Electronic Supplementary Information

Crystal Structures and Properties of High-nitrogen Energetic Salts Based on (*Z*)-1,1-diamino-2-nitro-2-(1*H*-tetrazol-5-yl)ethene

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Crystal Structure Analysis

Table S1. Bond lengths [Å] for **2**.

Atom	Atom	Lengths [Å]
O(1)	N(13)	1.2679(13)
O(2)	N(13)	1.2739(14)
O(3)	N(20)	1.2648(14)
O(4)	N(20)	1.2821(13)
N(1)	C(1)	1.3280(16)
N(2)	C(1)	1.3314(16)
N(3)	C(1)	1.3266(16)
N(4)	C(2)	1.3267(16)
N(5)	C(2)	1.3267(17)
N(6)	C(2)	1.3280(16)
N(7)	C(3)	1.3287(16)
N(8)	C(3)	1.3211(16)
N(9)	C(5)	1.3381(16)
N(9)	N(10)	1.3436(16)
N(10)	N(11)	1.3030(16)
N(11)	N(12)	1.3392(15)
N(12)	C(5)	1.3421(15)
N(13)	C(4)	1.3617(15)
N(14)	N(15)	1.3410(14)
N(14)	C(8)	1.3431(15)
N(15)	N(16)	1.3004(16)
N(16)	N(17)	1.3445(15)
N(17)	C(8)	1.3417(16)
N(18)	C(6)	1.3221(16)
N(19)	C(6)	1.3259(16)
N(20)	C(7)	1.3612(15)
C(3)	C(4)	1.4597(16)
C(4)	C(5)	1.4679(16)
C(6)	C(7)	1.4559(16)
C(7)	C(8)	1.4750(15)

Table S2. Bond angles [°] for **2**.

Atom	Atom	Atom	Angle/°
C(5)	N(9)	N(10)	104.80(11)
N(11)	N(10)	N(9)	110.05(11)
N(10)	N(11)	N(12)	109.15(11)
N(11)	N(12)	C(5)	105.43(10)
O(1)	N(13)	O(2)	117.45(10)
O(1)	N(13)	C(4)	120.57(10)
O(2)	N(13)	C(4)	121.98(10)
N(15)	N(14)	C(8)	105.32(10)
N(16)	N(15)	N(14)	109.16(10)
N(15)	N(16)	N(17)	110.35(10)
C(8)	N(17)	N(16)	104.49(10)
O(3)	N(20)	O(4)	117.56(10)
O(3)	N(20)	C(7)	120.25(10)
O(4)	N(20)	C(7)	122.19(10)
N(3)	C(1)	N(1)	119.45(12)
N(3)	C(1)	N(2)	120.61(11)
N(1)	C(1)	N(2)	119.92(12)
N(5)	C(2)	N(4)	119.77(12)
N(5)	C(2)	N(6)	120.35(12)
N(4)	C(2)	N(6)	119.87(12)
N(8)	C(3)	N(7)	118.15(11)
N(8)	C(3)	C(4)	121.62(11)
N(7)	C(3)	C(4)	120.23(11)
N(13)	C(4)	C(3)	119.99(10)
N(13)	C(4)	C(5)	118.90(10)
C(3)	C(4)	C(5)	121.05(10)
N(9)	C(5)	N(12)	110.56(11)
N(9)	C(5)	C(4)	126.82(11)
N(12)	C(5)	C(4)	122.58(11)
N(18)	C(6)	N(19)	118.71(11)
N(18)	C(6)	C(7)	119.21(11)
N(19)	C(6)	C(7)	122.07(11)
N(20)	C(7)	C(6)	120.03(10)
N(20)	C(7)	C(8)	118.80(10)
C(6)	C(7)	C(8)	121.17(10)
N(17)	C(8)	N(14)	110.67(10)
N(17)	C(8)	C(7)	127.36(11)
N(14)	C(8)	C(7)	121.93(10)

Table S3. Torsion angles [°] for **2**.

