Nitrogen-Rich 4,4'-Azobis(1,2,4-triazolone) Salts—Synthesis and Promising Properties of a New Family of High-Density Insensitive Materials

Jiaping Zhu,[a] Shaohua Jin,[a] Li Wan,[a] Lijie Li,[a] Chunyuan Zhang,[a] Shusen Chen [a], Qinghai Shu[a*]

[a] *School of Materials Science & Engineering, Beijing Institute of Technology, Beijing, China. Tel: +86–10–68918535; E‐mail:* qhshu121@bit.edu.cn

Figures

Figure

4,4'–azobis(1,2,4–triazolone), ZTO

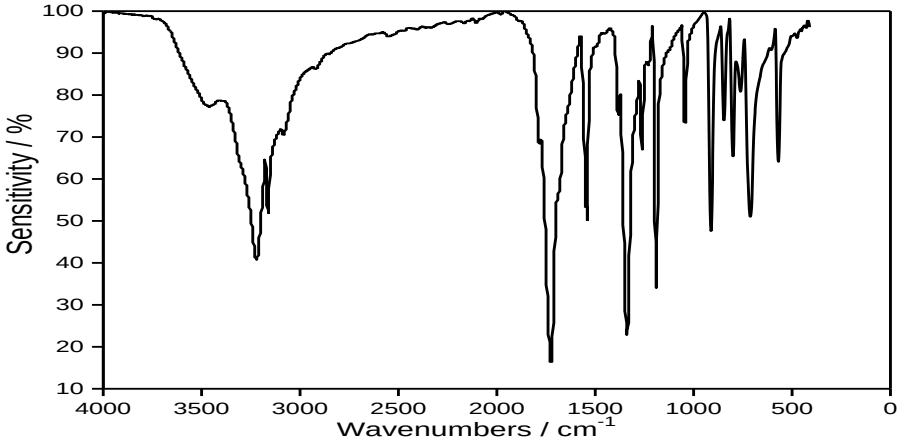

Figure S1. FTIR (KBr) spectrum of ZTO

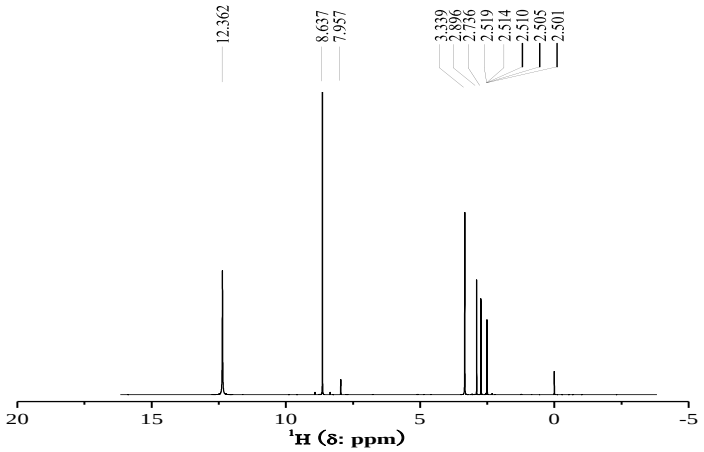

Figure S2. ^{1}H NMR spectrum (400 MHz, d_6–DMSO) of ZTO

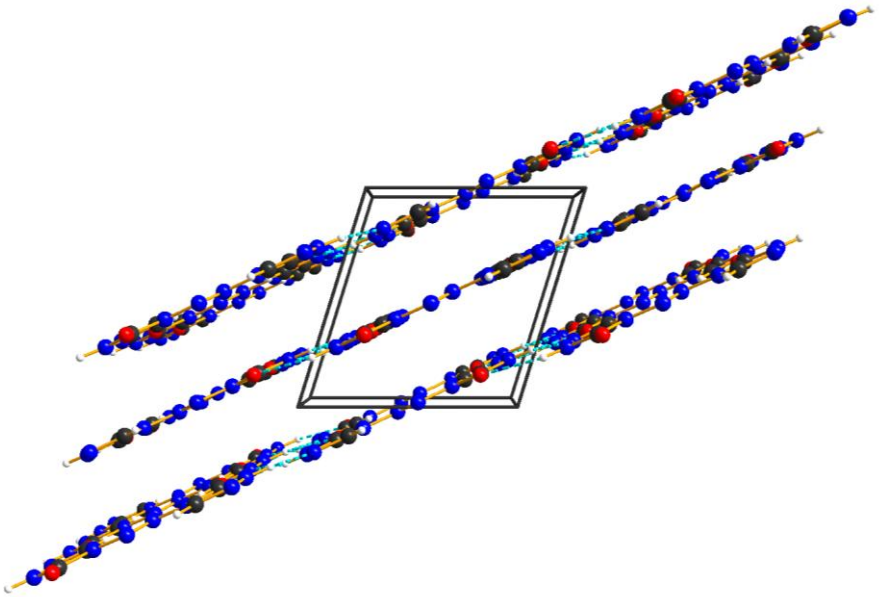

Figure S3. Packing cell of ZTO

Lithium salt (1)

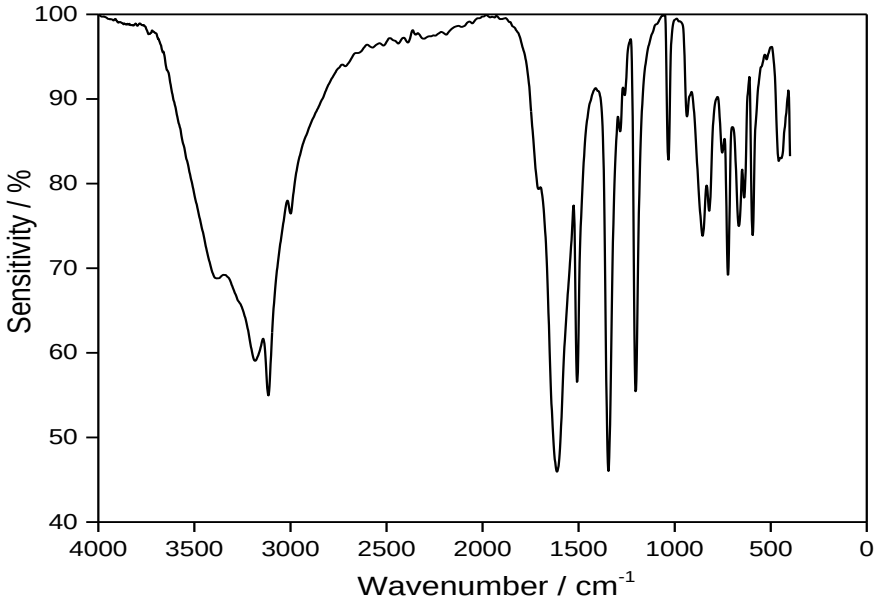

Figure S4. FTIR (KBr) spectrum of salt **1**

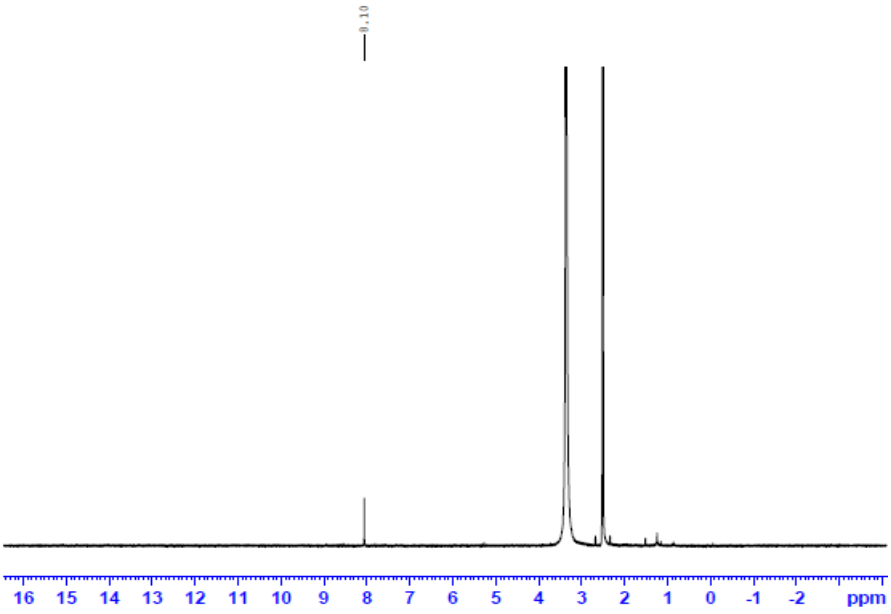

Figure S5. ^{1}H NMR spectrum (400 MHz, d_6–DMSO) of salt **1**

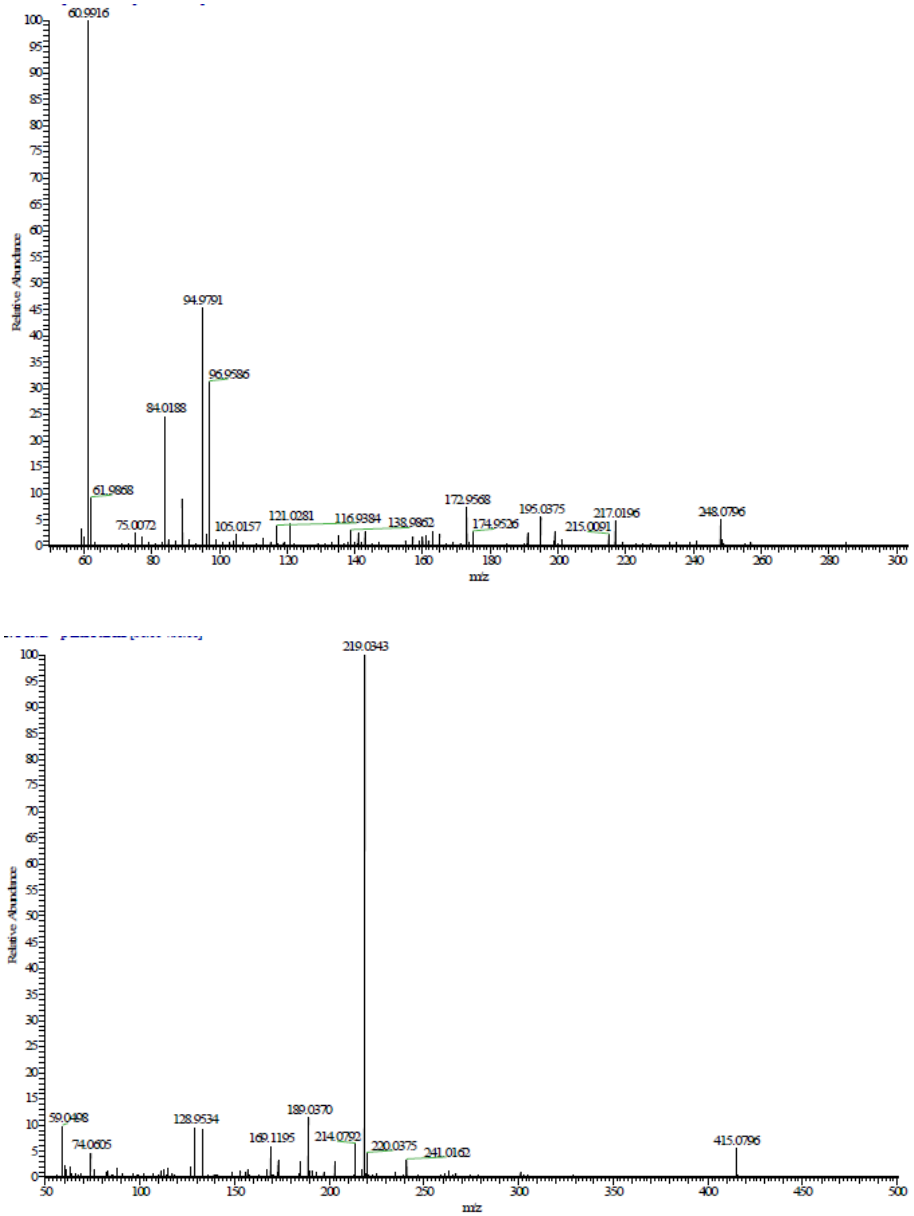

Figure S6. Negative (up) and Positive (down) ESI–MS of salt **1**

Sodium slat (2)

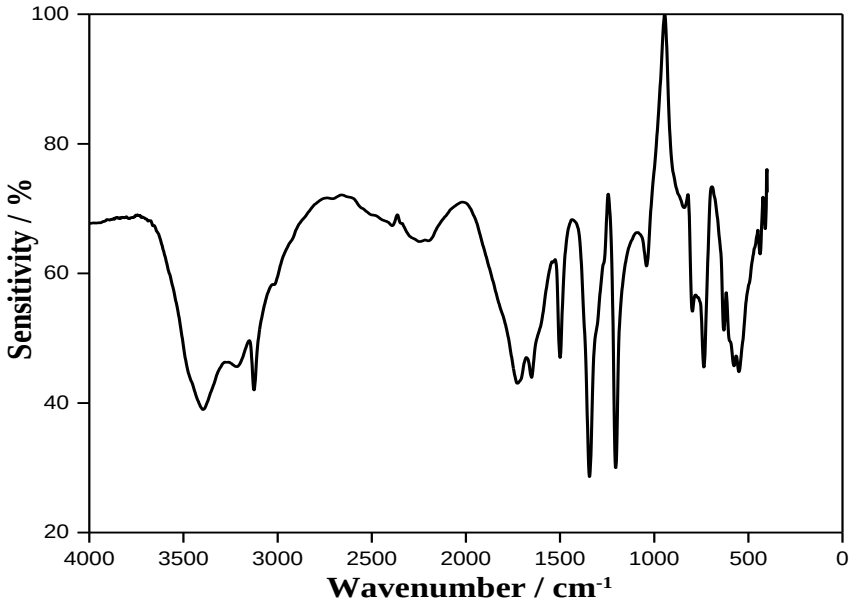

Figure S7. FTIR (KBr) spectrum of salt **2**

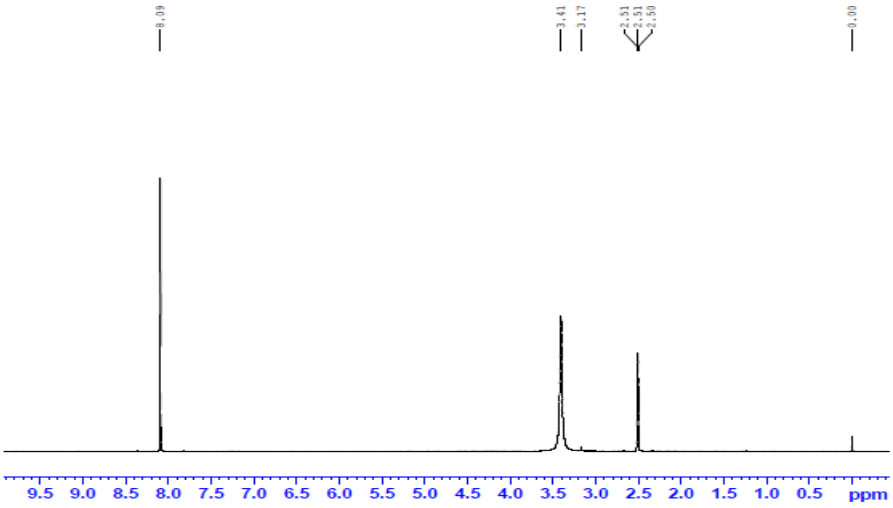

Figure S8. ^{1}H NMR spectrum (400 MHz, d_6–DMSO) of salt **2**

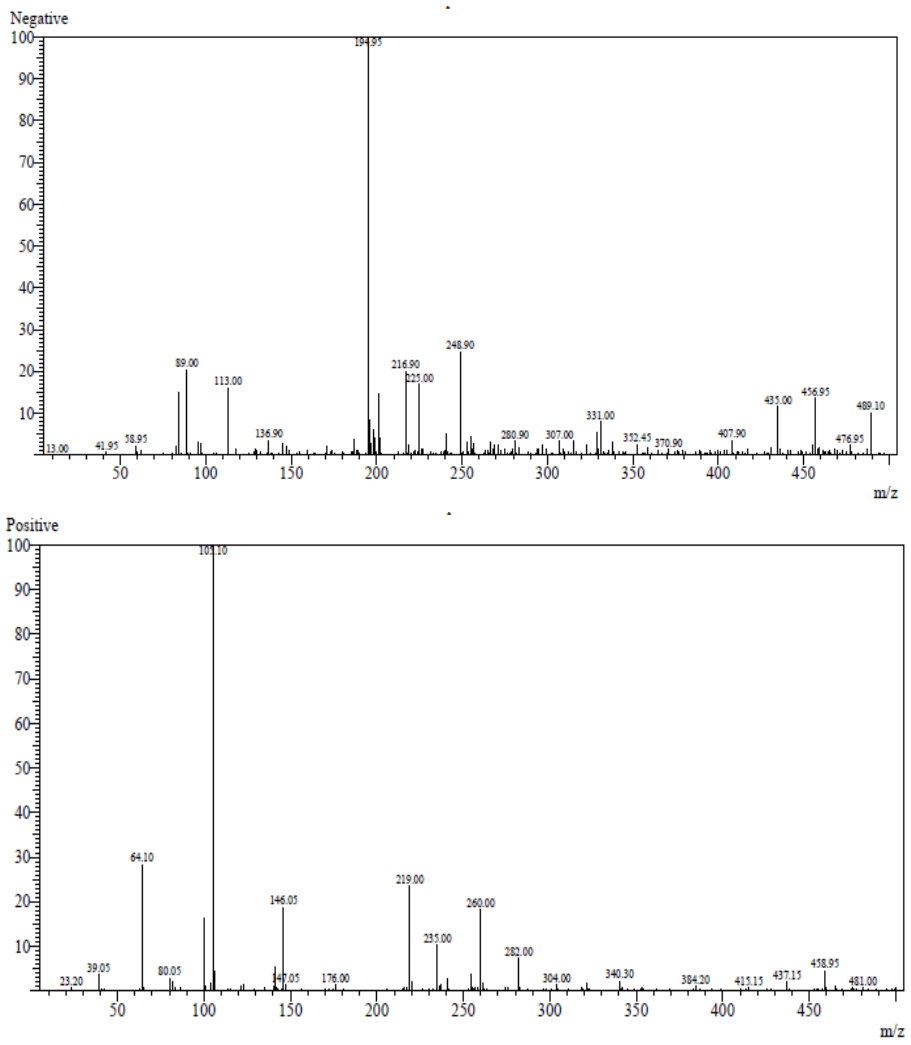

Figure S9. Negative (up) and Positive (down) ESI–MS of salt **2**

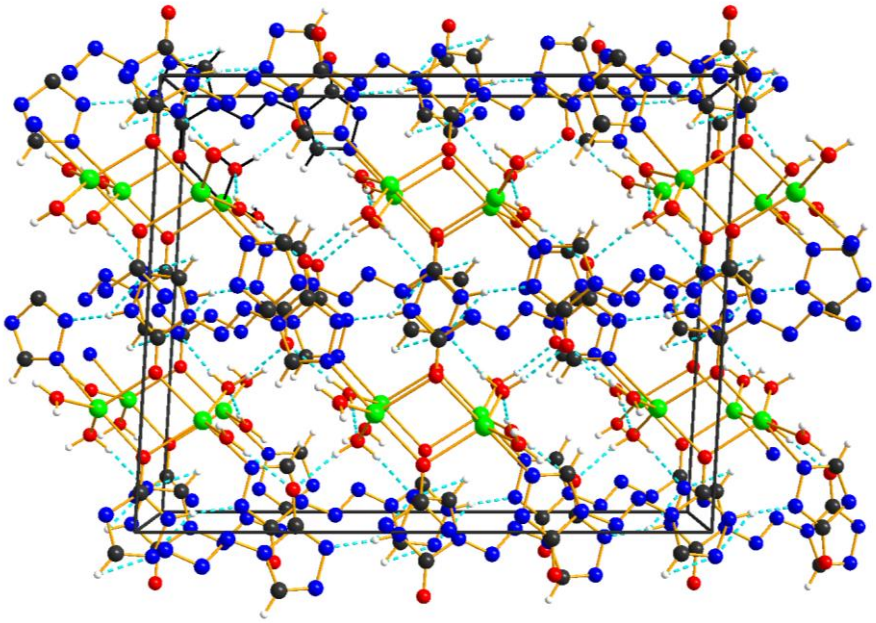

Figure S10. Packing cell of salt **2**

Potassium salt (3)

