Electronic Supplementary Material (ESI) for Chemical Science.

$^{79/81}$Br Nuclear Quadrupole Resonance Spectroscopic Characterization of Halogen Bonds in Supramolecular Assemblies

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List of Figures

$^{1}H \rightarrow ^{13}C$ Cross-Polarization Magic-Angle Spinning Solid-State NMR Spectra. B_0 = 9.4 T.

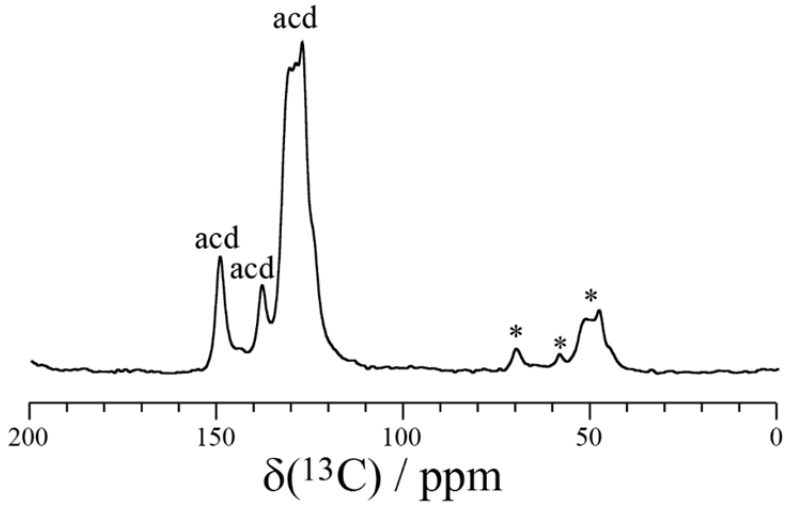

Figure S1. Experimental ^{13}C solid-state NMR spectrum of **2** (*p*-DBrTFB)(acridine). The "acd" labels denote the resonances assigned to acridine ($\delta(^{13}C)$ = 149.0 ± 0.3 ppm, 137.6 ± 0.3 ppm, 130.4 ± 0.5 ppm to 126.9 ± 0.4 ppm, left to right). The asterisks denote spinning sidebands.

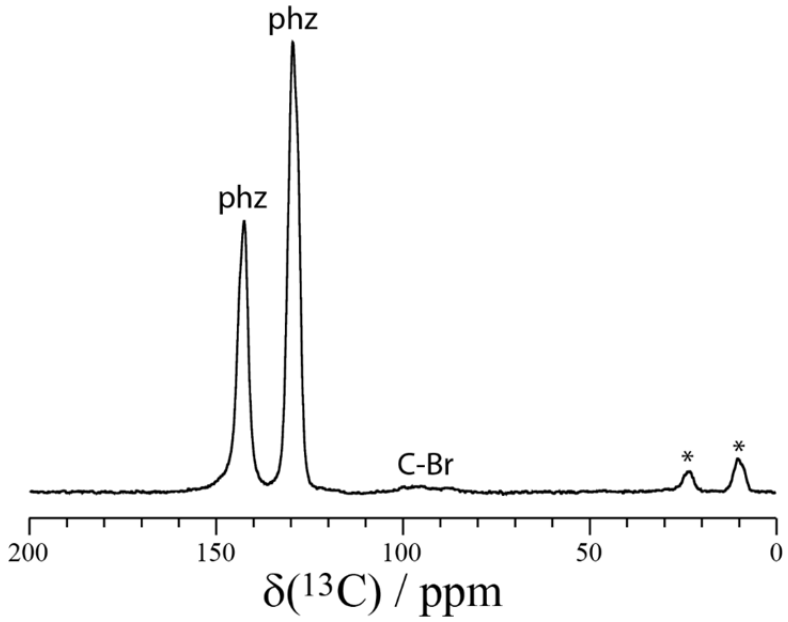

Figure S2. Experimental ^{13}C solid-state NMR spectrum of **3** (*p*-DBrTFB)(phenazine). The "phz" labels denote the resonances assigned to phenazine ($\delta(^{13}C)$ = 142.8 ± 0.6 ppm, 129.8 ± 0.7 ppm, left to right), whereas the "C-Br" label denotes the resonance assigned to the carbon covalently bonded to bromine ($\delta(^{13}C)$ = 100.8 ± 0.8 ppm to 85.8 ± 1.7 ppm). The asterisks denote spinning sidebands.