Atom	Atom	Atom	Atom	Angle/°
C(5)	N(9)	N(10)	N(11)	-0.80(15)
N(9)	N(10)	N(11)	N(12)	0.70(16)
N(10)	N(11)	N(12)	C(5)	-0.30(15)
C(8)	N(14)	N(15)	N(16)	-0.59(14)
N(14)	N(15)	N(16)	N(17)	0.58(14)
N(15)	N(16)	N(17)	C(8)	-0.31(14)
O(1)	N(13)	C(4)	C(3)	-179.18(10)
O(2)	N(13)	C(4)	C(3)	1.57(17)
O(1)	N(13)	C(4)	C(5)	3.59(16)
O(2)	N(13)	C(4)	C(5)	-175.66(10)
N(8)	C(3)	C(4)	N(13)	-0.35(17)
N(7)	C(3)	C(4)	N(13)	-179.28(10)
N(8)	C(3)	C(4)	C(5)	176.82(11)
N(7)	C(3)	C(4)	C(5)	-2.11(17)
N(10)	N(9)	C(5)	N(12)	0.61(15)
N(10)	N(9)	C(5)	C(4)	178.41(11)
N(11)	N(12)	C(5)	N(9)	-0.21(15)
N(11)	N(12)	C(5)	C(4)	-178.12(11)
N(13)	C(4)	C(5)	N(9)	19.10(18)
C(3)	C(4)	C(5)	N(9)	-158.10(12)
N(13)	C(4)	C(5)	N(12)	-163.34(11)
C(3)	C(4)	C(5)	N(12)	19.46(17)
O(3)	N(20)	C(7)	C(6)	-176.40(10)
O(4)	N(20)	C(7)	C(6)	3.79(17)
O(3)	N(20)	C(7)	C(8)	3.95(16)
O(4)	N(20)	C(7)	C(8)	-175.86(10
N(18)	C(6)	C(7)	N(20)	178.84(11)
N(19)	C(6)	C(7)	N(20)	-1.66(18)
N(18)	C(6)	C(7)	C(8)	-1.52(17)
N(19)	C(6)	C(7)	C(8)	177.98(11)
N(16)	N(17)	C(8)	N(14)	-0.07(14)
N(16)	N(17)	C(8)	C(7)	177.64(11)
N(15)	N(14)	C(8)	N(17)	0.41(14)
N(15)	N(14)	C(8)	C(7)	-177.45(10)
N(20)	C(7)	C(8)	N(17)	15.07(18)
C(6)	C(7)	C(8)	N(17)	-164.58(12)
N(20)	C(7)	C(8)	N(14)	-167.45(11)
C(6)	C(7)	C(8)	N(14)	12.90(17)

Table S4. Hydrogen bonds for **2** [Å and °].

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N(1)	H(1A)	O(3)	0.87(2)	2.03(2)	2.8854(15)	167.5(18)
N(1)	H(1B)	N(9)[1]	0.85(2)	2.55(2)	3.2389(16)	138.6(16)
N(1)	H(1B)	N(10)[1]	0.85(2)	2.33(2)	3.0994(16)	150.6(17)
N(2)	H(2B)	O(1)[1]	0.880(19)	2.428(18)	3.1031(15)	133.8(15)
N(2)	H(2B)	N(9)[1]	0.880(19)	2.197(19)	3.0158(16)	154.5(16)
N(2)	H(2A)	N(16)[2]	0.897(18)	2.186(18)	3.0525(16)	162.3(15)
N(3)	H(3B)	N(15)[2]	0.822(19)	2.292(19)	3.0892(16)	163.5(16)
N(3)	H(3A)	O(4)	0.812(18)	2.119(19)	2.9164(15)	167.5(15)
N(4)	H(4A)	O(2)	0.82(2)	2.02(2)	2.8334(15)	173.7(18)
N(4)	H(4B)	N(10)[3]	0.81(2)	2.69(2)	3.3621(17)	141.3(17)
N(4)	H(4B)	N(11)[3]	0.81(2)	2.25(2)	3.0355(17)	164.5(17)
N(5)	H(5A)	O(1)[4]	0.89(2)	2.25(2)	2.9672(14)	137.9(15)
N(5)	H(5B)	O(1)	0.900(19)	2.06(2)	2.9573(15)	171.1(17)
N(5)	H(5B)	O(2)	0.900(19)	2.650(19)	3.3399(15)	134.1(15)
N(6)	H(6A)	N(10)[3]	0.86(2)	2.12(2)	2.9703(17)	169.7(16)
N(6)	H(6B)	O(3)[5]	0.84(2)	2.49(2)	3.0459(15)	124.1(17)
N(6)	H(6B)	N(9)[4]	0.84(2)	2.56(2)	3.2199(17)	136.5(18)
N(7)	H(7A)	O(3)	0.904(19)	2.458(18)	3.0951(14)	127.8(14)
N(7)	H(7A)	N(17)	0.904(19)	2.173(19)	3.0318(16)	158.2(16)
N(7)	H(7B)	N(12)	0.874(18)	1.978(18)	2.6921(16)	138.1(15)
N(8)	H(8A)	O(2)	0.924(18)	1.804(18)	2.5266(15)	133.0(16)
N(8)	H(8B)	N(16)	0.92(2)	2.18(2)	3.0064(16)	149.4(16)
N(8)	H(8B)	N(17)	0.92(2)	2.44(2)	3.1748(16)	137.8(16)
N(18)	H(18A)	N(14)	0.89(2)	1.91(2)	2.6312(15)	136.9(17)
N(18)	H(18B)	N(15)[6]	0.859(19)	2.408(18)	3.0371(15)	130.5(15)
N(19)	H(19A)	N(11)[7]	0.87(2)	2.37(2)	3.0210(16)	131.5(17)
N(19)	H(19B)	O(4)	0.93(2)	1.81(2)	2.5412(16)	134.1(18)

[1]2-X,-Y,-Z;[2]+X,+Y,-1+Z; [3]+X,+Y,1+Z; [4]3-X,-Y,1-Z; [5]2-X,-Y,1-Z; [6]-X,1-Y,1-Z; [7]1-X,1-Y,-Z

Table S5. Bond lengths [Å] for **3**.

