

Intramolecular H···S interactions in metal di-(isopropyl)dithiocarbamate complexes

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Electronic Supplementary Information

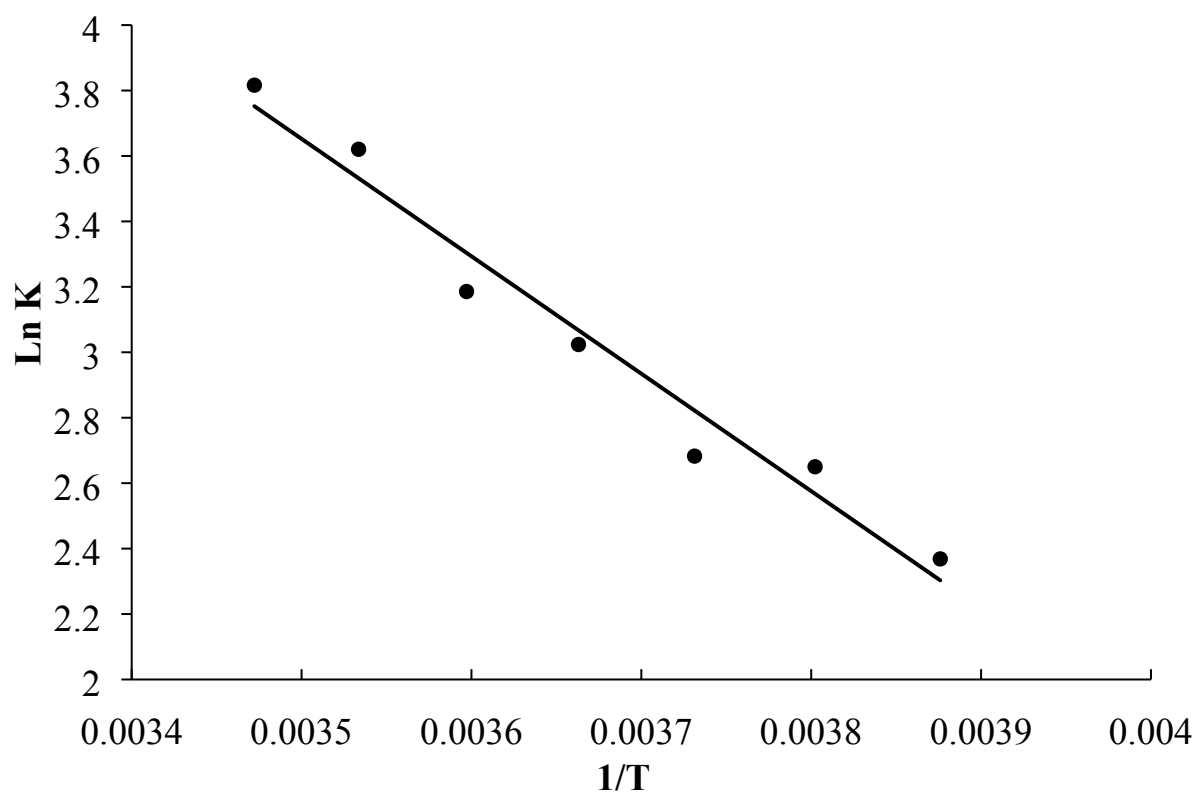


Figure S1: Arrhenius plot for exchange of isopropyl methyl groups in $\text{Na}(\text{dipdte}) \cdot 5\text{H}_2\text{O}$.

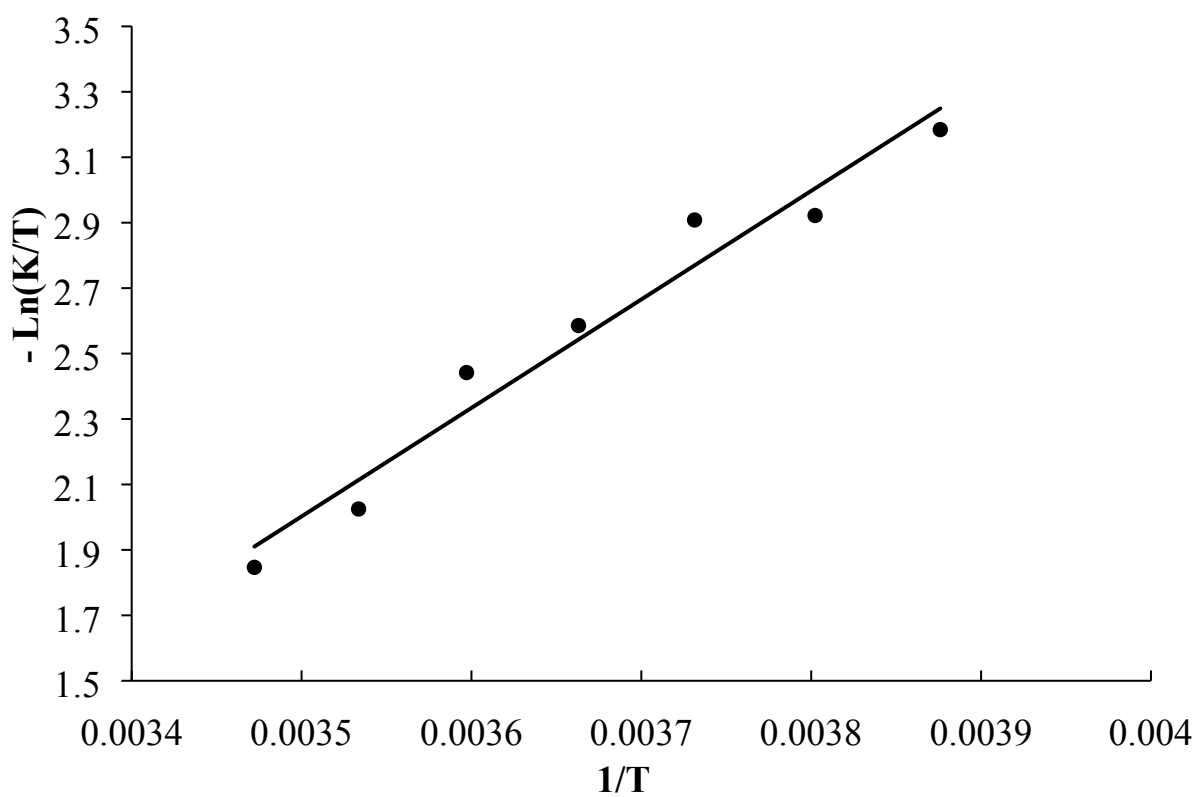


Figure S2: Eyring plot for exchange of isopropyl methyl groups in $\text{Na}(\text{dipdte}) \cdot 5\text{H}_2\text{O}$.

Table S1: Selected data obtained from CSD database survey of metal dipdtp complexes.