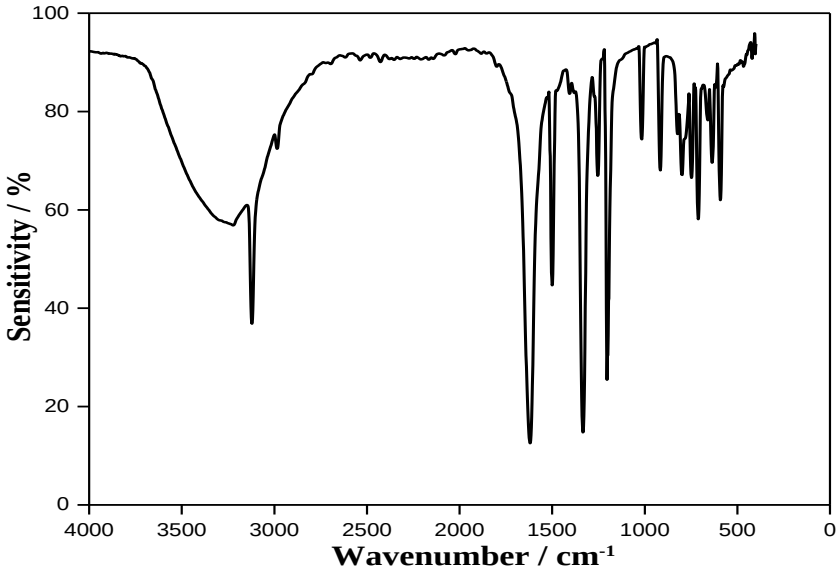

Figure S11. FTIR (KBr) spectrum of salt **3**

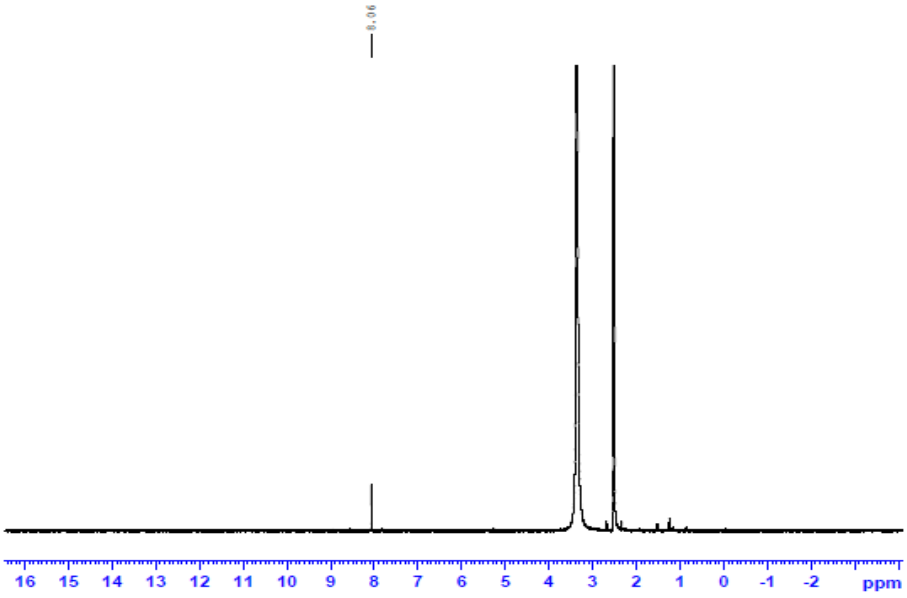

Figure S12. ^{1}H NMR spectrum (400 MHz, d_6–DMSO) of salt **3**

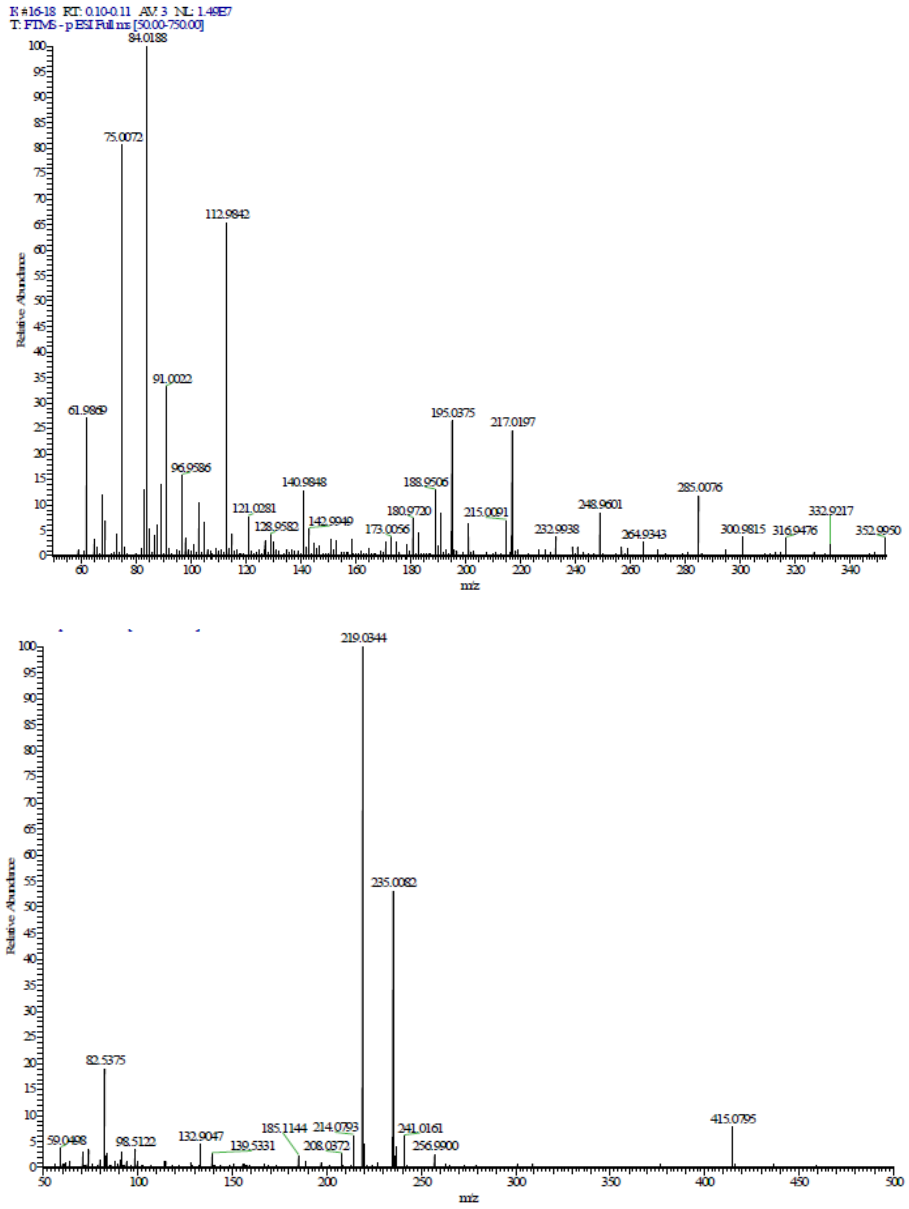

Figure S13. Negative (up) and Positive (down) ESI–MS of salt **3**

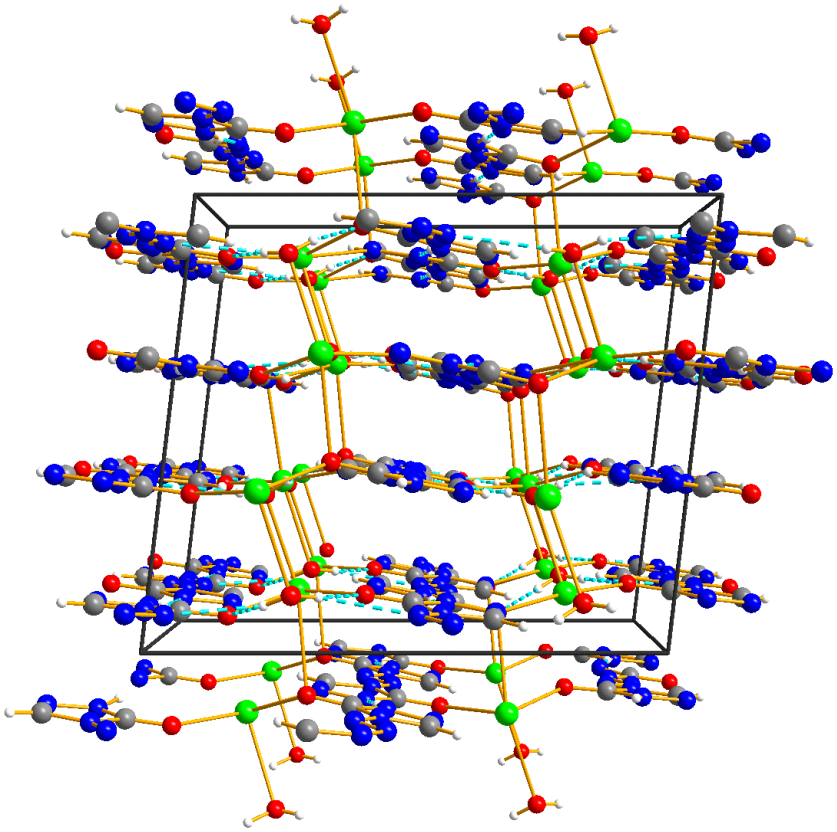

Figure S14. Packing cell of salt **3**

Caesium salt (4)

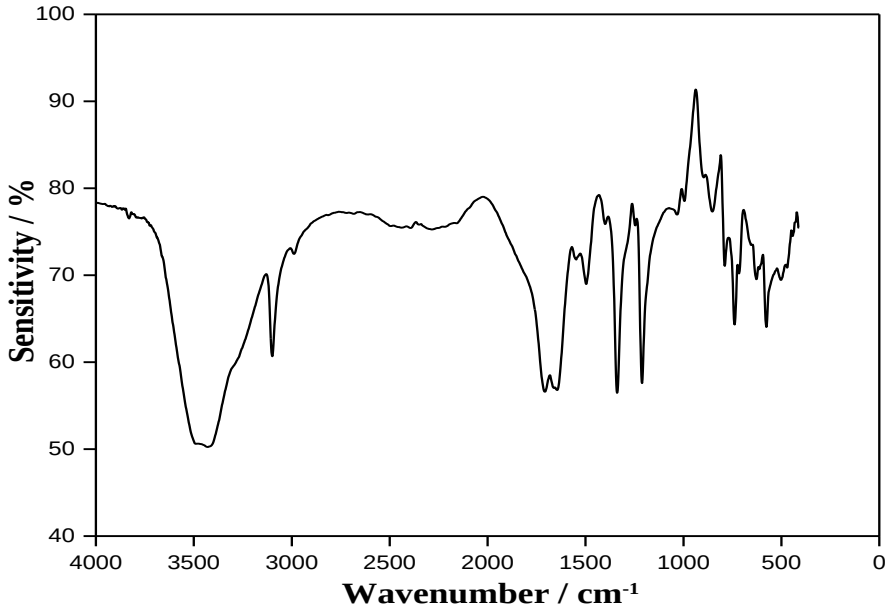

Figure S15. FTIR (KBr) spectrum of salt **4**

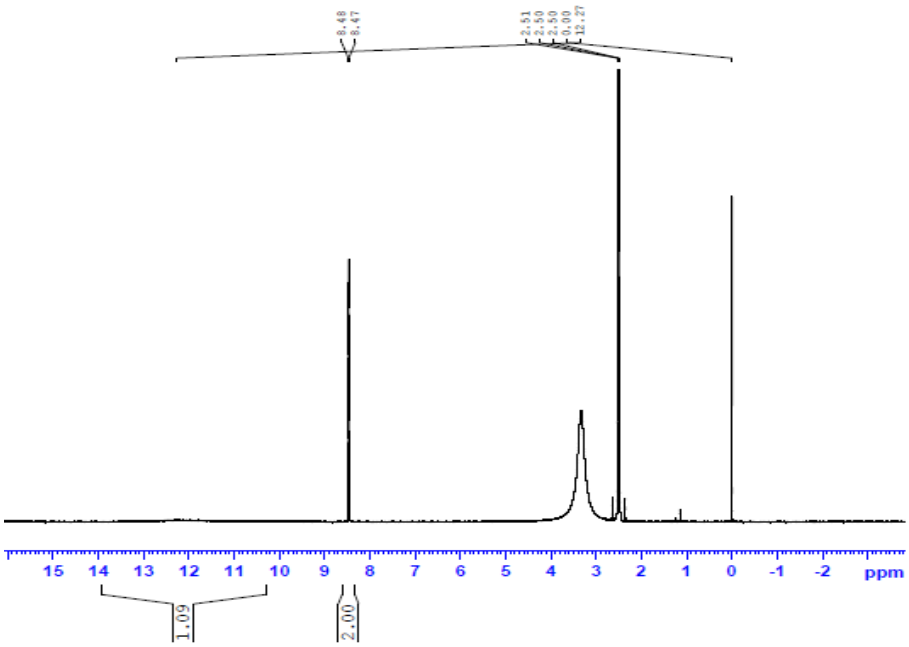

Figure S16. ^{1}H NMR spectrum (400 MHz, d_6–DMSO) of salt **4**

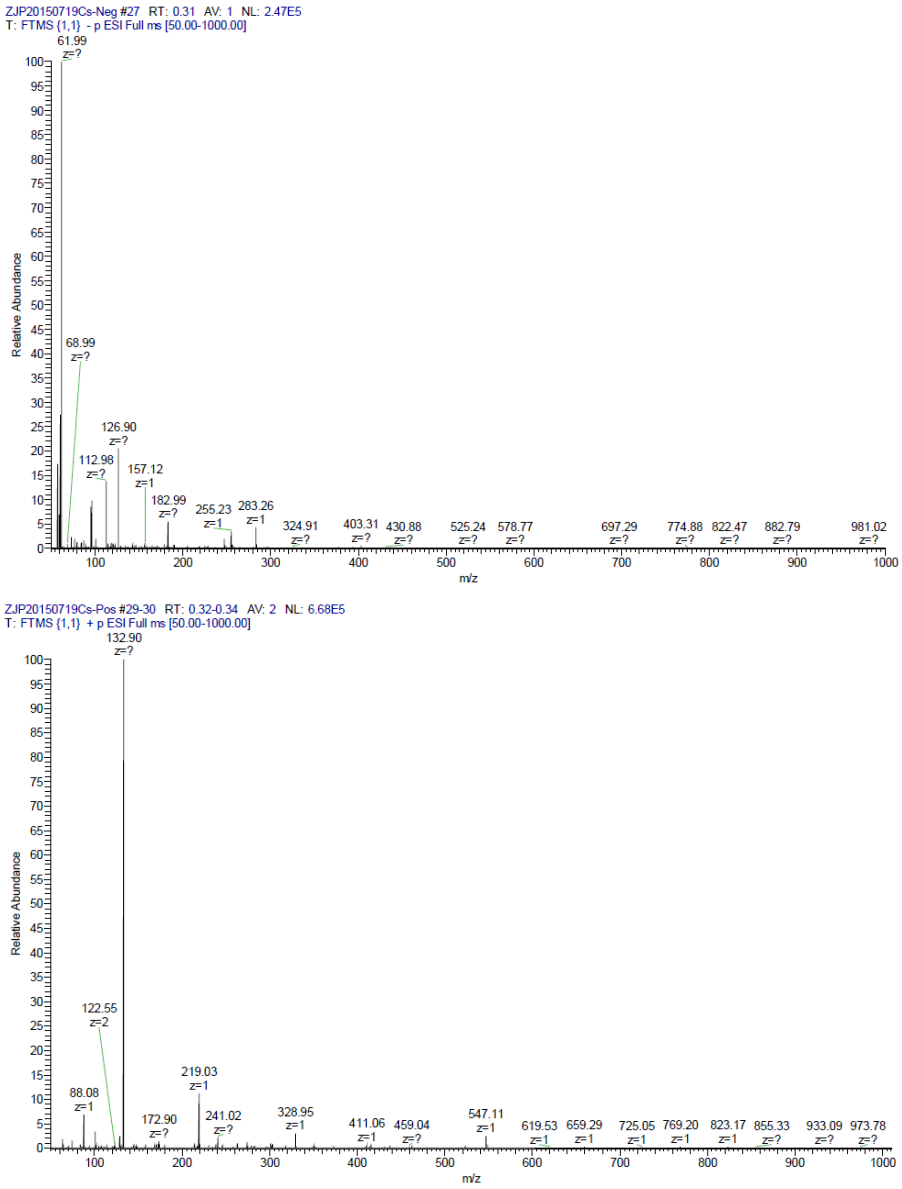

Figure S17. Negative (up) and Positive (down) ESI–MS of salt **4**

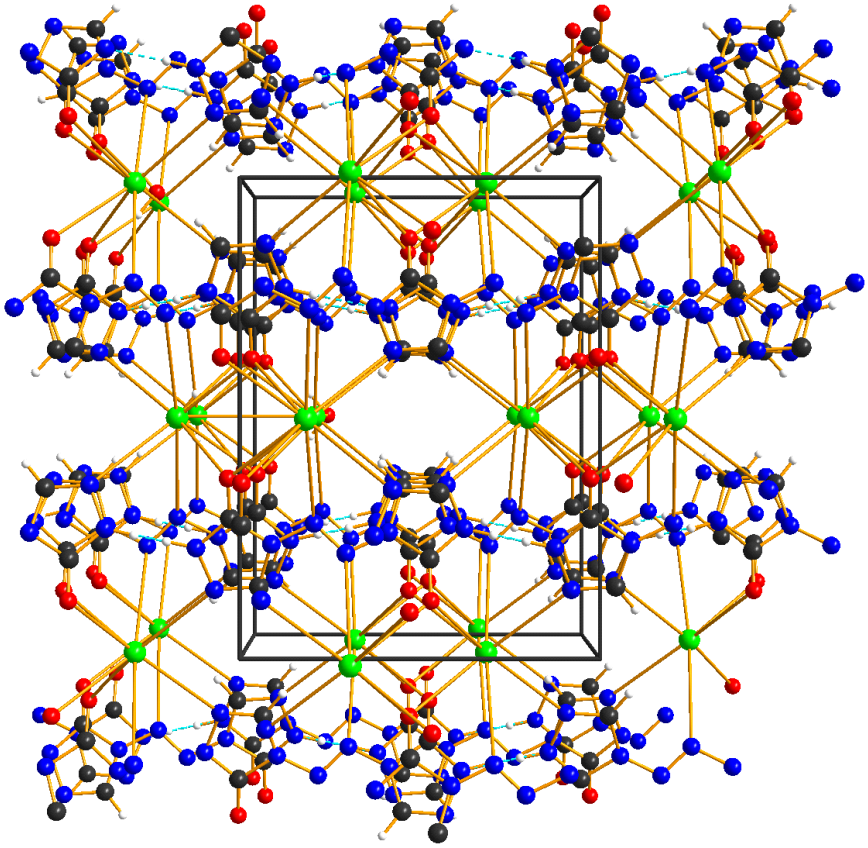

Figure S18. Packing cell of salt **4**

Hydrazine salt (5)

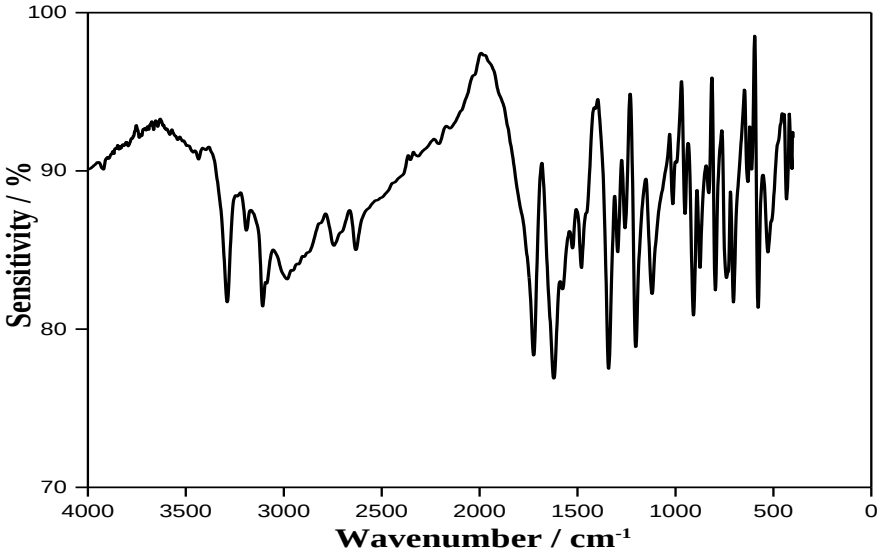

Figure S19. FTIR (KBr) spectrum of salt **5**

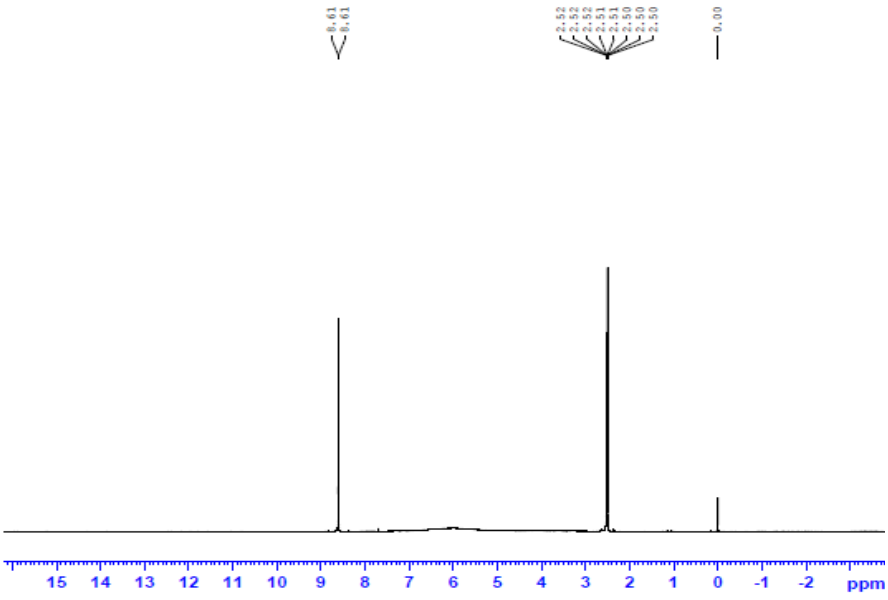

Figure S20. ^{1}H NMR spectrum (400 MHz, d_6–DMSO) of salt **5**

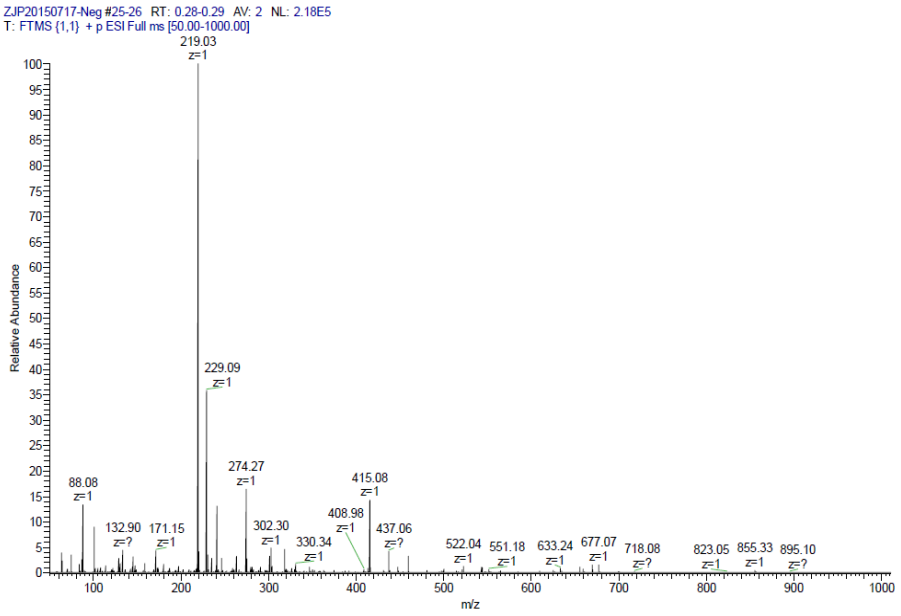

Figure S21. Negative ESI–MS of salt **5**

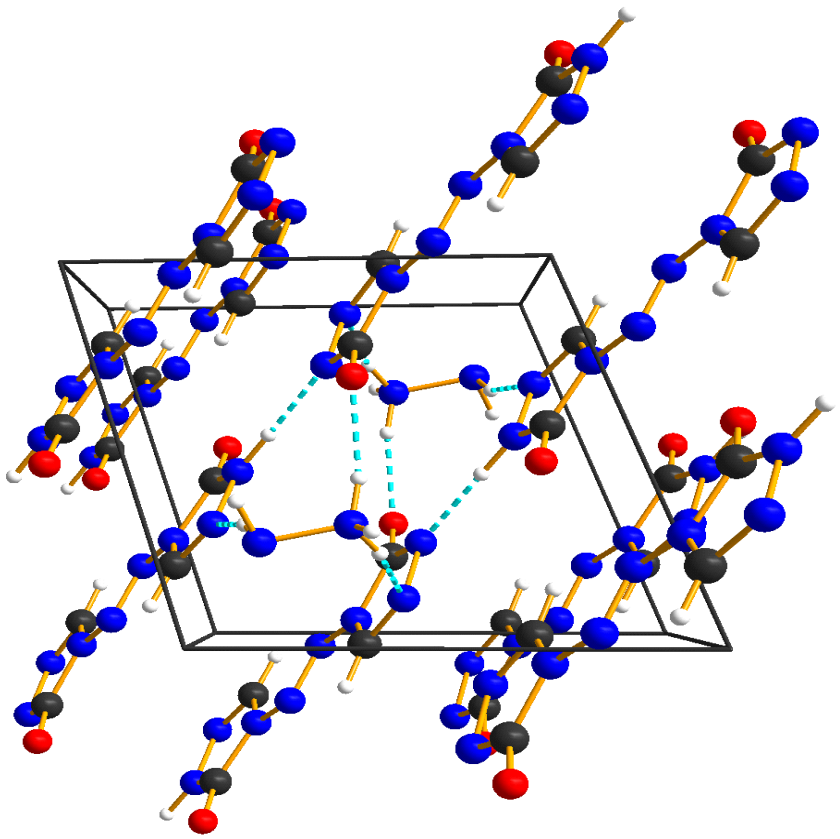

Figure S22. Packing cell of salt **5**

Magnesium salt (6)

