VT NMR Allows a Direct Observation of Carboxylate Shift in Zinc Carboxylate Complexes

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Table S1 - Crystal Data and Details of the Structure Determination for 1a
[Zn4(CH3COO)6(bdmap)2]

Crystal Data			
Chemical Formula of Asymmetric Unit	C13 H26 N2 O7 Zn2		
Empirical Formula	C26 H52 N4 O14 Zn4		
Formula Weight	906.28		
Crystal System	Monoclinic		
Space group	P21/c	(No. 14)	
a, b, c [Angstrom]	10.8650(10)	19.237(2)	10.0540(10)
alpha, beta, gamma [deg]	90	114.4420(10)	90
V [Ang**3]	1913.1(3)		
Z	4		
D(calc) [g/cm**3]	1.573		
F(000)	936		
Mu(MoKa) [/mm]	2.5		
Crystal Size [mm]	0.29 x	0.44 x	0.61
Data Collection			
Temperature (K)	293		
Radiation [Angstrom]	MoKa	0.71070	
Theta Min-Max [Deg]	2.1,	28.0	
Dataset	-14: 14 ; -25: 25 ; -13: 13		
Tot., Uniq. Data, R(int)	18518,	4610,	0.034
Observed data [I > 2.5 sigma(I)]	2502		
Refinement			
Refinement method	Full-matrix least-squares on F		
Nref, Npar	2487,	217	
R, wR, Goodness-of-fit [I > 2.5 sigma(I)]	0.061,	0.073,	0.991
R, wR, Goodness-of-fit (all data)	0.124,	0.184,	1.85
Max. and Av. Shift/Error	0.01,	0.00	
Min. and Max. resd. dens. [e/Ang^3]	-0.92,	0.94	

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for 1a [Zn4(CH3COO)6(bdmap)2]

Atom	x	y	z	U(eq) [Ang^2]
Zn1	0.71292(8)	0.56814(4)	0.59022(8)	0.0465(3)
Zn2	0.62581(8)	0.42328(4)	0.68565(8)	0.0421(3)
O1	0.6657(6)	0.5924(3)	0.7564(6)	0.0581(17)
O1'	0.5682(5)	0.6091(2)	0.4157(6)	0.0509(16)
O2	0.5939(6)	0.4931(3)	0.8155(6)	0.0544(17)
O3	0.8986(6)	0.5258(3)	0.6979(7)	0.0667(19)
O4	0.8386(5)	0.4382(3)	0.8017(6)	0.0612(17)
O5	0.6404(4)	0.4698(2)	0.5147(5)	0.0413(12)
O6	0.6892(9)	0.3655(3)	0.4615(9)	0.084(3)
N1'	0.6547(7)	0.3248(3)	0.7853(8)	0.055(2)
N2'	0.8163(8)	0.6639(4)	0.5720(10)	0.069(3)
C1	0.6194(7)	0.5566(4)	0.8300(7)	0.047(2)
C1'	0.5318(12)	0.2832(5)	0.6764(15)	0.085(4)
C2	0.5882(10)	0.5946(5)	0.9434(10)	0.066(3)
C2'	0.5891(9)	0.6764(4)	0.3780(9)	0.056(2)
C3	0.9248(8)	0.4746(4)	0.7823(8)	0.055(2)
C3'	0.7087(13)	0.7072(5)	0.494(2)	0.131(7)
C4	1.0718(10)	0.4564(7)	0.8664(11)	0.081(4)
C5	0.6869(7)	0.4273(4)	0.4451(8)	0.048(2)
C6	0.7394(10)	0.4612(6)	0.3428(10)	0.070(3)
C11'	0.7656(13)	0.2844(5)	0.7827(14)	0.086(4)
C12'	0.670(3)	0.3325(8)	0.9344(18)	0.150(11)
C21'	0.898(2)	0.6913(9)	0.722(2)	0.146(8)
C22'	0.9110(16)	0.6527(7)	0.509(2)	0.120(7)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S3 - Bond Distances (Angstrom) and Bond Angles (Degrees) for 1a [Zn4(CH3COO)6(bdmap)2]

Zn1	-O1	1.995(6)	C5	-C6	1.515(13)		
Zn1	-O1'	1.972(5)	C1'	-H11'	1.0453		
Zn1	-O3	2.024(7)	C1'	-H12'	1.0441		
Zn1	-O5	2.069(4)	C2	-H21	1.0240		
Zn1	-N2'	2.204(8)	C2	-H22	1.0468		
Zn2	-O2	2.001(6)	C2	-H23	1.0454		
Zn2	-O4	2.135(6)	C2'	-H21'	1.0449		
Zn2	-O5	2.001(5)	C3'	-H31'	1.0394		
Zn2	-N1'	2.105(6)	C3'	-H32'	1.0498		
Zn2	-O1'_a	2.023(6)	C4	-H41	1.0366		
O1	-C1	1.258(10)	C4	-H42	1.0360		
O1'	-C2'	1.394(9)	C4	-H43	1.0431		
O2	-C1	1.248(10)	C6	-H61	0.9137		
O3	-C3	1.254(10)	C6	-H62	1.0392		
O4	-C3	1.248(11)	C6	-H63	1.0409		
O5	-C5	1.306(9)	C11'	-H11'1	0.9503		
O6	-C5	1.199(10)	C11'	-H11'2	1.0372		
N1'	-C1'	1.553(15)	C11'	-H11'3	1.0612		
N1'	-C11'	1.443(16)	C12'	-H12'1	0.9435		
N1'	-C12'	1.45(2)	C12'	-H12'2	1.0707		
N2'	-C3'	1.385(17)	C12'	-H12'3	1.0457		
N2'	-C21'	1.49(2)	C21'	-H21'1	0.8990		
N2'	-C22'	1.43(2)	C21'	-H21'2	1.0604		
C1	-C2	1.506(12)	C21'	-H21'3	1.0403		
C1'	-C2'_a	1.426(16)	C22'	-H22'1	1.0227		
C2'	-C3'	1.465(19)	C22'	-H22'2	1.0566		
C3	-C4	1.507(14)	C22'	-H22'3	1.0457		

O1	-Zn1	-O1'	105.4(2)	Zn1	-O5	-C5	126.6(5)
O1	-Zn1	-O3	101.0(3)	Zn2	-O5	-C5	111.5(4)
O1	-Zn1	-O5	109.3(2)	Zn2	-N1'	-C1'	102.3(6)
O1	-Zn1	-N2'	101.0(3)	Zn2	-N1'	-C11'	115.9(6)

O1'	-Zn1	-O3	152.6(3)	Zn2	-N1'	-C12'	109.4(7)
O1'	-Zn1	-O5	89.80(18)	C1'	-N1'	-C11'	101.0(8)
O1'	-Zn1	-N2'	80.7(3)	C1'	-N1'	-C12'	118.7(14)
O3	-Zn1	-O5	88.4(2)	C11'	-N1'	-C12'	109.6(13)
O3	-Zn1	-N2'	87.2(3)	Zn1	-N2'	-C3'	102.1(7)
O5	-Zn1	-N2'	149.7(3)	Zn1	-N2'	-C21'	108.7(9)
O2	-Zn2	-O4	89.7(2)	Zn1	-N2'	-C22'	113.3(7)
O2	-Zn2	-O5	110.9(2)	C3'	-N2'	-C21'	111.7(11)
O2	-Zn2	-N1'	109.0(3)	C3'	-N2'	-C22'	115.7(12)
O1'_a	-Zn2	-O2	96.3(2)	C21'	-N2'	-C22'	105.3(13)
O4	-Zn2	-O5	87.5(2)	O1	-C1	-O2	126.2(7)
O4	-Zn2	-N1'	86.9(3)	O1	-C1	-C2	116.7(7)
O1'_a	-Zn2	-O4	169.7(2)	O2	-C1	-C2	117.1(7)
O5	-Zn2	-N1'	139.6(2)	N1'	-C1'	-C2'_a	112.1(8)
O1'_a	-Zn2	-O5	98.1(2)	O1'	-C2'	-C3'	110.5(8)
O1'_a	-Zn2	-N1'	83.2(3)	O1'	-C2'	-C1'_a	112.5(9)
Zn1	-O1	-C1	131.9(5)	C1'_a	-C2'	-C3'	117.2(9)
Zn1	-O1'	-C2'	117.0(5)	O3	-C3	-O4	124.9(8)
Zn1	-O1'	-Zn2_a	127.3(2)	O3	-C3	-C4	117.0(9)
Zn2_a	-O1'	-C2'	113.7(5)	O4	-C3	-C4	118.1(8)
Zn2	-O2	-C1	130.0(6)	N2'	-C3'	-C2'	118.1(8)
Zn1	-O3	-C3	125.1(6)	O5	-C5	-O6	122.5(8)
Zn2	-O4	-C3	134.7(5)	O5	-C5	-C6	115.6(7)
Zn1	-O5	-Zn2	104.3(2)	O6	-C5	-C6	121.9(9)
N1'	-C1'	-H11'	108.98	H61	-C6	-H62	110.80
N1'	-C1'	-H12'	108.91	H61	-C6	-H63	110.65
H11'	-C1'	-H12'	108.73	H62	-C6	-H63	109.47
C2'_a	-C1'	-H11'	108.88	N1'	-C11'	-H11'1	104.94
C2'_a	-C1'	-H12'	109.18	N1'	-C11'	-H11'2	111.91
C1	-C2	-H21	108.96	N1'	-C11'	-H11'3	110.20
C1	-C2	-H22	109.08	H11'1	-C11'	-H11'2	111.88
C1	-C2	-H23	109.16	H11'1	-C11'	-H11'3	109.84
H21	-C2	-H22	110.49	H11'2	-C11'	-H11'3	108.06
H21	-C2	-H23	110.61	N1'	-C12'	-H12'1	117.33
H22	-C2	-H23	108.52	N1'	-C12'	-H12'2	105.59
O1'	-C2'	-H21'	105.13	N1'	-C12'	-H12'3	107.17
C3'	-C2'	-H21'	105.15	H12'1	-C12'	-H12'2	108.68
C1'_a	-C2'	-H21'	105.17	H12'1	-C12'	-H12'3	110.78
N2'	-C3'	-H31'	107.85	H12'2	-C12'	-H12'3	106.71
N2'	-C3'	-H32'	107.25	N2'	-C21'	-H21'1	111.94
C2'	-C3'	-H31'	107.45	N2'	-C21'	-H21'2	107.76
C2'	-C3'	-H32'	107.19	N2'	-C21'	-H22'3	109.38
H31'	-C3'	-H32'	108.76	H21'1	-C21'	-H21'2	107.93
C3	-C4	-H41	107.43	H21'1	-C21'	-H22'3	108.52
C3	-C4	-H42	107.47	H21'2	-C21'	-H22'3	111.34
C3	-C4	-H43	116.86	N2'	-C22'	-H21'3	102.90
H41	-C4	-H42	110.04	N2'	-C22'	-H22'1	111.08
H41	-C4	-H43	107.46	N2'	-C22'	-H22'2	111.39
H42	-C4	-H43	107.50	H21'3	-C22'	-H22'1	111.42
C5	-C6	-H61	105.36	H21'	-C22'	-H22'2	112.31
C5	-C6	-H62	110.38	H22'1	-C22'	-H22'2	107.76
C5	-C6	-H63	110.12				