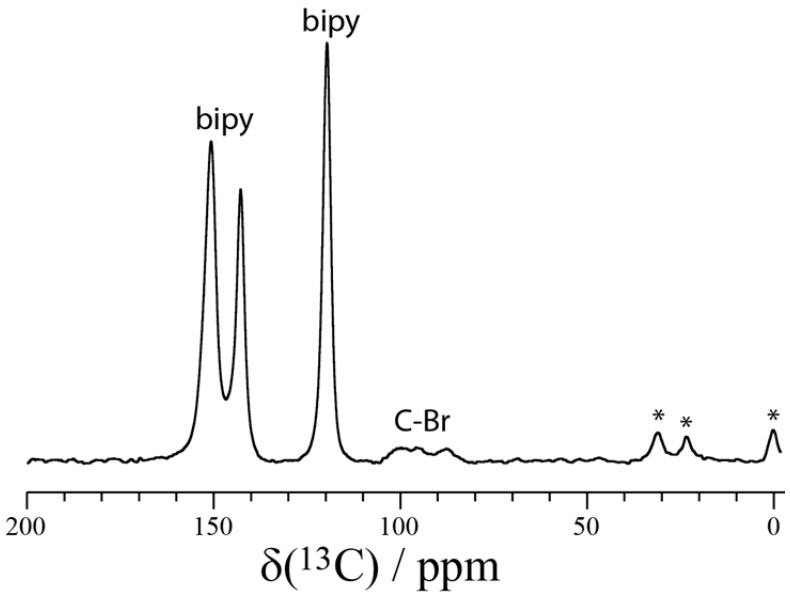

Figure S3. Experimental ^{13}C solid-state NMR spectrum of **4** (*p*-DBrTFB)(bipy). The "bipy" labels denote the resonances assigned to phenazine ($\delta(^{13}C)$ = 150.9 ± 0.4 ppm, 142.9 ± 0.4 ppm, 119.88 ± 0.2 ppm, left to right), whereas the "C-Br" label denotes the resonance assigned to the carbon covalently bonded to bromine ($\delta(^{13}C)$ = 103.3 ± 1.6 ppm to 85.3 ± 1.3 ppm). The asterisks denote spinning sidebands.

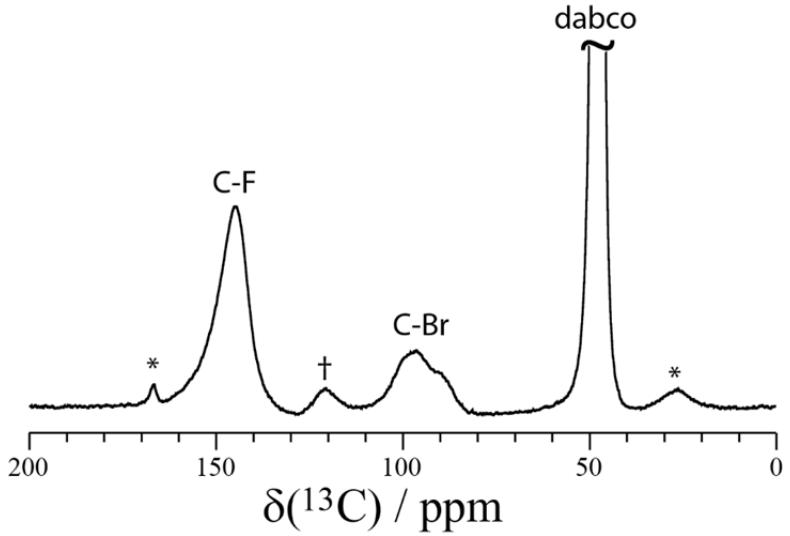

Figure S4. Experimental ^{13}C solid-state NMR spectrum of **5** (*p*-DBrTFB)(dabco). The "dabco" label denotes the resonance assigned to dabco ($\delta(^{13}C)$ = 47.6 ± 0.1 ppm), whereas the "C-Br" label denotes the resonance assigned to the carbon covalently bonded to bromine ($\delta(^{13}C)$ = 102.6 ± 1.3 ppm to 85.3 ± 2.1 ppm), and the "C-F" symbol denotes the carbon covalently bonded to fluorine ($\delta(^{13}C)$ = 102.6 ± 1.3 ppm). The asterisks denote spinning sidebands. The dagger indicates a trace impurity.