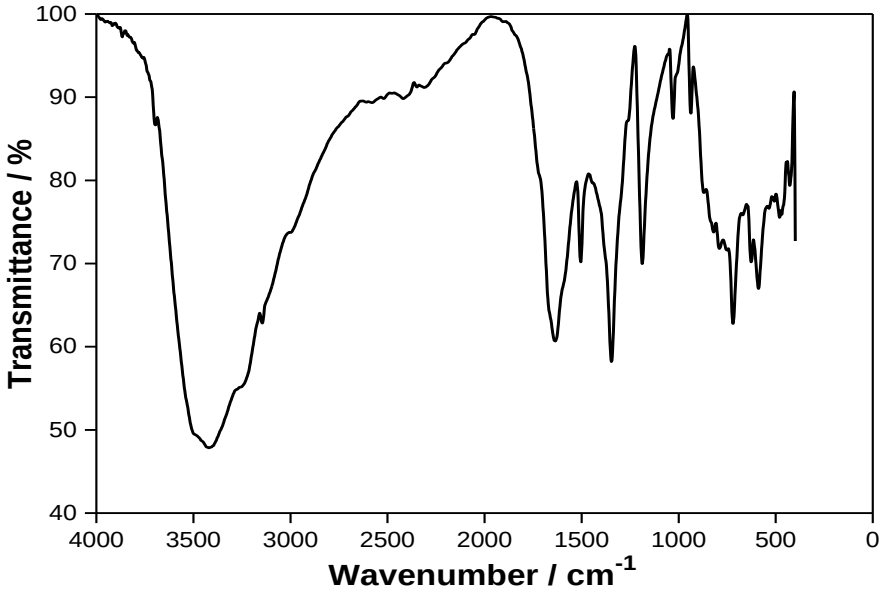

Figure S23. FTIR (KBr) spectrum of salt **6**

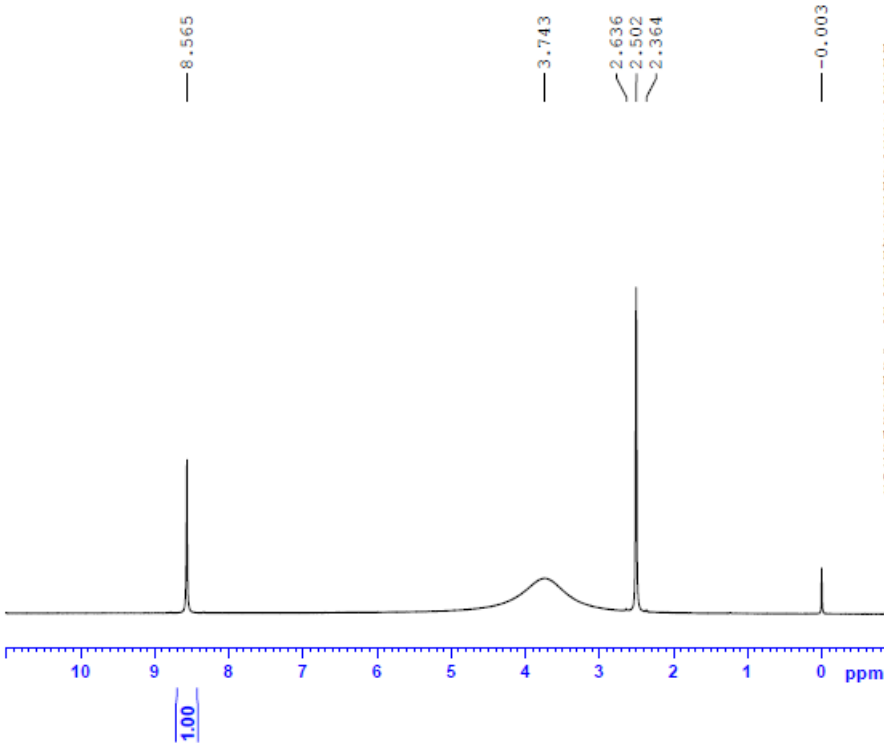

Figure S24. ^{1}H NMR spectrum (400 MHz, d_6–DMSO) of salt **6.**

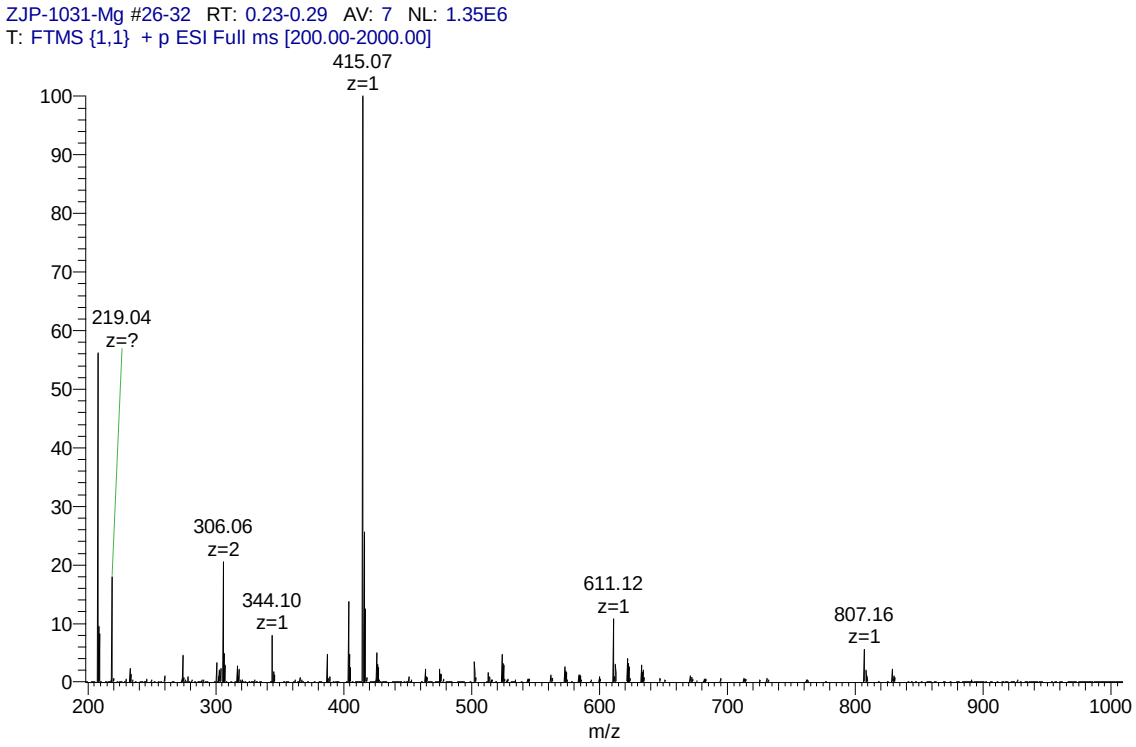

Figure S25. ESI – MS of salt **6**

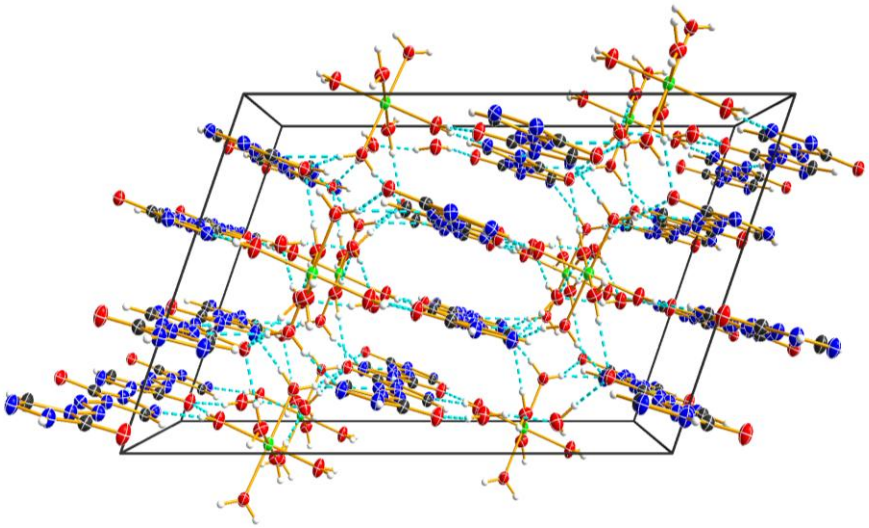

Figure S26. Packing cell of salt **6**

Calcium salt (7)

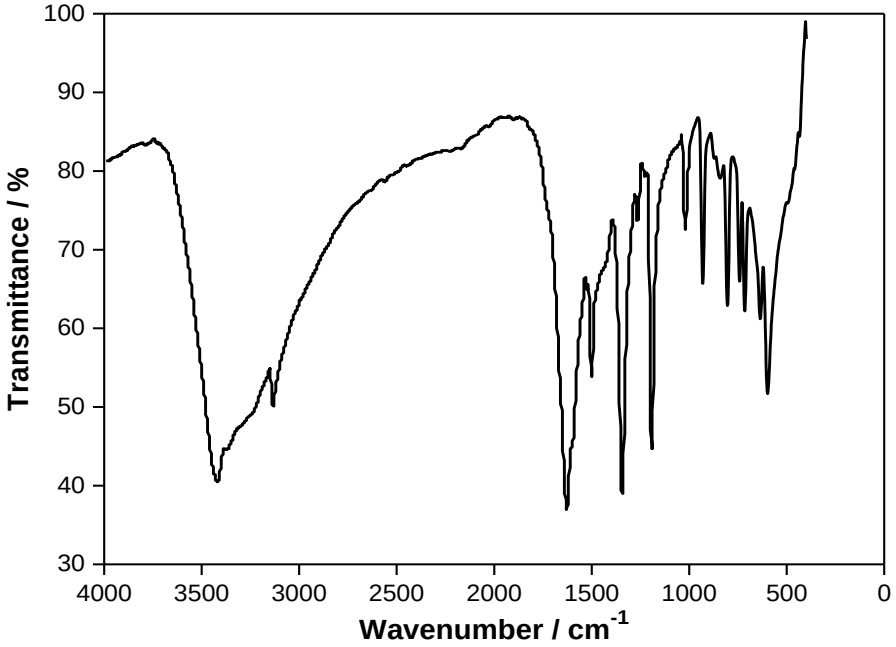

Figure S27. FTIR (KBr) spectrum of salt **7**

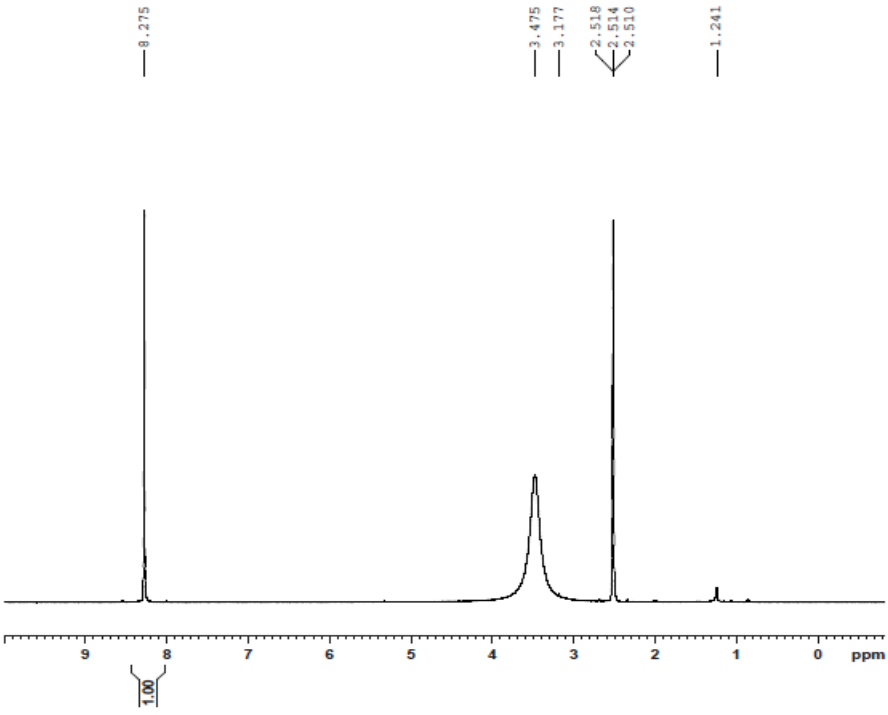

Figure S28. ^{1}H NMR spectrum (400 MHz, d_6–DMSO) of salt **7**

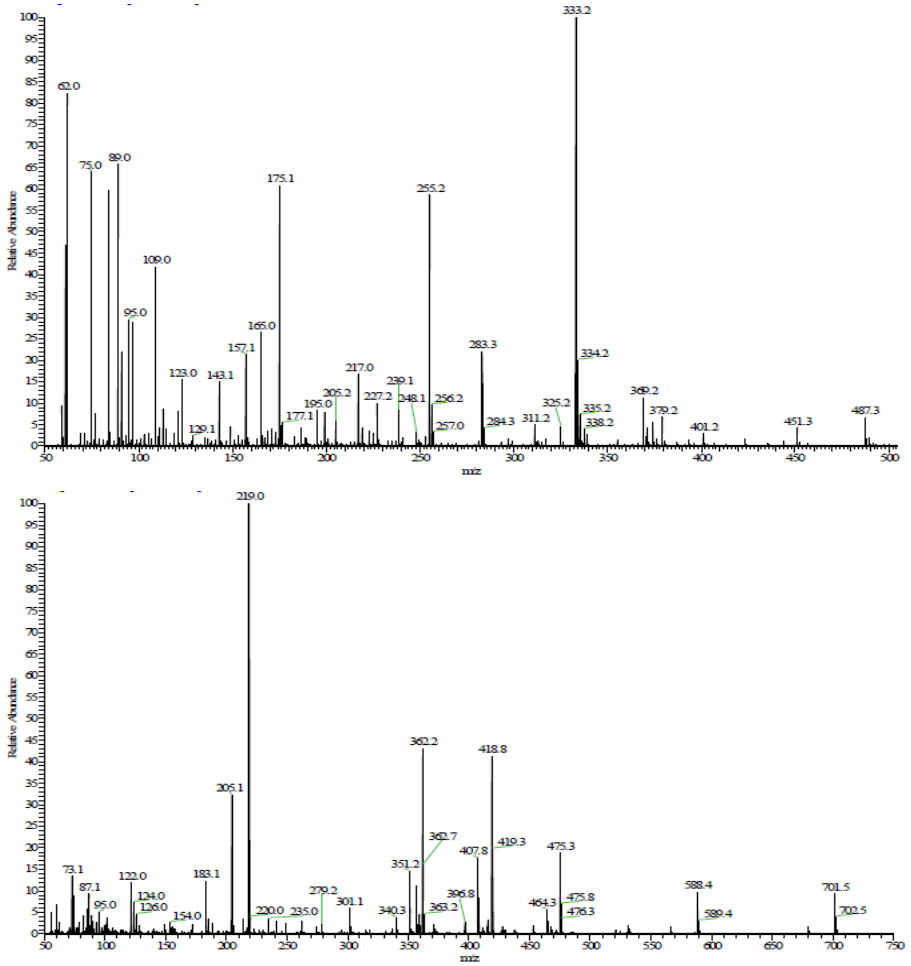

Figure 29. Negative (up) and Positive (down) ESI–MS of salt **7**

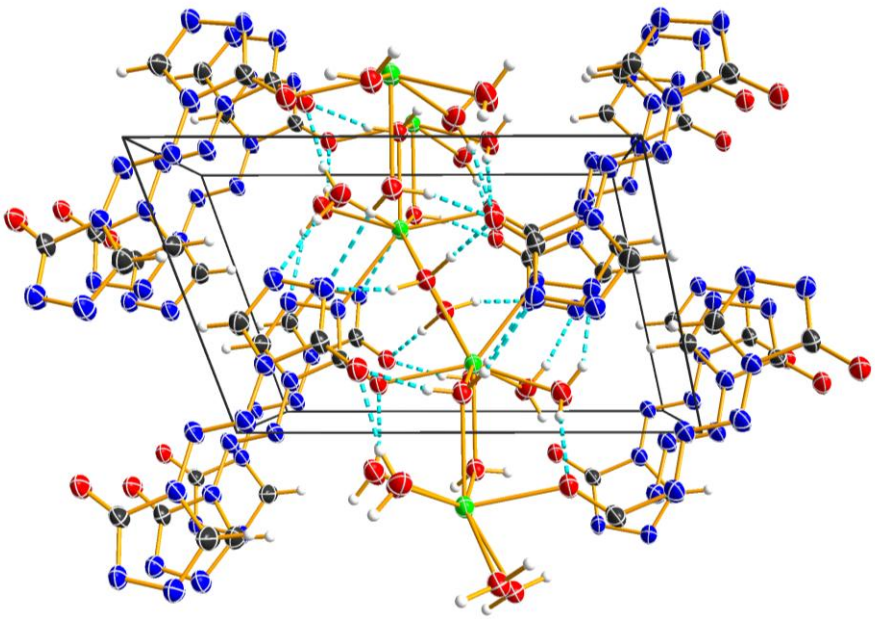

Figure S30. Packing cell of salt **7**

Strontium salt (8)

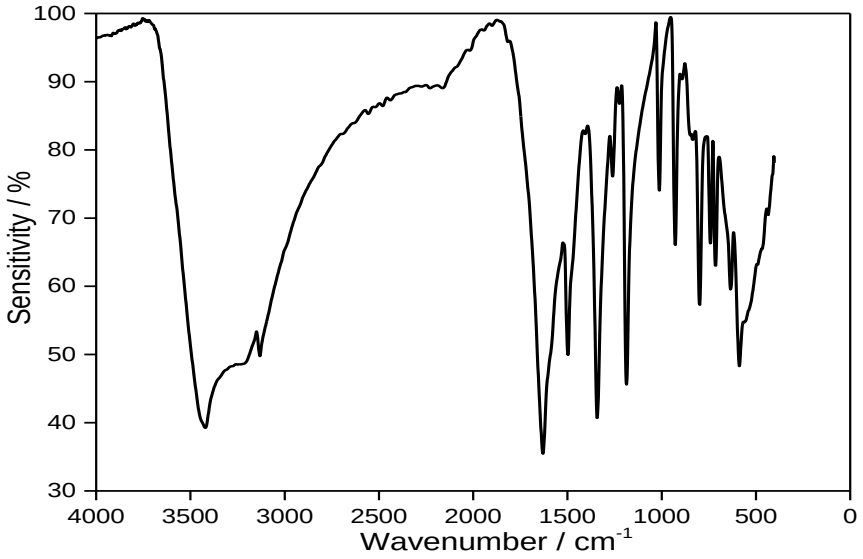

Figure 31. FTIR (KBr) spectrum of salt **8**

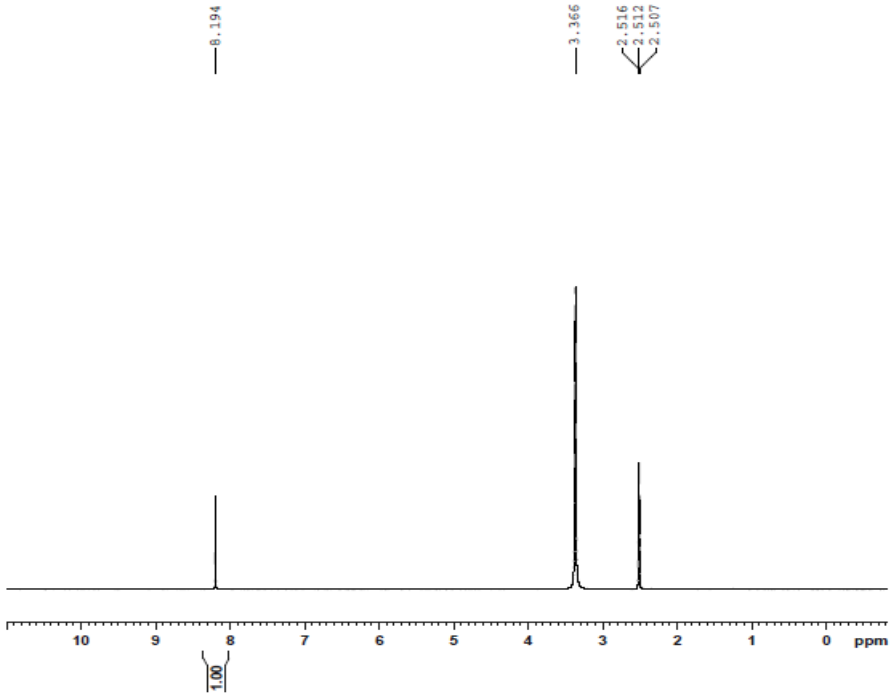

Figure S32. ^{1}H NMR spectrum (400 MHz, d_6–DMSO) of salt **8**

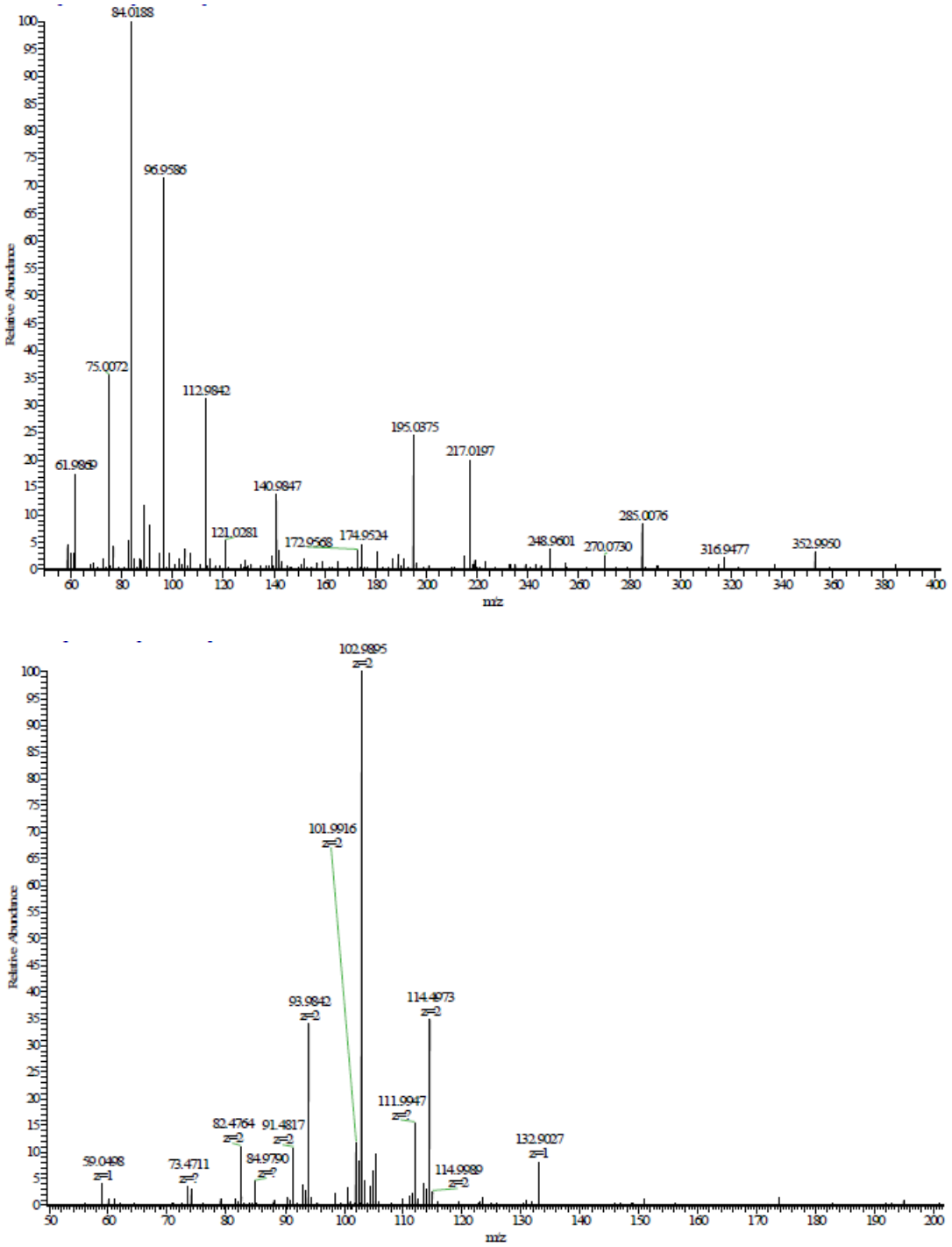

Figure 33. Negative (up) and Positive (down) ESI–MS of salt **8**

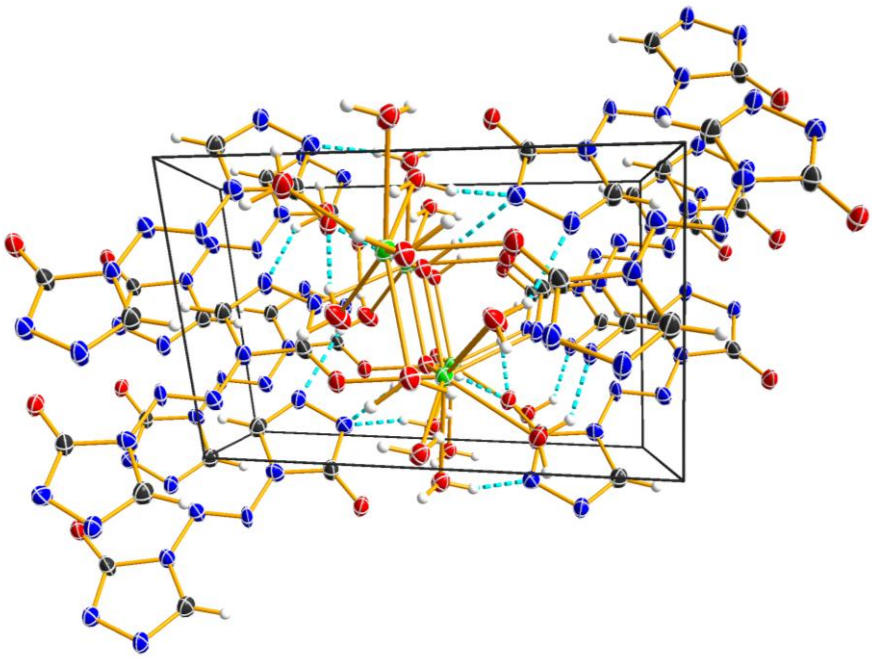

Figure S34. Packing cell of salt **8**

Barium salt (9)