CSD Refcode	CSD number	Metal	C1-N1-C2	C1-N1-C5	C2-S1	C5-S2	C1-N1	S1-C1-S2
AFELEE	908263	Au	119.4	123.5	2.998	3.195	1.305	109.46
CEXZEM	924188	In	120.88	124.07	3.008	3.101	1.329	116.15
DUHPEC	754186	Zn	119.9	124.9	3.006	3.126	1.34	115.69
FERROJ	1154897	Mo	119.2	123.6	3.006	3.201	1.323	109.2
GOPRIM	1170146	Nd	120.1	123.5	2.941	3.098	1.324	116.5
IPTCMO	1180752	Mo	120.8	123.113	3.042	3.116	1.309	109.95
IPTCNI10	1180754	Ni	119.5	124.2	3.037	3.174	1.311	108.38
IPTCZN	1180758	Zn	121.38	124.19	3.017	3.096	1.326	115.99
JAKNEO	1182236	Be	120.32	123.91	3.042	3.152	1.324	111.73
JERDUF	1184894	Co	117	123	3.117	3.121	1.322	108.7
LITJUT	144058	Zn	122.2	123.3	3.046	3.072	1.34	115.6
LITKAA01	118972	Zn	121.1	123.7	3.027	3.099	1.342	115.7
MIFDEK	162242	Sn	121.1	123.8	3.005	3.139	1.329	115
NDTCCU02	111990	Cu	120.1	124.1	3.018	3.162	1.321	111.3
PRCBFE	1237953	Fe	119.07	123.32	3.046	3.166	1.315	108.1
QIWMAK	145420	W	120.1	122.1	3.018	3.17	1.327	109.3
QIYTIK	638242	Cd	121.01	124.59	2.995	3.128	1.336	117.25
QUKCII	139236	Ni	118.8	124.8	3.04	3.219	1.314	107.2
RAHKUI	833598	Au	119.5	123.4	3.027	3.153	1.293	109
RAZBEB	827580	Au	119.8	123.9	3.03	3.174	1.3	109.37
SUVTUY	131014	Cd	122.3	123.5	3.018	3.084	1.327	117.31
TISFIK	1271462	In	120.4	124.4	2.994	3.098	1.317	116.5
UFEWEH01	135544	Pd	120.8	123.5	3.029	3.173	1.307	109.9
XAJWOU	139090	Ni	120.87	123.53	3.077	3.177	1.312	108.12
XUJHEP	196553	Cr	118.48	123.73	3.017	3.217	1.335	108.11
YECXAF	1300618	In	120.7	123.9	2.991	3.117	1.33	116.5
YEFIQ	856056	Ni	119.2	123.7	3.054	3.21	1.324	106.47
YEFVUC	868305	Pd	119.1	124.7	3.037	3.185	1.31	108.2

Table S2. Complete set of bond lengths (Å) and angles (°) for Na(dipdte)·5H₂O.

S1-C1	1.7484(16)	C5-C6	1.522(2)
S2-C1	1.7145(17)	Na1-O4	2.3891(13)
N1-C2	1.492(2)	Na1-O1	2.4492(14)
N1-C1	1.345(2)	Na1-O2	2.4207(13)
N1-C5	1.496(2)	Na1-O5	2.3859(15)
C2-C3	1.524(2)	Na1-O3	2.3879(14)
C2-C4	1.519(2)	Na1-O3 ¹	2.4278(14)
C5-C7	1.525(2)	O3-Na1 ¹	2.4278(14)
C2-N1-C5	113.38(12)	O4-Na1-O3 ¹	84.60(5)
C2-N1-C5	113.38(12)	O4-Na1-O3 ¹	84.60(5)
C1-N1-C2	122.01(13)	O2-Na1-O1	95.54(5)
C1-N1-C5	124.59(14)	O2-Na1-O3 ¹	80.40(5)
N1-C2-C3	111.51(13)	O5-Na1-O4	96.85(5)
N1-C2-C4	111.23(13)	O5-Na1-O1	88.03(5)
C4-C2-C3	112.74(15)	O5-Na1-O2	98.83(5)
S2-C1-S1	118.11(9)	O5-Na1-O3	97.38(5)
N1-C1-S1	120.25(12)	O5-Na1-O3 ¹	175.04(5)
N1-C1-S2	121.63(12)	O3-Na1-O4	85.89(5)
N1-C5-C7	113.60(13)	O3 ¹ -Na1-O1	87.17(5)
N1-C5-C6	113.02(13)	O3-Na1-O1	174.47(5)
C6-C5-C7	113.36(15)	O3-Na1-O2	84.83(5)
O4-Na1-O1	92.33(5)	O3-Na1-O3 ¹	87.45(5)
O4-Na1-O2	162.67(5)	Na1-O3-Na1 ¹	92.55(5)
C2-N1-C1-S1	-2.19(18)	C1-N1-C5-C7	-65.41(19)
C2-N1-C1-S2	179.00(10)	C1-N1-C5-C6	65.6(2)
C2-N1-C5-C7	116.30(15)	C5-N1-C2-C3	61.13(17)
C2-N1-C5-C6	-112.71(16)	C5-N1-C2-C4	-65.66(17)
C1-N1-C2-C3	-117.20(16)	C5-N1-C1-S1	179.67(10)
C1-N1-C2-C4	116.01(16)	C5-N1-C1-S2	0.9(2)