Atom	Atom	Lengths [Å]
O1	N7	1.294(4)
O2	N7	1.267(4)
N1	N2	1.343(4)
N1	C4	1.344(4)
N2	N3	1.313(5)
N3	N4	1.350(4)
N4	C4	1.334(5)
N5	C2	1.313(5)
N6	C2	1.329(5)
N7	C3	1.350(4)
N8	C1	1.320(5)
N9	C1	1.315(5)
N10	C1	1.340(5)
N10	N11	1.409(5)
C2	C3	1.460(5)
C3	C4	1.472(5)

Table S6. Bond angles [°] for **3**.

Atom	Atom	Atom	Angle/°
N2	N1	C4	104.9(3)
N3	N2	N1	109.2(3)
N2	N3	N4	109.9(3)
C4	N4	N3	104.5(3
O2	N7	O1	117.8(3)
O2	N7	C3	120.9(3)
O1	N7	C3	121.2(3)
C1	N10	N11	118.4(4)
N9	C1	N8	120.5(4)
N9	C1	N10	120.0(4)
N8	C1	N10	119.5(4)
N5	C2	N6	119.0(3)
N5	C2	C3	123.0(4)
N6	C2	C3	117.9(3)
N7	C3	C2	121.5(3)
N7	C3	C4	119.1(3)
C2	C3	C4	119.0(3)
N4	C4	N1	111.5(3)
N4	C4	C3	127.3(3)
N1	C4	C3	121.2(3)

Table S7. Torsion angles [°] for **3**.

Atom	Atom	Atom	Atom	Angle/°
C4	N1	N2	N3	-0.2(4)
N1	N2	N3	N4	0.4(4)
N2	N3	N4	C4	-0.4(4)
N11	N10	C1	N9	5.1(6)
N11	N10	C1	N8	-175.8(4)
O2	N7	C3	C2	178.2(4)
O1	N7	C3	C2	-1.5(5)
O2	N7	C3	C4	-9.3(5)
O1	N7	C3	C4	171.0(3)
N5	C2	C3	N7	16.5(5)
N6	C2	C3	N7	-164.3(3)
N5	C2	C3	C4	-156.0(3)
N6	C2	C3	C4	23.3(5)
N3	N4	C4	N1	0.3(4)
N3	N4	C4	C3	-179.1(3)
N2	N1	C4	N4	0.0(4)
N2	N1	C4	C3	179.3(3)
N7	C3	C4	N4	52.2(5)
C2	C3	C4	N4	-135.1(4)
N7	C3	C4	N1	-127.1(4)
C2	C3	C4	N1	45.6(5)

Table S8. Hydrogen bonds for **3** [Å and °].

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N5	H5A	N3[1]	0.86	2.56	3.277(5)	140.9
N5	H5A	N4[1]	0.86	2.06	2.879(5)	158.5
N5	H5B	O1	0.86	2.03	2.621(5)	125.5
N6	H6A	O2[1]	0.86	2.25	3.020(5)	148.6
N6	H6A	N4[1]	0.86	2.69	3.362(5)	135.5
N6	H6B	N1[2]	0.86	2.30	3.010(5)	140.2
N8	H8A	O1	0.86	2.03	2.889(4)	176.3
N8	H8B	N2[3]	0.86	2.32	2.983(5)	133.9
N9	H9A	O2	0.86	2.11	2.967(5)	171.1
N9	H9B	N1[4]	0.86	2.48	3.142(5)	134.2
N10	H10	N3[5]	0.86	2.15	2.933(5)	150.3
N11	H11B	O1[6]	0.83(5)	2.50(5)	3.230(6)	147(5)

[1]-X,1/2+Y,1-Z; [2]-1+X,+Y,+Z; [3]+X,+Y,1+Z; [4]1-X,-1/2+Y,1-Z; [5]1+X,+Y,1+Z; [6]1-X,-1/2+Y,2-Z

Table S9. Bond lengths [Å] for **5**.

Atom	Atom	Lengths [Å]
O(1)	N(15)	1.2708(15)
O(2)	N(15)	1.2658(15)
N(2)	C(4)	1.3238(18)
N(2)	N(3)	1.4139(17)
N(4)	C(4)	1.3253(16)
N(4)	N(5)	1.4104(16)
N(6)	C(4)	1.3284(18)
N(6)	N(7)	1.4135(15)
N(9)	C(3)	1.3149(16)
N(10)	C(3)	1.3253(16)
N(11)	C(1)	1.3353(17)
N(11)	N(12)	1.3385(16)
N(12)	N(13)	1.3107(17)
N(13)	N(14)	1.3381(17)
N(14)	C(1)	1.3363(17)
N(15)	C(2)	1.3513(17)
C(1)	C(2)	1.4711(17)
C(2)	C(3)	1.4475(17)

Table S10. Bond angles [°] for **5**.