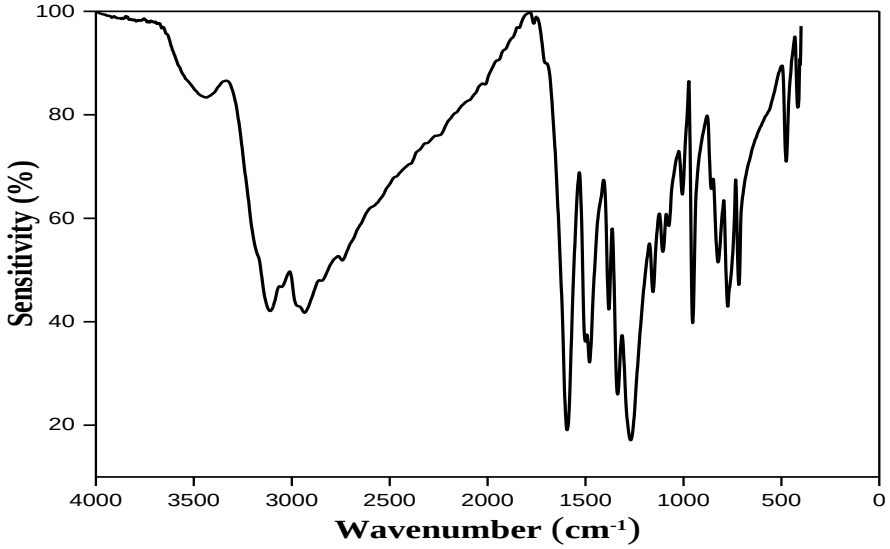

Figure S35. FTIR (KBr) spectrum of salt **9**

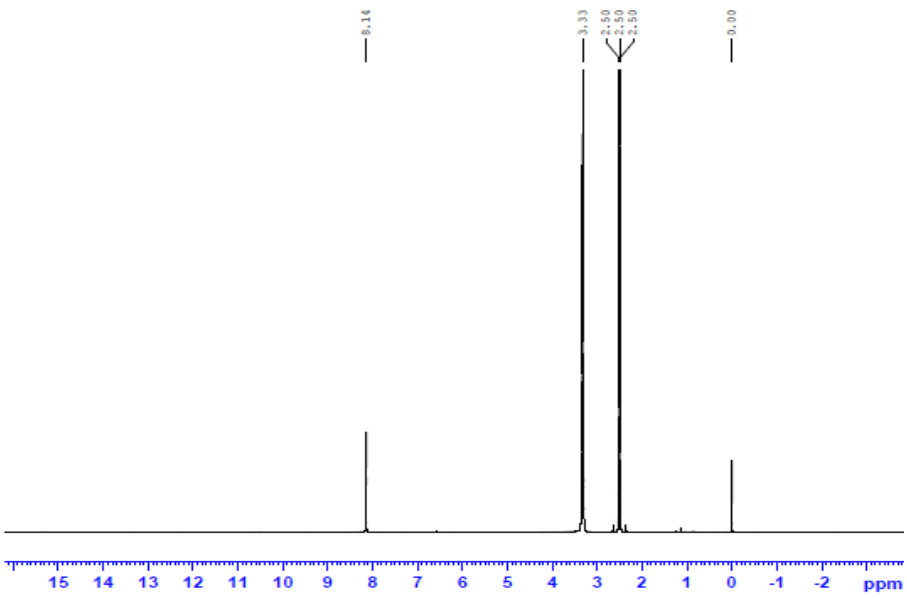

Figure S36. ^{1}H NMR spectrum (400 MHz, d_6–DMSO) of salt **9**

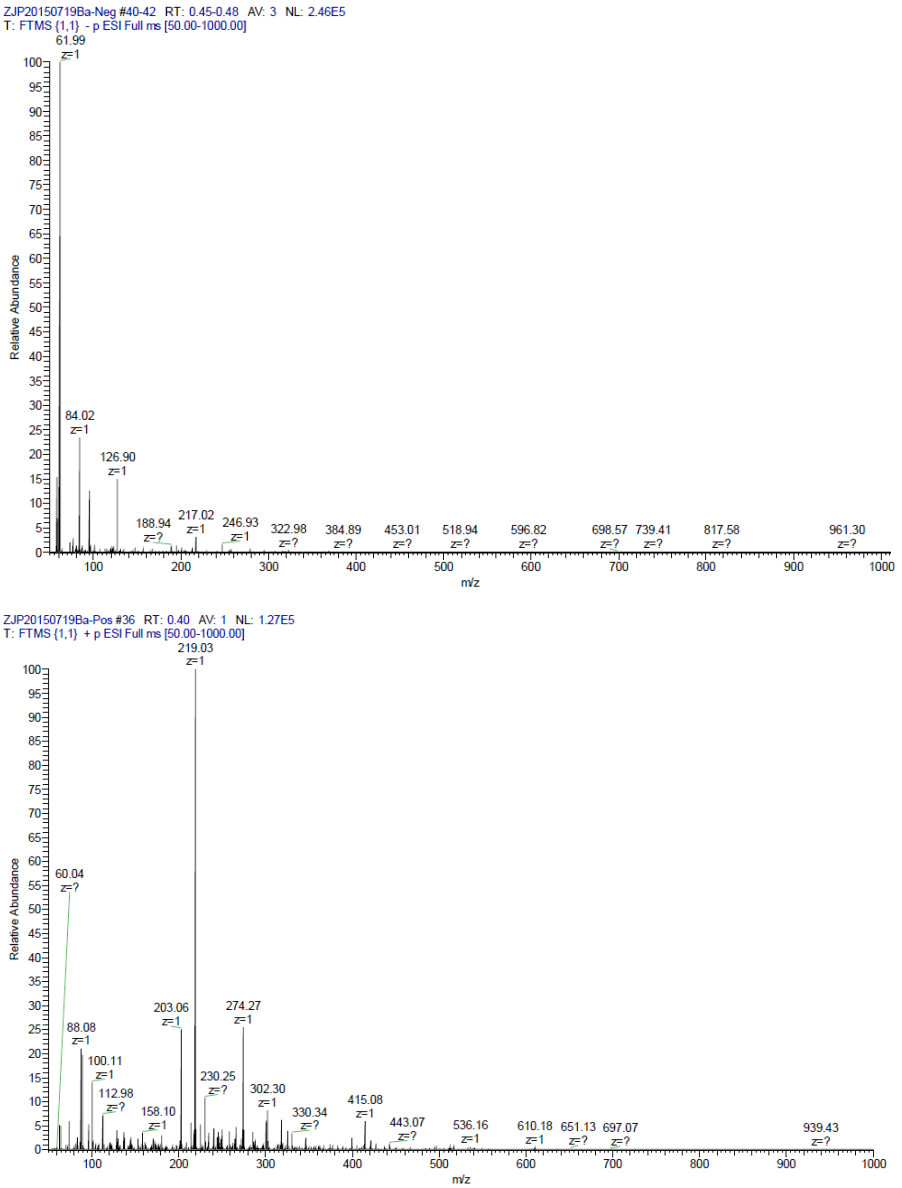

Figure S37. Negative (up) and Positive (down) ESI–MS of salt **9**

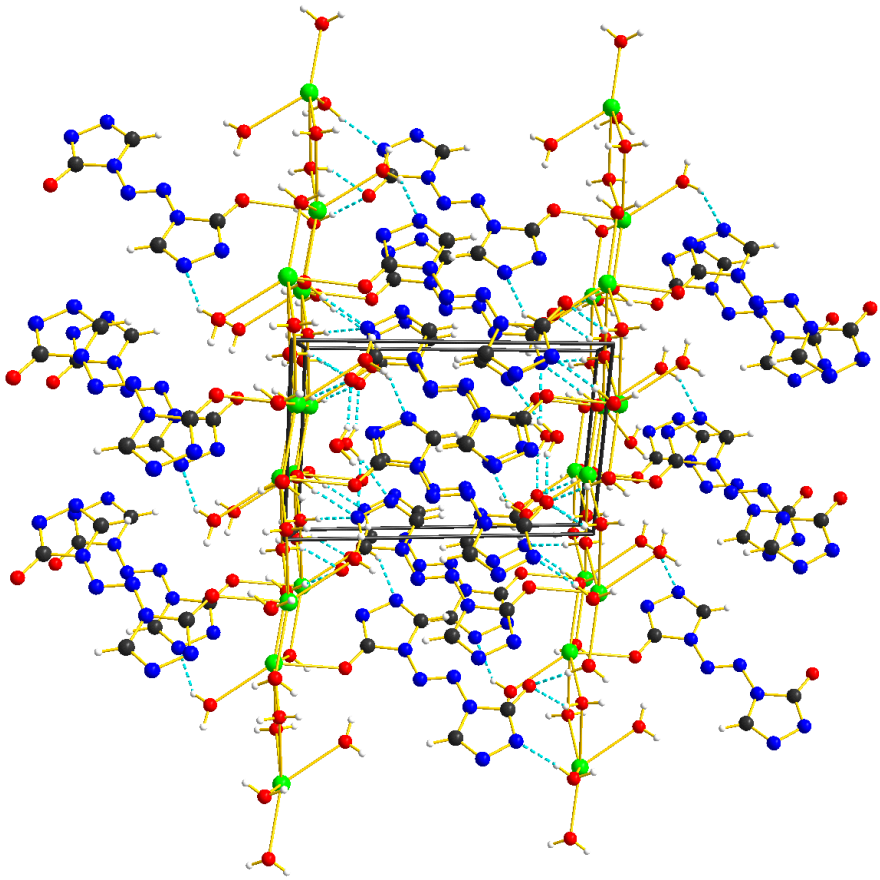

Figure S38. Packing cell of salt **9**

Thermal analysis

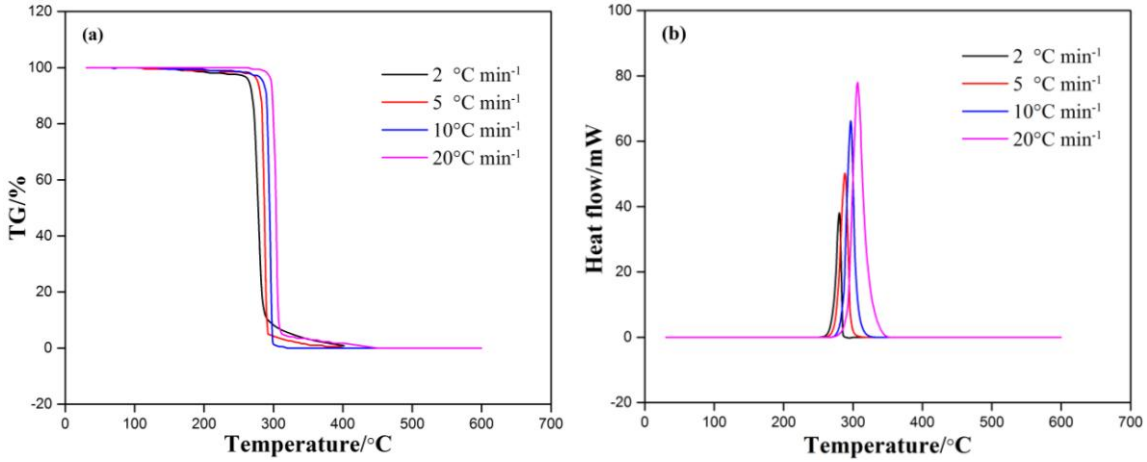

Figure S39. TG (a) and DTA (b) of ZTO at different heating rates

5

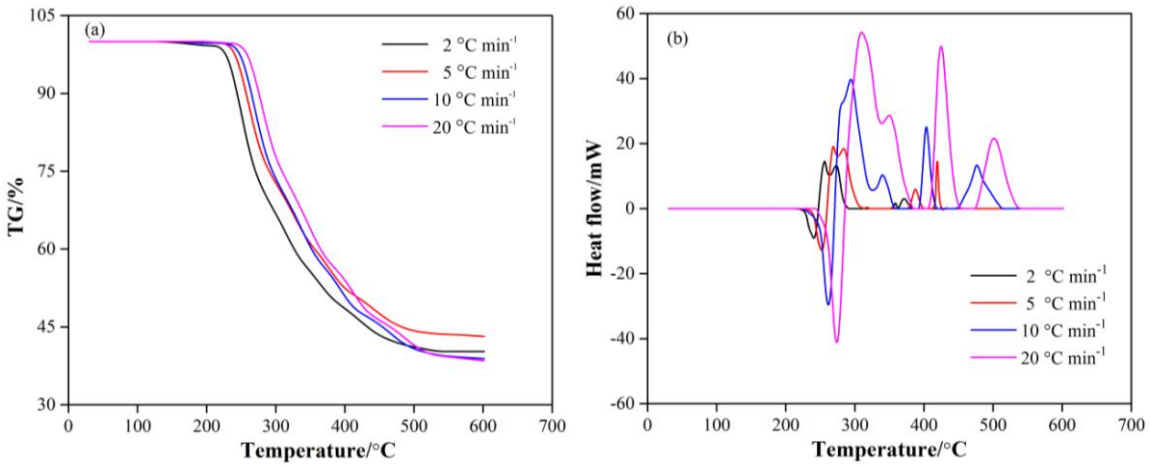

Figure S40. TG (a) and DTA (b) of **1** at different heating rates

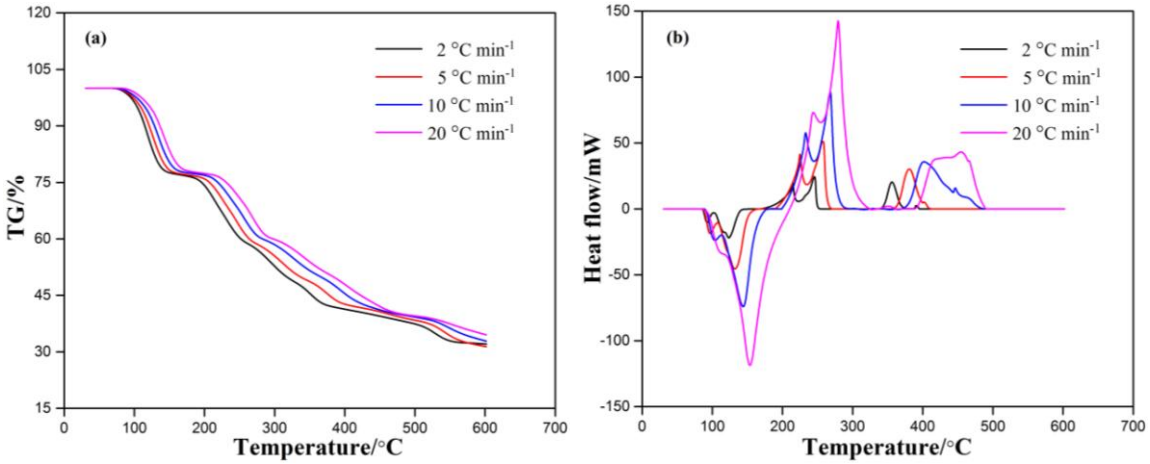

Figure S41. TG (a) and DTA (b) of **2** at different heating rates

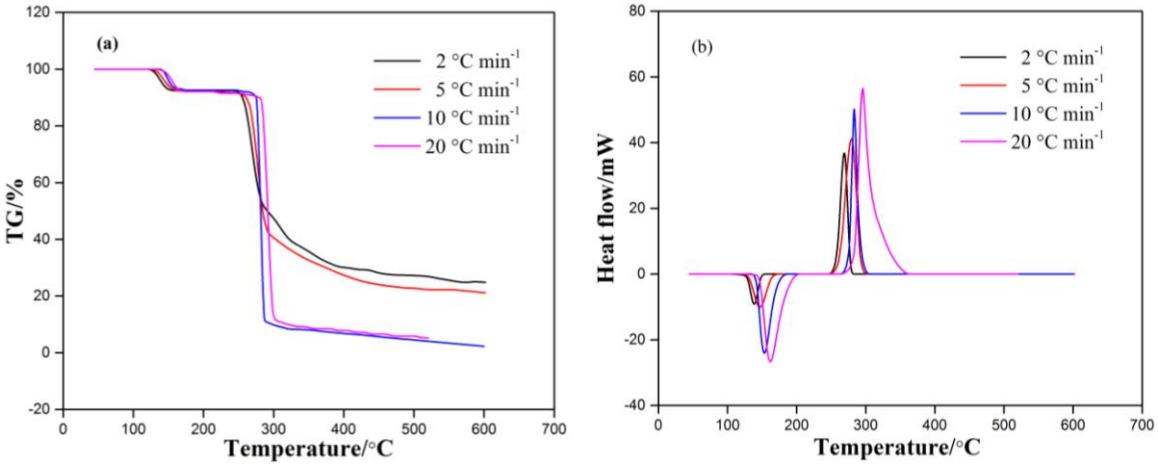

Figure S42. TG (a) and DTA (b) of **3** at different heating rates

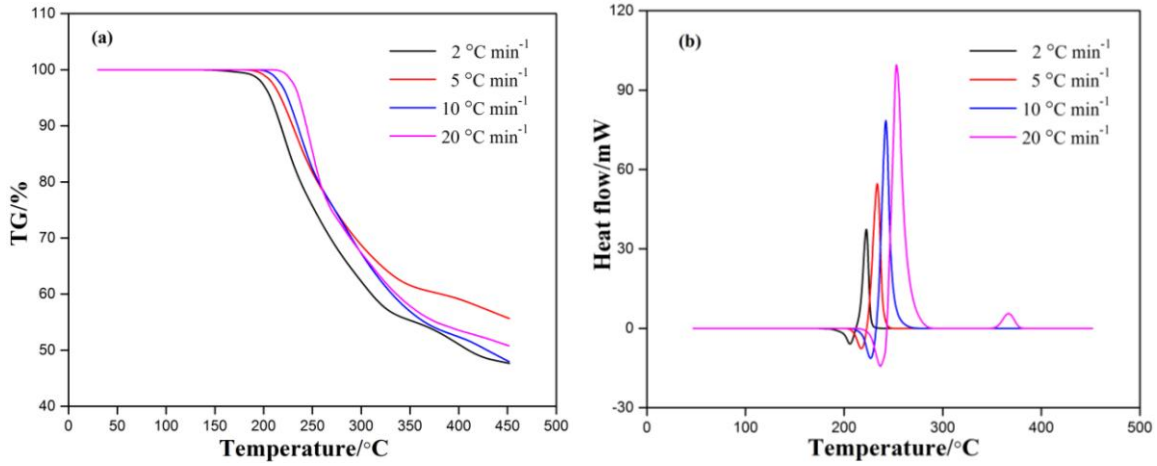

Figure S43. TG (a) and DTA (b) of **4** at different heating rates

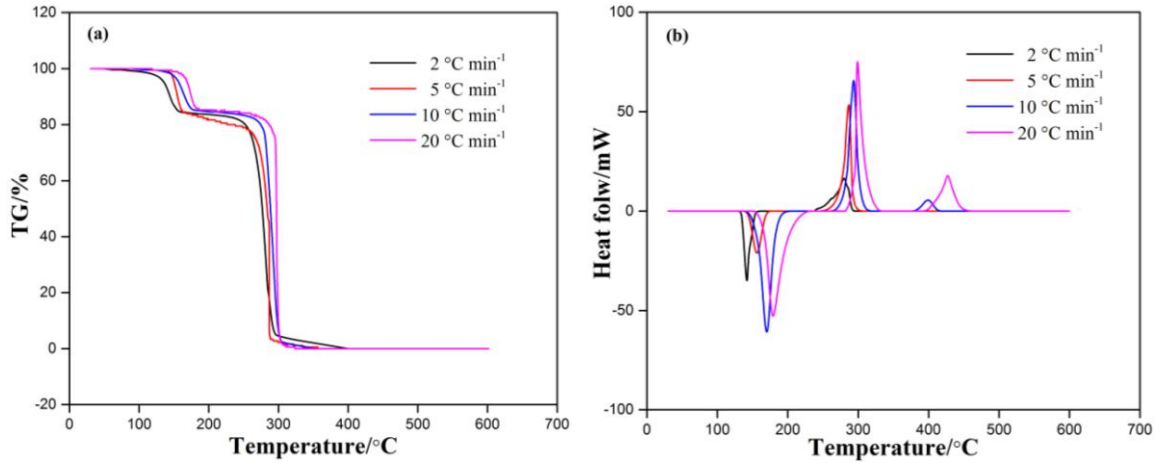

Figure S44. TG (a) and DTA (b) of **5** at different heating rates

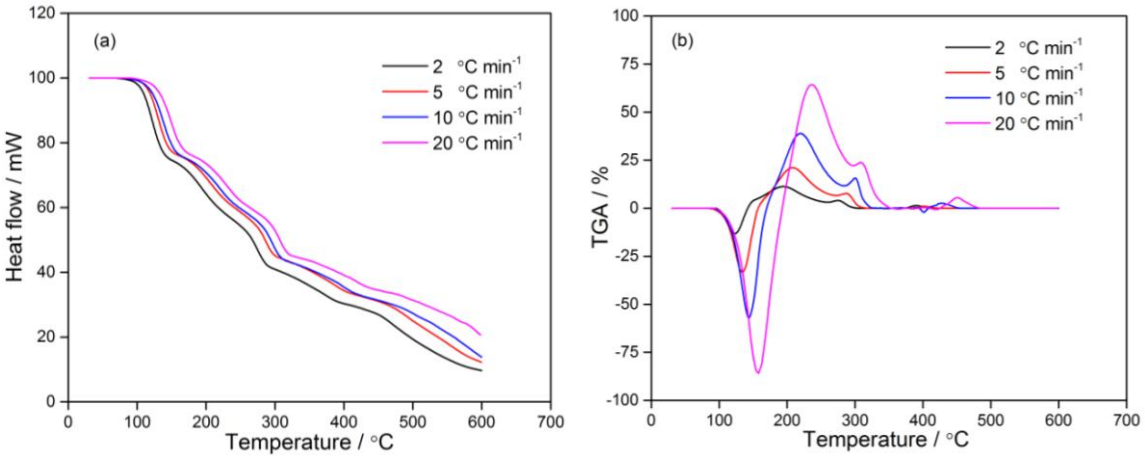

Figure S45. TG (a) and DTA (b) of **6** at different heating rates

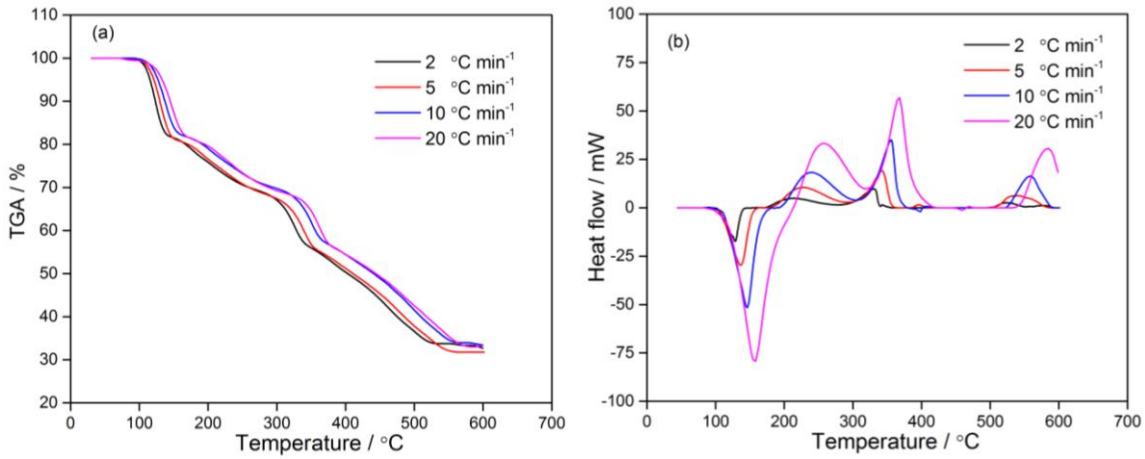

Figure S46. TG (a) and DTA (b) of **7** at different heating rates

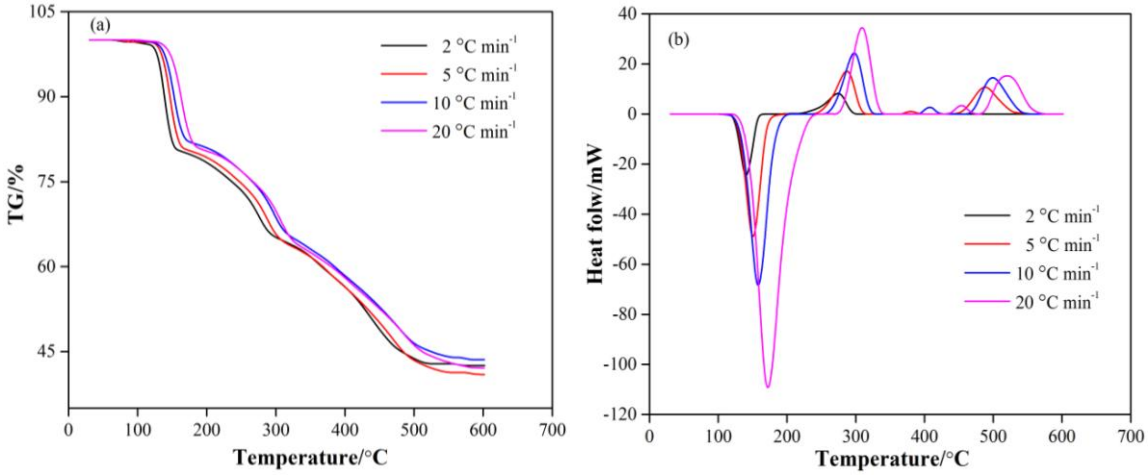

Figure S47. TG (a) and DTA (b) of **8** at different heating rates

5

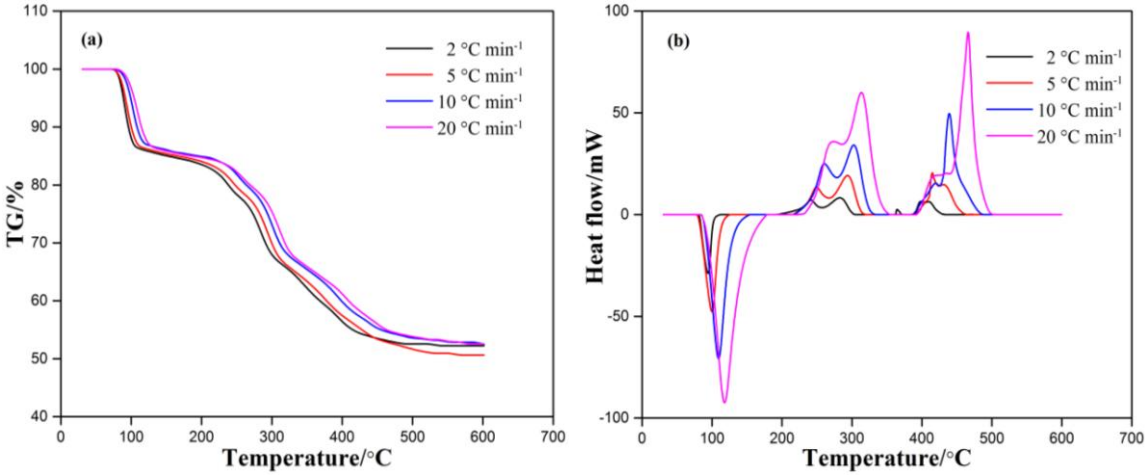

Figure S48. TG (a) and DTA (b) of **9** at different heating rates

Table

Table S1 Crystal structure solution and refinement for ZTO and its salts **2**–**9**.