Table S4 - Interesting Distances(Angstrom)for 1a [Zn4(CH3COO)6(bdmap)2]

Zn1	-O2	3.363(6)	Zn1	-O4	3.199(6)
Zn2	-O1	3.320(6)	Zn2	-O3	3.520(7)
Zn2	-O6	2.841(9)	Zn1	-Zn2	3.215(1)

Table S5 - (An)isotropic Displacement Parameters for 1a [Zn4(CH3COO)6(bdmap)2]

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Zn1	0.0495(5)	0.0458(4)	0.0444(4)	0.0025(3)	0.0197(3)	-0.0043(3)
Zn2	0.0509(5)	0.0390(4)	0.0395(4)	0.0029(3)	0.0219(3)	0.0022(3)
O1	0.068(3)	0.059(3)	0.050(3)	-0.003(2)	0.027(3)	0.003(2)
O1'	0.058(3)	0.041(2)	0.052(3)	0.006(2)	0.021(2)	-0.009(2)
O2	0.065(3)	0.053(3)	0.052(3)	-0.008(2)	0.031(2)	0.000(2)
O3	0.046(3)	0.073(3)	0.070(4)	0.019(3)	0.013(3)	-0.002(3)
O4	0.048(3)	0.075(3)	0.052(3)	0.014(3)	0.012(2)	0.000(2)
O5	0.045(2)	0.042(2)	0.041(2)	-0.0005(18)	0.022(2)	0.0011(18)
O6	0.128(6)	0.053(3)	0.100(5)	-0.006(3)	0.075(5)	0.015(4)
N1'	0.058(4)	0.048(3)	0.068(4)	0.017(3)	0.034(3)	0.014(3)
N2'	0.060(4)	0.056(4)	0.091(5)	-0.005(4)	0.032(4)	-0.014(3)
C1	0.045(4)	0.056(4)	0.038(3)	-0.003(3)	0.014(3)	0.005(3)
C1'	0.083(7)	0.059(5)	0.122(9)	0.013(5)	0.050(7)	0.008(5)
C2	0.071(5)	0.066(5)	0.064(5)	-0.014(4)	0.031(4)	0.010(4)
C2'	0.068(5)	0.043(3)	0.057(4)	0.009(3)	0.025(4)	-0.010(3)
C3	0.049(4)	0.064(4)	0.048(4)	-0.005(3)	0.017(3)	0.004(3)
C3'	0.080(7)	0.048(5)	0.26(2)	0.046(8)	0.065(10)	0.000(5)
C4	0.054(5)	0.123(8)	0.059(5)	0.020(5)	0.015(4)	0.015(5)
C5	0.052(4)	0.050(4)	0.046(3)	-0.001(3)	0.025(3)	0.009(3)
C6	0.071(5)	0.099(7)	0.056(5)	-0.001(4)	0.043(4)	0.002(5)
C11'	0.111(8)	0.058(5)	0.104(8)	0.020(5)	0.060(7)	0.034(5)
C12'	0.31(3)	0.100(9)	0.099(9)	0.045(8)	0.071(13)	-0.083(12)
C22'	0.111(9)	0.091(8)	0.212(17)	0.045(9)	0.122(11)	0.012(7)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms.
Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Translation of Symmetry Code to Equiv.Pos

a =[3666.00] = 1-x,1-y,1-z
b =[3767.00] = 2-x,1-y,2-z
c =[4554.00] = x,1/2-y,-1/2+z
d =[3667.00] = 1-x,1-y,2-z
e =[4564.00] = x,3/2-y,-1/2+z
f =[3766.00] = 2-x,1-y,1-z
g =[4555.00] = x,1/2-y,1/2+z
h =[4565.00] = x,3/2-y,1/2+z

Table S6 - Crystal Data and Details of the Structure Determination for 2a [Zn4(CH3CH2COO)6(bdmap)2]

Crystal Data			
Chemical Formula of Asymmetric Unit			C16 H32 N2 O7 Zn2
Empirical Formula			C32 H64 N4 O14 Zn4
Formula Weight			990.43
Crystal System			Monoclinic
Space group		P21/c	(No. 14)
a, b, c [Angstrom]	11.647(7)	10.178(2)	19.630(10)
alpha, beta, gamma [deg]	90	106.97(5)	90
V [Ang**3]			2225.7(19)
Z			4
D(calc) [g/cm**3]			1.478
F(000)			1032
Mu(MoKa) [/mm]			2.2
Crystal Size [mm]		0.17 x 0.23 x 0.27	
Data Collection			
Temperature (K)			293
Radiation [Angstrom]		MoKa	0.71070
Theta Min-Max [Deg]			1.8, 27.9
Dataset		-3: 15 ; -13: 13 ; -25: 24	
Tot., Uniq. Data, R(int)		12749, 5293, 0.045	
Observed data [I > 2.5 sigma(I)]			1709
Refinement			
Refinement method		Full-matrix least-squares on F	
Nref, Npar			1708, 244
R, wR, Goodness-of-fit [I > 2.5 sigma(I)]		0.0420, 0.047, 0.95	
R, wR, Goodness-of-fit (all data)		0.2, 0.268, 2.998	
Max. and Av. Shift/Error			0.003, 0.0002
Min. and Max. resd. dens. [e/Ang^3]			-2.21, 1.26

Table S7 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for 2a [Zn4(CH3CH2COO)6(bdmap)2]

Atom	x	y	z	U(eq) [Ang^2]
Zn1	0.19199(9)	0.08045(11)	0.48477(5)	0.0488(3)
Zn2	0.12082(9)	-0.07031(11)	0.61292(5)	0.0473(3)
O1	0.2329(6)	-0.1074(6)	0.4782(3)	0.063(3)
O1'	0.0513(5)	0.1292(5)	0.4039(3)	0.0504(19)
O2	0.1804(6)	-0.2158(6)	0.5642(3)	0.062(3)
O3	0.3317(6)	0.1436(7)	0.5663(3)	0.069(2)
O4	0.3103(6)	0.0017(8)	0.6485(3)	0.073(3)
O5	0.0857(5)	0.0926(5)	0.5539(2)	0.0436(17)
O6	0.0710(7)	0.1817(6)	0.6536(3)	0.073(3)
N1'	0.1392(7)	-0.1290(7)	0.7196(3)	0.052(3)
N2'	0.2876(7)	0.1603(7)	0.4124(4)	0.058(3)
C1	0.2305(8)	-0.2055(9)	0.5161(5)	0.054(3)
C1'	0.0150(9)	-0.1184(9)	0.7234(4)	0.061(4)
C2	0.3548(15)	-0.4076(16)	0.5639(10)	0.138(8)
C2'	0.0760(8)	0.1739(8)	0.3415(4)	0.050(3)
C3	0.3612(8)	0.0953(11)	0.6290(5)	0.060(4)
C3'	0.2004(10)	0.1349(9)	0.3417(5)	0.062(3)
C4	0.4388(17)	0.264(3)	0.7177(14)	0.209(13)
C5	0.0776(8)	0.1952(8)	0.5929(4)	0.049(3)
C6	0.0641(13)	0.4394(10)	0.6029(6)	0.093(5)
C11'	0.1843(10)	-0.2655(10)	0.7306(6)	0.077(4)
C12	0.2969(12)	-0.3284(10)	0.5015(7)	0.090(5)
C12'	0.2172(11)	-0.0424(10)	0.7748(5)	0.076(4)
C21'	0.4015(10)	0.0906(12)	0.4192(6)	0.085(4)
C22'	0.3110(9)	0.3018(10)	0.4257(6)	0.071(4)
C34	0.4638(11)	0.1624(14)	0.6819(6)	0.095(5)
C56	0.0804(9)	0.3267(8)	0.5585(5)	0.058(3)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S8 - Bond Distances (Angstrom) and Bond Angles (Degrees) for 2a [Zn4(CH3CH2COO)6(bdmap)2]