Atom	Atom	Atom	Angle/°
C(4)	N(2)	N(3)	118.94(11)
C(4)	N(4)	N(5)	118.81(11)
C(4)	N(4)	N(5)	118.21(11)
C(1)	N(11)	N(12)	104.88(11)
N(13)	N(12)	N(11)	109.44(10)
N(12)	N(13)	N(14)	109.62(10)
C(1)	N(14)	N(13)	104.76(11)
O(2)	N(15)	O(1)	118.16(11)
O(2)	N(15)	C(2)	122.63(11)
O(1)	N(15)	C(2)	119.21(12)
N(11)	C(1)	N(14)	111.29(11)
N(11)	C(1)	C(2)	122.24(11)
N(14)	C(1)	C(2)	126.43(12)
N(15)	C(2)	C(3)	120.61(11)
N(15)	C(2)	C(1)	118.41(11)
C(3)	C(2)	C(1)	120.93(10)
N(9)	C(3)	N(10)	118.90(11)
N(9)	C(3)	C(2)	121.97(11)
N(10)	C(3)	C(2)	119.11(11)
N(2)	C(4)	N(4)	120.35(12)
N(2)	C(4)	N(6)	119.90(11)
N(4)	C(4)	N(6)	119.74(11)

Table S11. Torsion angles [°] for **5**.

Atom	Atom	Atom	Atom	Angle/°
C(1)	N(11)	N(12)	N(13)	-0.27(13)
N(11)	N(12)	N(13)	N(14)	0.38(13)
N(12)	N(13)	N(14)	C(1)	-0.33(13)
N(12)	N(11)	C(1)	N(14)	0.06(14)
N(12)	N(11)	C(1)	C(2)	-178.07(10)
N(13)	N(14)	C(1)	N(11)	0.16(14)
N(13)	N(14)	C(1)	C(2)	178.19(11)
O(2)	N(15)	C(2)	C(3)	2.86(19)
O(1)	N(15)	C(2)	C(3)	-177.75(13)
O(2)	N(15)	C(2)	C(1)	-179.82(11)
O(1)	N(15)	C(2)	C(1)	-0.43(19)
N(11)	C(1)	C(2)	N(15)	-131.56(13)
N(14)	C(1)	C(2)	N(15)	50.62(17)
N(11)	C(1)	C(2)	C(3)	45.76(16)
N(14)	C(1)	C(2)	C(3)	-132.07(13)
N(15)	C(2)	C(3)	N(9)	17.81(18)
C(1)	C(2)	C(3)	N(9)	159.44(12)
N(15)	C(2)	C(3)	N(10)	-163.71(13)
C(1)	C(2)	C(3)	N(10)	19.03(17)
N(3)	N(2)	C(4)	N(4)	6.46(18)
N(3)	N(2)	C(4)	N(6)	-174.59(11)
N(5)	N(4)	C(4)	N(2)	-179.91(11)
N(5)	N(4)	C(4)	N(6)	1.13(18)
N(7)	N(6)	C(4)	N(2)	-9.37(18)
N(7)	N(6)	C(4)	N(4)	169.60(12)

Table S12. Hydrogen bonds for **5** [Å and °].

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N2	H2	N11[1]	0.837	2.202	2.930	145.47
N4	H4	N12$_2$	0.863	2.451	3.079	130.06
N6	H6	N3[3]	0.877	2.343	3.213	171.44
N9	H9A	O1[4]	0.860	1.950	2.800	169.46
N9	H9B	O1[5]	0.860	2.627	3.273	132.85
N9	H9B	O2	0.860	2.020	2.607	124.71
N10	H10A	N14[6]	0.860	2.350	3.156	156.01
N10	H10B	N11	0.860	2.592	3.040	113.55
N10	H10B	N13[7]	0.860	2.234	3.062	161.59
N3	H3B	O2[8]	0.927	2.367	3.146	141.57
N3	H3B	N5[9]	0.927	2.480	3.049	119.84
N5	H5A	N14[10]	0.896	2.359	3.194	155.16
N5	H5B	N7[11]	0.929	2.524	3.154	125.36
N5	H5B	N11[12]	0.929	2.462	3.202	136.67
N7	H7A	N12[13]	0.922	2.259	3.143	160.67
N7	H7B	O2	0.886	2.189	2.897	136.54

[1]-x+1, -y+1, -z+1; [2]-x, -y+1, -z+1; [3]-x, y+1/2, -z+3/2; [4] x+1, y, z; [5]-x+1, -y+1, -z+1; [6]x+1, y, z; [7]-x+1, -y+2, -z+1; [8]-x+1, y-1/2, -z+3/2 [9]-x, y-1/2, -z+3/2; [10]-x, y-1/2, -z+3/2; [11]x-1, y, z; [12] -x, -y+1, -z+1; [13]-x, -y+1, -z+1

