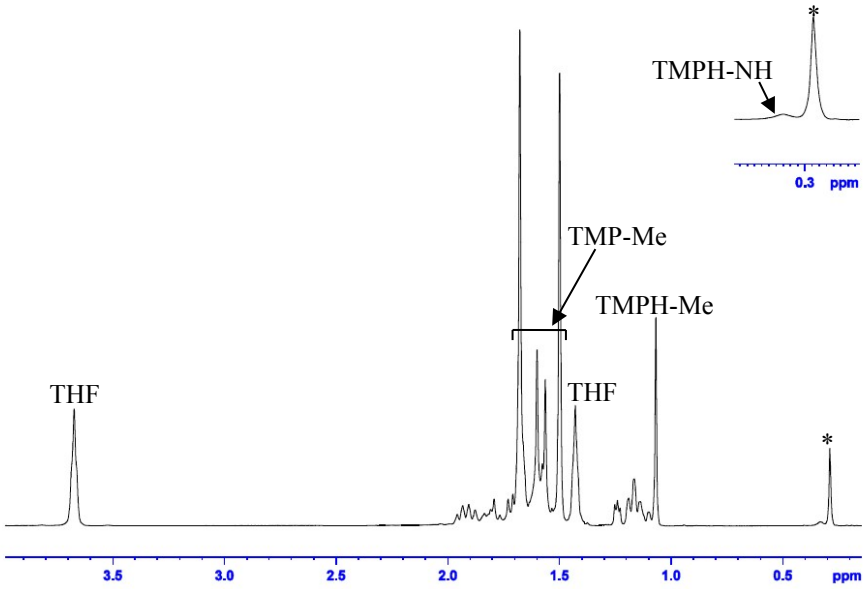

Figure S9 ^{1}H NMR spectrum of $\mathbf{10}_2$. Inset: NH peak attributable to trace TMPH and vacuum grease (*).

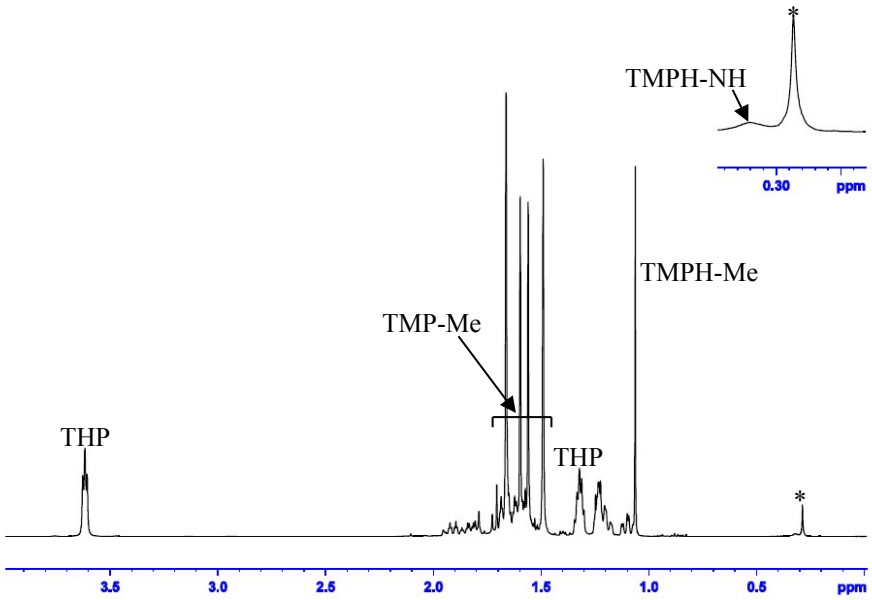

Figure S10 ^{1}H NMR spectrum of $\mathbf{11}_2$. Inset: NH peak attributable to trace TMPH and vacuum grease (*).

