



STRUCTURAL
CHEMISTRY

Volume 78 (2022)

Supporting information for article:

^{77}Se and ^{125}Te solid-state NMR and X-ray diffraction structural study of chalcogen-bonded 3,4-dicyano-1,2,5-chalcogenodiazole cocrystals

Tamali Nag, Jeffrey S. Ovens and David L. Bryce

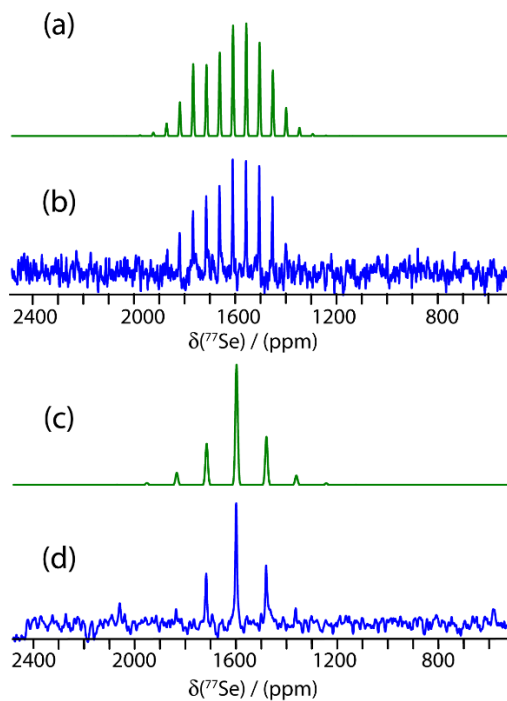
S1. Additional solid-state NMR spectra

Figure S1 ^{77}Se CP/MAS NMR experiments acquired with proton decoupling at $B_0 = 9.4$ T for cocystal **1a**. Experimental spectra are shown in blue and simulated spectra are shown in green. Top: MAS rate = 4 kHz; bottom: MAS rate = 9 kHz.

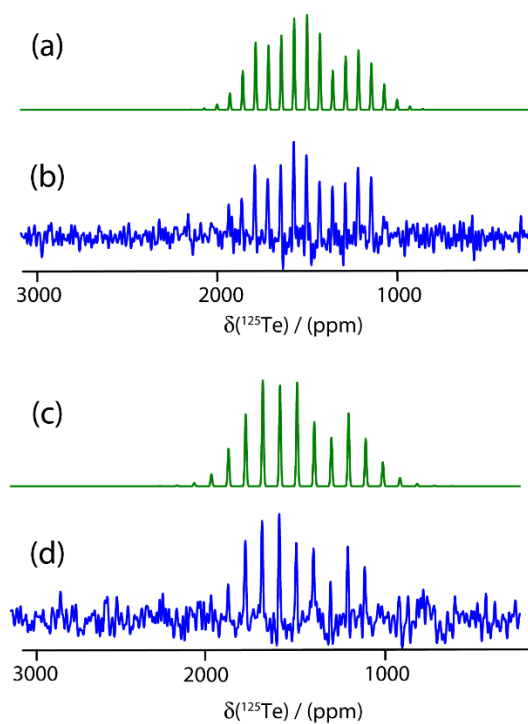


Figure S2 ^{125}Te Bloch decay MAS NMR experiments acquired with proton decoupling at $B_0 = 9.4$ T for cocystal **2c**. Experimental spectra are shown in blue and simulated spectra are shown in green. Top: MAS rate = 9 kHz; bottom: MAS rate = 12 kHz.

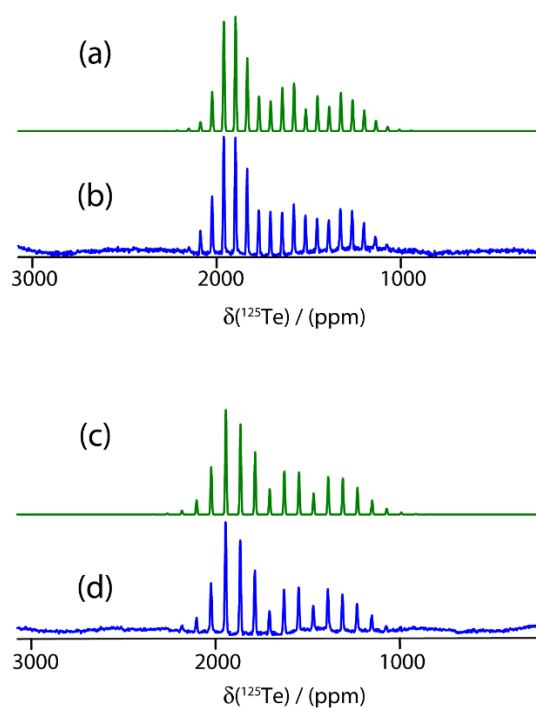


Figure S3 ^{125}Te Bloch decay MAS NMR experiments acquired with proton decoupling at $B_0 = 9.4$ T for cocystal **2b**. Experimental spectra are shown in blue and simulated spectra are shown in green. Top: MAS rate = 8 kHz; bottom: MAS rate = 10 kHz.