Symmetry Code: ¹1-X,1-Y,1-Z

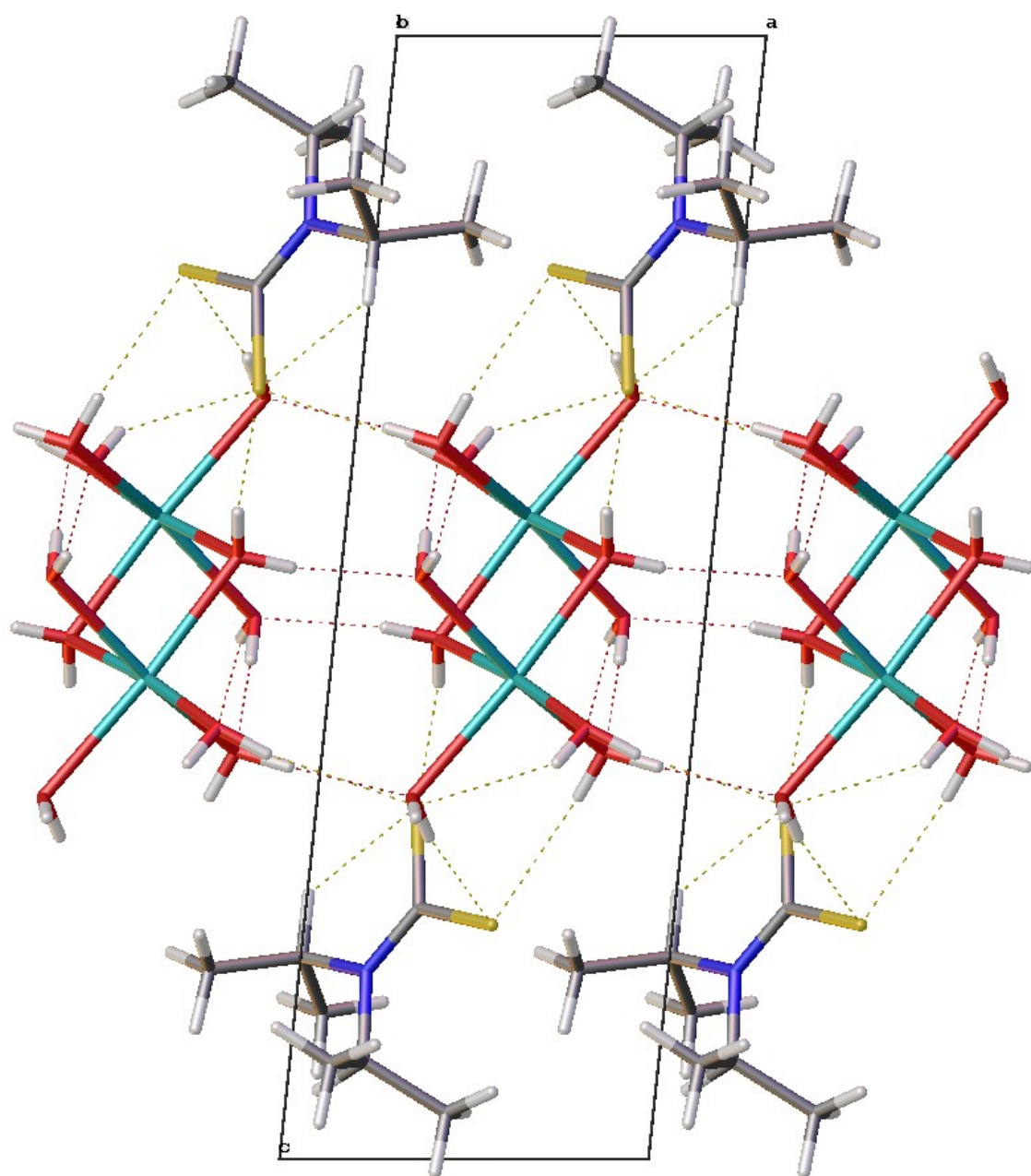


Figure S3. Molecular packing diagram as viewed along the *b* axis, showing layered morphology of Na(dipdte)·5H₂O.

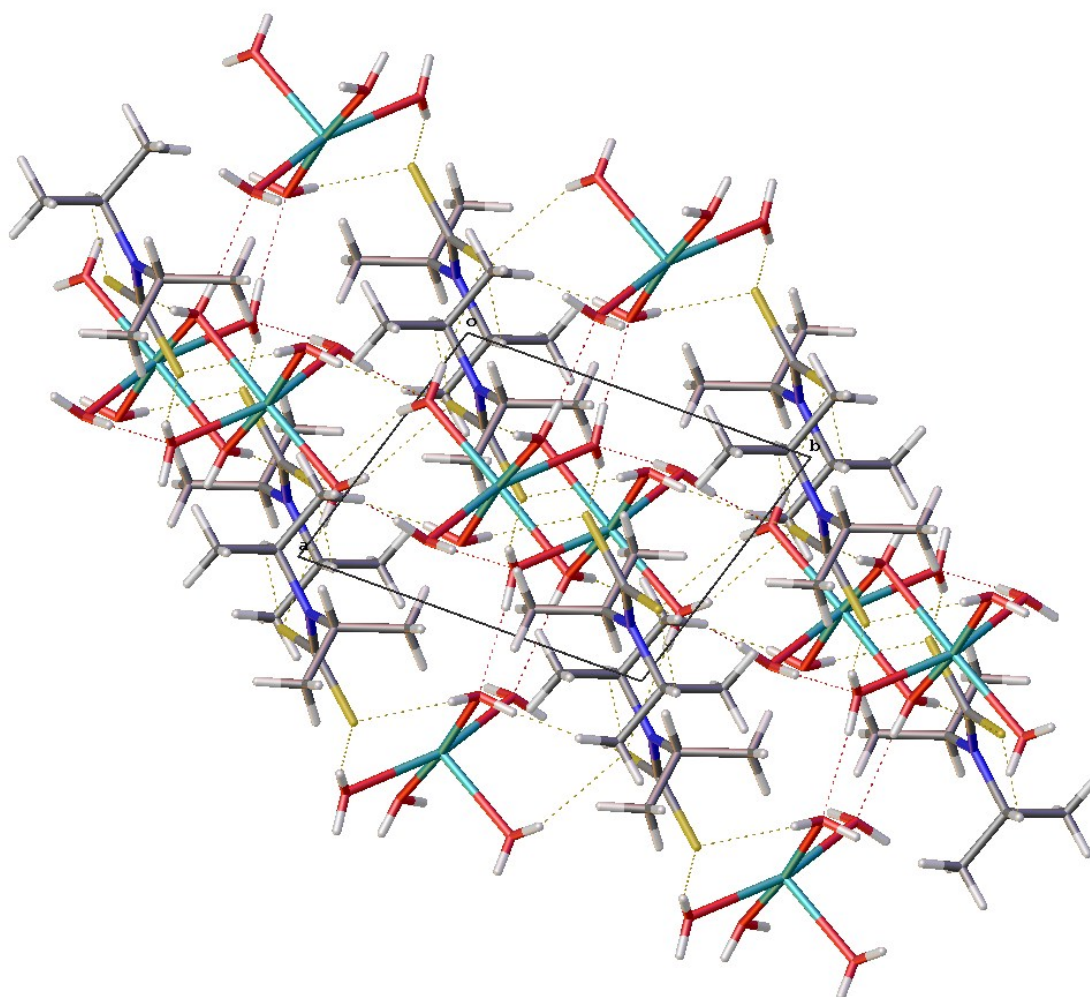


Figure S4. Molecular packing diagram as viewed along the *c* axis, showing layered morphology of Na(dipdte)·5H₂O.