Zn1	-O1	1.984(6)	C4	-C34	1.33(3)
Zn1	-O1'	1.983(6)	C5	-C56	1.504(12)
Zn1	-O3	2.025(7)	C6	-C56	1.486(14)
Zn1	-O5	2.090(5)	C1'	-H11'	1.0584
Zn1	-N2'	2.200(8)	C1'	-H12'	1.0533
Zn2	-O2	1.994(6)	C2	-H21	1.0550
Zn2	-O4	2.235(7)	C2	-H22	1.0493
Zn2	-O5	1.996(5)	C2	-H23	1.0427
Zn2	-N1'	2.128(6)	C2'	-H21'	1.0498
Zn2	-O1'_a	2.025(6)	C3'	-H31'	1.0544
O1	-C1	1.250(11)	C3'	-H32'	1.0465
O1'	-C2'	1.413(10)	C4	-H41	1.0574
O2	-C1	1.251(12)	C4	-H42	1.0499
O3	-C3	1.276(11)	C4	-H43	1.0520
O4	-C3	1.240(13)	C6	-H61	0.9866
O5	-C5	1.314(9)	C6	-H62	1.0508
O6	-C5	1.224(10)	C6	-H63	1.0453
N1'	-C1'	1.474(14)	C11'	-H11'1	1.0429
N1'	-C11'	1.479(13)	C11'	-H11'2	1.0434
N1'	-C12'	1.484(12)	C11'	-H11'3	1.0537
N2'	-C3'	1.484(13)	C12	-H121	1.0571
N2'	-C21'	1.476(15)	C12	-H122	1.0421
N2'	-C22'	1.475(13)	C12'	-H12'1	1.0468
C1	-C12	1.541(15)	C12'	-H12'2	1.0370
C1'	-C2'_a	1.509(12)	C12'	-H12'3	1.0506
C2	-C12	1.46(2)	C21'	-H21'1	1.0621
C2'	-C3'	1.501(15)	C21'	-H21'2	1.0452
C3	-C34	1.499(16)	C21'	-H21'3	1.0412
C22'	-H22'1	1.0268	C34	-H342	1.0661
C22'	-H22'2	0.9749	C56	-H561	1.0554
C22'	-H22'3	1.0527	C56	-H562	1.0393
C34	-H341	1.0636			

O1	-Zn1	-O1'	110.3(2)	Zn1	-O5	-C5	125.6(5)
O1	-Zn1	-O3	101.8(3)	Zn2	-O5	-C5	111.1(4)
O1	-Zn1	-O5	107.4(2)	Zn2	-N1'	-C1'	102.2(5)
O1	-Zn1	-N2'	97.9(3)	Zn2	-N1'	-C11'	109.7(6)
O1'	-Zn1	-O3	147.0(3)	Zn2	-N1'	-C12'	114.6(6)
O1'	-Zn1	-O5	89.8(2)	C1'	-N1'	-C11'	111.9(8)
O1'	-Zn1	-N2'	81.2(3)	C1'	-N1'	-C12'	108.7(7)
O3	-Zn1	-O5	87.7(2)	C11'	-N1'	-C12'	109.6(8)
O3	-Zn1	-N2'	87.2(3)	Zn1	-N2'	-C3'	101.7(6)
O5	-Zn1	-N2'	154.7(2)	Zn1	-N2'	-C21'	112.0(6)
O2	-Zn2	-O4	86.7(3)	Zn1	-N2'	-C22'	110.4(6)
O2	-Zn2	-O5	112.3(2)	C3'	-N2'	-C21'	110.7(8)
O2	-Zn2	-N1'	108.3(3)	C3'	-N2'	-C22'	112.1(7)
O1'_a	-Zn2	-O2	99.7(3)	C21'	-N2'	-C22'	109.8(8)
O4	-Zn2	-O5	85.7(3)	O1	-C1	-O2	127.8(9)
O4	-Zn2	-N1'	88.7(3)	O1	-C1	-C12	116.0(9)
O1'_a	-Zn2	-O4	171.2(2)	O2	-C1	-C12	116.3(9)
O5	-Zn2	-N1'	138.5(2)	N1'	-C1'	-C2'_a	112.8(7)
O1'_a	-Zn2	-O5	97.2(2)	O1'	-C2'	-C3'	110.7(7)
O1'_a	-Zn2	-N1'	83.6(3)	O1'	-C2'	-C1'_a	109.9(7)
Zn1	-O1	-C1	133.1(6)	C1'_a	-C2'	-C3'	110.0(7)
Zn1	-O1'	-C2'	116.4(5)	O3	-C3	-O4	125.1(9)
Zn1	-O1'	-Zn2_a	127.1(3)	O3	-C3	-C34	115.4(9)
Zn2_a	-O1'	-C2'	113.4(5)	O4	-C3	-C34	119.5(9)
Zn2	-O2	-C1	127.2(6)	N2'	-C3'	-C2'	110.7(8)
Zn1	-O3	-C3	124.6(7)	O5	-C5	-O6	120.9(7)
Zn2	-O4	-C3	132.3(6)	O5	-C5	-C56	115.5(7)
Zn1	-O5	-Zn2	105.5(3)	O6	-C5	-C56	123.6(8)
C1	-C12	-C2	115.3(12)	C56	-C6	-H61	115.39
C3	-C34	-C4	117.8(14)	C56	-C6	-H62	108.96
C5	-C56	-C6	113.6(8)	C56	-C6	-H63	109.60
N1'	-C1'	-H11'	109.15	H61	-C6	-H62	106.99
N1'	-C1'	-H12'	109.79	H61	-C6	-H63	107.42
H11'	-C1'	-H12'	107.07	H62	-C6	-H63	108.24
C2'_a	-C1'	-H11'	108.97	N1'	-C11'	-H11'1	109.68
C2'_a	-C1'	-H12'	108.88	N1'	-C11'	-H11'2	110.25
C12	-C2	-H21	108.52	N1'	-C11'	-H11'3	112.75
C12	-C2	-H22	109.50	H11'1	-C11'	-H11'2	108.97
C12	-C2	-H23	116.42	H11'1	-C11'	-H11'3	107.56
H21	-C2	-H22	107.63	H11'2	-C11'	-H11'3	107.52
H21	-C2	-H23	107.00	C1	-C12	-H121	108.45
H22	-C2	-H23	107.44	C1	-C12	-H122	109.15
O1'	-C2'	-H21'	106.38	C2	-C12	-H121	107.30
C3'	-C2'	-H21'	109.83	C2	-C12	-H122	108.44
C1'_a	-C2'	-H21'	109.90	H121	-C12	-H122	108.00
N2'	-C3'	-H31'	109.24	N1'	-C12'	-H12'1	110.66
N2'	-C3'	-H32'	109.80	N1'	-C12'	-H12'2	110.79
C2'	-C3'	-H31'	109.56	N1'	-C12'	-H12'3	108.35
C2'	-C3'	-H32'	109.66	H12'1	-C12'	-H12'2	109.18
H31'	-C3'	-H32'	107.87	H12'1	-C12'	-H12'3	108.54
C34	-C4	-H41	108.05	H12'2	-C12'	-H12'3	109.28
C34	-C4	-H42	109.87	N2'	-C21'	-H21'1	109.97
C34	-C4	-H43	119.11	N2'	-C21'	-H21'2	111.07
H41	-C4	-H42	107.40	N2'	-C21'	-H21'3	111.95
H41	-C4	-H43	105.64	H21'1	-C21'	-H21'2	107.39
H42	-C4	-H43	106.18	H21'1	-C21'	-H21'3	107.50
H21'2	-C21'	-H21'3	108.79	C4	-C34	-H341	121.60
N2'	-C22'	-H22'1	106.38	C4	-C34	-H342	101.29
N2'	-C22'	-H22'2	114.08	H341	-C34	-H342	100.50
N2'	-C22'	-H22'3	113.03	C5	-C56	-H561	108.66
H22'1	-C22'	-H22'2	112.87	C5	-C56	-H562	109.44
H22'1	-C22'	-H22'3	109.05	C6	-C56	-H561	107.74
H22'2	-C22'	-H22'3	101.47	C6	-C56	-H562	108.93
C3	-C34	-H341	108.96	H561	-C56	-H562	108.33
C3	-C34	-H342	102.59				

Table S9 - Interesting Distances(Angstrom)for 2a [Zn4(CH3CH2COO)6(bdmap)2]

Zn1	-O2	3.415(6)	Zn1	-O4	3.207(6)
Zn2	-O1	3.295(7)	Zn2	-O3	3.595(7)
Zn2	-O6	2.797(7)	Zn1	-Zn2	3.254(2)

Table S10 - Anisotropic Displacement Parameters for 2a [Zn4(CH3CH2COO)6(bdmap)2]

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Zn1	0.0631(7)	0.0454(6)	0.0427(5)	0.0014(5)	0.0231(5)	-0.0006(6)
Zn2	0.0637(7)	0.0403(5)	0.0428(5)	0.0020(5)	0.0231(5)	0.0017(6)
O1	0.093(5)	0.044(4)	0.061(4)	0.002(3)	0.037(4)	0.007(3)
O1'	0.066(4)	0.053(3)	0.039(3)	0.005(2)	0.026(3)	0.002(3)
O2	0.085(5)	0.041(4)	0.072(4)	-0.004(3)	0.042(4)	0.009(3)
O3	0.064(4)	0.080(4)	0.062(4)	-0.001(4)	0.017(3)	-0.016(4)
O4	0.070(5)	0.079(5)	0.064(4)	0.012(4)	0.009(4)	-0.008(4)
O5	0.060(3)	0.036(3)	0.039(3)	-0.002(2)	0.021(3)	-0.001(3)
O6	0.138(6)	0.043(3)	0.056(4)	-0.004(3)	0.055(4)	-0.007(4)
N1'	0.068(5)	0.044(4)	0.041(4)	0.003(3)	0.013(4)	-0.007(4)
N2'	0.064(5)	0.056(5)	0.062(5)	0.004(4)	0.032(4)	-0.003(4)
C1	0.049(6)	0.049(6)	0.068(6)	-0.013(5)	0.023(5)	-0.002(5)
C1'	0.090(8)	0.056(6)	0.044(5)	0.005(4)	0.030(5)	-0.009(5)
C2	0.145(14)	0.099(11)	0.185(16)	0.014(12)	0.073(12)	0.018(11)
C2'	0.070(6)	0.039(4)	0.044(4)	0.001(4)	0.023(4)	-0.007(4)
C3	0.053(6)	0.078(8)	0.045(5)	-0.003(5)	0.007(4)	0.001(5)
C3'	0.087(7)	0.059(6)	0.055(5)	0.001(4)	0.043(5)	-0.003(5)
C4	0.122(14)	0.26(3)	0.24(2)	-0.16(2)	0.043(14)	-0.042(16)
C5	0.073(6)	0.037(5)	0.044(5)	-0.004(4)	0.029(5)	0.000(4)
C6	0.165(11)	0.041(5)	0.083(7)	0.008(5)	0.052(7)	0.008(7)
C11'	0.093(8)	0.059(6)	0.073(6)	0.009(5)	0.014(6)	0.002(6)
C12	0.127(10)	0.045(6)	0.116(10)	0.000(6)	0.063(9)	0.012(7)
C12'	0.106(8)	0.070(7)	0.049(5)	-0.007(5)	0.016(5)	-0.028(6)
C21'	0.076(7)	0.090(8)	0.104(8)	0.019(7)	0.049(6)	0.021(7)
C22'	0.073(7)	0.055(6)	0.084(7)	0.005(5)	0.021(6)	-0.005(5)
C34	0.072(8)	0.124(11)	0.077(7)	-0.033(7)	0.004(6)	-0.011(8)
C56	0.089(7)	0.033(4)	0.055(5)	0.003(4)	0.025(5)	0.000(5)

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms.
Astar(i) are Reciprocal Axial Lengths and h(i)are the Reflection Indices.