	ZTO	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**
Chemical formula	$C_4H_4N_8O_2$	$C_4H_7N_8NaO_4$	$C_8H_{10}N_{16}K_2O_6$	$C_4H_5CsN_8O_3$	$C_4H_8N_{10}O_2$	$C_8H_{26}N_{16}O_{14}Mg$	$C_8H_{26}N_{16}O_{14}Ca$	$C_4H_{10}N_8O_6Sr$	$C_8H_{20}N_{16}O_{12}Ba_2$
Mw /g mol^{-1}	196.15	254.17	504.52	344.05	228.20	594.76	612.56	699.58	807.08
Crystal size /mm	0.37×0.20×0.14	0.18×0.17×0.16	0.37×0.16×0.15	0.21×0.20×0.19	0.22×0.20×0.18	0.19×0.11×0.07	0.13×0.09×0.05	0.09×0.06×0.03	0.22×0.12×0.08
Crystal system	Monoclinic	Monoclinic	Monoclinic	Orthorhombic	Triclinic	Monoclinic	Triclinic	Triclinic	Triclinic
Crystal group	*P*2$_1$/*c*	*C*2/*c*	*P*2$_1$/*c*	*Pnna*	*P*–1	*C*2/*c*	*P*–1	*P*–1	*P*–1
a/ Å	7.581(3)	19.421(15)	14.345(4)	6.8101(13)	7.7212(5)	19.528(5)	7.555(3)	7.603(3)	7.6249(18)
b/ Å	6.325(3)	6.514(5)	10.332(3)	13.764(3)	8.2866(5)	10.445(3)	7.692(3)	7.714(2)	7.8460(16)
c/ Å	7.891(4)	15.382(12)	12.600(4)	10.311(2)	8.3755(5)	12.557(3)	11.022(5)	11.324(4)	11.723(3)
α/ °	90	90	90	90	62.6840(10)	90	75.555(15)	73.482(16)	70.520(8)
β/ °	107.344(5)	93.234(16)	96.748(3)	90	71.5710(10)	110.294(2)	87.243(16)	86.381(18)	85.079(10)
γ/ °	90	90	90	90	83.2530(10)	90	61.775(12)	63.029(9)	64.007(7)
v/ Å^3	361.1(3)	1943(3)	1854.7(9)	966.6(3)	451.47(5)	2402(11)	544.7(4)	565.8(3)	592.8(2)
z	2	8	4	4	2	4	1	2	1
$\rho_{calc.}$ /g cm^{-3}	1.804	1.738	1.807	2.378	1.679	1.644	1.867	2.077	2.261
μ mm^{-1}	0.150	0.187	0.584	3.842	0.138	0.173	0.622	4.809	3.392
F(000)	200	1040	1024	656	236	1240	316	352	388
θ range / °	2.81–31.51	2.10–24.86	2.56–31.48	2.47–25.01	2.77–25.14	3.06–31.49	3.07–31.53	3.09–31.49	2.98–31.50
Λ (Mokα)/Å	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Temp. /K	153(2)	293(2)	153(2)	296(2)	296(2)	153(2)	153(2)	153(2)	153(2)
Refl. collected	3404	4338	22348	5565	2911	11865	8063	8470	8849
Refl. unique	1194	1668	6095	850	1602	3922	3488	3665	3870
R (int)	0.0218	0.0669	0.0455	0.0153	0.0107	0.0256	0.0811	0.0844	0.0310
Data /rest. /param.	1194/0/68	1668/4/170	6095/0/314	850/0/74	1602/0/158	3922/0/222	3488/13/194	3665/12/190	3870/14/205
GOOF	1.003	1.091	1.003	1.067	1.048	1.002	0.842	0.897	1.000
R_1, wR_2 [$I>2\sigma(I)$]	R_1 = 0.0392	R_1 = 0.0631	R_1 = 0.0545	R_1 = 0.0133	R_1 = 0.0359	R_1 = 0.0387	R_1 = 0.0801	R_1 = 0.0701	R_1 = 0.0332
	wR_2 = 0.0968	wR_2 = 0.1552	wR_2 = 0.1371	wR_2 = 0.0323	wR_2 = 0.0962	wR_2 = 0.0932	wR_2 = 0.2191	wR_2 = 0.1832	wR_2 = 0.0734
R_1, wR_2 (all data)	R_1 = 0.0484	R_1 = 0.0779	R_1 = 0.0713	R_1 = 0.0149	R_1 = 0.0398	R_1 = 0.0547	R_1 = 0.1105	R_1 = 0.0885	R_1 = 0.0369
	wR_2 = 0.1040	wR_2 = 0.1660	wR_2 = 0.1515	wR_2 = 0.0335	wR_2 = 0.0998	wR_2 = 0.1014	wR_2 = 0.2421	wR_2 = 0.1900	wR_2 = 0.0762
Index range	–11⩽h⩽11	–22⩽h⩽22	–19⩽h⩽20	–7⩽h⩽8	–9⩽h⩽9	–28⩽h⩽28	–11⩽h⩽11	–11⩽h⩽11	–10⩽h⩽11
	–9⩽k⩽5	–7⩽k⩽7	–15⩽k⩽15	–16⩽k⩽16	–9⩽k⩽9	–15⩽k⩽14	–11⩽k⩽11	–11⩽k⩽11	–11⩽k⩽11
	–11⩽l⩽11	–12⩽l⩽17	–18⩽l⩽15	–10⩽l⩽12	–9⩽l⩽9	–18⩽l⩽18	–16⩽l⩽16	–16⩽l⩽16	–17⩽l⩽17
CCDC numbers	1048057	1063734	1420716	1420255	1413030	1435798	1439859	1440023	1415595

Table S2. Selected bond distances (Å) of ZTO and its salts

Compound	Bond	length	Bond	length	Bond	length
ZTO	C(1)–N(1)	1.2952	C(2)–N(2)	1.3596	N(4)–N(4$^{\#1}$)	1.2525
	C(1)–N(3)	1.3760	C(2)–N(3)	1.4112	C(2)–O(1)	1.2144
	N(1)–N(2)	1.3815	N(3)–N(4)	1.3707		
2	Na(1)–O(4)	2.319(4)	N(1)–C(1)	1.325(4)	C(3)–N(6)	1.392(4)
	Na(1)–O(1)	2.329(3)	N(1)–N(2)	1.380(4)	N(4)–N(5)	1.236(4)
	Na(1)–O(1$^{\#1}$)	2.392(3)	C(1)–N(3)	1.387(4)	C(4)–N(8)	1.277(5)
	Na(1)–O(3)	2.419(4)	O(2)–C(3)	1.228(4)	C(4)–N(6)	1.365(5)
	Na(1)–N(8$^{\#2}$)	2.527(3)	N(2)–C(2)	1.270(5)	N(5)–N(6)	1.355(4)
	Na(1)–Na(1$^{\#1}$)	3.647(4)	C(2)–N(3)	1.369(4)	N(7)–N(8)	1.393(4)
	O(1)–C(1)	1.221(4)	N(3)–N(4)	1.362(4)	N(8)–Na(1$^{\#3}$)	2.527(3)
	O(1)–Na(1$^{\#1}$)	2.392(3)	C(3)–N(7)	1.314(5)		
3	K(1)–O(4$^{\#1}$)	2.6811(15)	O(2)–K(1$^{\#2}$)	2.6820(15)	N(7)–N(8)	1.413(2)
	K(1)–O(2$^{\#2}$)	2.6820(15)	O(3)–C(5)	1.245(2)	N(8)–C(4)	1.302(2)
	K(1)–O(5)	2.7302(19)	O(3)–K(2$^{\#4}$)	2.6643(15)	N(8)–K(2$^{\#1}$)	2.8651(18)
	K(1)–O(1)	2.8063(18)	O(4)–C(7)	1.226(2)	N(9)–C(5)	1.336(2)
	K(1)–N(10)	2.9004(18)	O(4)–K(1$^{\#5}$)	2.6811(15)	N(9)–N(10)	1.407(2)
	K(1)–N(2$^{\#3}$)	2.9724(17)	N(1)–C(1)	1.342(2)	N(10)–C(6)	1.296(2)
	K(1)–C(1)	3.408(2)	N(1)–N(2)	1.391(2)	N(11)–N(12)	1.357(2)
	K(1)–K(2)	4.1531(11)	N(2)–C(2)	1.296(2)	N(11)–C(6)	1.386(2)
	K(2)–O(3$^{\#4}$)	2.6642(15)	N(2)–K(1$^{\#3}$)	2.9724(17)	N(11)–C(5)	1.413(2)
	K(2)–O(1)	2.7159(15)	N(3)–N(4)	1.375(2)	N(12)–N(13)	1.250(2)
	K(2)–O(6)	2.7686(19)	N(3)–C(2)	1.385(2)	N(13)–N(14)	1.371(2)
	K(2)–N(8$^{\#5}$)	2.8651(18)	N(3)–C(1)	1.395(2)	N(14)–C(8)	1.384(2)
	K(2)–N(16$^{\#6}$)	2.9789(18)	N(4)–N(5)	1.248(2)	N(14)–C(7)	1.405(2)
	K(2)–N(10)	3.019(2)	N(5)–N(6)	1.360(2)	N(15)–C(7)	1.345(2)
	K(2)–C(6)	3.495(2)	N(6)–C(4)	1.382(2)	N(15)–N(16)	1.395(2)
	O(1)–C(1)	1.237(2)	N(6)–C(3)	1.410(2)	N(16)–C(8)	1.302(2)
	O(2)–C(3)	1.251(2)	N(7)–C(3)	1.334(2)	N(16)–K(2$^{\#6}$)	2.9789(18)
4	O(1)–C(2)	1.228(2)	Cs(1)–N(1$^{\#5}$)	3.2825(16)	N(1)–N(2)	1.399(2)
	O(1)–Cs(1$^{\#1}$)	3.0910(13)	Cs(1)–N(1$^{\#6}$)	3.2825(16)	N(1)–Cs(1$^{\#8}$)	3.2825(16)
	O(1)–Cs(1)	3.2208(14)	Cs(1)–O(2$^{\#7}$)	3.4169(7)	N(2)–C(2)	1.337(2)
	O(2)–Cs(1)	3.4169(7)	Cs(1)–N(4$^{\#1}$)	3.5214(16)	N(3)–N(4)	1.3684(19)
	O(2)–Cs(1$^{\#2}$)	3.4169(7)	Cs(1)–N(4$^{\#3}$)	3.5214(16)	N(3)–C(1)	1.383(2)
	Cs(1)–O(1$^{\#3}$)	3.0910(13)	Cs(1)–C(2)	3.7696(18)	N(3)–C(2)	1.409(2)
	Cs(1)–O(1$^{\#1}$)	3.0910(13)	Cs(1)–C(2$^{\#4}$)	3.7696(18)	N(4)–N(4$^{\#9}$)	1.253(3)
	Cs(1)–O(1$^{\#4}$)	3.2208(14)	N(1)–C(1)	1.286(2)	N(4)–Cs(1$^{\#1}$)	3.5214(16)
5	C(1) –O(1)	1.2543(18)	C(3)–O(2)	1.2225(19)	N(4)–N(5)	1.2495(19)
	C(1)–N(1)	1.3268(19)	C(3)–N(8)	1.345(2)	N(5)–N(6)	1.3767(17)
	C(1)–N(3)	1.4039(19)	C(3)–N(6)	1.4039(19)	N(7)–N(8)	1.3824(19)
	C(2)–N(2)	1.292(2)	C(4)–N(7)	1.282(2)	N(9)–N(10)	1.439(2)
	C(2)–N(3)	1.3758(19)	C(4)–N(6)	1.378(2)		

Table S2 (continued)

Compound	Bond	length	Bond	length	Bond	length
6	Mg(1)–O(5)	2.0575(10)	O(2)–C(3)	1.2640(15)	N(4)–N(5)	1.2526(14)
	Mg(1)–O(5$^{\#1}$)	2.0576(10)	N(1)–C(1)	1.3455(15)	N(5)–N(6)	1.3676(13)
	Mg(1)–O(4)	2.0593(10)	N(1)–N(2)	1.3860(14)	N(6)–C(4)	1.3794(14)
	Mg(1)–O(4$^{\#1}$)	2.0594(10)	N(2)–C(2)	1.2948(16)	N(6)–C(3)	1.4046(14)
	Mg(1)–O(3$^{\#1}$)	2.1023(10)	N(3)–N(4)	1.3789(13)	N(7)–C(3)	1.3289(15)
	Mg(1)–O(3)	2.1023(10)	N(3)–C(2)	1.3816(15)	N(7)–N(8)	1.4071(14)
	O(1)–C(1)	1.2388(15)	N(3)–C(1)	1.3938(14)	N(8)–C(4)	1.2966(15)
7	Ca(1)–O(1)	2.404(3)	O(1)–C(1)	1.258(4)	N(3)–C(1)	1.409(4)
	Ca(1)–O(5)	2.426(3)	O(2)–C(3)	1.259(4)	N(4)–N(5)	1.257(4)
	Ca(1)–O(6)	2.429(3)	O(3)–Ca(1)#1	2.523(3)	N(5)–N(6)	1.369(4)
	Ca(1)–O(3)	2.511(3)	O(4)–Ca(1)#2	2.584(3)	N(6)–C(4)	1.390(4)
	Ca(1)–O(3)#1	2.523(3)	N(1)–C(1)	1.342(4)	N(6)–C(3)	1.404(4)
	Ca(1)–O(4)	2.577(3)	N(1)–N(2)	1.404(4)	N(7)–C(3)	1.324(4)
	Ca(1)–O(4)#2	2.584(3)	N(1)–Ca(1)#1	2.591(3)	N(7)–N(8)	1.408(4)
	Ca(1)–N(1)#1	2.591(3)	N(2)–C(2)	1.300(5)	N(8)–C(4)	1.298(5)
	Ca(1)–Ca(1)#1	4.0521(18)	N(3)–C(2)	1.367(4)		
	Ca(1)–Ca(1)#2	4.2154(19)	N(3)–N(4)	1.385(4)		
8	Sr(1) – O(1)#1	2.540(4)	N(1) – C(1)	1.338(7)	N(7) – C(3)	1.334(7)
	Sr(1) – O(5)	2.578(4)	N(1) – N(2)	1.397(6)	N(7) – N(8)	1.403(6)
	Sr(1) – O(3)#1	2.591(4)	N(2) – C(2)	1.309(7)	N(8) – C(4)	1.303(7)
	Sr(1) – O(6)	2.607(5)	N(3) – N(4)	1.380(6)	C(1) – O(1)	1.263(7)
	Sr(1) – O(4)#2	2.643(4)	N(3) – C(2)	1.383(7)	C(3) – O(2)	1.261(6)
	Sr(1) – O(3)	2.661(4)	N(3) – C(1)	1.420(7)	O(1) – Sr(1)#1	2.540(4)
	Sr(1) – O(4)	2.671(4)	N(4) – N(5)	1.239(6)	O(3) – Sr(1)#1	2.591(4)
	Sr(1) – N(1)	2.747(5)	N(5) – N(6)	1.376(6)	O(4) – Sr(1)#2	2.643(4)
	Sr(1) – Sr(1)#1	4.2239(15)	N(6) – C(4)	1.388(7)		
	Sr(1) – Sr(1)#2	4.2894(17)	N(6) – C(3)	1.392(7)		
9	Ba(1)–O(3$^{\#1}$)	2.708(2)	C(1)–O(1)	1.261(4)	N(1)–N(2)	1.410(4)
	Ba(1)–O(2)	2.709(2)	C(1)–N(1)	1.332(4)	N(2)–C(2)	1.297(4)
	Ba(1)–O(4)	2.724(2)	C(1)–N(3)	1.392(4)	N(8)–C(3)	1.339(4)
	Ba(1)–O(6)	2.766(2)	C(4)–N(7)	1.300(4)	N(8)–N(7)	1.411(4)
	Ba(1)–O(4$^{\#2}$)	2.796(2)	C(4)–N(6)	1.378(4)	N(8)–Ba(1$^{\#1)}$	2.915(3)
	Ba(1)–O(3)	2.827(2)	O(2)–C(3)	1.255(4)	O(3)–Ba(1$^{\#1}$)	2.708(2)
	Ba(1)–O(5)	2.895(3)	N(5)–N(4)	1.248(3)	O(4)–Ba(1$^{\#2}$)	2.796(2)
	Ba(1)–N(8$^{\#1}$)	2.915(3)	N(5)–N(6)	1.370(3)	O(5)–Ba(1$^{\#3}$)	3.175(3)
	Ba(1)–O(5$^{\#3}$)	3.175(3)	N(4)–N(3)	1.377(3)	N(1)–N(2)	1.4049(18)
	Ba(1)–Ba(1$^{\#2}$)	4.3889(10)	N(3)–C(2)	1.380(4)	N(3)–N(4)	1.3698(17)
	Ba(1)–Ba(1$^{\#1}$)	4.4470(9)	N(6)–C(3)	1.411(4)		

Table S3. The selected bond angle (°) of ZTO and its salts

ZTO	C(1)–N(1)–N(2)	105.48(8)	C(1)–N(3)–C(2)	109.10(9)	O(1)–C(2)–N(3)	127.92(9)
	C(2)–N(2)–N(1)	113.56(9)	N($4^{\#1}$)–N(4)–N(3)	110.12(11)	N(2)–C(2)–N(3)	101.42(9)
	N(4)–N(3)–C(1)	130.70(8)	N(1)–C(1)–N(3)	110.43(9)		
	N(4)–N(3)–C(2)	120.19(9)	O(1)–C(2)–N(2)	130.66(10)		
2	O(4)–Na(1)–O(1)	110.68(12)	O(1)–Na(1)–O(3)	88.37(11)	N(2)–C(2)–N(3)	109.9(3)
	O(4)–Na(1)–O($1^{\#1}$)	100.88(12)	O($1^{\#1}$)–Na(1)–O(3)	123.31(11)	N(4)–N(3)–C(2)	129.3(3)
	O(1)–Na(1)–O($1^{\#1}$)	77.48(11)	O(4)–Na(1)–N($8^{\#2}$)	84.06(12)	N(4)–N(3)–C(1)	122.7(3)
	O(4)–Na(1)–O(3)	135.05(13)	O(1)–Na(1)–N($8^{\#2}$)	164.98(12)	C(2)–N(3)–C(1)	107.9(3)
	O(1)–Na(1)–O(3)	88.37(11)	O($1^{\#1}$)–Na(1)–N($8^{\#2}$)	103.23(12)	O(2)–C(3)–N(7)	130.2(3)
	O($1^{\#1}$)–Na(1)–O(3)	123.31(11)	O(3)–Na(1)–N($8^{\#2}$)	78.68(11)	O(2)–C(3)–N(6)	124.6(3)
	O(4)–Na(1)–N($8^{\#2}$)	84.06(12)	O(4)–Na(1)–Na($1^{\#1}$)	118.16(9)	N(7)–C(3)–N(6)	105.2(3)
	O(1)–Na(1)–N($8^{\#2}$)	164.98(12)	O(1)–Na(1)–Na($1^{\#1}$)	40.06(7)	N(5)–N(4)–N(3)	109.2(3)
	O($1^{\#1}$)–Na(1)–N($8^{\#2}$)	103.23(12)	O($1^{\#1}$)–Na(1)–Na($1^{\#1}$)	38.80(7)	N(8)–C(4)–N(6)	109.7(3)
	O(3)–Na(1)–N($8^{\#2}$)	78.68(11)	O(3)–Na(1)–Na($1^{\#1}$)	102.77(8)	N(4)–N(5)–N(6)	113.2(3)
	O(4)–Na(1)–Na($1^{\#1}$)	118.16(9)	N($8^{\#2}$)–Na(1)–Na($1^{\#1}$)	135.70(10)	N(5)–N(6)–C(4)	132.6(3)
	O(1)–Na(1)–Na(1)#1	40.06(7)	C(1)–O(1)–Na(1)	132.4(2)	N(5)–N(6)–C(3)	119.7(3)
	O($1^{\#1}$)–Na(1)–Na($1^{\#1}$)	38.80(7)	C(1)–O(1)–Na($1^{\#1}$)	126.0(2)	C(4)–N(6)–C(3)	107.7(3)
	O(3)–Na(1)–Na($1^{\#1}$)	102.77(8)	Na(1)–O(1)–Na($1^{\#1}$)	101.14(11)	C(3)–N(7)–N(8)	110.3(3)
	N($8^{\#2}$)–Na(1)–Na($1^{\#1}$)	135.70(10)	C(1)–N(1)–N(2)	111.2(3)	C(4)–N(8)–N(7)	107.2(3)
	O(4)–Na(1)–O(1)	110.68(12)	O(1)–C(1)–N(1)	129.3(3)	C(4)–N(8)–Na($1^{\#3}$)	135.8(3)
	O(4)–Na(1)–O($1^{\#1}$)	100.88(12)	O(1)–C(1)–N(3)	126.6(3)	N(7)–N(8)–Na($1^{\#3}$)	115.9(2)
	O(1)–Na(1)–O($1^{\#1}$)	77.48(11)	N(1)–C(1)–N(3)	104.1(3)		
	O(4)–Na(1)–O(3)	135.05(13)	C(2)–N(2)–N(1)	106.9(3)		
3	O($4^{\#1}$)–K(1)–O($2^{\#2}$)	84.33(5)	N(10)–K(1)–C(1)	101.14(5)	O($3^{\#4}$)–K(2)–N(10)	92.22(5)
	O($4^{\#1}$)–K(1)–O(5)	83.81(5)	N($2^{\#3}$)–K(1)–C(1)	76.00(5)	O(1)–K(2)–N(10)	86.34(5)
	O($2^{\#2}$)–K(1)–O(5)	96.61(5)	O($4^{\#1}$)–K(1)–K(2)	85.02(4)	O(6)–K(2)–N(10)	171.04(5)
	O($4^{\#1}$)–K(1)–O(1)	78.47(5)	O($2^{\#2}$)–K(1)–K(2)	123.73(4)	N($8^{\#5}$)–K(2)–N(10)	83.20(5)
	O($2^{\#2}$)–K(1)–O(1)	83.33(5)	O(5)–K(1)–K(2)	136.63(4)	N($16^{\#6}$)–K(2)–N(10)	77.88(5)
	O(5)–K(1)–O(1)	162.20(5)	O(1)–K(1)–K(2)	40.41(3)	O($3^{\#4}$)–K(2)–C(6)	106.55(5)
	O($4^{\#1}$)–K(1)–N(10)	94.30(5)	N(10)–K(1)–K(2)	46.62(4)	O(1)–K(2)–C(6)	102.76(5)
	O($2^{\#2}$)–K(1)–N(10)	170.34(5)	N($2^{\#3}$)–K(1)–K(2)	86.12(4)	O(6)–K(2)–C(6)	157.50(5)
	O(5)–K(1)–N(10)	92.74(5)	C(1)–K(1)–K(2)	55.92(4)	N($8^{\#5}$)–K(2)–C(6)	68.93(5)
	O(1)–K(1)–N(10)	87.02(5)	O($3^{\#4}$)–K(2)–O(1)	86.65(5)	N($16^{\#6}$)–K(2)–C(6)	62.12(5)
	O($4^{\#1}$)–K(1)–N($2^{\#3}$)	167.51(5)	O($3^{\#4}$)–K(2)–O(6)	93.88(5)	N(10)–K(2)–C(6)	21.38(4)
	O($2^{\#2}$)–K(1)–N($2^{\#3}$)	93.32(5)	O(1)–K(2)–O(6)	87.45(5)	O($3^{\#4}$)–K(2)–K(1)	89.72(4)
	O(5)–K(1)–N($2^{\#3}$)	108.66(5)	O($3^{\#4}$)–K(2)–N($8^{\#5}$)	175.40(5)	O(1)–K(2)–K(1)	42.06(3)
	O(1)–K(1)–N($2^{\#3}$)	89.08(5)	O(1)–K(2)–N($8^{\#5}$)	93.48(5)	O(6)–K(2)–K(1)	129.11(4)
	N(10)–K(1)–N($2^{\#3}$)	85.95(5)	O(6)–K(2)–N($8^{\#5}$)	90.73(5)	N($8^{\#5}$)–K(2)–K(1)	87.31(4)
	O($4^{\#1}$)–K(1)–C(1)	91.73(5)	O($3^{\#4}$)–K(2)–N($16^{\#6}$)	93.27(5)	N($16^{\#6}$)–K(2)–K(1)	122.17(4)
	O($2^{\#2}$)–K(1)–C(1)	69.40(5)	O(1)–K(2)–N(16)$^{\#6}$	164.21(5)	N(10)–K(2)–K(1)	44.29(4)
	O(5)–K(1)–C(1)	165.72(5)	O(6)–K(2)–N($16^{\#6}$)	108.30(5)	C(6)–K(2)–K(1)	61.78(4)
	O(1)–K(1)–C(1)	20.13(4)	N($8^{\#5}$) –K(2)–N($16^{\#6}$)	85.35(5)	C(1)–O(1)–K(2)	127.55(12)
	C(1)–O(1)–K(1)	108.54(12)	C(2)–N(2)–K($1^{\#3}$)	141.44(13)	N(9)–N(10)–K(2)	101.50(11)
	K(2)–O(1)–K(1)	97.53(5)	N(7)–N(8)–K(2)#1	109.46(11)	K(1)–N(10)–K(2)	89.09(5)
	C(3)–O(2)–K($1^{\#2}$)	133.39(12)	C(5)–N(9)–N(10)	109.20(15)	O(1)–C(1)–N(3)	126.72(17)
	C(5)–O(3)–K($2^{\#4}$)	133.70(12)	C(6)–N(10)–N(9)	108.46(16)	N(1)–C(1)–N(3)	103.20(15)
	C(7)–O(4)–K($1^{\#5}$)	130.79(12)	C(6)–N(10)–K(1)	138.71(14)	O(1)–C(1)–K(1)	51.33(10)
	C(1)–N(1)–N(2)	112.66(15)	N(9)–N(10)–K(1)	108.72(11)	N(1)–C(1)–K(1)	110.96(12)
	C(2)–N(2)–N(1)	105.58(16)	C(6)–N(10)–K(2)	100.51(13)	N(3)–C(1)–K(1)	113.86(12)