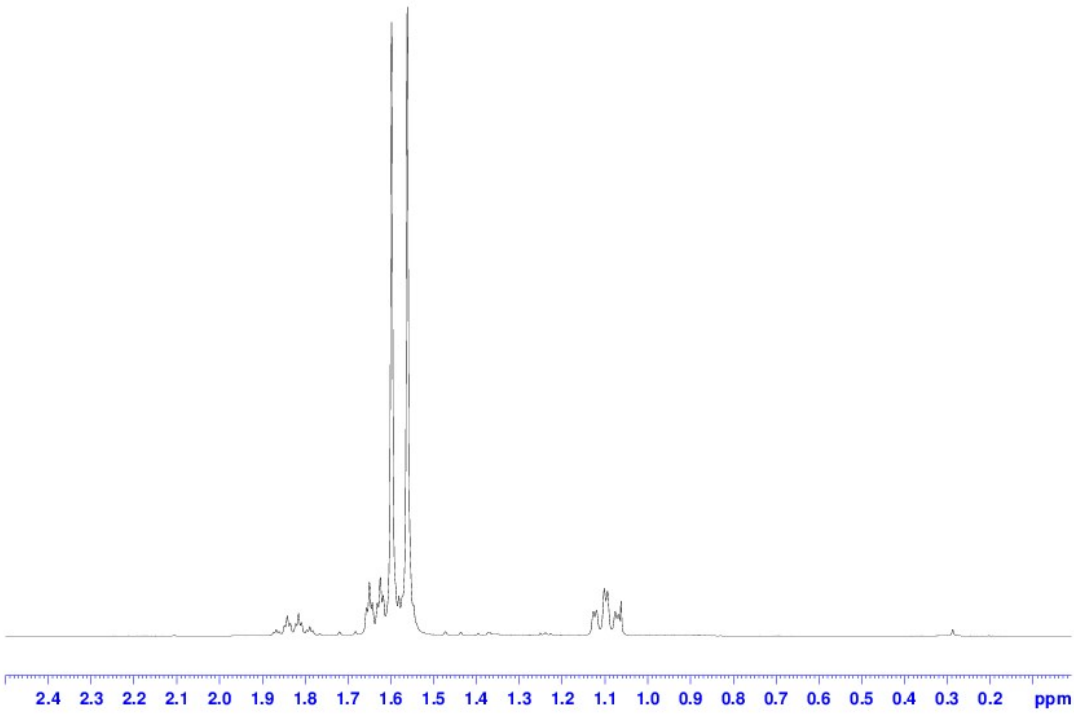

Figure S11 ^{1}H NMR spectrum of $\mathbf{12}_2$, establishing the position of the TMP-Me resonances in a Gilman cuprate.

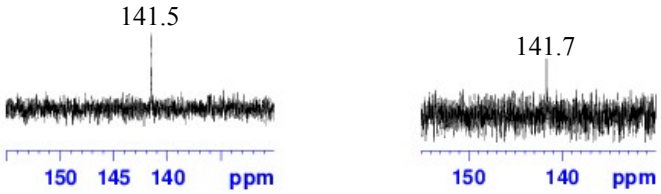

Figure S12 ^{13}C NMR spectra of the SCN region of $\mathbf{10}_2$ (left) and $\mathbf{11}_2$ (right). In either case the sample concentration is 50 mg/0.7 mL. All other peaks were unchanged relative to the values observed for 20 mg/0.7 mL samples (see manuscript Figure 6 and Experimental Section)

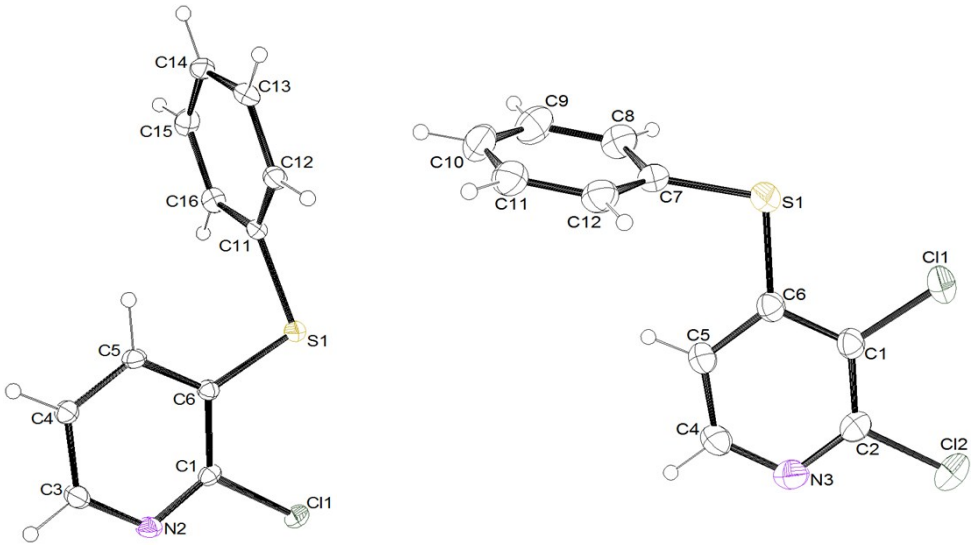

Figure S13 ORTEP diagrams (30% probability) of compounds **15c** and **16c**.