NMR Spectra

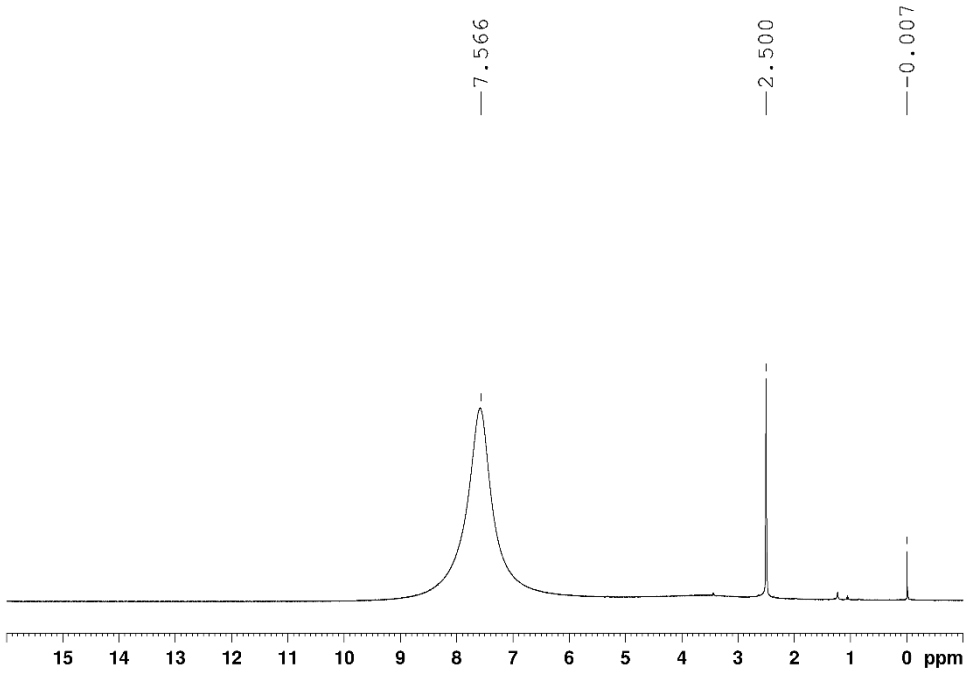

Figure S1. ^{1}H NMR spectrum of **2**.

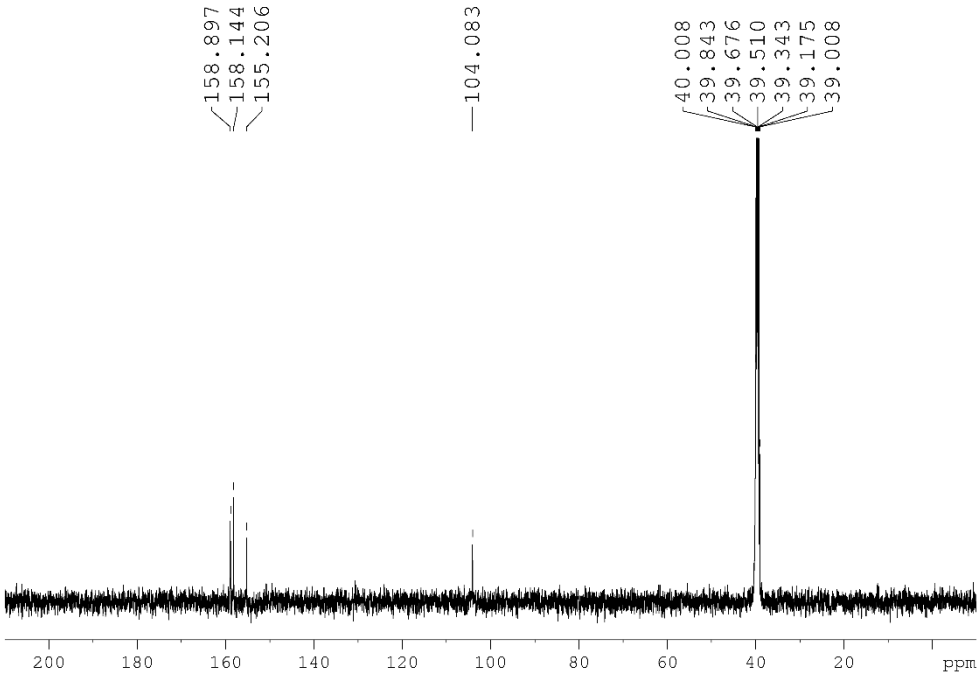

Figure S2. ^{13}C NMR spectrum of **2**.