Translation of Symmetry Code to Equiv.Pos

a =[3556.00] = -x,-y,1-z
b =[2556.00] = -x,1/2+y,3/2-z
c =[1565.00] = x,1+y,z
d =[3656.00] = 1-x,-y,1-z
e =[4545.00] = x,-1/2-y,1/2+z
f =[1545.00] = x,-1+y,z
g =[2546.00] = -x,-1/2+y,3/2-z
h =[4554.00] = x,1/2-y,-1/2+z
i =[4544.00] = x,-1/2-y,-1/2+z
j =[4555.00] = x,1/2-y,1/2+z
k =[3566.00] = -x,1-y,1-z

Table S11 - Crystal Data and Details of the Structure Determination
for 1-catena [Zn4(CH3COO)6(bdmap)2]n.2CD2Cl2

Crystal Data			
Chemical Formula of Asymmetric Unit		C14 H26 D2 N2 O7 Cl2 Zn2	
Formula Weight			540.05
Crystal System			Monoclinic
Space group		P21/n	(No. 14)
a, b, c [Angstrom]	10.7671(2)	13.4855(3)	15.5292(4)
alpha, beta, gamma [deg]	90	90.7610(10)	90
V [Ang**3]			2254.64(9)
Z			4
D(obs), D(calc) [g/cm**3]			1.591
F(000)			1104
Mu(MoKa) [/mm]			2.4
Crystal Size [mm]		0.10 x 0.15 x 0.30	
Data Collection			
Temperature (K)			200
Radiation [Angstrom]		MoKa	0.71073
Theta Min-Max [Deg]			2.0, 27.5
Dataset		-13: 13 ; -17: 17 ; -20: 20	
Tot., Uniq. Data, R(int)		9663, 5130, 0.030	
Observed data [I > 2.0 sigma(I)]			3879
Refinement			
Nref, Npar			5130, 367
R, wR, S		0.0398, 0.0987, 1.04	
w = 1/[^2^(FO^2^)+(0.0395P)^2^+2.5944P] WHERE P=(FO^2^+2FC^2^)/3'			
Max. and Av. Shift/Error			0.01, 0.00
Min. and Max. resd. dens. [e/Ang^3]			-0.49, 0.61

Table S12 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for 1-catena [Zn4(CH3COO)6(bdmap)2]n 2CD2Cl2

Atom	x	y	z	U(eq) [Ang^2]
Zn1	0.19396(3)	0.89467(2)	0.21425(2)	0.0283(1)
Zn2	0.19693(3)	0.62920(2)	0.21857(2)	0.0297(1)
O1	0.2150(2)	0.90281(16)	0.34371(14)	0.0392(7)
O1'	0.11648(18)	0.75987(13)	0.20703(14)	0.0317(6)
O2	0.2665(2)	1.05508(16)	0.38919(15)	0.0441(8)
O3	0.3654(2)	0.84559(15)	0.18066(17)	0.0440(8)
O4	0.3732(2)	0.68704(16)	0.22113(18)	0.0487(8)
O5	0.25404(19)	1.03758(14)	0.18507(13)	0.0309(6)
O6	0.2118(3)	0.97841(19)	0.05642(17)	0.0567(9)
N1'	-0.0035(2)	0.57822(18)	0.2201(2)	0.0406(9)
N2'	-0.0070(2)	0.94187(17)	0.20566(18)	0.0341(8)
C1	0.2308(3)	0.9672(2)	0.4008(2)	0.0346(10)
C1'	-0.0685(3)	0.6653(2)	0.1841(3)	0.0449(13)
C2	0.2064(5)	0.9369(3)	0.4930(3)	0.0637(16)
C2'	-0.0129(3)	0.7601(2)	0.2204(2)	0.0342(10)
C3	0.4206(3)	0.7651(2)	0.1943(2)	0.0359(10)
C3'	-0.0692(3)	0.8497(2)	0.1762(3)	0.0409(11)
C4	0.5596(4)	0.7631(3)	0.1792(4)	0.0664(16)
C5	0.2460(3)	1.0473(2)	0.1021(2)	0.0387(10)
C6	0.2745(5)	1.1483(4)	0.0660(4)	0.0681(19)
C11'	-0.0293(4)	0.4904(3)	0.1657(3)	0.0524(13)
C12'	-0.0453(4)	0.5569(3)	0.3079(3)	0.0519(14)
C21'	-0.0406(4)	1.0237(3)	0.1465(3)	0.0439(13)
C22'	-0.0496(4)	0.9694(3)	0.2922(3)	0.0433(11)
*Cl2	0.7965(4)	0.7744(2)	0.4163(2)	0.1167(18)
C7	0.7142(11)	0.7445(4)	0.4953(4)	0.140(5)
*Cl1A	0.6523(10)	0.7683(3)	0.4162(5)	0.178(5)
*Cl1	0.5329(4)	0.76847(18)	0.45172(16)	0.0752(12)
*Cl2A	0.9119(5)	0.7779(2)	0.4734(2)	0.0929(16)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Starred Atom sites have a S.O.F less than 1.0

Table S13 - Bond Distances (Angstrom) and Bond Angles (Degrees) for 1-catena [Zn4(CH3COO)6(bdmap)2]n 2CD2Cl2

Zn1	-O1	2.023(2)	C3	-C4	1.518(5)
Zn1	-O1'	2.0026(18)	C5	-C6	1.506(6)
Zn1	-O3	2.035(2)	C1'	-H11'	0.95(3)
Zn1	-O5	2.0846(19)	C1'	-H12'	0.96(3)
Zn1	-N2'	2.258(2)	C2	-H2B	1.01(9)
Zn2	-O1'	1.9707(18)	C2	-H2A	0.78(9)
Zn2	-O4	2.052(2)	C2	-H2C	0.85(9)
Zn2	-N1'	2.265(2)	C2'	-H21'	0.97(5)
Zn2	-O2_b	1.993(2)	C3'	-H32'	0.92(4)
Zn2	-O5_b	2.006(2)	C3'	-H31'	0.94(3)
Cl1A	-C7	1.426(11)	C4	-H4C	0.84(10)
Cl2	-C7	1.575(9)	C4	-H4A	0.83(9)
O1	-C1	1.251(4)	C4	-H4B	1.02(11)
O1'	-C2'	1.411(4)	C6	-H62	1.04(8)
O2	-C1	1.260(4)	C6	-H61	0.88(6)
O3	-C3	1.254(4)	C6	-H6	0.74(8)
O4	-C3	1.244(4)	C11'	-H112	0.97(5)
O5	-C5	1.297(4)	C11'	-H111	0.97(4)
O6	-C5	1.223(4)	C11'	-H113	0.98(4)
N1'	-C11'	1.479(5)	C12'	-H122	0.90(4)
N1'	-C12'	1.470(5)	C12'	-H121	0.97(4)
N1'	-C1'	1.473(4)	C12'	-H123	1.01(4)
N2'	-C22'	1.473(5)	C21'	-H212	1.03(4)
N2'	-C3'	1.481(4)	C21'	-H213	0.95(5)
N2'	-C21'	1.478(5)	C21'	-H211	0.96(4)
C1	-C2	1.515(6)	C22'	-H223	0.98(4)
C1'	-C2'	1.517(4)	C22'	-H221	1.06(4)
C2'	-C3'	1.512(4)	C22'	-H222	1.01(4)
C7	-D7A	0.78(8)	C7	-D7B	0.94(8)

