Electronic Supplementary Information: Central-Transition Double-Quantum Sideband NMR Spectroscopy of Half-Integer Quadrupolar Nuclei: Estimating Internuclear Distances and Probing Clusters within Multi-Spin Networks

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S1 ^{11}B Spin Systems in bis(catecholato)diboron

Table S1 lists the probabilities of finding a particular pattern of occupancy by the ^{11}B isotope (80.1 % natural abundance) in the 4 boron site system shown in Fig. 2b.

Sites Solely Occupied by ^{11}B	Probability
$(1,2,3,4)$	41.2 %
$(1,2,3)$ or $(1,2,4)$	20.5 %
$(1,3,4)$ or $(2,3,4)$	20.5 %
$(1,3)$ or $(2,4)$	5.1 %
$(1,4)$ or $(2,3)$	5.1 %
$(1,2)$	2.5 %

Table S1: ^{11}B occupancy probalilities in the 4 boron system shown in Fig. 2b.

S2 Dipolar Coupling Multipliticies

Table S2 collects the internuclear distances and dipolar couplings for the samples used in this study, bis(catecholato)diboron ($C_{12}H_8B_2O_4$), Na_2SO_4 and α-Al_2O_3. As each sample solely features one crystallographically unique B, Al or Na site, respectively, the indices j and k are given by $j = k = 1$ in each case and thus dropped for clarity, i. e., $r = r_{11}$, $b = b_{11}$, $\Omega^{\mathrm{DD}} = \Omega^{\mathrm{DD}}_{11}$, $\beta^{\mathrm{DD}} = \beta^{\mathrm{DD}}_{11}$, and $\gamma^{\mathrm{DD}} = \gamma^{\mathrm{DD}}_{11}$. The listed internuclear distances r and dipolar coupling constants b correspond to ^{11}B–^{11}B pairs for bis(catecholato)diboron, to ^{23}Na–^{23}Na pairs for Na_2SO_4, and to ^{27}Al–^{27}Al pairs for α-Al_2O_3. In all cases the multiplicity M and number of dipolar interactions that result in unique NMR responses N (see section 2.2.2) are given together with the Euler angles $\Omega^{\mathrm{DD}} = \{0, \beta^{\mathrm{DD}}, \gamma^{\mathrm{DD}}\}$.

Sample	r	$-b/2\pi$	M	N	$\{\beta^{\mathrm{DD}}, \gamma^{\mathrm{DD}}\}$
	[pm]	[Hz]			[°]
$C_{12}H_8B_2O_4$	168	2619	2	1	$\{53.6, 42.5\}$
	382	222	2	1	$\{85.7, 166.1\}$
	475	116	4	1	$\{98.6, -180.0\}$
	601	57.0	1	1	$\{73.5, 9.1\}$
	621	51.7	2	2	$\{167.4, 42.5\}$, $\{12.6, 137.5\}$
Na_2SO_4	321	253	4	2	$\{122.2, 117.7\}$, $\{23.2, -4.7\}$
	360	181	4	4	$\{98.7, -163.5\}$, $\{98.7, -16.5\}$, $\{60.2, -133.4\}$, $\{143.1, 6.5\}$
	361	180	2	1	$\{118.3, -90\}$
	420	113.5	8	4	$\{73.9, 32.4\}$, $\{106.1, 57.9\}$, $\{73.9, 147.6\}$, $\{33.7, 157.1\}$
	508	64.2	4	4	$\{69.4, 44.2\}$, $\{96.2, 64.9\}$, $\{69.4, 135.8\}$, $\{35.8, 136.2\}$
	549	50.8	4	4	$\{121.6, 177\}$, $\{71, -25.9\}$, $\{41.4, -104\}$, $\{161.5, 59.6\}$
	572	44.9	8	2	$\{90, 102.8\}$, $\{44.5, -112.4\}$
	587	41.6	4	1	$\{142.6, 135.2\}$
	590	40.9	8	4	$\{53.7, 11\}$, $\{101.4, 143.8\}$, $\{126.3, 79.3\}$, $\{170.8, 21.6\}$
α-Al_2O_3	266	436	2	1	$\{0, 0\}$
	279	375	6	3	$\{79.9, 60\}$, $\{79.9, -60\}$, $\{100.1, 0\}$
	322	245	6	3	$\{58.6, 60\}$, $\{58.6, -60\}$, $\{121.4, 0.\}$
	350	191	12	3	$\{128.2, 60\}$, $\{128.2, -60\}$, $\{51.8, 0\}$
	384	144	2	1	$\{0, 0\}$
	476	75.7	15	3	$\{90, 90\}$, $\{90, 30\}$, $\{90, -30\}$
	513	60.5	12	3	$\{32.4, 60\}$, $\{32.4, -60\}$, $\{32.4, 180.\}$
	545	50.4	18	6	$\{60.8, 90\}$, $\{60.8, -90\}$, $\{60.8, 30\}$, $\{60.8, -30\}$
					$\{60.8, 150\}$, $\{60.8, -150\}$
	552	48.6	3	1	$\{84.9, 0\}$, $\{84.9, 120\}$, $\{84.9, -120\}$
	555	47.8	6	3	$\{29.7, 0\}$, $\{29.7, 120\}$, $\{29.7, -120\}$
	575	43.1	9	3	$\{73, 0\}$, $\{73, 120\}$, $\{73, -120\}$
	591	39.6	9	3	$\{111.5, 0\}$, $\{111.5, 120\}$, $\{111.5, -120\}$

Table S2: Internuclear distances and dipolar couplings for the samples used in this study, bis(catecholato)diboron ($C_{12}H_8B_2O_4$), Na_2SO_4 and α-Al_2O_3.