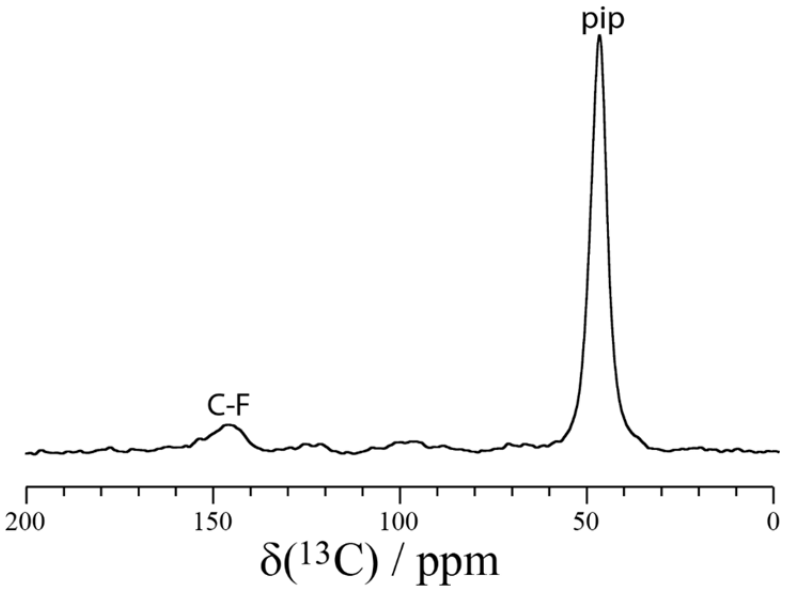

Figure S5. Experimental ^{13}C solid-state NMR spectrum of **6** (*p*-DBrTFB)(pip). The "pip" label denotes the resonance assigned to piperazine ($\delta(^{13}C)$ = 46.5 ± 0.4 ppm), whereas the "C-F" label denotes the resonance assigned the carbon covalently bonded to fluorine ($\delta(^{13}C)$ = 145.9 ± 2.3 ppm). The asterisks denote spinning sidebands.

Powder X-ray Diffraction

Powder X-ray diffractograms were acquired using a Rigaku Ultima IV Diffractometer operating at room temperature (298 ± 1 K) with a copper source and a diffracted beam monochromator.

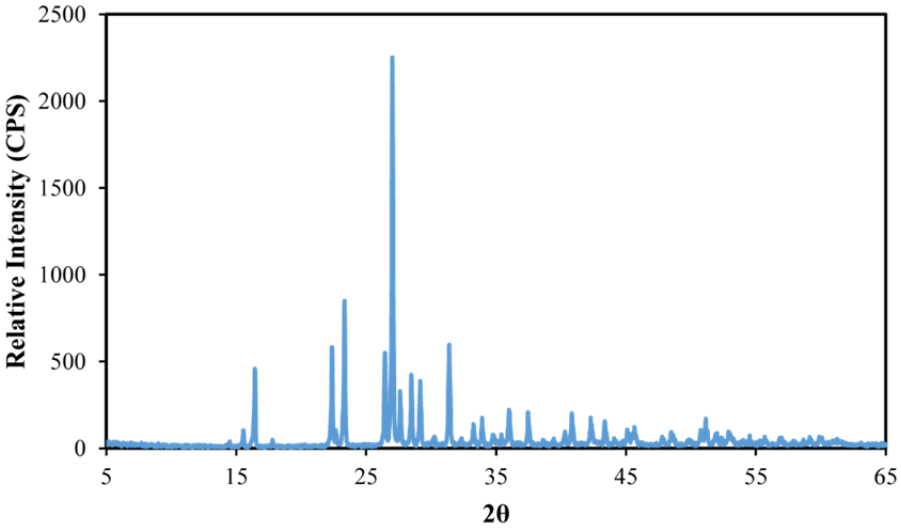

Figure S6. Experimental powder X-ray diffraction of sample **1**.