O1	-Zn1	-O1'	98.39(9)	Zn1	-O5	-Zn2_a	119.12(10)
O1	-Zn1	-O3	100.51(10)	Zn2_a	-O5	-C5	133.82(18)
O1	-Zn1	-O5	97.75(8)	Zn2	-N1'	-C1'	101.65(17)
O1	-Zn1	-N2'	97.93(9)	Zn2	-N1'	-C11'	114.1(2)
O1'	-Zn1	-O3	93.96(8)	Zn2	-N1'	-C12'	111.9(2)
O1'	-Zn1	-O5	163.18(8)	C1'	-N1'	-C11'	109.7(3)
O1'	-Zn1	-N2'	81.63(8)	C1'	-N1'	-C12'	111.0(3)
O3	-Zn1	-O5	87.70(8)	C11'	-N1'	-C12'	108.4(3)
O3	-Zn1	-N2'	161.48(10)	Zn1	-N2'	-C3'	102.16(17)
O5	-Zn1	-N2'	91.52(8)	Zn1	-N2'	-C21'	118.3(2)
O1'	-Zn2	-O4	93.85(8)	Zn1	-N2'	-C22'	109.1(2)
O1'	-Zn2	-N1'	81.64(8)	C3'	-N2'	-C21'	109.2(3)
O1'	-Zn2	-O2_b	117.62(9)	C3'	-N2'	-C22'	110.4(3)
O1'	-Zn2	-O5_b	136.86(9)	C21'	-N2'	-C22'	107.6(3)
O4	-Zn2	-N1'	175.02(9)	O1	-C1	-O2	126.2(3)
O2_b	-Zn2	-O4	90.80(10)	O1	-C1	-C2	117.3(3)
O4	-Zn2	-O5_b	89.17(9)	O2	-C1	-C2	116.5(3)
O2_b	-Zn2	-N1'	93.18(10)	N1'	-C1'	-C2'	110.3(3)
O5_b	-Zn2	-N1'	92.67(9)	O1'	-C2'	-C1'	109.2(2)
O2_b	-Zn2	-O5_b	105.34(9)	O1'	-C2'	-C3'	109.0(2)
Zn1	-O1	-C1	139.0(2)	C1'	-C2'	-C3'	110.5(3)
Zn1	-O1'	-Zn2	128.63(10)	O3	-C3	-O4	126.4(3)
Zn1	-O1'	-C2'	113.64(15)	O3	-C3	-C4	117.1(3)
Zn2	-O1'	-C2'	114.97(15)	O4	-C3	-C4	116.5(3)
Zn2_a	-O2	-C1	131.0(2)	N2'	-C3'	-C2'	110.7(3)
Zn1	-O3	-C3	131.9(2)	O5	-C5	-O6	121.0(3)
Zn2	-O4	-C3	134.3(2)	O5	-C5	-C6	116.7(3)
Zn1	-O5	-C5	107.01(17)	O6	-C5	-C6	122.2(3)
N1'	-C1'	-H11'	113.7(17)	H6	-C6	-H61	103(8)
N1'	-C1'	-H12'	105.8(17)	H6	-C6	-H62	94(8)
C2'	-C1'	-H11'	110.7(17)	H61	-C6	-H62	118(5)
C2'	-C1'	-H12'	104.2(17)	N1'	-C11'	-H111	107(2)
H11'	-C1'	-H12'	111(3)	N1'	-C11'	-H112	110(2)
C1	-C2	-H2A	114(7)	N1'	-C11'	-H113	111(2)
C1	-C2	-H2B	113(5)	H111	-C11'	-H112	104(3)
C1	-C2	-H2C	112(6)	H111	-C11'	-H113	112(3)
H2A	-C2	-H2B	109(9)	H112	-C11'	-H113	113(3)
H2A	-C2	-H2C	106(10)	N1'	-C12'	-H121	109(2)
H2B	-C2	-H2C	103(9)	N1'	-C12'	-H122	110(3)

O1'	-C2'	-H21'	111(2)	N1'	-C12'	-H123	109.5(18)
C1'	-C2'	-H21'	108.9(17)	H121	-C12'	-H122	106(3)
C3'	-C2'	-H21'	108.3(17)	H121	-C12'	-H123	109(3)
N2'	-C3'	-H31'	104.3(18)	H122	-C12'	-H123	112(3)
N2'	-C3'	-H32'	107(2)	N2'	-C21'	-H211	111(2)
C2'	-C3'	-H31'	108.2(17)	N2'	-C21'	-H212	106(2)
C2'	-C3'	-H32'	111(2)	N2'	-C21'	-H213	108(2)
H31'	-C3'	-H32'	116(3)	H211	-C21'	-H212	111(3)
C3	-C4	-H4A	107(6)	H211	-C21'	-H213	108(3)
C3	-C4	-H4B	99(6)	H212	-C21'	-H213	113(3)
C3	-C4	-H4C	119(7)	N2'	-C22'	-H221	106.1(17)
H4A	-C4	-H4B	84(8)	N2'	-C22'	-H222	110(3)
H4A	-C4	-H4C	134(9)	N2'	-C22'	-H223	109(2)
H4B	-C4	-H4C	83(8)	H221	-C22'	-H222	112(3)
C5	-C6	-H6	114(6)	H221	-C22'	-H223	106(3)
C5	-C6	-H61	106(4)	H222	-C22'	-H223	113(3)
C5	-C6	-H62	121(4)	Cl2	-C7	-D7A	123(6)
Cl2	-C7	-D7B	101(5)	Cl1A	-C7	-D7B	118(5)
Cl1A	-C7	-D7A	122(6)	D7A	-C7	-D7B	117(8)

Table S14 - (An)isotropic Displacement Parameters for 1-catena [Zn4(CH3COO)6(bdmap)2]n 2CD2Cl2

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Zn1	0.0298(2)	0.0203(2)	0.0347(2)	-0.0007(1)	-0.0004(1)	-0.0002(1)
Zn2	0.0313(2)	0.0211(2)	0.0368(2)	0.0008(1)	-0.0001(2)	0.0018(1)
O1	0.0517(14)	0.0314(11)	0.0342(12)	0.0016(9)	-0.0078(10)	-0.0028(10)
O1'	0.0267(10)	0.0213(10)	0.0470(13)	-0.0024(9)	-0.0031(9)	0.0005(8)
O2	0.0594(15)	0.0333(12)	0.0396(13)	-0.0008(10)	0.0046(11)	-0.0097(11)
O3	0.0379(13)	0.0244(11)	0.0699(17)	0.0031(11)	0.0131(11)	0.0036(9)
O4	0.0322(12)	0.0311(12)	0.0829(19)	0.0179(12)	0.0023(12)	-0.0009(9)
O5	0.0383(12)	0.0226(10)	0.0318(11)	0.0013(8)	0.0011(9)	-0.0010(8)
O6	0.0709(18)	0.0491(15)	0.0498(16)	-0.0173(13)	-0.0093(13)	0.0003(13)
N1'	0.0335(14)	0.0221(12)	0.066(2)	-0.0008(12)	-0.0060(13)	0.0001(10)
N2'	0.0326(14)	0.0219(12)	0.0476(16)	-0.0007(11)	-0.0038(12)	0.0013(10)
C1	0.0376(17)	0.0344(17)	0.0318(16)	0.0026(13)	-0.0048(13)	- 0.0021(13)
C1'	0.0315(19)	0.0277(16)	0.075(3)	-0.0033(17)	-0.0132(18)	-0.0007(13)
C2	0.102(4)	0.054(2)	0.035(2)	0.0063(18)	-0.001(2)	-0.019(2)
C2'	0.0284(15)	0.0220(14)	0.052(2)	-0.0038(13)	-0.0050(14)	-0.0005(11)
C3	0.0339(16)	0.0275(15)	0.0463(19)	-0.0015(13)	0.0058(14)	0.0013(13)
C3'	0.0328(19)	0.0307(17)	0.059(2)	-0.0040(16)	-0.0087(17)	0.0034(13)
C4	0.042(2)	0.038(2)	0.120(4)	0.006(2)	0.030(2)	0.0030(17)
C5	0.0430(19)	0.0355(17)	0.0377(18)	0.0015(14)	0.0020(14)	0.0027(14)
C6	0.089(4)	0.060(3)	0.055(3)	0.027(2)	-0.007(3)	-0.014(3)
C11'	0.042(2)	0.0268(18)	0.088(3)	-0.0112(19)	-0.013(2)	-0.0028(15)
C12'	0.040(2)	0.037(2)	0.079(3)	0.002(2)	0.010(2)	-0.0020(17)
C21'	0.037(2)	0.0334(18)	0.061(3)	0.0089(17)	-0.0080(18)	0.0062(15)
C22'	0.038(2)	0.0362(19)	0.056(2)	-0.0062(17)	0.0068(17)	0.0030(15)

==========

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms.
Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Translation of Symmetry Code to Equiv.Pos

a =[2555.00] = 1/2-x,1/2+y,1/2-z
b =[2545.00] = 1/2-x,-1/2+y,1/2-z
c =[4464.00] = -1/2+x,3/2-y,-1/2+z
d =[3676.00] = 1-x,2-y,1-z
e =[4464.00] = -1/2+x,3/2-y,-1/2+z
j =[1455.00] = -1+x,y,z
k =[4464.00] = -1/2+x,3/2-y,-1/2+z
l =[1455.00] = -1+x,y,z
m =[1655.00] = 1+x,y,z
n =[3676.00] = 1-x,2-y,1-z
o =[4565.00] = 1/2+x,3/2-y,1/2+z