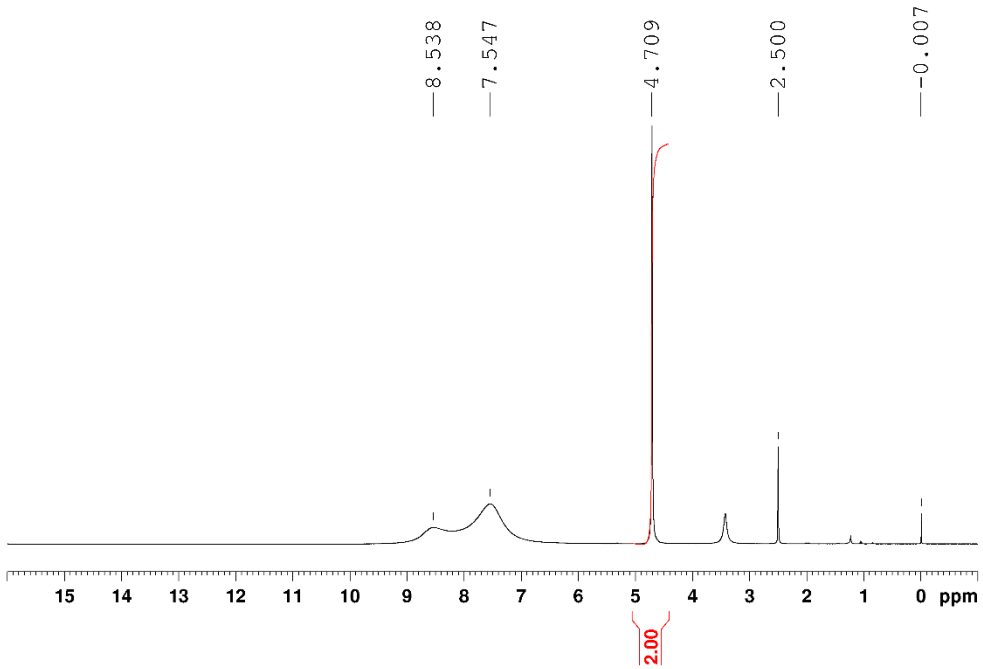

Figure S3. ^{1}H NMR spectrum of **3**.

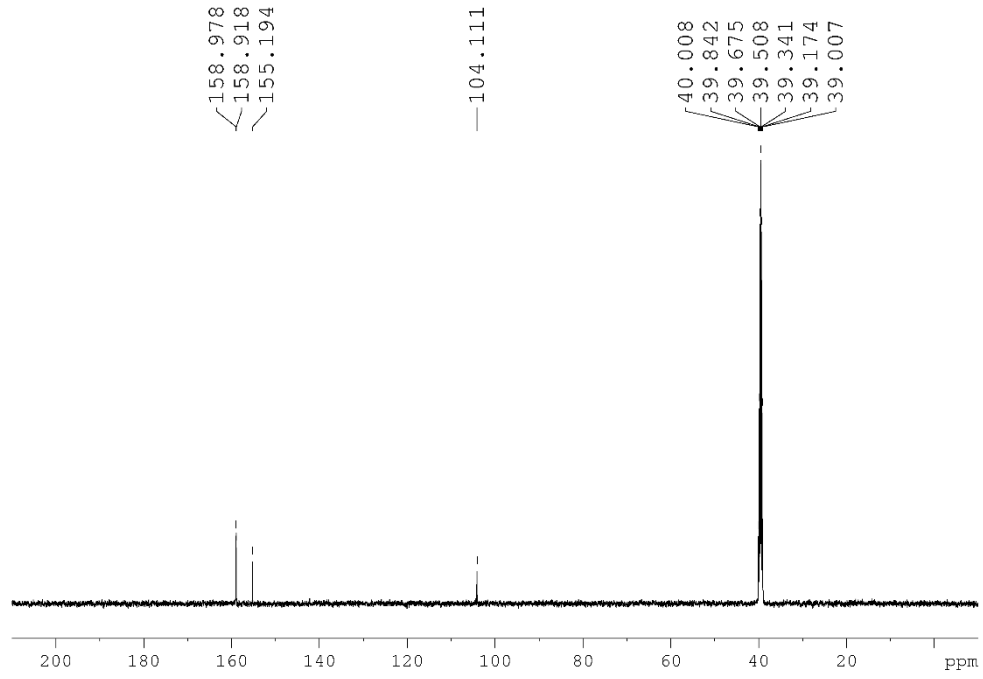

Figure S4. ^{13}C NMR spectrum of **3**.