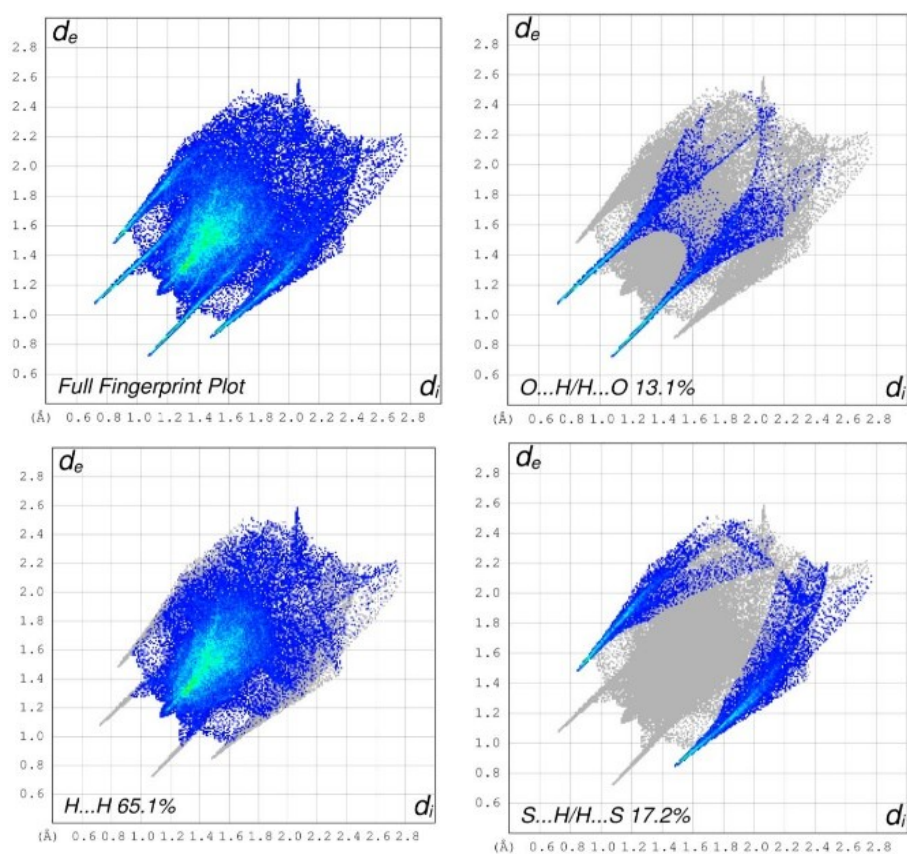


Figure S5: Two-dimensional fingerprint plots for the Hirshfeld surface of $\text{Na}(\text{dipdte}) \cdot 5\text{H}_2\text{O}$.

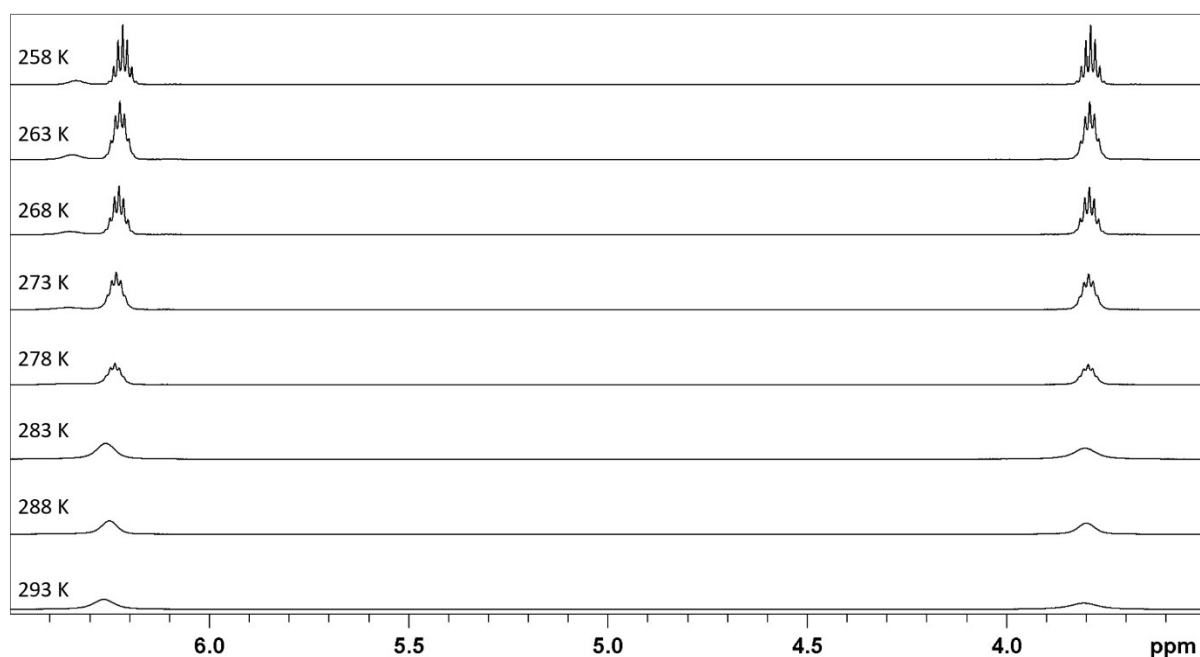


Figure S6: Overlaid variable temperature ^1H NMR spectra acquired at 600 MHz for an acetonitrile- d_3 solution of $\text{Na}(\text{dipdte}) \cdot 5\text{H}_2\text{O}$ in the region of 6.5 to 3.5 ppm.