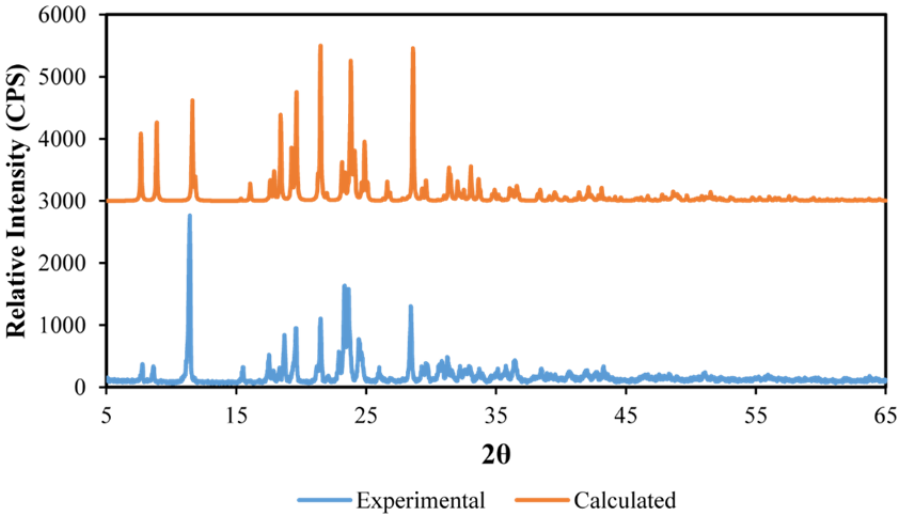

Figure S7. Experimental powder X-ray diffraction of sample **2** with the calculated pattern overlaid.

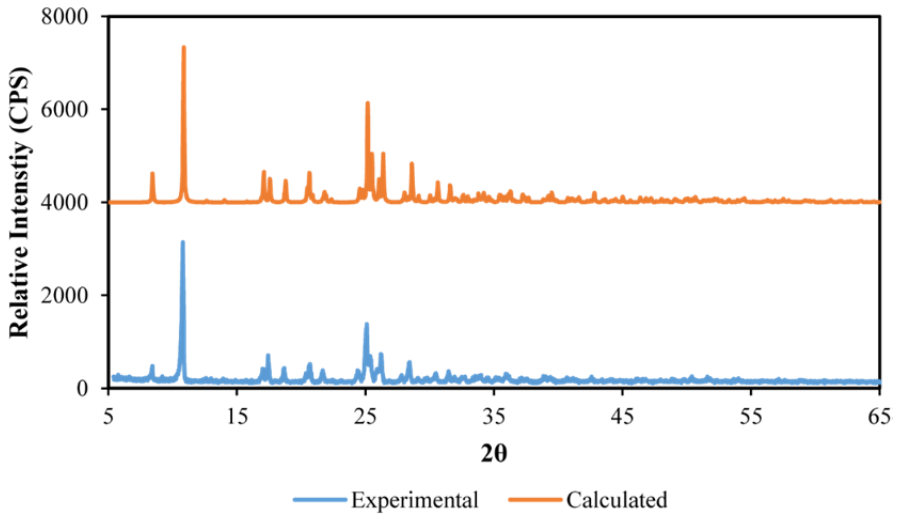

Figure S8. Experimental powder X-ray diffraction of sample **3** with the calculated pattern overlaid.