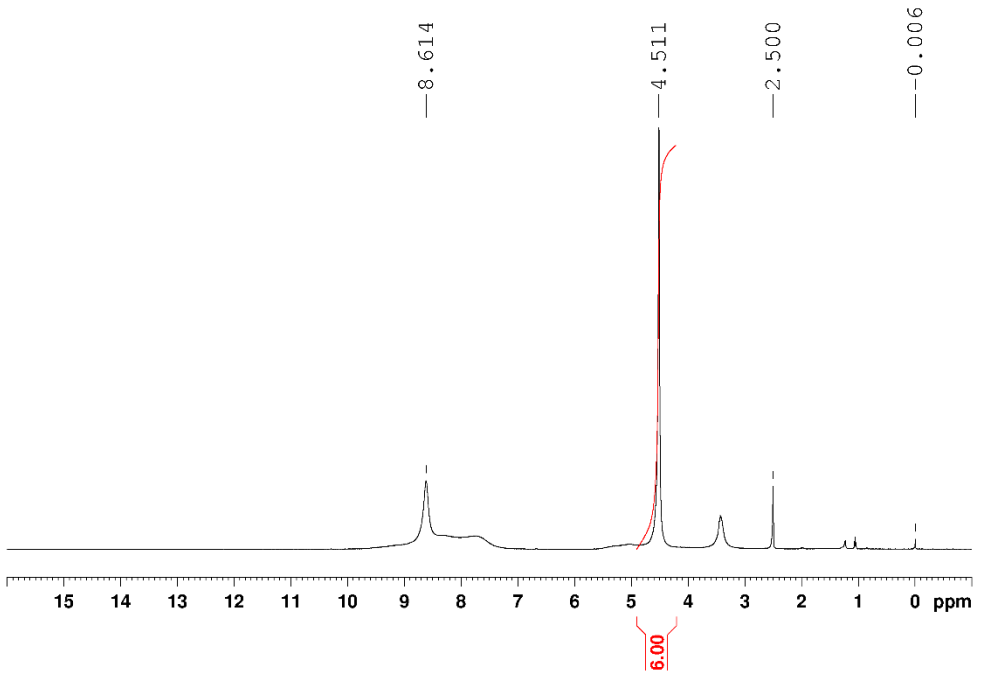

Figure S5. ^{1}H NMR spectrum of **5**.

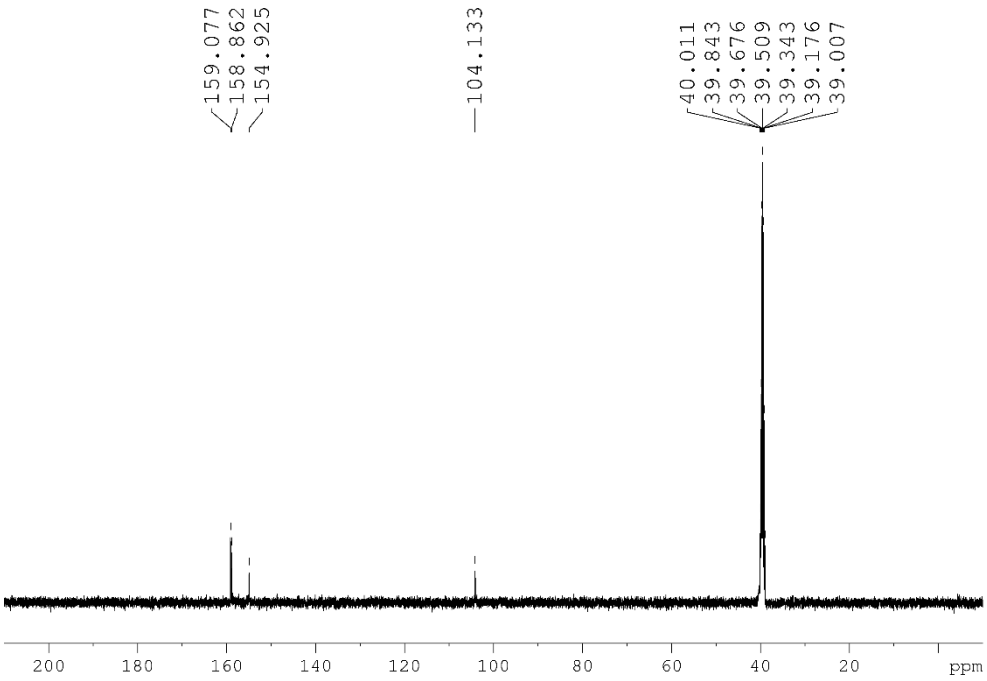

Figure S6. ^{13}C NMR spectrum of **5**.

DSC Plot

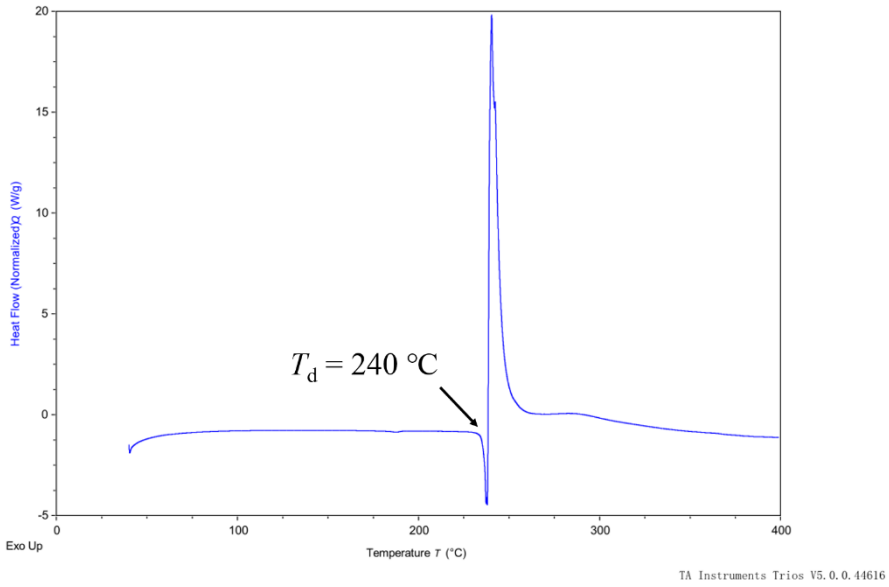

Figure S7. DSC plot of **2**.