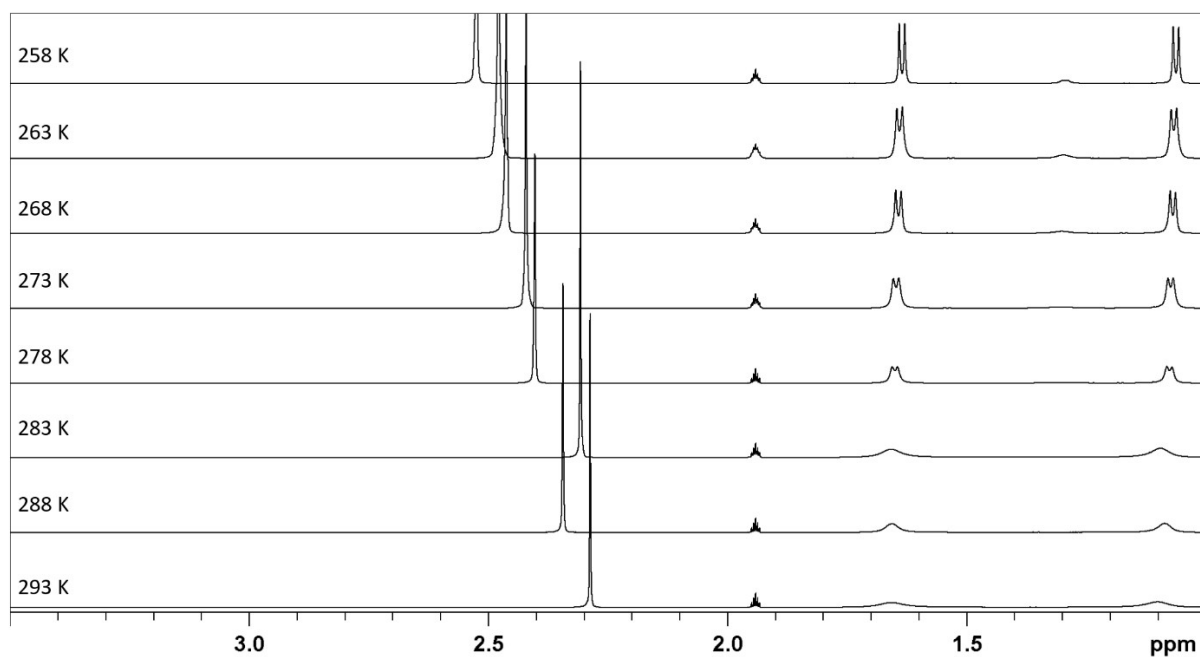


Figure S7: Overlaid variable temperature ^1H NMR spectra acquired at 600 MHz for an acetonitrile- d_3 solution of $\text{Na}(\text{dipdte}) \cdot 5\text{H}_2\text{O}$ in the region of 3.5 to 1.0 ppm.

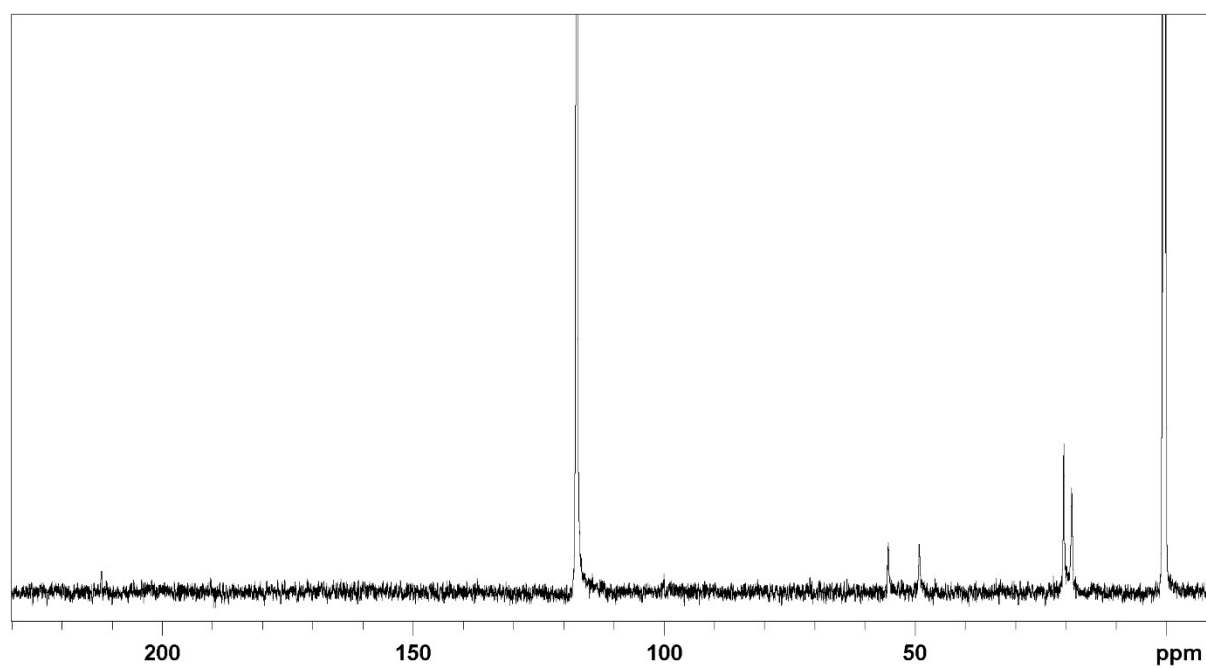


Figure S8: 150 MHz ^{13}C NMR spectrum of $\text{Na(dipdte)} \cdot 5\text{H}_2\text{O}$ in $\text{acetonitrile-}d_3$ acquired at 293 K.

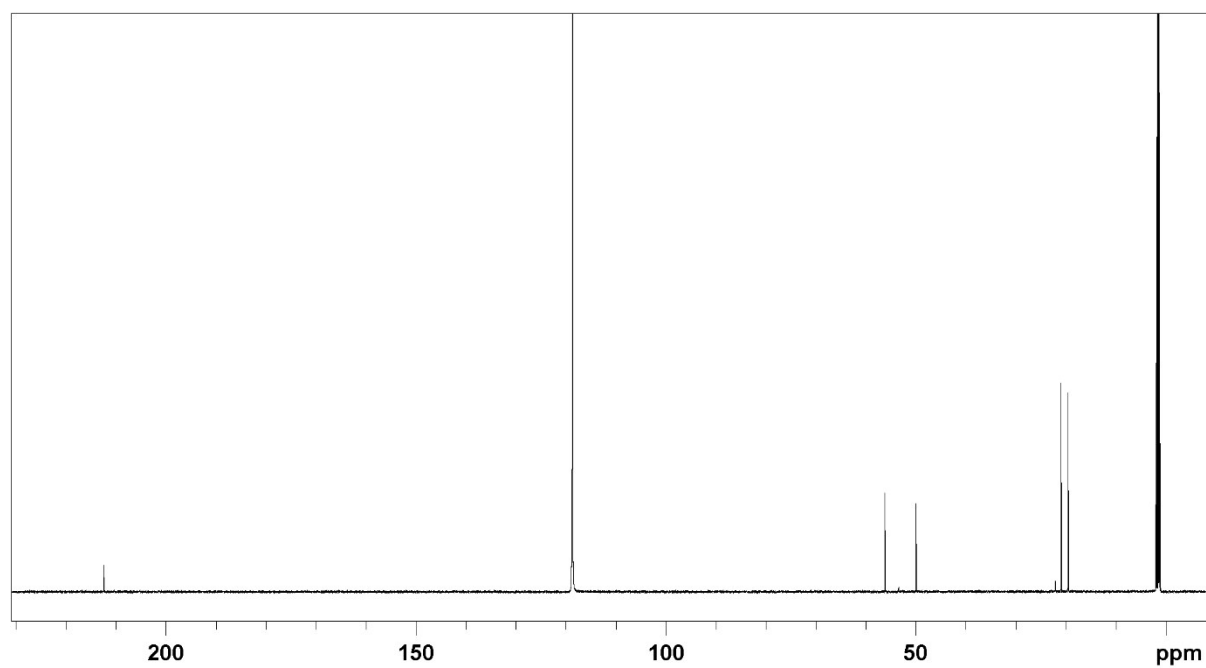


Figure S9: 150 MHz ^{13}C NMR spectrum of $\text{Na(dipdte)} \cdot 5\text{H}_2\text{O}$ in $\text{acetonitrile-}d_3$ acquired at 258 K.