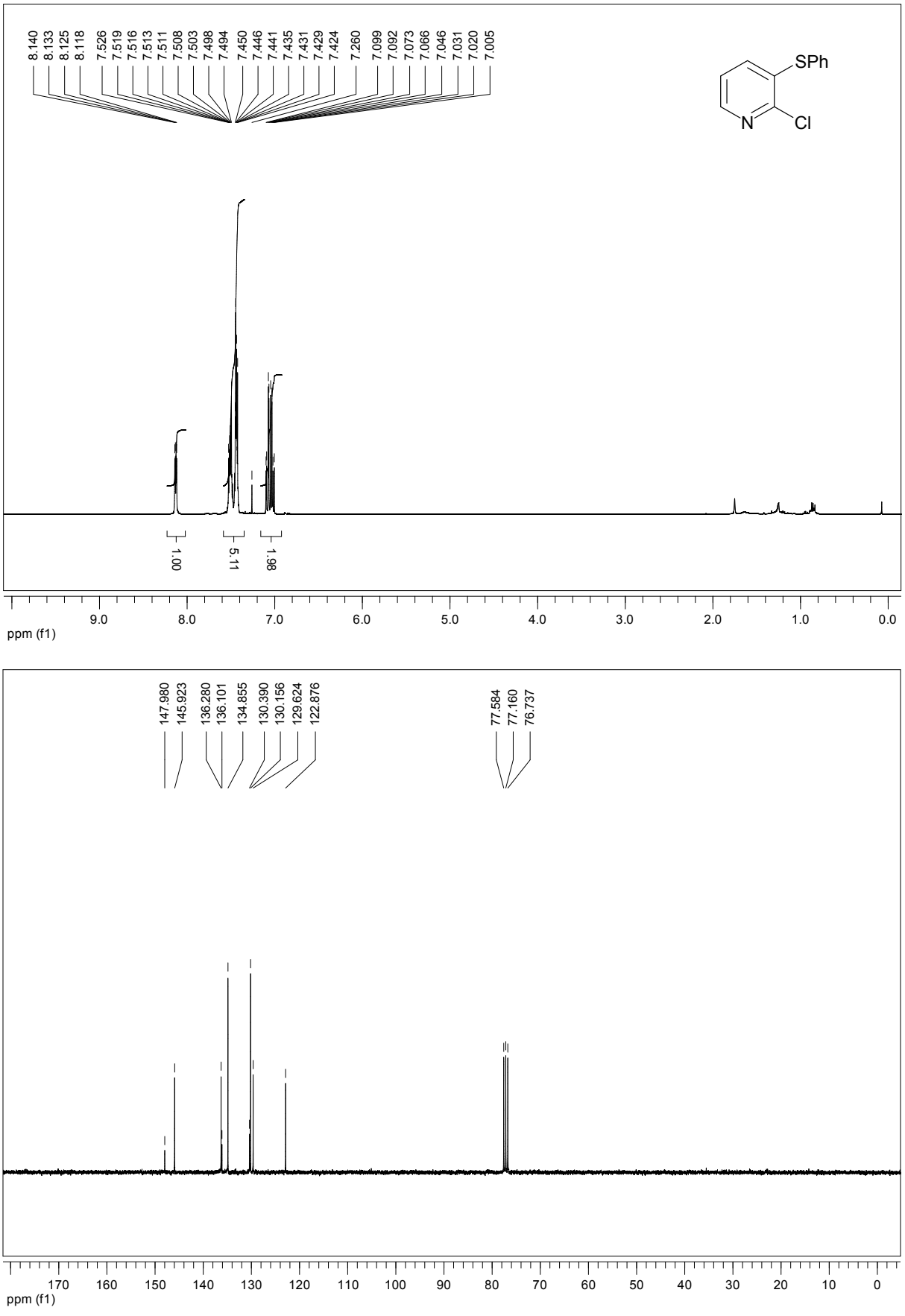

Figure S14 ^{1}H and ^{13}C NMR spectra of 2-chloro-3-(phenylsulfanyl)pyridine **15c**.