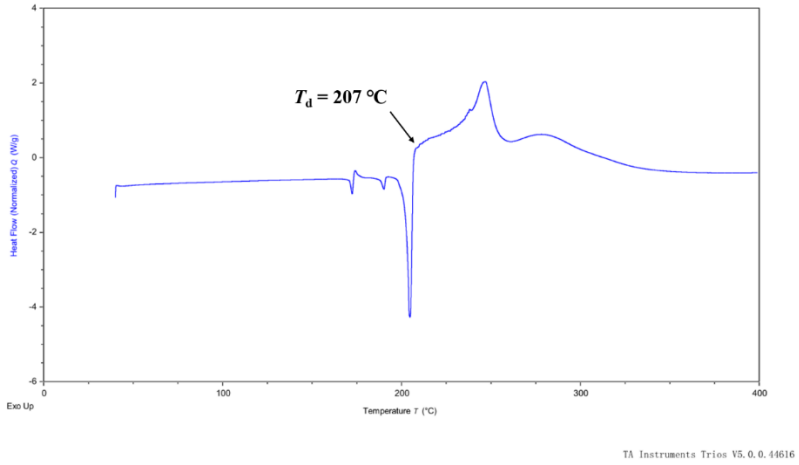

Figure S8. DSC plot of **3**.

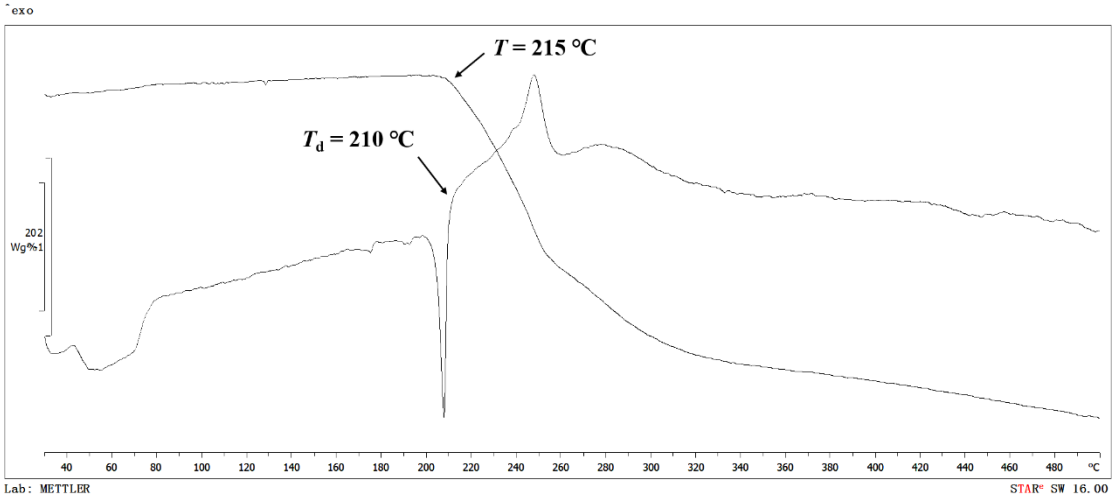

Figure S9. TG-DSC plot of **3**.

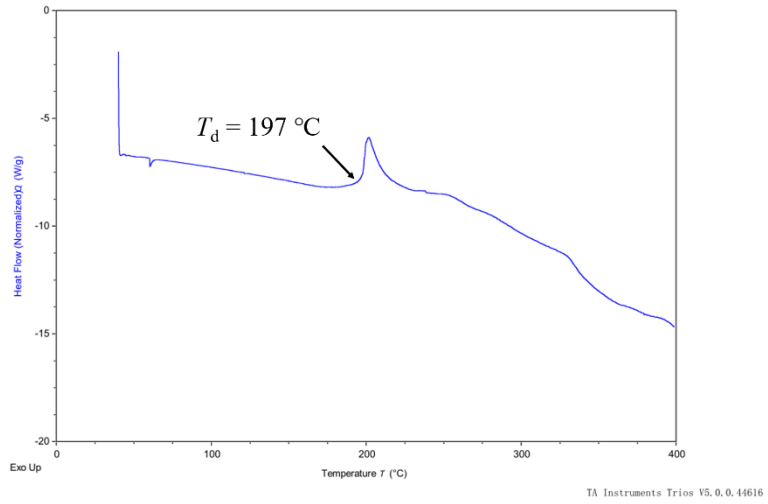

Figure S10. DSC plot of **5**.

Table S13. Lattice Energy for Heat of Formation.

Compounds	ΔH_L (kJ/mol)	ΔH_f^{Cation} (kJ/mol)	ΔH_f^{anion} (kJ/mol)	ΔH_f^{298} (kJ/mol)
G-TzFOX	492.29	575.85	147.14	230.70
AG-TzFOX	482.79	667.41	147.14	331.75
TAG-TzFOX	466.47	871.47	147.14	552.15