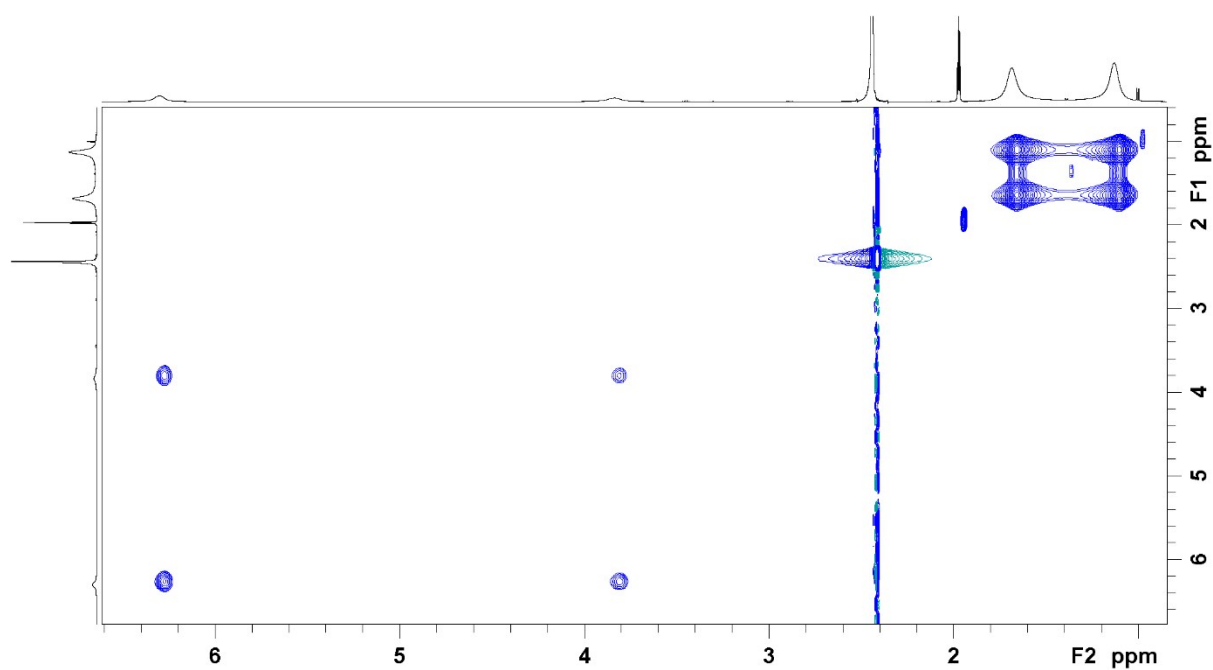


Figure S10: 600 MHz ^1H 2D-NOESY spectrum of $\text{Na}(\text{dipdte})\cdot 5\text{H}_2\text{O}$ in acetonitrile- d_3 acquired at 293 K with a mixing time of 100 ms.

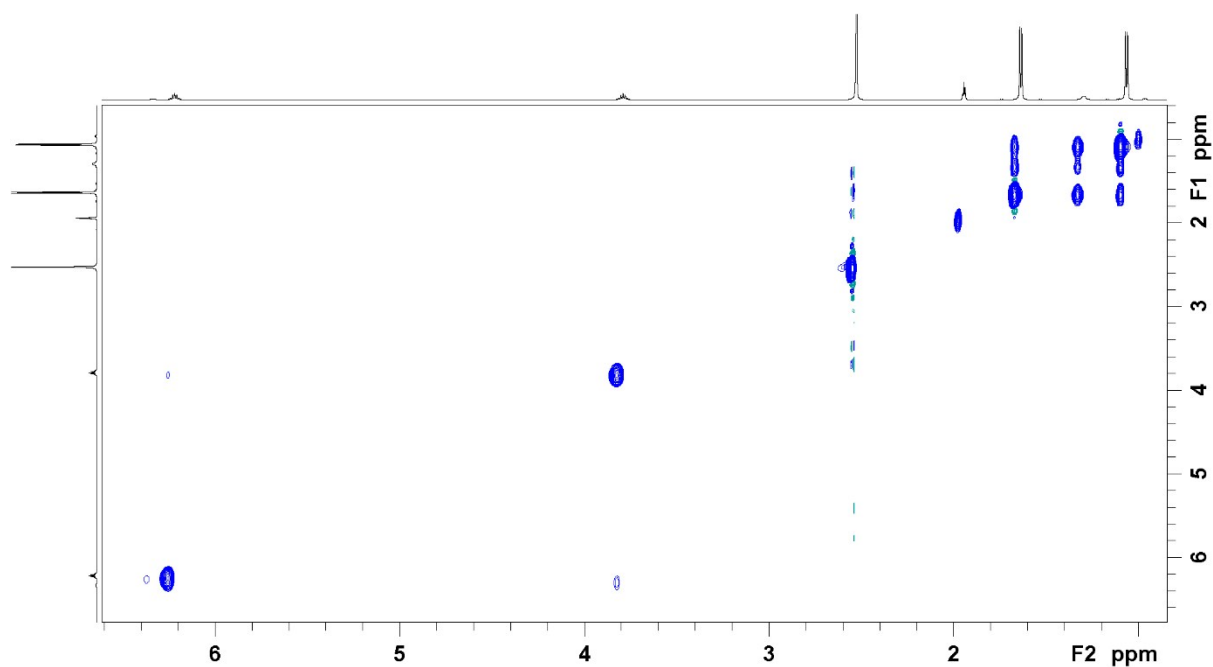


Figure S11: 600 MHz ^1H 2D-NOESY spectrum of $\text{Na}(\text{dipdte})\cdot 5\text{H}_2\text{O}$ in acetonitrile- d_3 acquired at 258 K with a mixing time of 100 ms.