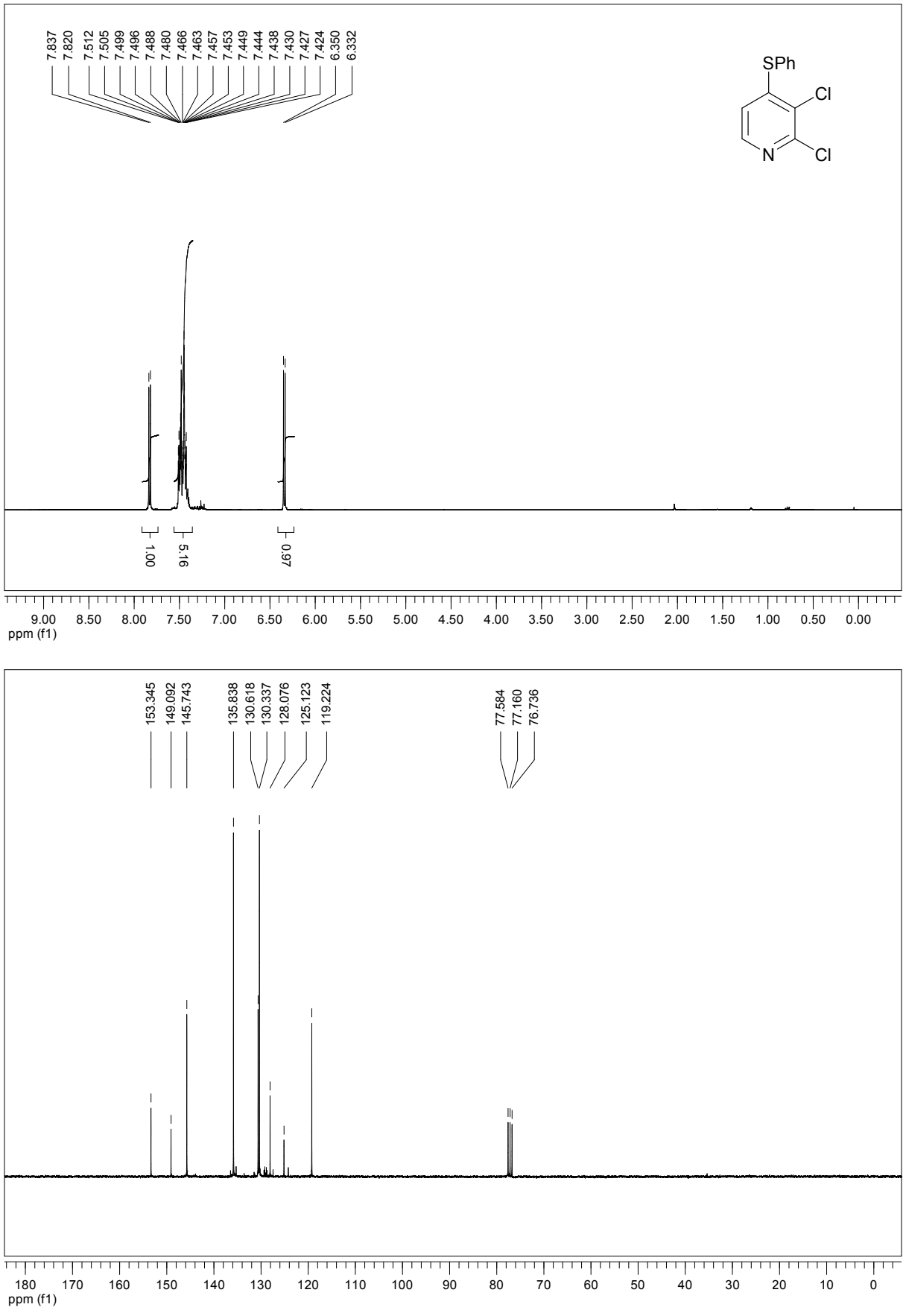

Figure S15 ^{1}H and ^{13}C NMR spectra of 2,3-dichloro-4-(phenylsulfanyl)pyridine **16c**.