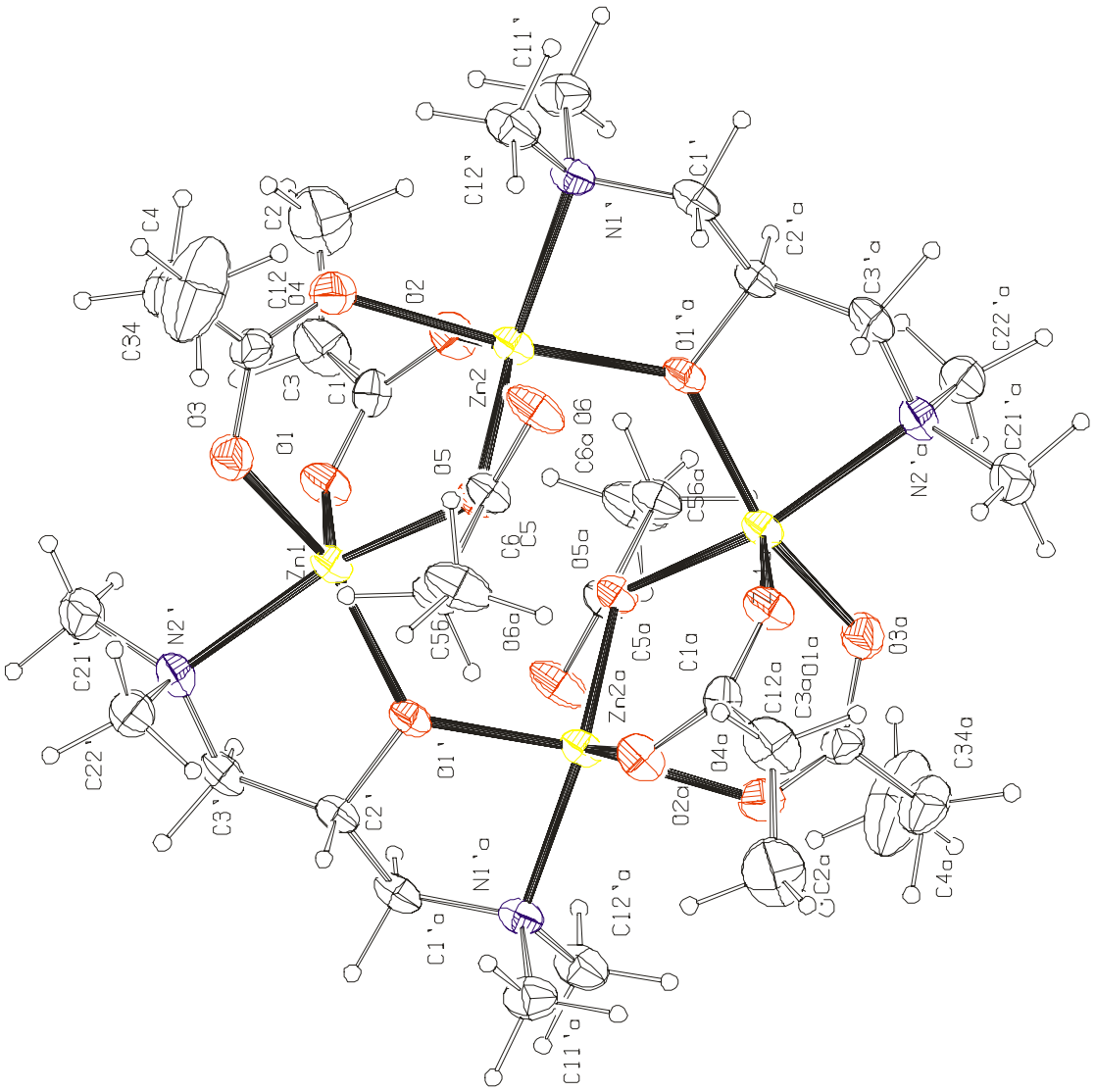


Figure S1. Molecular structure of **2a**. Distances in Å: Zn1-Zn2 3.254(2), Zn1-Zn2a 3.589(3), Zn1-O1 1.984(6), Zn1-O3 2.025(7), Zn1-N2' 2.200(8), Zn2-O2 1.994(6), Zn2-O4 2.235(7), Zn2-N1' 2.128(6), Zn1-O5 2.090(5), Zn2-O5 1.996(5). Representative torsion angles (°): O(1′)-C(2′)-C(3′)-N(2′) = 44.7(9), O(1′a)-C(2′a)-C(1′)-N(1′) = 45.8(9).

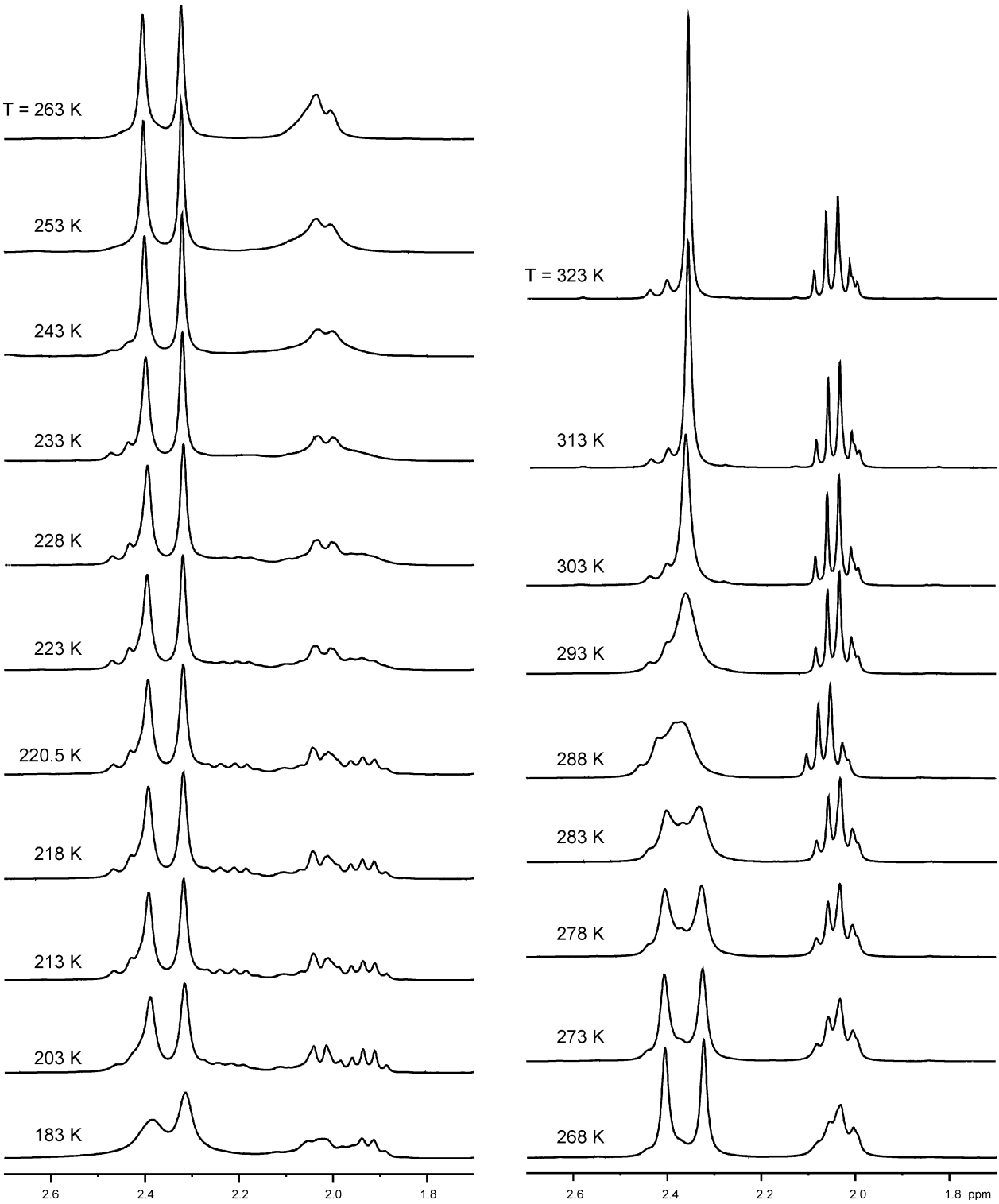


Figure S2. Variable temperature ^{1}H NMR spectra of **2** (0.005 M solution) in THF-d_8.

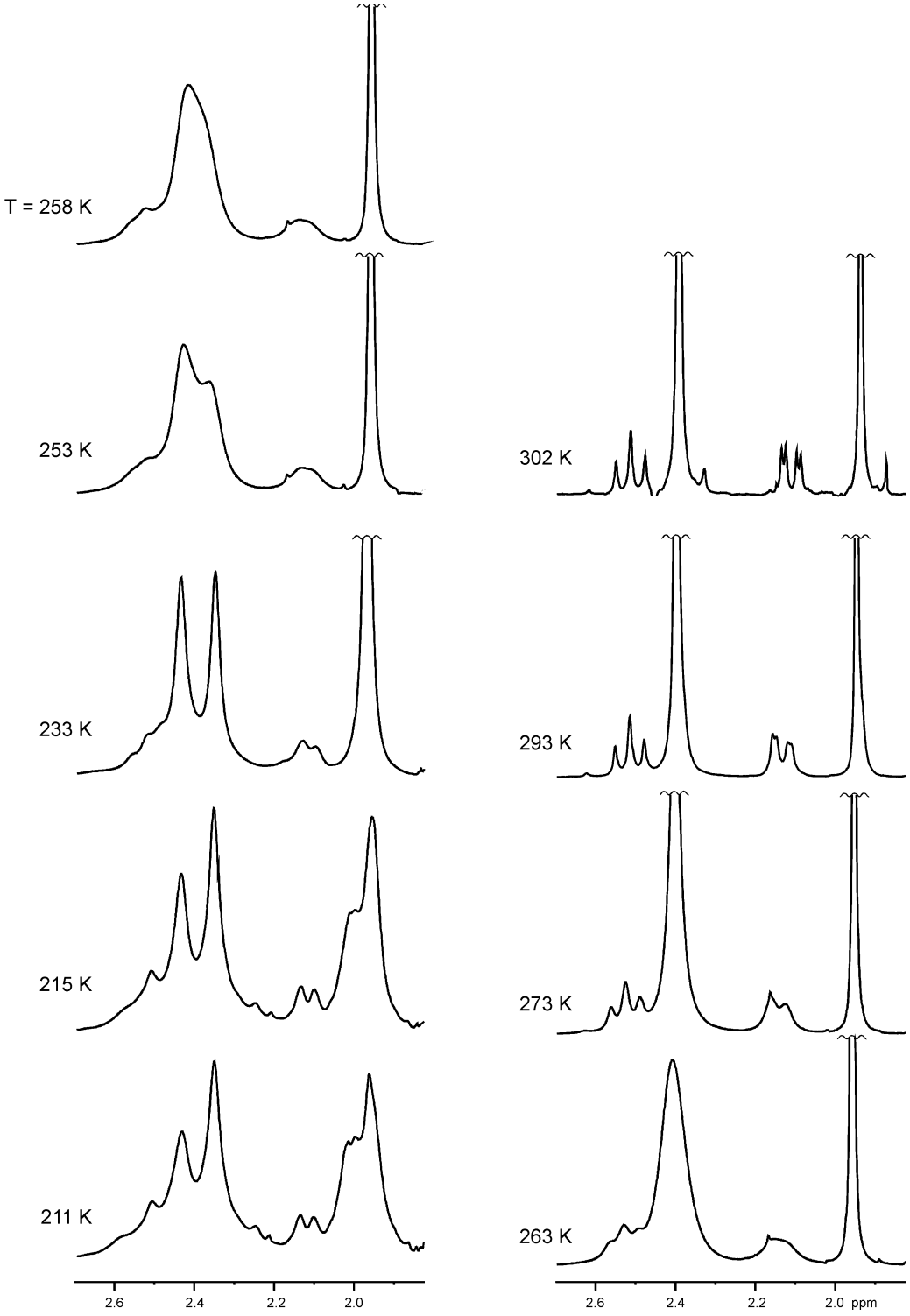


Figure S3. Variable temperature ^{1}H NMR spectra of **1** (0.01 M solution) in $CDCl_3$.