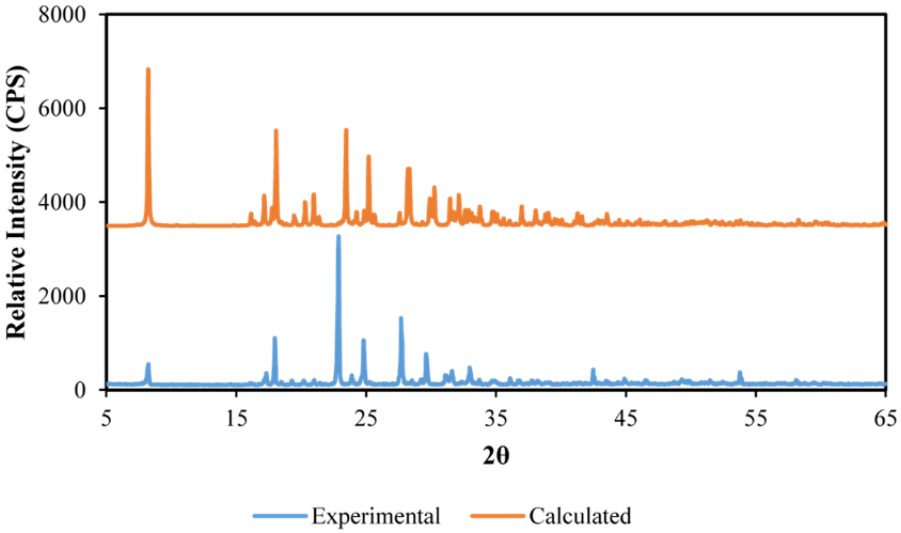

Figure S9. Experimental powder X-ray diffraction of sample **4** with the calculated pattern overlaid.

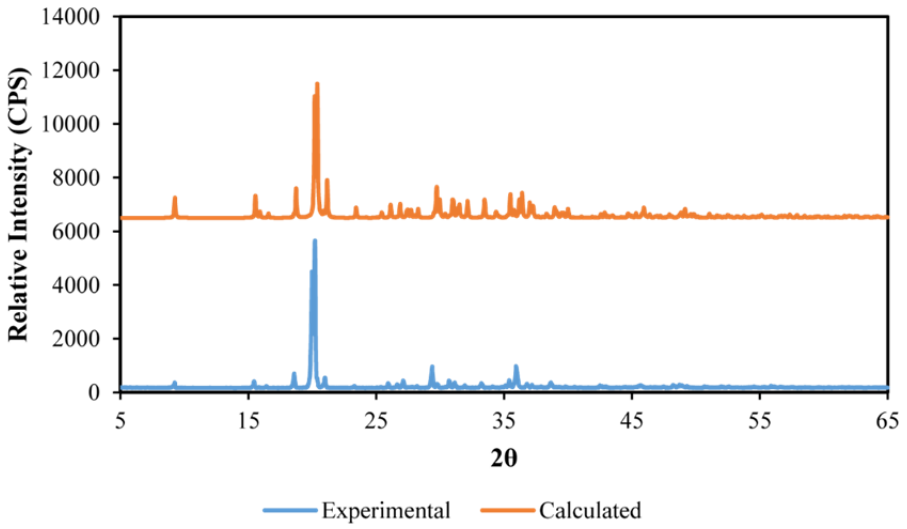

Figure S10. Experimental powder X-ray diffraction of sample **5** with the calculated pattern overlaid.

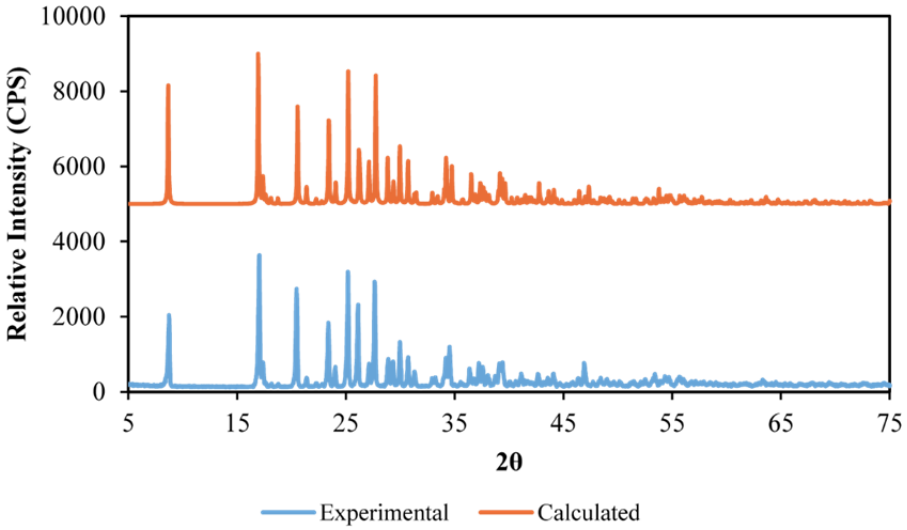

Figure S11. Experimental powder X-ray diffraction of sample **6** with the calculated pattern overlaid.