Table S3. (continued)

	N(2)–C(2)–N(3)	110.04(17)	C(4)–N(8)–N(7)	107.64(16)	O(1)–C(1)–N(1)	130.07(17)
	O(2)–C(3)–N(7)	129.53(17)	C(4)–N(8)–K(2)#1	141.36(14)	N(7)–C(3)–N(6)	106.34(16)
	O(2)–C(3)–N(6)	124.13(16)	N(12)–N(11)–C(6)	131.35(15)	N(8)–C(4)–N(6)	109.71(17)
	N(1)–N(2)–K($1^{\#3}$)	112.12(11)	N(12)–N(11)–C(5)	121.02(15)	O(3)–C(5)–N(9)	130.42(17)
	N(4)–N(3)–C(2)	131.62(15)	C(6)–N(11)–C(5)	107.48(15)	O(3)–C(5)–N(11)	123.75(16)
	N(4)–N(3)–C(1)	119.74(15)	N(13)–N(12)–N(11)	111.44(15)	N(9)–C(5)–N(11)	105.83(16)
	C(2)–N(3)–C(1)	108.51(15)	N(12)–N(13)–N(14)	110.92(15)	N(10)–C(6)–N(11)	109.03(17)
	N(5)–N(4)–N(3)	110.89(15)	N(13)–N(14)–C(8)	131.78(15)	N(10)–C(6)–K(2)	58.12(11)
	N(4)–N(5)–N(6)	111.78(15)	N(13)–N(14)–C(7)	119.31(15)	N(11)–C(6)–K(2)	113.12(12)
	N(5)–N(6)–C(4)	131.88(15)	C(8)–N(14)–C(7)	108.89(15)	O(4)–C(7)–N(15)	130.68(17)
	N(5)–N(6)–C(3)	120.90(15)	C(7)–N(15)–N(16)	113.05(15)	O(4)–C(7)–N(14)	126.70(17)
	C(4)–N(6)–C(3)	107.11(15)	C(8)–N(16)–K($2^{\#6}$)	142.09(13)	N(15)–C(7)–N(14)	102.62(15)
	C(3)–N(7)–N(8)	109.18(15)	N(15)–N(16)–K($2^{\#6}$)	112.39(11)	N(16)–C(8)–N(14)	109.97(16)
4	C(2)–O(1)–Cs($1^{\#1}$)	129.08(11)	O(1)–Cs(1)–O(2)	50.82(4)	N($1^{\#5}$)–Cs(1)–N($4^{\#3}$)	107.26(4)
	C(2)–O(1)–Cs(1)	107.11(11)	N($1^{\#5}$)–Cs(1)–O(2)	105.60(4)	N($1^{\#6}$)–Cs(1)–N($4^{\#3}$)	68.57(4)
	Cs($1^{\#1}$)–O(1)–Cs(1)	110.65(4)	N($1^{\#6}$) –Cs(1)–O(2)	66.93(4)	O(2)–Cs(1)–N($4^{\#3}$)	120.74(3)
	Cs(1)–O(2)–Cs($1^{\#2}$)	170.45(7)	O($1^{\#3}$)–Cs(1)–O($2^{\#7}$)	70.49(4)	O($2^{\#7}$)–Cs(1)–N($4^{\#3}$)	58.74(3)
	O($1^{\#3}$)–Cs(1)–O($1^{\#1}$)	85.53(5)	O($1^{\#1}$)–Cs(1)–O($2^{\#7}$)	117.14(4)	N($4^{\#1}$)–Cs(1)–N($4^{\#3}$)	174.66(5)
	O($1^{\#3}$)–Cs(1)–O($1^{\#4}$)	69.35(4)	O($1^{\#4}$)–Cs(1)–O($2^{\#7}$)	50.82(4)	O($1^{\#3}$)–Cs(1)–C(2)	56.00(4)
	O($1^{\#1}$)–Cs(1)–O($1^{\#4}$)	66.47(2)	O(1)–Cs(1)–O($2^{\#7}$)	135.81(3)	O($1^{\#1}$)–Cs(1)–C(2)	84.50(4)
	O($1^{\#3}$)–Cs(1)–O(1)	66.47(2)	N($1^{\#5}$)–Cs(1)–O($2^{\#7}$)	66.93(4)	O($1^{\#4}$)–Cs(1)–C(2)	119.57(4)
	O($1^{\#1}$)–Cs(1)–O(1)	69.35(4)	N($1^{\#6}$)–Cs(1)–O($2^{\#7}$)	105.60(4)	O(1)–Cs(1)–C(2)	18.15(4)
	O($1^{\#4}$) –Cs(1)–O(1)	118.40(5)	O(2)–Cs(1)–O($2^{\#7}$)	170.45(7)	N($1^{\#5}$)–Cs(1)–C(2)	158.84(4)
	O($1^{\#3}$)–Cs(1)–N($1^{\#5}$)	137.25(4)	O($1^{\#3}$)–Cs(1)–N($4^{\#1}$)	135.26(3)	N($1^{\#6}$)–Cs(1)–C(2)	74.09(4)
	O($1^{\#1}$)–Cs(1)–N($1^{\#5}$)	110.44(4)	O($1^{\#1}$)–Cs(1)–N($4^{\#1}$)	50.07(3)	O(2)–Cs(1)–C(2)	64.30(3)
	O($1^{\#4}$)–Cs(1)–N($1^{\#5}$)	80.94(4)	O($1^{\#4}$)–Cs(1)–N($4^{\#1}$)	85.49(4)	O($2^{\#7}$)–Cs(1)–C(2)	120.53(3)
	O(1)–Cs(1)–N($1^{\#5}$)	155.95(4)	O(1)–Cs(1)–N($4^{\#1}$)	97.26(4)	N($4^{\#1}$)–Cs(1)–C(2)	115.23(4)
	O($1^{\#3}$)–Cs(1)–N($1^{\#6}$)	110.44(4)	N($1^{\#5}$)–Cs(1)–N($4^{\#1}$)	68.57(4)	N($4^{\#3}$)–Cs(1)–C(2)	67.37(4)
	O($1^{\#1}$)–Cs(1)–N($1^{\#6}$)	137.25(4)	N($1^{\#6}$)–Cs(1)–N($4^{\#1}$)	107.26(4)	O($1^{\#3}$)–Cs(1)–C($2^{\#4}$)	84.50(4)
	O($1^{\#4}$)–Cs(1)–N($1^{\#6}$)	155.95(4)	O(2)–Cs(1)–N($4^{\#1}$)	58.74(3)	O($1^{\#1}$)–Cs(1)–C($2^{\#4}$)	56.00(4)
	O(1)–Cs(1)–N($1^{\#6}$)	80.94(4)	O($2^{\#7}$)–Cs(1)–N($4^{\#1}$)	120.74(3)	O($1^{\#4}$)–Cs(1)–C($2^{\#4}$)	18.15(4)
	N($1^{\#5}$)–Cs(1)–N($1^{\#6}$)	84.88(6)	O($1^{\#3}$)–Cs(1)–N($4^{\#3}$)	50.07(3)	O(1)–Cs(1)–C($2^{\#4}$)	119.57(4)
	O($1^{\#3}$)–Cs(1)–O(2)	117.14(4)	O($1^{\#1}$)–Cs(1)–N($4^{\#3}$)	135.26(3)	N($1^{\#5}$)–Cs(1)–C($2^{\#4}$)	74.09(4)
	O($1^{\#1}$)–Cs(1)–O(2)	70.49(4)	O($1^{\#4}$)–Cs(1)–N($4^{\#3}$)	97.25(4)	N($1^{\#6}$)–Cs(1)–C($2^{\#4}$)	158.84(4)
	O($1^{\#4}$)–Cs(1)–O(2)	135.81(3)	O(1)–Cs(1)–N($4^{\#3}$)	85.49(4)	O(2)–Cs(1)–C($2^{\#4}$)	120.53(3)
	O($2^{\#7}$)–Cs(1)–C($2^{\#4}$)	64.30(3)	N(4)–N(3)–C(1)	131.30(15)	O(1)–C(2)–N(2)	130.38(17)
	N($4^{\#1}$)–Cs(1)–C($2^{\#4}$)	67.37(4)	N(4)–N(3)–C(2)	120.68(15)	O(1)–C(2)–N(3)	125.31(16)
	N($4^{\#3}$)–Cs(1)–C($2^{\#4}$)	115.23(4)	C(1)–N(3)–C(2)	107.65(14)	N(2)–C(2)–N(3)	104.30(16)
	C(1)–N(1)–N(2)	106.95(15)	N($4^{\#9}$)–N(4)–N(3)	110.65(19)	O(1)–C(2)–Cs(1)	54.75(9)
	C(1)–N(1)–Cs($1^{\#8}$)	141.34(13)	N($4^{\#9}$)–N(4)–Cs($1^{\#1}$)	128.45(11)	N(2)–C(2)–Cs(1)	93.35(10)
	N(2)–N(1)–Cs($1^{\#8}$)	110.93(10)	N(3)–N(4)–Cs($1^{\#1}$)	110.64(10)	N(3)–C(2)–Cs(1)	133.28(11)
	C(2)–N(2)–N(1)	111.02(14)	N(1)–C(1)–N(3)	110.07(16)	N(4)–N(5)–N(6)	109.57(12)
5	O(1)–C(1)–N(1)	130.10(14)	N(7)–C(4)–N(6)	110.61(14)	N(5)–N(6)–C(4)	130.40(12)
	O(1)–C(1)–N(3)	123.39(13)	C(1)–N(1)–N(2)	108.57(12)	N(5)–N(6)–C(3)	121.31(12)
	N(1)–C(1)–N(3)	106.51(13)	C(2)–N(2)–N(1)	108.55(12)	C(4)–N(6)–C(3)	108.27(12)
	N(2)–C(2)–N(3)	109.07(14)	N(4)–N(3)–C(2)	131.88(12)	C(4)–N(7)–N(8)	105.77(12)
	O(2)–C(3)–N(8)	130.30(14)	N(4)–N(3)–C(1)	120.77(12)	C(3)–N(8)–N(7)	112.91(13)
	O(2)–C(3)–N(6)	127.27(14)	C(2)–N(3)–C(1)	107.30(12)		
	N(8)–C(3)–N(6)	102.42(13)	N(5)–N(4)–N(3)	111.21(12)		

Table S3. (continued)

6	O(5)–Mg(1)–O(5$^{\#1}$)	180.0	O(4)–Mg(1)–O(3)	88.41(4)	C(4)–N(6)–C(3)	107.32(9)
	O(5)–Mg(1)–O(4)	87.30(4)	O(4)#1–Mg(1)–O(3)	91.59(4)	C(3)–N(7)–N(8)	108.48(9)
	O(5$^{\#1}$) –Mg(1)–O(4)	92.70(4)	O(3)#1–Mg(1)–O(3)	180.00(5)	C(4)–N(8)–N(7)	108.62(9)
	O(5)–Mg(1)–O(4$^{\#1}$)	92.70(4)	C(1)–N(1)–N(2)	111.91(9)	O(1)–C(1)–N(1)	130.75(10)
	O(5$^{\#1}$) –Mg(1)–O(4$^{\#1}$)	87.30(4)	C(2)–N(2)–N(1)	106.40(9)	O(1)–C(1)–N(3)	125.80(10)
	O(4)–Mg(1)–O(4$^{\#1}$)	180.00(5)	N(4)–N(3)–C(2)	131.80(9)	N(1)–C(1)–N(3)	103.45(10)
	O(5)–Mg(1)–O(3$^{\#1}$)	89.70(4)	N(4)–N(3)–C(1)	119.54(9)	N(2)–C(2)–N(3)	109.64(10)
	O(5$^{\#1}$) –Mg(1)–O(3$^{\#1}$)	90.30(4)	C(2)–N(3)–C(1)	108.59(9)	O(2)–C(3)–N(7)	130.75(10)
	O(4)–Mg(1)–O(3$^{\#1}$)	91.59(4)	N(5)–N(4)–N(3)	110.60(9)	O(2)–C(3)–N(6)	122.58(10)
	O(4)#1–Mg(1)–O(3$^{\#1}$)	88.41(4)	N(4)–N(5)–N(6)	110.84(9)	N(7)–C(3)–N(6)	106.66(10)
	O(5)–Mg(1)–O(3)	90.30(4)	N(5)–N(6)–C(4)	131.75(9)	N(8)–C(4)–N(6)	108.91(10)
	O(5)#1–Mg(1)–O(3)	89.70(4)	N(5)–N(6)–C(3)	120.75(9)		
7	O(1)–Ca(1)–O(5)	118.21(10)	O(3)–Ca(1)–N(1)#1	69.31(9)	C(1)–N(1)–N(2)	107.7(3)
	O(1)–Ca(1)–O(6)	143.96(9)	O(3)#1–Ca(1)–N(1)#1	73.56(9)	C(1)–N(1)–Ca(1)#1	134.8(2)
	O(5)–Ca(1)–O(6)	74.60(10)	O(4)–Ca(1)–N(1)#1	106.52(10)	N(2)–N(1)–Ca(1)#1	117.2(2)
	O(1)–Ca(1)–O(3)	74.61(9)	O(4)#2–Ca(1)–N(1)#1	140.93(9)	C(2)–N(2)–N(1)	109.4(3)
	O(5)–Ca(1)–O(3)	139.92(9)	O(1)–Ca(1)–Ca(1)#1	73.26(7)	C(2)–N(3)–N(4)	129.0(3)
	O(6)–Ca(1)–O(3)	118.83(10)	O(5)–Ca(1)–Ca(1)#1	107.14(7)	C(2)–N(3)–C(1)	108.0(3)
	O(1)–Ca(1)–O(3)#1	78.55(9)	O(6)–Ca(1)–Ca(1)#1	138.44(8)	N(4)–N(3)–C(1)	123.0(3)
	O(5)–Ca(1)–O(3)#1	73.26(9)	O(3)–Ca(1)–Ca(1)#1	36.50(6)	N(5)–N(4)–N(3)	109.5(3)
	O(6)–Ca(1)–O(3)#1	136.20(9)	O(3)#1–Ca(1)–Ca(1)#1	36.29(6)	N(4)–N(5)–N(6)	111.7(3)
	O(3)–Ca(1)–O(3)#1	72.79(9)	O(4)–Ca(1)–Ca(1)#1	114.60(7)	N(5)–N(6)–C(4)	131.7(3)
	O(1)–Ca(1)–O(4)	83.61(9)	O(4)#2–Ca(1)–Ca(1)#1	151.39(7)	N(5)–N(6)–C(3)	121.8(3)
	O(5)–Ca(1)–O(4)	137.20(9)	N(1)#1–Ca(1)–Ca(1)#1	66.73(7)	C(4)–N(6)–C(3)	106.4(3)
	O(6)–Ca(1)–O(4)	68.26(9)	O(1)–Ca(1)–Ca(1)#2	79.75(7)	C(3)–N(7)–N(8)	108.2(3)
	O(3)–Ca(1)–O(4)	78.80(8)	O(5)–Ca(1)–Ca(1)#2	108.47(7)	C(4)–N(8)–N(7)	108.7(3)
	O(3)#1–Ca(1)–O(4)	149.54(8)	O(6)–Ca(1)–Ca(1)#2	64.24(7)	O(1)–C(1)–N(1)	129.8(3)
	O(1)–Ca(1)–O(4)#2	79.68(9)	O(3)–Ca(1)–Ca(1)#2	111.25(6)	O(1)–C(1)–N(3)	123.9(3)
	O(5)–Ca(1)–O(4)#2	77.59(9)	O(3)#1–Ca(1)–Ca(1)#2	155.85(7)	N(1)–C(1)–N(3)	106.3(3)
	O(6)–Ca(1)–O(4)#2	70.16(9)	O(4)–Ca(1)–Ca(1)#2	35.30(6)	N(2)–C(2)–N(3)	108.6(3)
	O(3)–Ca(1)–O(4)#2	141.73(9)	O(4)#2–Ca(1)–Ca(1)#2	35.19(6)	O(2)–C(3)–N(7)	129.1(3)
	O(3)#1–Ca(1)–O(4)#2	128.96(9)	N(1)#1–Ca(1)–Ca(1)#2	130.53(7)	O(2)–C(3)–N(6)	123.2(3)
	O(4)–Ca(1)–O(4)#2	70.50(10)	Ca(1)#1–Ca(1)–Ca(1)#2	142.45(4)	N(7)–C(3)–N(6)	107.6(3)
	O(1)–Ca(1)–N(1)#1	139.38(9)	C(1)–O(1)–Ca(1)	133.8(2)	N(8)–C(4)–N(6)	109.0(3)
	O(5)–Ca(1)–N(1)#1	81.16(10)	Ca(1)–O(3)–Ca(1)#1	107.21(9)		
	O(6)–Ca(1)–N(1)#1	72.78(10)	Ca(1)–O(4)–Ca(1)#2	109.50(10)		
8	O(1)#1–Sr(1)–O(5)	144.78(13)	O(6)–Sr(1)–N(1)	81.19(16)	C(2)–N(2)–N(1)	109.4(4)
	O(1)#1–Sr(1)–O(3)#1	80.25(13)	O(4)#2–Sr(1)–N(1)	138.62(13)	N(4)–N(3)–C(2)	129.8(5)
	O(5)–Sr(1)–O(3)#1	134.97(13)	O(3)–Sr(1)–N(1)	68.82(13)	N(4)–N(3)–C(1)	122.8(4)
	O(1)#1–Sr(1)–O(6)	124.66(16)	O(4)–Sr(1)–N(1)	101.99(14)	C(2)–N(3)–C(1)	107.3(4)
	O(5)–Sr(1)–O(6)	74.27(15)	O(1)#1–Sr(1)–Sr(1)#1	71.85(9)	N(5)–N(4)–N(3)	110.2(4)
	O(3)#1–Sr(1)–O(6)	75.64(13)	O(5)–Sr(1)–Sr(1)#1	134.18(10)	N(4)–N(5)–N(6)	111.6(5)
	O(1)#1–Sr(1)–O(4)#2	84.41(13)	O(3)#1–Sr(1)–Sr(1)#1	37.03(9)	N(5)–N(6)–C(4)	132.0(5)
	O(5)–Sr(1)–O(4)#2	70.08(13)	O(6)–Sr(1)–Sr(1)#1	109.94(10)	N(5)–N(6)–C(3)	121.3(5)
	O(3)#1–Sr(1)–O(4)#2	133.57(13)	O(4)#2–Sr(1)–Sr(1)#1	155.34(9)	C(4)–N(6)–C(3)	106.7(4)
	O(6)–Sr(1)–O(4)#2	77.94(14)	O(3)–Sr(1)–Sr(1)#1	35.89(8)	C(3)–N(7)–N(8)	108.1(4)
	O(1)#1–Sr(1)–O(3)	70.75(13)	O(4)–Sr(1)–Sr(1)#1	109.62(9)	C(4)–N(8)–N(7)	108.4(5)
	O(5)–Sr(1)–O(3)	114.72(14)	N(1)–Sr(1)–Sr(1)#1	65.92(10)	O(1)–C(1)–N(1)	130.7(5)
	O(3)#1–Sr(1)–O(3)	72.92(14)	O(1)#1–Sr(1)–Sr(1)#2	81.47(9)	O(1)–C(1)–N(3)	123.0(5)

Table S3. (continued)