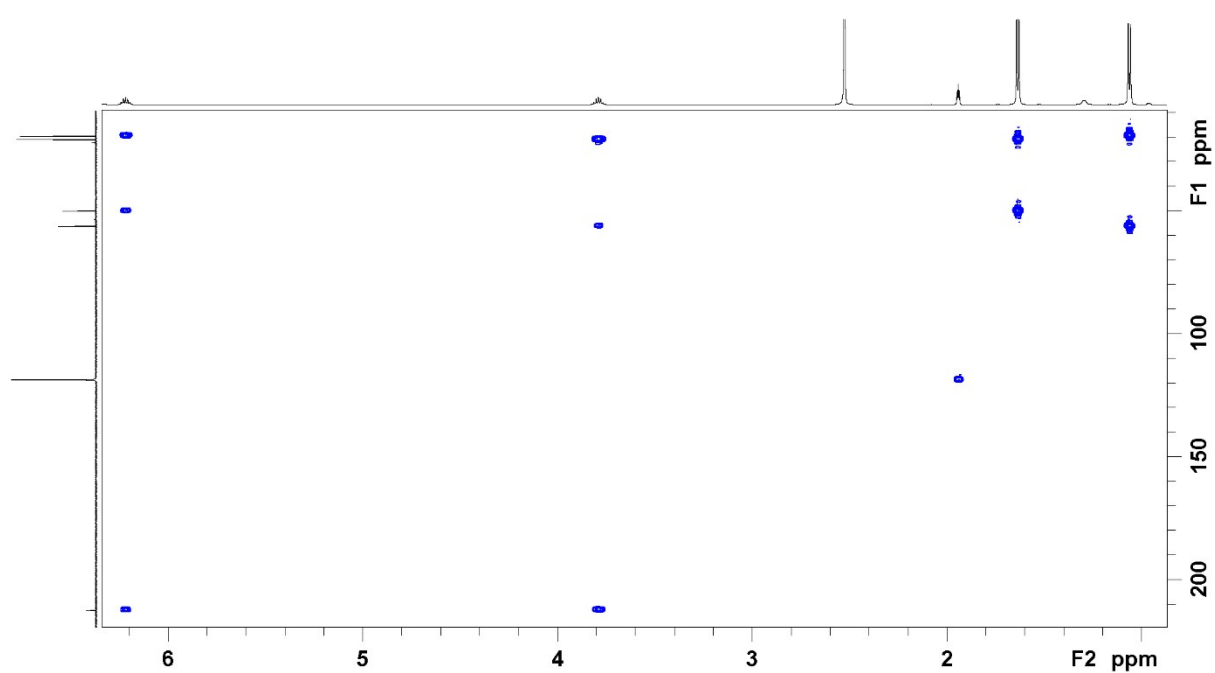


Figure S12: 600 MHz ^1H - ^{13}C HMBC spectrum of Na(dipdte)- $5\text{H}_2\text{O}$ in acetonitrile- d_3 acquired at 258 K.

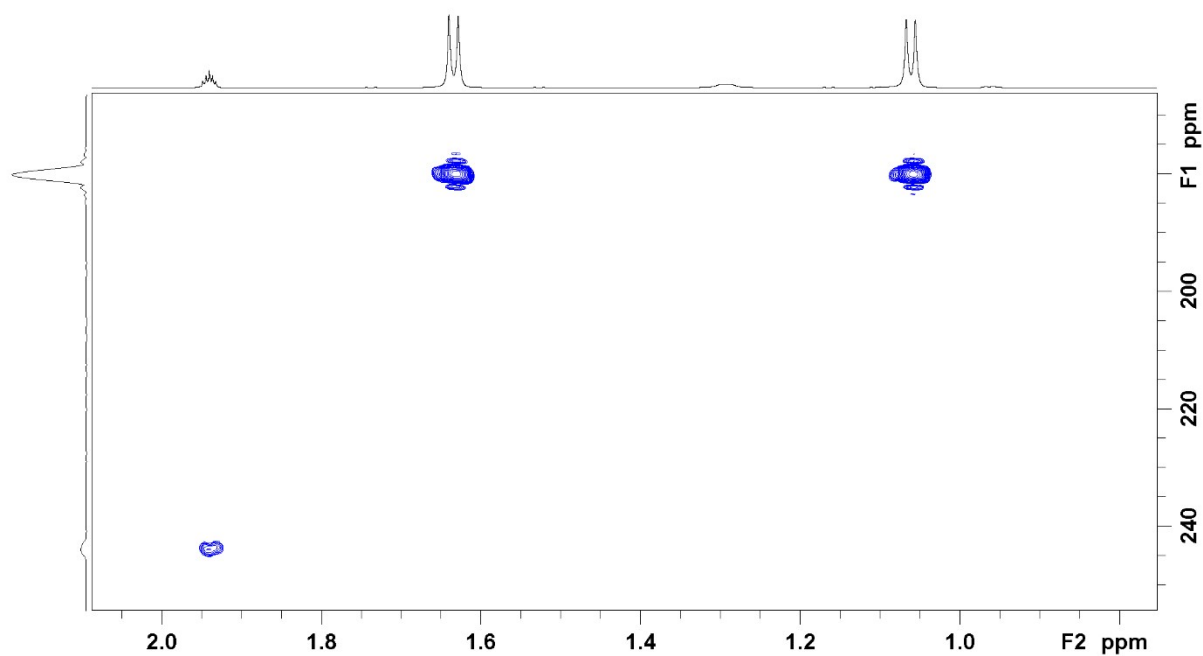


Figure S13. 600 MHz ^1H - ^{15}N HMBC spectrum of Na(dipdte)- $5\text{H}_2\text{O}$ in acetonitrile- d_3 acquired at 258 K.

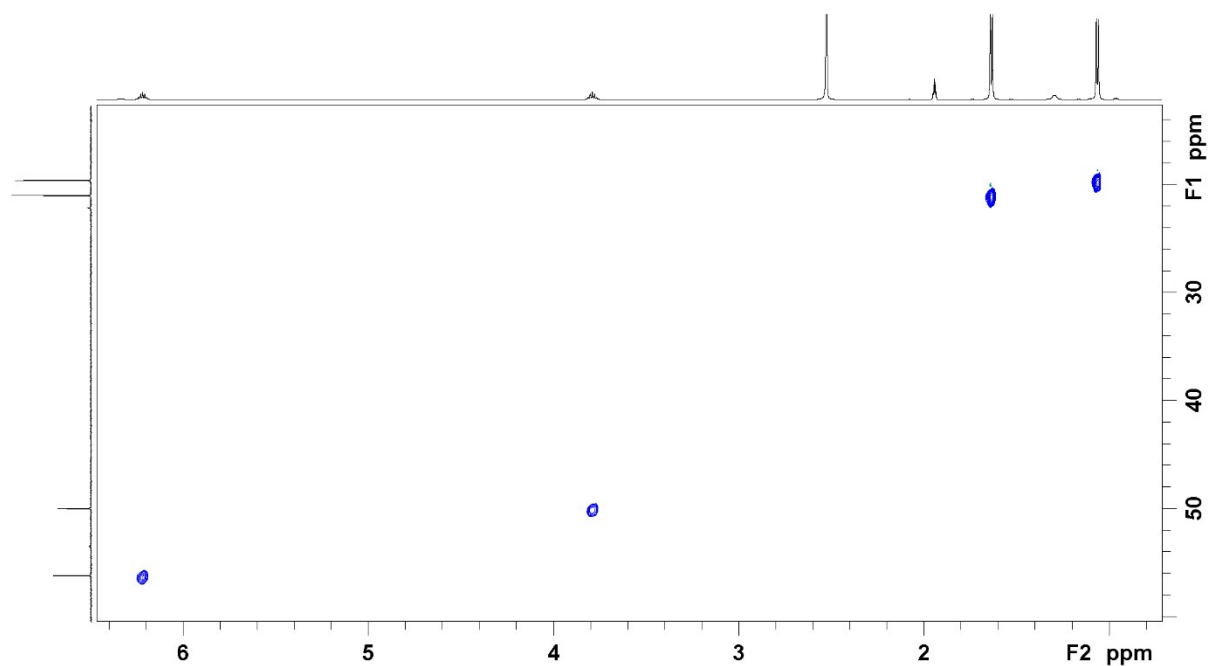


Figure S14: 600 MHz ^{13}C - ^1H HSQC spectrum of Na(dipdte) $\cdot$ 5H $_2$ O in acetonitrile- d_3 acquired at 258 K.