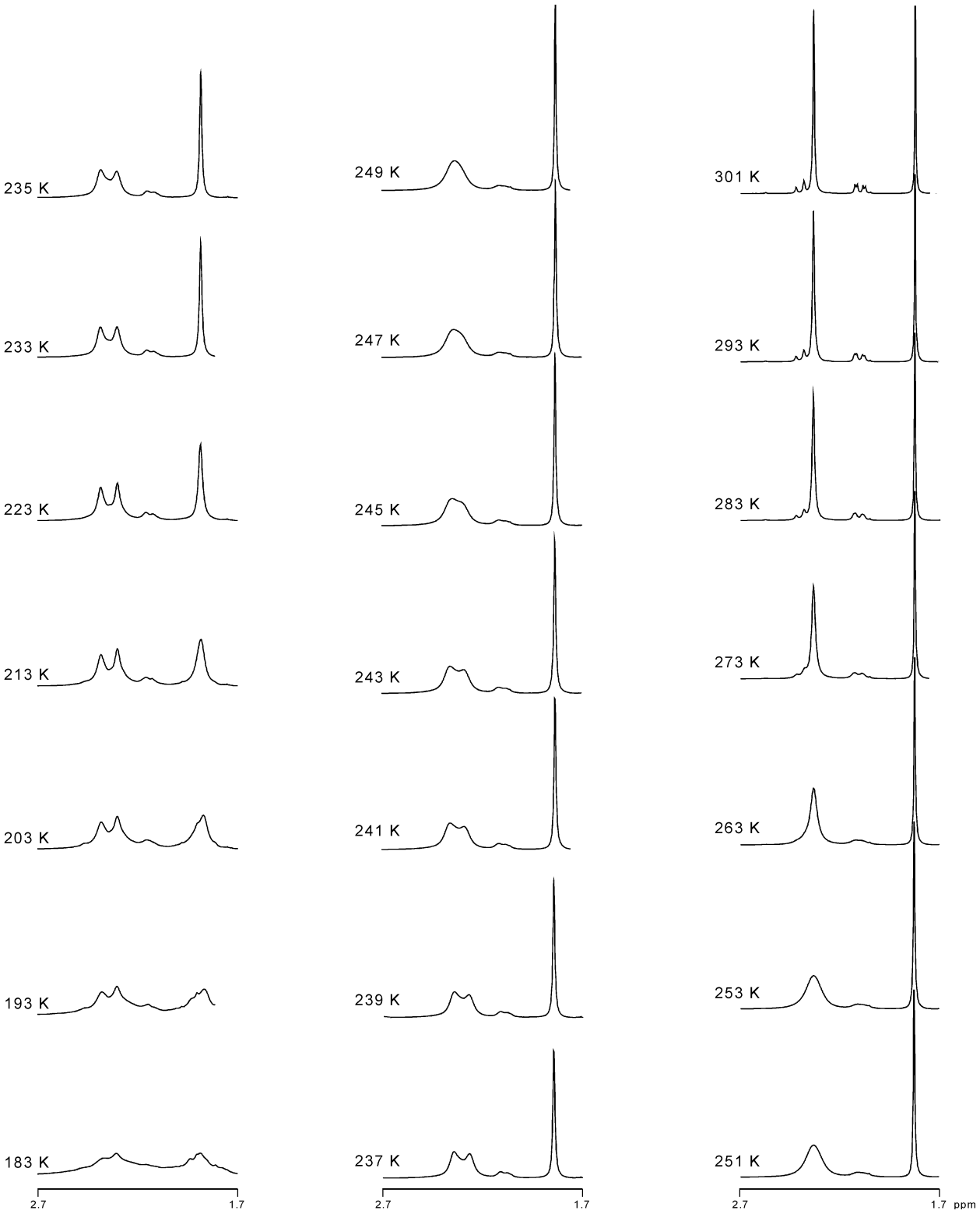


Figure S4. Variable temperature ^{1}H NMR spectra of **1** (0.01 M solution) in CD_2Cl_2

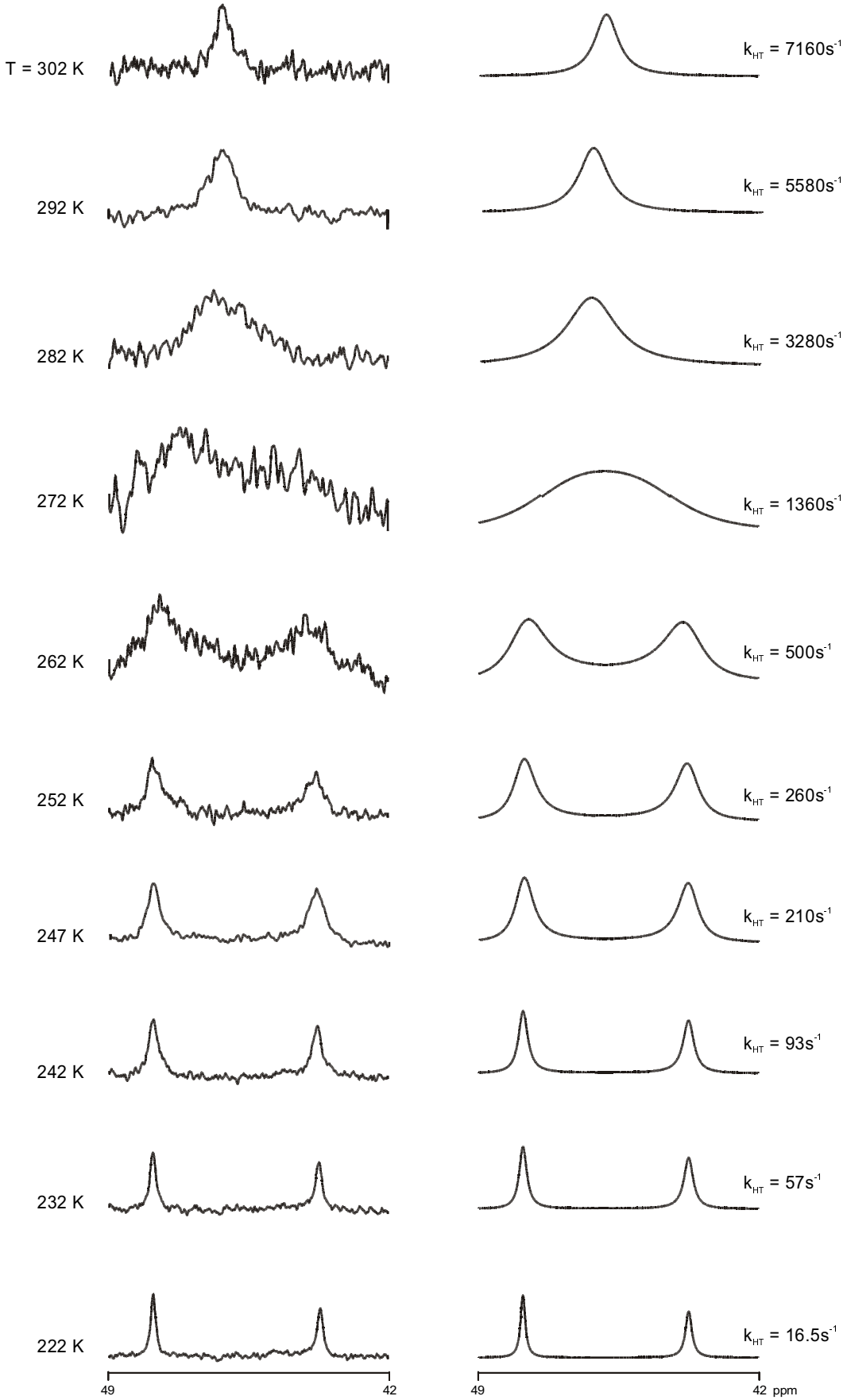


Figure S5. Observed (left) and simulated (right) variable temperature ^{13}C NMR spectra of **1** (0.08 M solution) in CD_2Cl_2.