8	O(4)#2–Sr(1)–O(3)	140.49(12)	O(3)#1–Sr(1)–Sr(1)#2	160.28(9)	N(2)–C(2)–N(3)	108.4(5)
	O(1)#1–Sr(1)–O(4)	81.85(13)	O(6)–Sr(1)–Sr(1)#2	109.39(10)	O(2)–C(3)–N(7)	128.4(5)
	O(5)–Sr(1)–O(4)	67.75(14)	O(4)#2–Sr(1)–Sr(1)#2	36.40(9)	O(2)–C(3)–N(6)	124.0(5)
	O(3)#1–Sr(1)–O(4)	146.07(12)	O(3)–Sr(1)–Sr(1)#2	107.72(8)	N(7)–C(3)–N(6)	107.7(5)
	O(6)–Sr(1)–O(4)	137.73(13)	O(4)–Sr(1)–Sr(1)#2	35.96(9)	N(8)–C(4)–N(6)	109.1(5)
	O(4)#2–Sr(1)–O(4)	72.35(15)	N(1)–Sr(1)–Sr(1)#2	126.28(11)	C(1)–O(1)–Sr(1)#1	133.8(4)
	O(3)–Sr(1)–O(4)	74.05(12)	Sr(1)#1–Sr(1)–Sr(1)#2	140.27(3)	Sr(1)#1–O(3)–Sr(1)	107.08(14)
	O(1)#1–Sr(1)–N(1)	136.36(14)	C(1)–N(1)–N(2)	108.6(4)	Sr(1)#2–O(4)–Sr(1)	107.65(15)
	O(5)–Sr(1)–N(1)	70.03(14)	C(1)–N(1)–Sr(1)	133.6(4)		
	O(3)#1–Sr(1)–N(1)	72.89(13)	N(2)–N(1)–Sr(1)	116.8(3)		
9	O($3^{\#1}$)–Ba(1)–O(2)	82.47(7)	O(5)–Ba(1)–N($8^{\#1}$)	81.32(8)	Ba($1^{\#2}$)–Ba(1)–Ba($1^{\#1}$)	136.302(10)
	O($3^{\#1}$)–Ba(1)–O(4)	141.87(7)	O($3^{\#1}$)–Ba(1)–O($5^{\#3}$)	74.69(6)	O(1)–C(1)–N(1)	128.5(3)
	O(2)–Ba(1)–O(4)	92.60(7)	O(2)–Ba(1)–O($5^{\#3}$)	67.27(7)	O(1)–C(1)–N(3)	124.2(3)
	O($3^{\#1}$) –Ba(1)–O(6)	132.96(7)	O(4)–Ba(1)–O($5^{\#3}$)	68.64(6)	N(1)–C(1)–N(3)	107.4(2)
	O(2)–Ba(1)–O(6)	142.32(8)	O(6)–Ba(1)–O($5^{\#3}$)	126.62(7)	N(7)–C(4)–N(6)	109.0(3)
	O(4)–Ba(1)–O(6)	67.57(7)	O($4^{\#2}$)–Ba(1)–O($5^{\#3}$)	127.01(6)	C(3)–O(2)–Ba(1)	133.3(2)
	O($3^{\#1}$)–Ba(1)–O($4^{\#2}$)	139.42(6)	O(3)–Ba(1)–O($5^{\#3}$)	124.53(6)	N(4)–N(5)–N(6)	110.5(2)
	O(2)–Ba(1)–O($4^{\#2}$)	77.90(7)	O(5)–Ba(1)–O($5^{\#3}$)	66.36(8)	N(5)–N(4)–N(3)	111.2(2)
	O(4)–Ba(1)–O($4^{\#2}$)	74.66(7)	N($8^{\#1}$)–Ba(1)–O($5^{\#3}$)	136.18(7)	N(4)–N(3)–C(2)	132.9(3)
	O(6)–Ba(1)–O($4^{\#2}$)	66.30(8)	O($3^{\#1}$)–Ba(1)–Ba($1^{\#2}$)	166.39(5)	N(4)–N(3)–C(1)	120.2(2)
	O($3^{\#1}$)–Ba(1)–O(3)	73.08(8)	O(2)–Ba(1)–Ba($1^{\#2}$)	83.95(5)	C(2)–N(3)–C(1)	106.9(2)
	O(2)–Ba(1)–O(3)	64.75(7)	O(4)–Ba(1)–Ba($1^{\#2}$)	37.90(5)	N(5)–N(6)–C(4)	131.2(3)
	O(4)–Ba(1)–O(3)	137.96(7)	O(6)–Ba(1)–Ba($1^{\#2}$)	60.47(6)	N(5)–N(6)–C(3)	121.6(2)
	O(6)–Ba(1)–O(3)	108.36(8)	O($4^{\#2}$)–Ba(1)–Ba($1^{\#2}$)	36.76(4)	C(4)–N(6)–C(3)	107.1(2)
	O($4^{\#2}$)–Ba(1)–O(3)	66.46(6)	O(3)–Ba(1)–Ba($1^{\#2}$)	101.91(5)	C(1)–N(1)–N(2)	108.2(2)
	O($3^{\#1}$)–Ba(1)–O(5)	79.03(7)	O(5)–Ba(1)–Ba($1^{\#2}$)	109.91(5)	C(2)–N(2)–N(1)	108.0(2)
	O(2)–Ba(1)–O(5)	133.09(7)	N($8^{\#1}$)–Ba(1)–Ba($1^{\#2}$)	120.03(6)	C(3)–N(8)–N(7)	107.7(2)
	O(4)–Ba(1)–O(5)	77.12(7)	O($5^{\#3}$)–Ba(1)–Ba($1^{\#2}$)	99.06(4)	C(3)–N(8)–Ba($1^{\#1}$)	133.2(2)
	O(6)–Ba(1)–O(5)	75.40(8)	O($3^{\#1}$)–Ba(1)–Ba($1^{\#1}$)	37.45(5)	N(7)–N(8)–Ba($1^{\#1}$)	117.71(17)
	O($4^{\#2}$)–Ba(1)–O(5)	138.74(6)	O(2)–Ba(1)–Ba($1^{\#1}$)	69.46(5)	C(4)–N(7)–N(8)	109.1(3)
	O(3)–Ba(1)–O(5)	144.33(6)	O(4)–Ba(1)–Ba($1^{\#1}$)	161.99(5)	O(2)–C(3)–N(8)	130.2(3)
	O($3^{\#1}$)–Ba(1)–N($8^{\#1}$)	70.59(7)	O(6)–Ba(1)–Ba($1^{\#1}$)	127.96(5)	O(2)–C(3)–N(6)	122.9(3)
	O(2)–Ba(1)–N($8^{\#1}$)	131.27(7)	O($4^{\#2}$) –Ba(1)–Ba($1^{\#1}$)	102.04(4)	N(8)–C(3)–N(6)	107.0(2)
	O(4)–Ba(1)–N($8^{\#1}$)	133.22(7)	O(3)–Ba(1)–Ba($1^{\#1}$)	35.63(5)	N(2)–C(2)–N(3)	109.5(3)
	O(6)–Ba(1)–N($8^{\#1}$)	67.01(7)	O(5)–Ba(1)–Ba($1^{\#1}$)	113.61(5)	Ba($1^{\#1}$)–O(3)–Ba(1)	106.92(8)
	O($4^{\#2}$)–Ba(1)–N($8^{\#1}$)	96.80(7)	N($8^{\#1}$)–Ba(1)–Ba($1^{\#1}$)	64.40(5)	Ba(1)–O(4)–Ba($1^{\#2}$)	105.34(7)
	O(3)–Ba(1)–N($8^{\#1}$)	68.81(7)	O($5^{\#3}$)–Ba(1)–Ba($1^{\#1}$)	101.51(4)	Ba(1)–O(5)–Ba($1^{\#3}$)	113.64(8)

Table S4. Torsion angles (°) for ZTO and its salts

ZTO	C(1)–N(1)–N(2)–C(2)	–0.14(13)	N(4)–N(3)–C(1)–N(1)	–179.72(10)	N(4)–N(3)–C(2)–O(1)	–0.34(16)
	C(1)–N(3)–N(4)–N(4$^{\#1}$)	–1.07(18)	C(2)–N(3)–C(1)–N(1)	0.47(13)	C(1)–N(3)–C(2)–O(1)	179.49(11)
	C(2)–N(3)–N(4)–N(4$^{\#1}$)	178.72(11)	N(1)–N(2)–C(2)–O(1)	–179.60(11)	N(4)–N(3)–C(2)–N(2)	179.66(9)
	N(2)–N(1)–C(1)–N(3)	–0.21(12)	N(1)–N(2)–C(2)–N(3)	0.40(12)	C(1)–N(3)–C(2)–N(2)	–0.50(11)
2	O(4)–Na(1)–O(1)–C(1)	–77.9(3)	N(2)–N(1)–C(1)–N(3)	–0.7(4)	N(8)–C(4)–N(6)–N(5)	179.4(3)
	O(1$^{\#1}$)–Na(1)–O(1)–C(1)	–175.0(3)	C(1)–N(1)–N(2)–C(2)	0.5(4)	N(8)–C(4)–N(6)–C(3)	–0.7(4)
	O(3)–Na(1)–O(1)–C(1)	60.3(3)	N(1)–N(2)–C(2)–N(3)	0.0(4)	O(2)–C(3)–N(6)–N(5)	1.3(5)
	N(8$^{\#2}$)–Na(1)–O(1)–C(1)	90.6(5)	N(2)–C(2)–N(3)–N(4)	176.3(3)	N(7)–C(3)–N(6)–N(5)	–179.5(3)
	Na(1$^{\#1}$)–Na(1)–O(1)–C(1)	172.5(4)	N(2)–C(2)–N(3)–C(1)	–0.5(4)	O(2)–C(3)–N(6)–C(4)	–178.6(3)
	O(4)–Na(1)–O(1)–Na(1$^{\#1}$)	109.57(13)	O(1)–C(1)–N(3)–N(4)	2.0(5)	N(7)–C(3)–N(6)–C(4)	0.6(4)
	O(1$^{\#1}$)–Na(1)–O(1)–Na(1$^{\#1}$)	12.51(15)	N(1)–C(1)–N(3)–N(4)	–176.3(3)	O(2)–C(3)–N(7)–N(8)	178.8(3)
	O(3)–Na(1)–O(1)–Na(1$^{\#1}$)	–112.18(12)	O(1)–C(1)–N(3)–C(2)	179.0(3)	N(6)–C(3)–N(7)–N(8)	–0.4(4)
	N(8$^{\#2}$)–Na(1)–O(1)–Na(1$^{\#1}$)	–81.9(4)	N(1)–C(1)–N(3)–C(2)	0.7(4)	N(6)–C(4)–N(8)–N(7)	0.5(4)
	Na(1)–O(1)–C(1)–N(1)	–160.8(3)	C(2)–N(3)–N(4)–N(5)	1.0(5)	N(6)–C(4)–N(8)–Na(1$^{\#3}$)	–165.9(3)
	Na(1$^{\#1}$) –O(1)–C(1)–N(1)	10.1(5)	C(1)–N(3)–N(4)–N(5)	177.3(3)	C(3)–N(7)–N(8)–C(4)	–0.1(4)
	Na(1)–O(1)–C(1)–N(3)	21.3(5)	N(3)–N(4)–N(5)–N(6)	179.9(3)	C(3)–N(7)–N(8)–Na(1$^{\#3}$)	169.5(2)
	Na(1$^{\#1}$)–O(1)–C(1)–N(3)	–167.8(3)	N(4)–N(5)–N(6)–C(4)	0.3(5)	O(6)–K(2)–O(1)–C(1)	–52.27(16)
	N(2)–N(1)–C(1)–O(1)	–179.0(3)	N(4)–N(5)–N(6)–C(3)	–179.5(3)	N(8$^{\#5}$)–K(2)–O(1)–C(1)	38.31(16)
3	O(4$^{\#1}$)–K(1)–K(2)–O(3$^{\#4}$)	–7.26(5)	N(10)–K(1)–K(2)–N(16$^{\#6}$)	–0.23(6)	N(2$^{\#3}$)–K(1)–O(1)–C(1)	–48.74(12)
	O(2$^{\#2}$)–K(1)–K(2)–O(3$^{\#4}$)	–87.04(6)	N(2$^{\#3}$)–K(1)–K(2)–N(16$^{\#6}$)	87.86(6)	K(2)–K(1)–O(1)–C(1)	–133.84(13)
	O(5)–K(1)–K(2)–O(3$^{\#4}$)	68.26(7)	C(1)–K(1)–K(2)–N(16$^{\#6}$)	163.56(5)	O(4$^{\#1}$)–K(1)–O(1)–K(2)	–95.90(5)
	O(1)–K(1)–K(2)–O(3$^{\#4}$)	–85.31(6)	O(4$^{\#1}$)–K(1)–K(2)–N(10)	–100.72(6)	O(2$^{\#2}$)–K(1)–O(1)–K(2)	178.55(5)
	N(10)–K(1)–K(2)–O(3$^{\#4}$)	93.46(6)	O(2$^{\#2}$)–K(1)–K(2)–N(10)	179.50(6)	O(5)–K(1)–O(1)–K(2)	–90.58(16)
	N(2$^{\#3}$) –K(1)–K(2)–O(3$^{\#4}$)	–178.45(5)	O(5)–K(1)–K(2)–N(10)	–25.20(7)	N(10)–K(1)–O(1)–K(2)	–0.90(5)
	C(1)–K(1)–K(2)–O(3$^{\#4}$)	–102.75(5)	O(1)–K(1)–K(2)–N(10)	–178.77(6)	N(2$^{\#3}$) –K(1)–O(1)–K(2)	85.10(5)
	O(4$^{\#1}$)–K(1)–K(2)–O(1)	78.05(6)	N(2$^{\#3}$)–K(1)–K(2)–N(10)	88.09(6)	C(1)–K(1)–O(1)–K(2)	133.84(13)
	O(2$^{\#2}$)–K(1)–K(2)–O(1)	–1.73(6)	C(1)–K(1)–K(2)–N(10)	163.79(6)	C(1)–N(1)–N(2)–C(2)	–0.3(2)
	O(5)–K(1)–K(2)–O(1)	153.57(7)	O(4$^{\#1}$)–K(1)–K(2)–C(6)	–116.28(5)	C(1)–N(1)–N(2)–K(1$^{\#3}$)	171.42(12)
	N(10)–K(1)–K(2)–O(1)	178.77(6)	O(2$^{\#2}$)–K(1)–K(2)–C(6)	163.94(5)	C(2)–N(3)–N(4)–N(5)	–5.4(3)
	N(2$^{\#3}$) –K(1)–K(2)–O(1)	–93.14(6)	O(5)–K(1)–K(2)–C(6)	–40.75(7)	C(1)–N(3)–N(4)–N(5)	179.25(16)
	C(1)–K(1)–K(2)–O(1)	–17.44(6)	O(1)–K(1)–K(2)–C(6)	165.67(6)	N(3)–N(4)–N(5)–N(6)	–179.94(15)
	O(4$^{\#1}$) –K(1)–K(2)–O(6)	87.51(6)	N(10)–K(1)–K(2)–C(6)	–15.56(6)	N(4)–N(5)–N(6)–C(4)	–1.3(3)
	O(2$^{\#2}$) –K(1)–K(2)–O(6)	7.73(6)	N(2$^{\#3}$)–K(1)–K(2)–C(6)	72.53(5)	N(4)–N(5)–N(6)–C(3)	–177.07(16)
	O(5)–K(1)–K(2)–O(6)	163.03(7)	C(1)–K(1)–K(2)–C(6)	148.24(5)	C(3)–N(7)–N(8)–C(4)	0.2(2)
	O(1)–K(1)–K(2)–O(6)	9.46(6)	O(3$^{\#4}$) –K(2)–O(1)–C(1)	–146.30(16)	C(3)–N(7)–N(8)–K(2$^{\#1}$)	–168.81(12)
	N(10)–K(1)–K(2)–O(6)	–171.77(7)	N(16$^{\#6}$)–K(2)–O(1)–C(1)	123.5(2)	C(5)–N(9)–N(10)–C(6)	–0.3(2)
	N(2$^{\#3}$)–K(1)–K(2)–O(6)	–83.68(6)	N(10)–K(2)–O(1)–C(1)	121.26(16)	C(5)–N(9)–N(10)–K(1)	–162.02(13)
	C(1)–K(1)–K(2)–O(6)	–7.98(6)	C(6)–K(2)–O(1)–C(1)	107.48(16)	C(5)–N(9)–N(10)–K(2)	105.00(14)
	O(4$^{\#1}$)–K(1)–K(2)–N(8$^{\#5}$)	176.25(5)	K(1)–K(2)–O(1)–C(1)	120.40(17)	O(4$^{\#1}$)–K(1)–N(10)–C(6)	–176.0(2)
	O(2$^{\#2}$)–K(1)–K(2)–N(8$^{\#5}$)	96.48(6)	O(3$^{\#4}$)–K(2)–O(1)–K(1)	93.30(5)	O(2$^{\#2}$)–K(1)–N(10)–C(6)	102.5(3)
	O(5)–K(1)–K(2)–N(8$^{\#5}$)	–108.22(7)	O(6)–K(2)–O(1)–K(1)	–172.66(5)	O(5)–K(1)–N(10)–C(6)	–92.0(2)
	O(1)–K(1)–K(2)–N(8$^{\#5}$)	98.21(6)	N(8$^{\#5}$)–K(2)–O(1)–K(1)	–82.09(5)	O(1)–K(1)–N(10)–C(6)	105.8(2)
	N(10)–K(1)–K(2)–N(8$^{\#5}$)	–83.02(6)	N(16$^{\#6}$)–K(2)–O(1)–K(1)	3.11(19)	N(2$^{\#3}$)–K(1)–N(10)–C(6)	16.5(2)
	N(2$^{\#3}$)–K(1)–K(2)–N(8$^{\#5}$)	5.07(5)	N(10)–K(2)–O(1)–K(1)	0.86(5)	C(1)–K(1)–N(10)–C(6)	91.3(2)
	C(1)–K(1)–K(2)–N(8$^{\#5}$)	80.77(5)	C(6)–K(2)–O(1)–K(1)	–12.92(5)	K(2)–K(1)–N(10)–C(6)	105.0(2)
	O(4$^{\#1}$)–K(1)–K(2)–N(16$^{\#6}$)	–100.95(6)	O(4$^{\#1}$)–K(1)–O(1)–C(1)	130.26(12)	O(4$^{\#1}$)–K(1)–N(10)–N(9)	–22.86(13)
	O(2$^{\#2}$)–K(1)–K(2)–N(16$^{\#6}$)	179.27(5)	O(2$^{\#2}$)–K(1)–O(1)–C(1)	44.71(12)	O(2$^{\#2}$)–K(1)–N(10)–N(9)	–104.3(3)
	O(5)–K(1)–K(2)–N(16$^{\#6}$)	–25.43(7)	O(5)–K(1)–O(1)–C(1)	135.58(17)	O(5)–K(1)–N(10)–N(9)	61.14(12)
	O(1)–K(1)–K(2)–N(16$^{\#6}$)	–179.00(6)	N(10)–K(1)–O(1)–C(1)	–134.73(12)	O(1)–K(1)–N(10)–N(9)	–101.05(12)

Table S4. (Continued)

3	N(2$^{\#3}$)–K(1)–N(10)–N(9)	169.67(13)	N(4)–N(3)–C(1)–O(1)	–5.2(3)	K(2$^{\#4}$)–O(3)–C(5)–N(11)	–170.74(13)
	C(1)–K(1)–N(10)–N(9)	–115.47(12)	C(2)–N(3)–C(1)–O(1)	178.38(19)	N(10)–N(9)–C(5)–O(3)	179.3(2)
	K(2)–K(1)–N(10)–N(9)	–101.84(13)	N(4)–N(3)–C(1)–N(1)	175.88(16)	N(10)–N(9)–C(5)–N(11)	0.4(2)
	O(4$^{\#1}$)–K(1)–N(10)–K(2)	78.99(5)	C(2)–N(3)–C(1)–N(1)	–0.5(2)	N(12)–N(11)–C(5)–O(3)	4.6(3)
	O(2$^{\#2}$)–K(1)–N(10)–K(2)	–2.5(3)	N(4)–N(3)–C(1)–K(1)	–63.75(18)	C(6)–N(11)–C(5)–O(3)	–179.38(18)
	O(5)–K(1)–N(10)–K(2)	162.98(5)	C(2)–N(3)–C(1)–K(1)	119.87(13)	N(12)–N(11)–C(5)–N(9)	–176.38(16)
	O(1)–K(1)–N(10)–K(2)	0.80(4)	O(4$^{\#1}$)–K(1)–C(1)–O(1)	–48.43(12)	C(6)–N(11)–C(5)–N(9)	–0.4(2)
	N(2$^{\#3}$)–K(1)–N(10)–K(2)	–88.49(5)	O(2$^{\#2}$)–K(1)–C(1)–O(1)	–131.71(12)	N(9)–N(10)–C(6)–N(11)	0.1(2)
	C(1)–K(1)–N(10)–K(2)	–13.63(5)	O(5)–K(1)–C(1)–O(1)	–119.8(2)	K(1)–N(10)–C(6)–N(11)	153.30(15)
	O(3$^{\#4}$)–K(2)–N(10)–C(6)	133.09(13)	N(10)–K(1)–C(1)–O(1)	46.30(12)	K(2)–N(10)–C(6)–N(11)	–105.94(14)
	O(1)–K(2)–N(10)–C(6)	–140.41(13)	N(2$^{\#3}$)–K(1)–C(1)–O(1)	129.23(12)	N(9)–N(10)–C(6)–K(2)	106.01(16)
	O(6)–K(2)–N(10)–C(6)	–94.1(3)	K(2)–K(1)–C(1)–O(1)	34.37(10)	K(1)–N(10)–C(6)–K(2)	–100.8(2)
	N(8$^{\#5}$) –K(2)–N(10)–C(6)	–46.46(13)	O(4$^{\#1}$)–K(1)–C(1)–N(1)	–173.62(12)	N(12)–N(11)–C(6)–N(10)	175.62(18)
	N(16$^{\#6}$)–K(2)–N(10)–C(6)	40.22(13)	O(2$^{\#2}$)–K(1)–C(1)–N(1)	103.09(13)	C(5)–N(11)–C(6)–N(10)	0.2(2)
	K(1)–K(2)–N(10)–C(6)	–139.58(15)	O(5)–K(1)–C(1)–N(1)	115.0(2)	N(12)–N(11)–C(6)–K(2)	113.02(18)
	O(3$^{\#4}$)–K(2)–N(10)–N(9)	21.60(11)	O(1)–K(1)–C(1)–N(1)	–125.19(19)	C(5)–N(11)–C(6)–K(2)	–62.42(16)
	O(1)–K(2)–N(10)–N(9)	108.10(11)	N(10)–K(1)–C(1)–N(1)	–78.89(13)	O(3$^{\#4}$)–K(2)–C(6)–N(10)	–49.57(13)
	O(6)–K(2)–N(10)–N(9)	154.4(3)	N(2$^{\#3}$)–K(1)–C(1)–N(1)	4.03(12)	O(1)–K(2)–C(6)–N(10)	40.70(13)
	N(8$^{\#5}$)–K(2)–N(10)–N(9)	–157.95(11)	K(2)–K(1)–C(1)–N(1)	–90.82(12)	O(6)–K(2)–C(6)–N(10)	156.03(14)
	N(16$^{\#6}$)–K(2)–N(10)–N(9)	–71.27(11)	O(4$^{\#1}$)–K(1)–C(1)–N(3)	70.48(12)	N(8$^{\#5}$)–K(2)–C(6)–N(10)	129.52(14)
	C(6)–K(2)–N(10)–N(9)	–111.49(18)	O(2$^{\#2}$)–K(1)–C(1)–N(3)	–12.80(11)	N(16$^{\#6}$)–K(2)–C(6)–N(10)	–134.42(14)
	K(1)–K(2)–N(10)–N(9)	108.93(11)	O(5)–K(1)–C(1)–N(3)	–0.9(3)	K(1)–K(2)–C(6)–N(10)	30.92(12)
	O(3)$^{\#4}$–K(2)–N(10)–K(1)	–87.33(5)	O(1)–K(1)–C(1)–N(3)	118.91(19)	O(3$^{\#4}$)–K(2)–C(6)–N(11)	49.17(13)
	O(1)–K(2)–N(10)–K(1)	–0.83(4)	N(10)–K(1)–C(1)–N(3)	165.21(12)	O(1)–K(2)–C(6)–N(11)	139.45(12)
	O(6)–K(2)–N(10)–K(1)	45.5(3)	N(2$^{\#3}$)–K(1)–C(1)–N(3)	–111.87(13)	O(6)–K(2)–C(6)–N(11)	–105.22(16)
	N(8)$^{\#5}$–K(2)–N(10)–K(1)	93.12(6)	K(2)–K(1)–C(1)–N(3)	153.28(13)	N(8$^{\#5}$) –K(2)–C(6)–N(11)	–131.73(13)
	N(16)$^{\#6}$–K(2)–N(10)–K(1)	179.80(5)	N(1)–N(2)–C(2)–N(3)	0.0(2)	N(16$^{\#6}$) –K(2)–C(6)–N(11)	–35.67(12)
	C(6)–K(2)–N(10)–K(1)	139.58(15)	K(1$^{\#3}$)–N(2)–C(2)–N(3)	–167.70(14)	N(10)–K(2)–C(6)–N(11)	98.75(18)
	C(6)–N(11)–N(12)–N(13)	3.0(3)	N(4)–N(3)–C(2)–N(2)	–175.48(18)	K(1)–K(2)–C(6)–N(11)	129.66(13)
	C(5)–N(11)–N(12)–N(13)	177.88(16)	C(1)–N(3)–C(2)–N(2)	0.3(2)	K(1$^{\#5}$)–O(4)–C(7)–N(15)	–21.0(3)
	N(11)–N(12)–N(13)–N(14)	–178.14(15)	K(1$^{\#2}$)–O(2)–C(3)–N(7)	13.7(3)	K(1$^{\#5}$)–O(4)–C(7)–N(14)	158.98(14)
	N(12)–N(13)–N(14)–C(8)	–1.4(3)	K(1$^{\#2}$)–O(2)–C(3)–N(6)	–166.94(13)	N(16)–N(15)–C(7)–O(4)	179.0(2)
	N(12)–N(13)–N(14)–C(7)	–179.69(16)	N(8)–N(7)–C(3)–O(2)	178.6(2)	N(16)–N(15)–C(7)–N(14)	–1.0(2)
	C(7)–N(15)–N(16)–C(8)	0.7(2)	N(8)–N(7)–C(3)–N(6)	–0.8(2)	N(13)–N(14)–C(7)–O(4)	–0.4(3)
	C(7)–N(15)–N(16)–K(2$^{\#6}$)	178.55(12)	N(5)–N(6)–C(3)–O(2)	–1.7(3)	C(8)–N(14)–C(7)–O(4)	–179.09(19)
	K(2)–O(1)–C(1)–N(1)	–29.9(3)	C(4)–N(6)–C(3)–O(2)	–178.39(19)	N(13)–N(14)–C(7)–N(15)	179.60(16)
	K(1)–O(1)–C(1)–N(1)	85.7(2)	N(5)–N(6)–C(3)–N(7)	177.78(16)	C(8)–N(14)–C(7)–N(15)	0.9(2)
	K(2)–O(1)–C(1)–N(3)	151.58(14)	C(4)–N(6)–C(3)–N(7)	1.1(2)	N(15)–N(16)–C(8)–N(14)	–0.1(2)
	K(1)–O(1)–C(1)–N(3)	–92.8(2)	N(7)–N(8)–C(4)–N(6)	0.5(2)	K(2$^{\#6}$) –N(16)–C(8)–N(14)	–176.81(14)
	K(2)–O(1)–C(1)–K(1)	–115.59(15)	K(2$^{\#1}$)–N(8)–C(4)–N(6)	163.79(15)	N(13)–N(14)–C(8)–N(16)	–179.00(19)
	N(2)–N(1)–C(1)–O(1)	–178.30(19)	N(5)–N(6)–C(4)–N(8)	–177.16(19)	C(7)–N(14)–C(8)–N(16)	–0.6(2)
	N(2)–N(1)–C(1)–N(3)	0.5(2)	C(3)–N(6)–C(4)–N(8)	–1.0(2)		
	N(2)–N(1)–C(1)–K(1)	–121.81(13)	K(2$^{\#4}$)–O(3)–C(5)–N(9)	10.5(3)		
4	C(2)–O(1)–Cs(1)–O(1$^{\#3}$)	50.98(10)	C(2)–O(1)–Cs(1)–N(1$^{\#5}$)	–120.72(13)	C(2)–O(1)–Cs(1)–O(2$^{\#7}$)	37.01(13)
	Cs(1$^{\#1}$)–O(1)–Cs(1)–O(1$^{\#3}$)	–94.20(6)	Cs(1$^{\#1}$)–O(1)–Cs(1)–N(1$^{\#5}$)	94.11(9)	Cs(1$^{\#1}$)–O(1)–Cs(1)–O(2$^{\#7}$)	–108.17(6)
	C(2)–O(1)–Cs(1)–O(1$^{\#1}$)	145.17(14)	C(2)–O(1)–Cs(1)–N(1$^{\#6}$)	–66.10(12)	C(2)–O(1)–Cs(1)–N(4$^{\#1}$)	–172.51(11)
	Cs(1$^{\#1}$) O(1)–Cs(1)–O(1$^{\#1}$)	0.0	Cs(1$^{\#1}$)–O(1)–Cs(1)–N(1$^{\#6}$)	148.73(5)	Cs(1$^{\#1}$)–O(1)–Cs(1)–N(4$^{\#1}$)	42.32(5)
	C(2)–O(1)–Cs(1)–O(1$^{\#4}$)	98.70(11)	C(2)–O(1)–Cs(1)–O(2)	–133.64(13)	C(2)–O(1)–Cs(1)–N(4$^{\#3}$)	2.89(11)
	Cs(1$^{\#1}$)–O(1)–Cs(1)–O(1$^{\#4}$)	–46.47(3)	Cs(1$^{\#1}$) –O(1)–Cs(1)–O(2)	81.18(5)	Cs(1$^{\#1}$)–O(1)–Cs(1)–N(4$^{\#3}$)	–142.29(4)