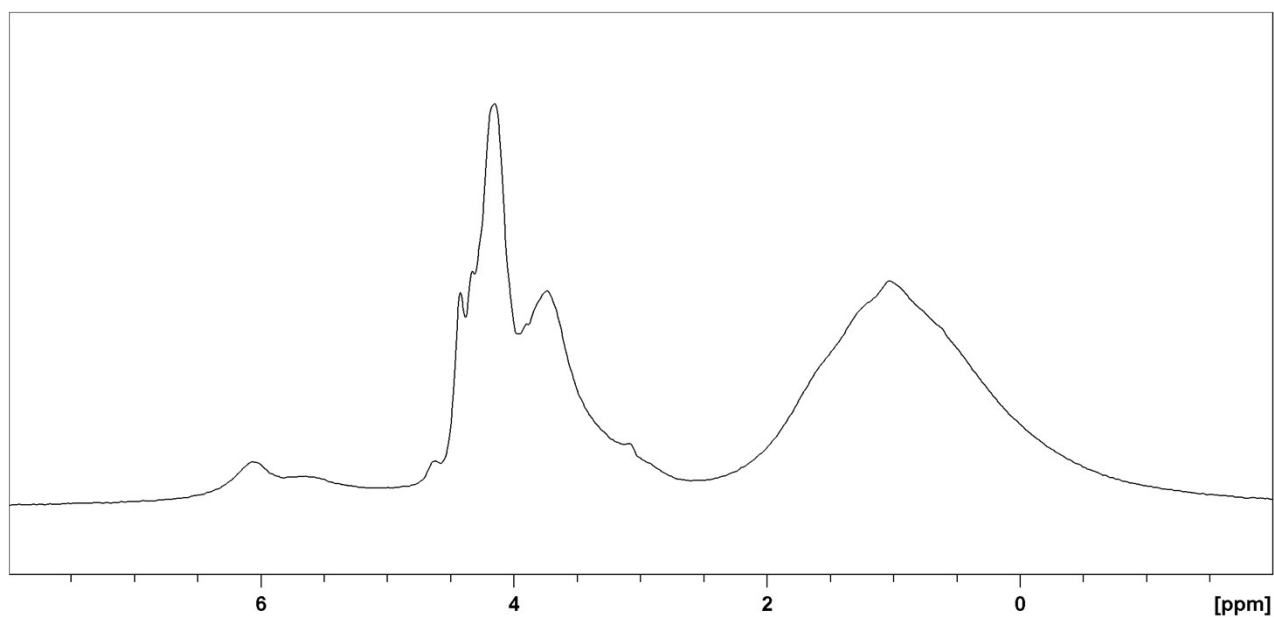


Figure S15: 700 MHz solid state ^1H NMR spectrum of Na(dipdte) $\cdot$ 5H $_2$ O acquired at 60 KHz MAS.

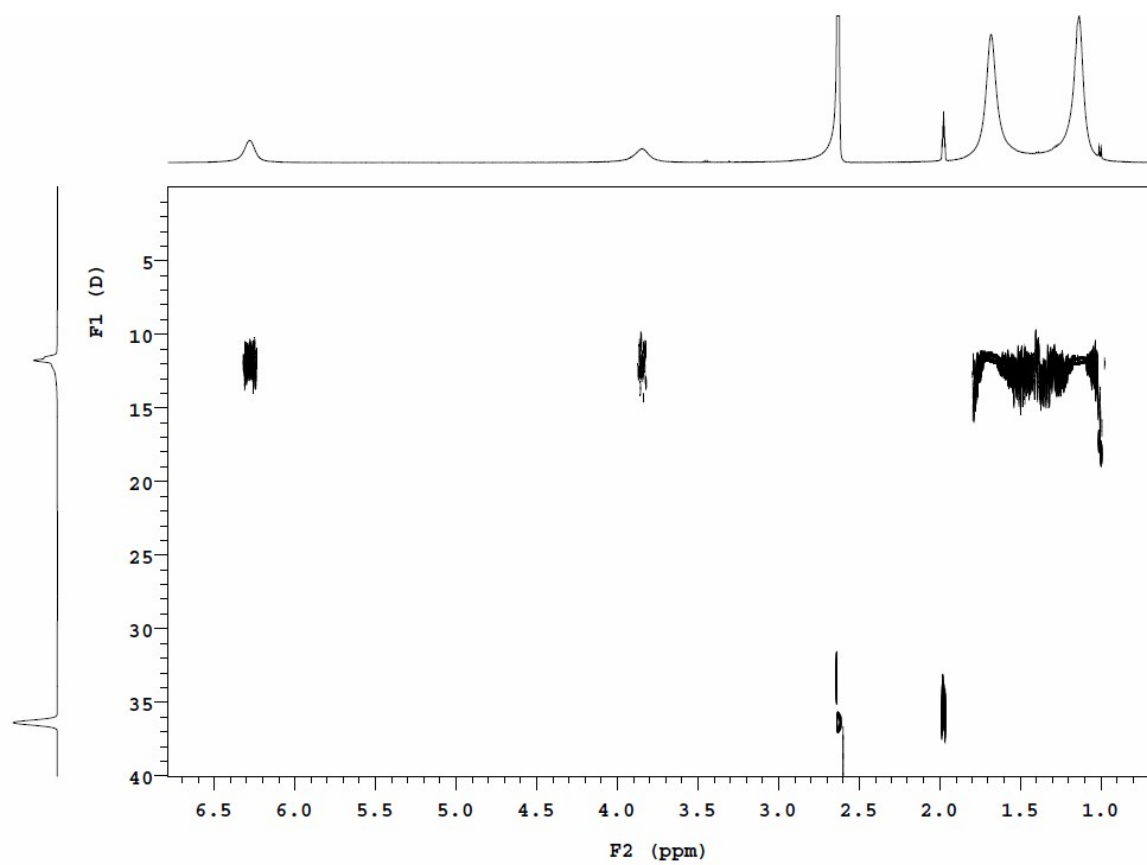


Figure S16: 500 MHz 2D-DOSY spectrum of Na(dipdte)·5H₂O in acetonitrile-*d*₃ at 293 K.