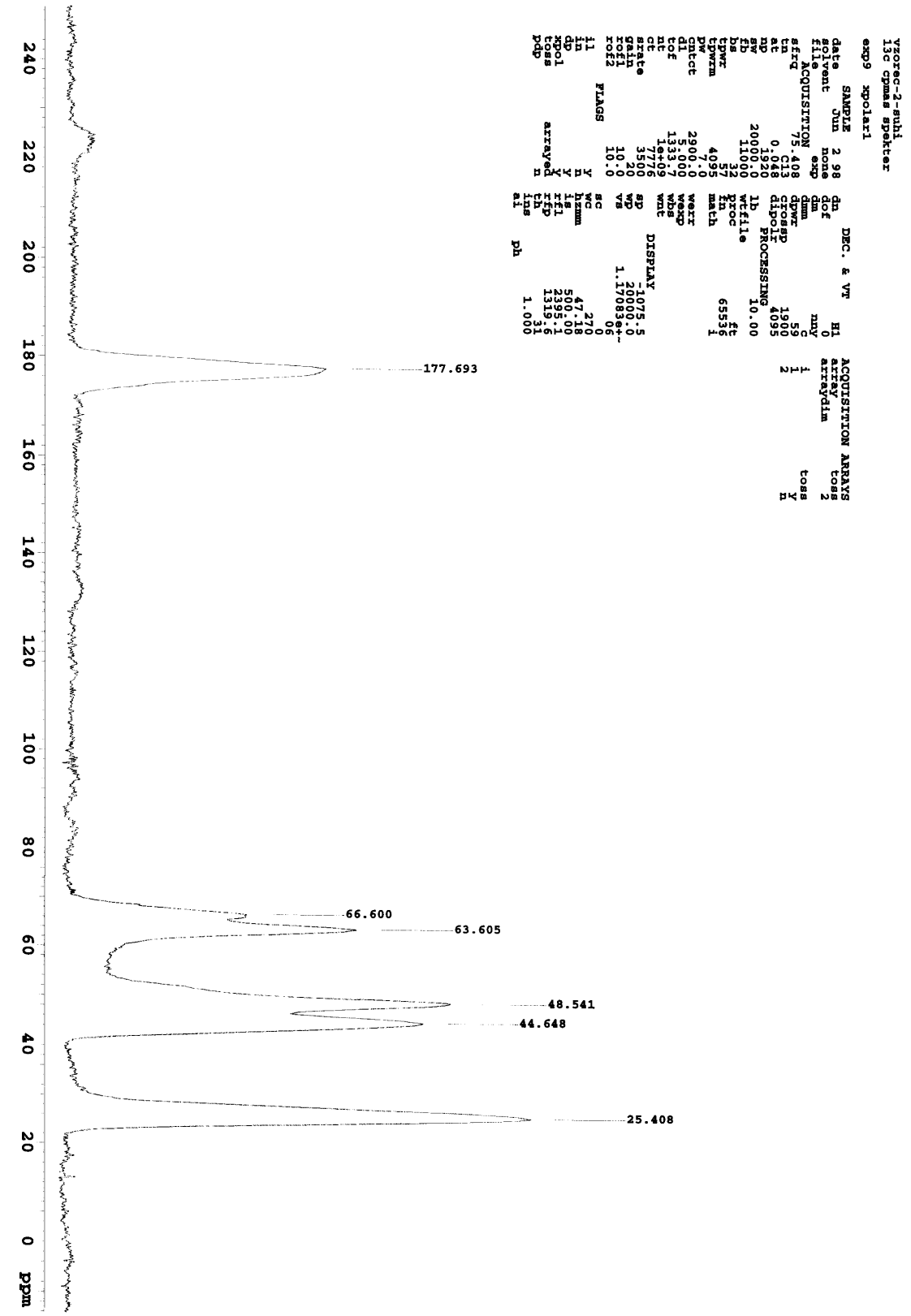


Figure S6. ^{13}C CPMAS (75.4 MHz) spectrum of **1.**

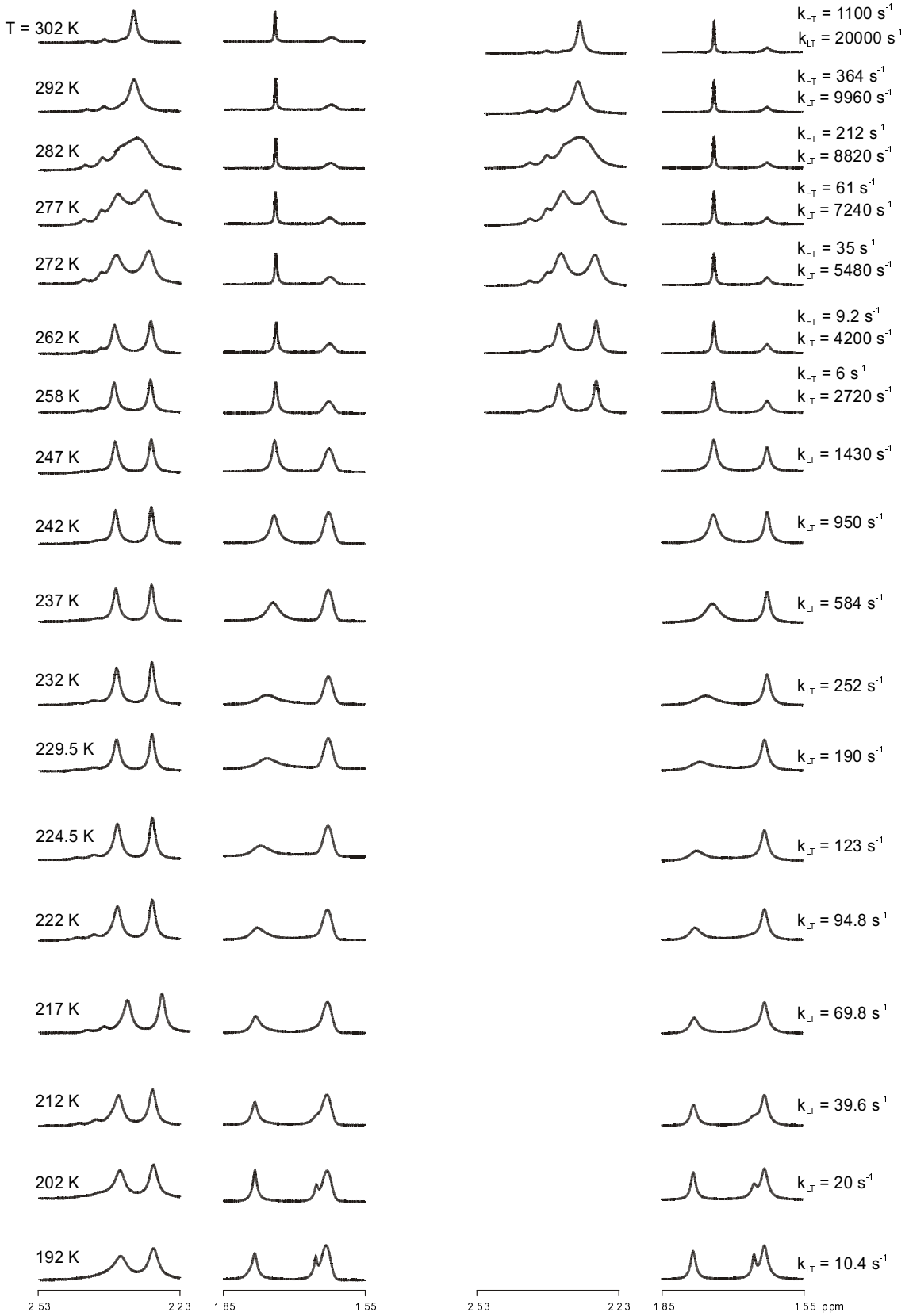


Figure S7.Observed (left) and simulated (right) variable temperature ^{1}H NMR spectra of **1** (0.005 M solution) in THF-d_8.The line-width used in simulation: $w_{1/2}$ (μ-1,1 acetate) = 1 Hz (T = 192–229.5 K), 0.6 Hz (T = 232–302 K), $w_{1/2}$ (μ-1,2 acetate) = 3 Hz (T = 192 K), 2 Hz (T = 202 K), 1.5 Hz (T = 212 K), 1 Hz (T = 212–229.5 K), 0.6 Hz (T = 232–302 K).

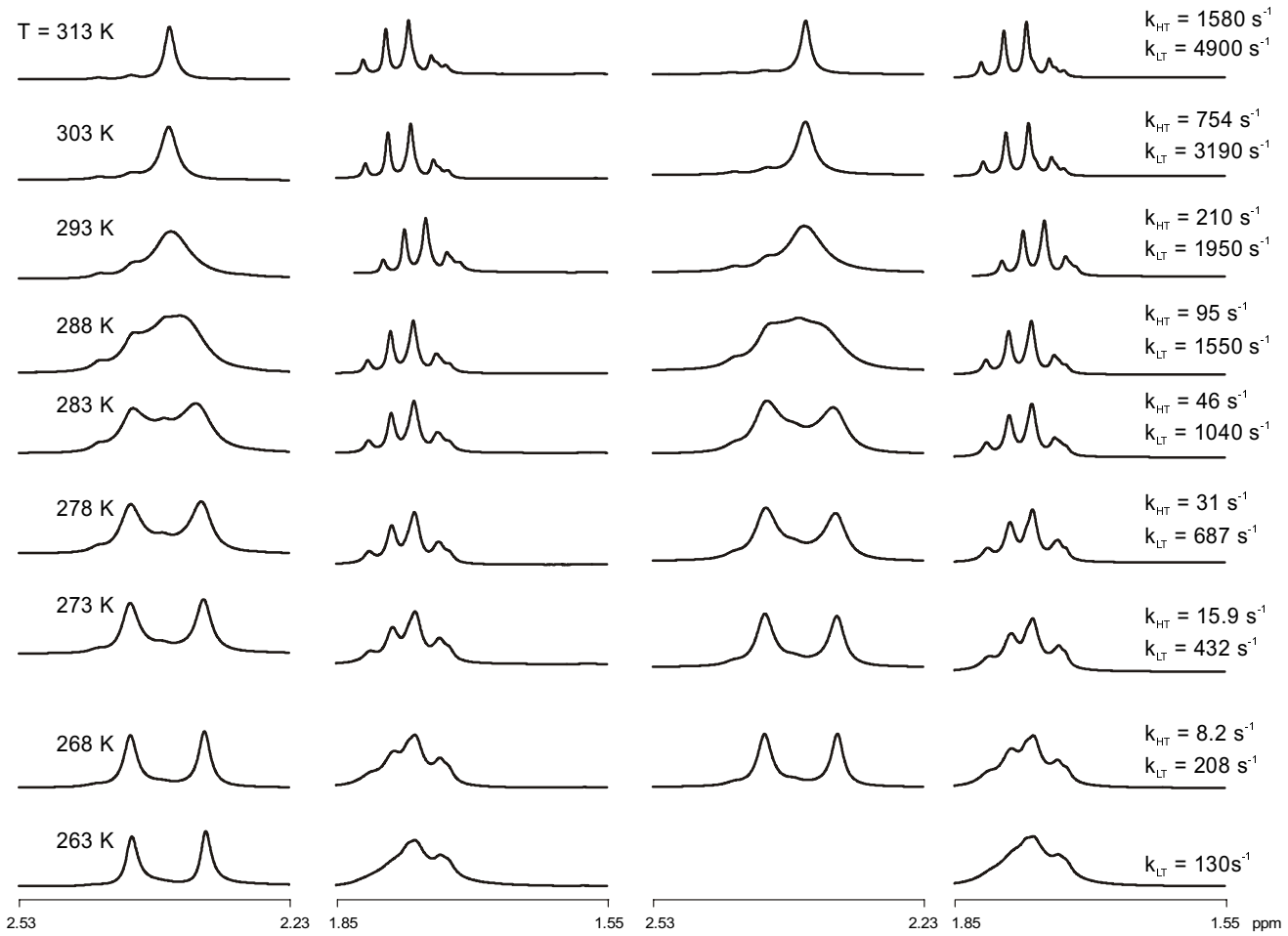


Figure S8. Observed (left) and simulated (right) variable temperature ^{1}H NMR spectra of **2** (0.005 M solution) in THF-d_8