Table S4. (Continued)

	Cs(1$^{\#1}$)–O(1)–Cs(1)–C(2)	–145.17(14)	Cs(1$^{\#1}$)–O(1)–C(2)–N(2)	–163.98(14)	O(1$^{\#3}$)–Cs(1)–C(2)–N(2)	100.34(11)
	C(2)–O(1)–Cs(1)–C(2$^{\#4}$)	119.43(12)	Cs(1)–O(1)–C(2)–N(2)	59.5(2)	O(1$^{\#1}$)–Cs(1)–C(2)–N(2)	–171.35(11)
	Cs(1$^{\#1}$)–O(1)–Cs(1)–C(2$^{\#4}$)	–25.74(6)	Cs(1$^{\#1}$)–O(1)–C(2)–N(3)	14.6(3)	O(1$^{\#4}$)–Cs(1)–C(2)–N(2)	129.70(10)
	Cs(1$^{\#2}$)–O(2)–Cs(1)–O(1$^{\#3}$)	–38.27(3)	Cs(1)–O(1)–C(2)–N(3)	–121.88(15)	O(1)–Cs(1)–C(2)–N(2)	–138.88(18)
	Cs(1$^{\#2}$)–O(2)–Cs(1)–O(1$^{\#1}$)	35.79(3)	Cs(1$^{\#1}$)–O(1)–C(2)–Cs(1)	136.49(15)	N(1$^{\#5}$)–Cs(1)–C(2)–N(2)	–35.00(18)
	Cs(1$^{\#2}$)–O(2)–Cs(1)–O(1$^{\#4}$)	49.37(5)	N(1)–N(2)–C(2)–O(1)	179.61(18)	N(1$^{\#6}$)–Cs(1)–C(2)–N(2)	–28.74(11)
	Cs(1$^{\#2}$)–O(2)–Cs(1)–O(1)	–43.04(4)	N(1)–N(2)–C(2)–N(3)	0.80(19)	O(2)–Cs(1)–C(2)–N(2)	–100.38(11)
	Cs(1$^{\#2}$)–O(2)–Cs(1)–N(1$^{\#5}$)	142.40(3)	N(1)–N(2)–C(2)–Cs(1)	–135.56(12)	O(2$^{\#7}$)–Cs(1)–C(2)–N(2)	70.27(12)
	Cs(1$^{\#2}$)–O(2)–Cs(1)–N(1$^{\#6}$)	–140.30(3)	N(4)–N(3)–C(2)–O(1)	6.8(3)	N(4$^{\#1}$)–Cs(1)–C(2)–N(2)	–130.66(11)
	Cs(1$^{\#2}$)–O(2)–Cs(1)–O(2$^{\#7}$)	180.0	C(1)–N(3)–C(2)–O(1)	–179.43(17)	N(4$^{\#3}$)–Cs(1)–C(2)–N(2)	44.24(10)
	Cs(1$^{\#2}$)–O(2)–Cs(1)–N(4$^{\#1}$)	90.23(4)	N(4)–N(3)–C(2)–N(2)	–174.30(15)	C(2$^{\#4}$)–Cs(1)–C(2)–N(2)	149.55(11)
	Cs(1$^{\#2}$)–O(2)–Cs(1)–N(4$^{\#3}$)	–95.97(3)	C(1)–N(3)–C(2)–N(2)	–0.53(18)	O(1$^{\#3}$)–Cs(1)–C(2)–N(3)	–12.93(14)
	Cs(1$^{\#2}$)–O(2)–Cs(1)–C(2)	–57.52(3)	N(4)–N(3)–C(2)–Cs(1)	–65.5(2)	O(1$^{\#1}$)–Cs(1)–C(2)–N(3)	75.38(15)
	Cs(1$^{\#2}$)–O(2)–Cs(1)–C(2$^{\#4}$)	61.94(4)	C(1)–N(3)–C(2)–Cs(1)	108.31(16)	O(1$^{\#4}$)–Cs(1)–C(2)–N(3)	16.43(17)
	C(1)–N(1)–N(2)–C(2)	–0.8(2)	O(1$^{\#3}$)–Cs(1)–C(2)–O(1)	–120.78(11)	O(1)–Cs(1)–C(2)–N(3)	107.9(2)
	Cs(1$^{\#8}$)–N(1)–N(2)–C(2)	171.31(11)	O(1$^{\#1}$)–Cs(1)–C(2)–O(1)	–32.47(13)	N(1$^{\#5}$)–Cs(1)–C(2)–N(3)	–148.27(14)
	C(1)–N(3)–N(4)–N(4$^{\#9}$)	20.58(19)	O(1$^{\#4}$)–Cs(1)–C(2)–O(1)	–91.43(12)	N(1$^{\#6}$)–Cs(1)–C(2)–N(3)	–142.01(16)
	C(2)–N(3)–N(4)–N(4$^{\#9}$)	–167.34(11)	N(1$^{\#5}$)–Cs(1)–C(2)–O(1)	103.87(15)	O(2)–Cs(1)–C(2)–N(3)	146.35(17)
	C(1)–N(3)–N(4)–Cs(1$^{\#1}$)	169.02(15)	N(1$^{\#6}$)–Cs(1)–C(2)–O(1)	110.14(12)	O(2$^{\#7}$)–Cs(1)–C(2)–N(3)	–43.00(17)
	C(2)–N(3)–N(4)–Cs(1$^{\#1}$)	–18.90(17)	O(2)–Cs(1)–C(2)–O(1)	38.50(11)	N(4$^{\#1}$)–Cs(1)–C(2)–N(3)	116.07(15)
	N(2)–N(1)–C(1)–N(3)	0.4(2)	O(2$^{\#7}$)–Cs(1)–C(2)–O(1)	–150.85(11)	N(4$^{\#3}$)–Cs(1)–C(2)–N(3)	–69.03(15)
	Cs(1$^{\#8}$)–N(1)–C(1)–N(3)	–167.73(13)	N(4$^{\#1}$)–Cs(1)–C(2)–O(1)	8.22(12)	C(2$^{\#4}$)–Cs(1)–C(2)–N(3)	36.28(14)
	N(4)–N(3)–C(1)–N(1)	172.92(16)	N(4$^{\#3}$)–Cs(1)–C(2)–O(1)	–176.88(12)		
	C(2)–N(3)–C(1)–N(1)	0.1(2)	C(2$^{\#4}$)–Cs(1)–C(2)–O(1)	–71.57(11)		
5	N(3)–C(1)–N(1)–N(2)	0.3(2)	O(1)–C(1)–N(3)–C(2)	–179.8(2)	N(2)–C(2)–N(3)–N(4)	177.4(2)
	O(1)–C(1)–N(1)–N(2)	179.7(2)	O(1)–C(1)–N(3)–N(4)	2.6(2)	N(8)–C(3)–N(6)–C(4)	–1.3(2)
	N(1)–C(1)–N(3)–C(2)	–0.3(2)	N(3)–C(2)–N(2)–N(1)	–0.1(2)	N(8)–C(3)–N(6)–C(4)	–179.7(1)
	N(1)–C(1)–N(3)–N(4)	–177.9(1)	N(2)–C(2)–N(3)–C(1)	0.2(2)	O(2)–C(3)–N(6)–C(4)	177.9(2)
	O(2)–C(3)–N(6)–N(5)	–0.5(3)	N(6)–C(4)–N(7)–N(8)	0.1(2)	N(4)–N(5)–N(6)–C(3)	177.3(1)
	N(6)–C(3)–N(8)–N(7)	1.4(2)	C(1)–N(1)–N(2)–C(2)	–0.1(2)	N(4)–N(5)–N(6)–C(4)	–0.7(2)
	O(2)–C(3)–N(8)–N(7)	–177.7(2)	C(1)–N(3)–N(4)–N(5)	177.4(1)	C(4)–N(7)–N(8)–C(3)	–1.0(2)
	N(7)–C(4)–N(6)–C(3)	0.8(2)	C(2)–N(3)–N(4)–N(5)	0.5(2)		
	N(7)–C(4)–N(6)–N(5)	179.0(1)	N(3)–N(4)–N(5)–N(6)	–179.8(1)		
6	C(1)–N(1)–N(2)–C(2)	–0.58(14)	N(4)–N(3)–C(1)–O(1)	2.52(18)	N(5)–N(6)–C(3)–O(2)	–4.98(16)
	C(2)–N(3)–N(4)–N(5)	–0.04(17)	C(2)–N(3)–C(1)–O(1)	179.90(12)	C(4)–N(6)–C(3)–O(2)	179.28(10)
	C(1)–N(3)–N(4)–N(5)	176.62(10)	N(4)–N(3)–C(1)–N(1)	–177.73(9)	N(5)–N(6)–C(3)–N(7)	175.14(9)
	N(3)–N(4)–N(5)–N(6)	–179.38(8)	C(2)–N(3)–C(1)–N(1)	–0.35(12)	C(4)–N(6)–C(3)–N(7)	–0.60(12)
	N(4)–N(5)–N(6)–C(4)	–6.24(16)	N(1)–N(2)–C(2)–N(3)	0.33(13)	N(7)–N(8)–C(4)–N(6)	–0.06(12)
	N(4)–N(5)–N(6)–C(3)	179.21(10)	N(4)–N(3)–C(2)–N(2)	176.95(11)	N(5)–N(6)–C(4)–N(8)	–174.68(10)
	C(3)–N(7)–N(8)–C(4)	–0.33(12)	C(1)–N(3)–C(2)–N(2)	0.01(14)	C(3)–N(6)–C(4)–N(8)	0.40(12)
	N(2)–N(1)–C(1)–O(1)	–179.70(12)	N(8)–N(7)–C(3)–O(2)	–179.30(11)		
	N(2)–N(1)–C(1)–N(3)	0.56(13)	N(8)–N(7)–C(3)–N(6)	0.57(12)		
7	O(5)–Ca(1)–O(1)–C(1)	–89.3(3)	Ca(1)#1–Ca(1)–O(1)–C(1)	11.5(3)	O(4)#2–Ca(1)–O(3)–Ca(1)#1	–132.07(12)
	O(6)–Ca(1)–O(1)–C(1)	167.7(3)	Ca(1)#2–Ca(1)–O(1)–C(1)	165.1(3)	N(1)#1–Ca(1)–O(3)–Ca(1)#1	78.48(10)
	O(3)–Ca(1)–O(1)–C(1)	49.5(3)	O(1)–Ca(1)–O(3)–Ca(1)#1	–82.52(10)	Ca(1)#2–Ca(1)–O(3)–Ca(1)#1	–154.76(7)
	O(3)#1–Ca(1)–O(1)–C(1)	–25.5(3)	O(5)–Ca(1)–O(3)–Ca(1)#1	33.23(18)	O(1)–Ca(1)–O(4)–Ca(1)#2	81.29(10)
	O(4)–Ca(1)–O(1)–C(1)	129.6(3)	O(6)–Ca(1)–O(3)–Ca(1)#1	133.79(10)	O(5)–Ca(1)–O(4)–Ca(1)#2	–44.11(17)
	O(4)#2–Ca(1)–O(1)–C(1)	–159.1(3)	O(3)#1–Ca(1)–O(3)–Ca(1)#1	0	O(6)–Ca(1)–O(4)–Ca(1)#2	–75.74(11)
	N(1)#1–Ca(1)–O(1)–C(1)	21.7(4)	O(4)–Ca(1)–O(3)–Ca(1)#1	–168.90(11)	O(3)–Ca(1)–O(4)–Ca(1)#2	156.80(11)

Table S4. (Continued)

7	O(3)#1–Ca(1)–O(4)–Ca(1)#2	135.52(15)	Ca(1)–O(1)–C(1)–N(1)	–8.5(6)	C(1)–N(3)–C(2)–N(2)	0.0(4)
	O(4)#2–Ca(1)–O(4)–Ca(1)#2	0	Ca(1)–O(1)–C(1)–N(3)	170.8(2)	N(8)–N(7)–C(3)–O(2)	–179.9(4)
	N(1)#1–Ca(1)–O(4)–Ca(1)#2	–138.95(10)	N(2)–N(1)–C(1)–O(1)	178.3(4)	N(8)–N(7)–C(3)–N(6)	–0.1(4)
	Ca(1)#1–Ca(1)–O(4)–Ca(1)#2	149.56(7)	Ca(1)#1–N(1)–C(1)–O(1)	–7.6(6)	N(5)–N(6)–C(3)–O(2)	–0.4(6)
	C(1)–N(1)–N(2)–C(2)	1.2(4)	N(2)–N(1)–C(1)–N(3)	–1.1(4)	C(4)–N(6)–C(3)–O(2)	180.0(3)
	Ca(1)#1–N(1)–N(2)–C(2)	–174.1(3)	Ca(1)#1–N(1)–C(1)–N(3)	172.9(2)	N(5)–N(6)–C(3)–N(7)	179.8(3)
	C(2)–N(3)–N(4)–N(5)	6.8(5)	C(2)–N(3)–C(1)–O(1)	–178.8(4)	C(4)–N(6)–C(3)–N(7)	0.2(4)
	C(1)–N(3)–N(4)–N(5)	–176.7(3)	N(4)–N(3)–C(1)–O(1)	4.1(6)	N(7)–N(8)–C(4)–N(6)	0.1(4)
	N(3)–N(4)–N(5)–N(6)	–178.2(3)	C(2)–N(3)–C(1)–N(1)	0.7(4)	N(5)–N(6)–C(4)–N(8)	–179.8(4)
	N(4)–N(5)–N(6)–C(4)	0.6(6)	N(4)–N(3)–C(1)–N(1)	–176.4(3)	C(3)–N(6)–C(4)–N(8)	–0.2(4)
	N(4)–N(5)–N(6)–C(3)	–179.0(3)	N(1)–N(2)–C(2)–N(3)	–0.7(4)	C(1)–N(3)–C(2)–N(2)	0.0(4)
	C(3)–N(7)–N(8)–C(4)	0.0(4)	N(4)–N(3)–C(2)–N(2)	176.9(4)		
8	O(1)#1–Sr(1)–N(1)–C(1)	33.3(6)	N(3)–N(4)–N(5)–N(6)	–179.4(4)	N(5)–N(6)–C(4)–N(8)	–179.3(6)
	O(5)–Sr(1)–N(1)–C(1)	–175.3(6)	N(4)–N(5)–N(6)–C(4)	–1.0(8)	C(3)–N(6)–C(4)–N(8)	–0.9(7)
	O(3)#1–Sr(1)–N(1)–C(1)	–21.3(5)	N(4)–N(5)–N(6)–C(3)	–179.1(5)	N(1)–C(1)–O(1)–Sr(1)#1	–13.5(10)
	O(6)–Sr(1)–N(1)–C(1)	–98.9(5)	C(3)–N(7)–N(8)–C(4)	–0.7(6)	N(3)–C(1)–O(1)–Sr(1)#1	165.7(4)
	O(4)#2–Sr(1)–N(1)–C(1)	–159.2(5)	N(2)–N(1)–C(1)–O(1)	179.2(6)	O(1)#1–Sr(1)–O(3)–Sr(1)#1	85.39(15)
	O(3)–Sr(1)–N(1)–C(1)	56.6(5)	Sr(1)–N(1)–C(1)–O(1)	–12.6(10)	O(5)–Sr(1)–O(3)–Sr(1)#1	–132.25(14)
	O(4)–Sr(1)–N(1)–C(1)	124.0(5)	N(2)–N(1)–C(1)–N(3)	0.0(6)	O(3)#1–Sr(1)–O(3)–Sr(1)#1	0
	Sr(1)#1–Sr(1)–N(1)–C(1)	17.7(5)	Sr(1)–N(1)–C(1)–N(3)	168.1(4)	O(6)–Sr(1)–O(3)–Sr(1)#1	–36.5(3)
	Sr(1)#2–Sr(1)–N(1)–C(1)	153.5(5)	N(4)–N(3)–C(1)–O(1)	2.7(9)	O(4)#2–Sr(1)–O(3)–Sr(1)#1	139.53(16)
	O(1)#1–Sr(1)–N(1)–N(2)	–159.3(3)	C(2)–N(3)–C(1)–O(1)	–179.4(6)	O(4)–Sr(1)–O(3)–Sr(1)#1	172.15(16)
	O(5)–Sr(1)–N(1)–N(2)	–7.9(4)	N(4)–N(3)–C(1)–N(1)	–178.0(5)	N(1)–Sr(1)–O(3)–Sr(1)#1	–77.82(16)
	O(3)#1–Sr(1)–N(1)–N(2)	146.1(4)	C(2)–N(3)–C(1)–N(1)	–0.1(6)	Sr(1)#2–Sr(1)–O(3)–Sr(1)#1	159.34(9)
	O(6)–Sr(1)–N(1)–N(2)	68.5(4)	N(1)–N(2)–C(2)–N(3)	–0.2(7)	O(1)#1–Sr(1)–O(4)–Sr(1)#2	–86.69(15)
	O(4)#2–Sr(1)–N(1)–N(2)	8.2(5)	N(4)–N(3)–C(2)–N(2)	177.9(5)	O(5)–Sr(1)–O(4)–Sr(1)#2	75.15(16)
	O(3)–Sr(1)–N(1)–N(2)	–136.0(4)	C(1)–N(3)–C(2)–N(2)	0.2(7)	O(3)#1–Sr(1)–O(4)–Sr(1)#2	–145.38(17)
	O(4)–Sr(1)–N(1)–N(2)	–68.6(4)	N(8)–N(7)–C(3)–O(2)	179.8(6)	O(6)–Sr(1)–O(4)–Sr(1)#2	47.5(3)
	Sr(1)#1–Sr(1)–N(1)–N(2)	–174.9(4)	N(8)–N(7)–C(3)–N(6)	0.2(6)	O(4)#2–Sr(1)–O(4)–Sr(1)#2	0
	Sr(1)#2–Sr(1)–N(1)–N(2)	–39.1(4)	N(5)–N(6)–C(3)–O(2)	–0.6(9)	O(3)–Sr(1)–O(4)–Sr(1)#2	–158.91(16)
	C(1)–N(1)–N(2)–C(2)	0.2(7)	C(4)–N(6)–C(3)–O(2)	–179.2(5)	N(1)–Sr(1)–O(4)–Sr(1)#2	137.51(15)
	Sr(1)–N(1)–N(2)–C(2)	–170.3(4)	N(5)–N(6)–C(3)–N(7)	179.0(5)	Sr(1)#1–Sr(1)–O(4)–Sr(1)#2	–154.04(10)
	C(2)–N(3)–N(4)–N(5)	5.0(8)	C(4)–N(6)–C(3)–N(7)	0.4(6)		
	C(1)–N(3)–N(4)–N(5)	–177.6(5)	N(7)–N(8)–C(4)–N(6)	1.0(7)		
9	O(3$^{\#1}$)–Ba(1)–O(2)–C(3)	6.1(3)	C(1)–N(1)–N(2)–C(2)	–0.5(4)	N(8$^{\#1}$)–Ba(1)–O(3)–Ba(1$^{\#1}$)	–75.25(8)
	O(4)–Ba(1)–O(2)–C(3)	148.1(3)	N(6)–C(4)–N(7)–N(8)	0.4(4)	O(5$^{\#3}$)–Ba(1)–O(3)–Ba(1$^{\#1}$)	57.02(10)
	O(6)–Ba(1)–O(2)–C(3)	–156.4(3)	C(3)–N(8)–N(7)–C(4)	–0.2(4)	Ba(1$^{\#2}$)–Ba(1)–O(3)–Ba(1$^{\#1}$)	166.93(5)
	O(4$^{\#2}$)–Ba(1)–O(2)–C(3)	–138.2(3)	Ba(1$^{\#1}$)–N(8)–N(7)–C(4)	168.0(2)	O(3$^{\#1}$)–Ba(1)–O(4)–Ba(1$^{\#2}$)	157.81(8)
	O(3)–Ba(1)–O(2)–C(3)	–68.7(3)	Ba(1)–O(2)–C(3)–N(8)	24.6(5)	O(2)–Ba(1)–O(4)–Ba(1$^{\#2}$)	76.70(8)
	O(5)–Ba(1)–O(2)–C(3)	73.3(3)	Ba(1)–O(2)–C(3)–N(6)	–155.0(2)	O(6)–Ba(1)–O(4)–Ba(1$^{\#2}$)	–70.26(9)
	N(8$^{\#1}$)–Ba(1)–O(2)–C(3)	–49.7(3)	N(7)–N(8)–C(3)–O(2)	–179.7(3)	O(4$^{\#2}$) –Ba(1)–O(4)–Ba(1$^{\#2}$)	0.0
	O(5$^{\#3}$)–Ba(1)–O(2)–C(3)	82.6(3)	Ba(1)#1–N(8)–C(3)–O(2)	14.5(5)	O(3)–Ba(1)–O(4)–Ba(1$^{\#2}$)	22.66(12)
	Ba(1$^{\#2}$)–Ba(1)–O(2)–C(3)	–175.0(3)	N(7)–N(8)–C(3)–N(6)	–0.1(3)	O(5)–Ba(1)–O(4)–Ba(1$^{\#2}$)	–149.58(8)
	Ba(1$^{\#1}$)–Ba(1)–O(2)–C(3)	–30.3(3)	Ba(1)#1–N(8)–C(3)–N(6)	–165.8(2)	N(8$^{\#1}$)–Ba(1)–O(4)–Ba(1$^{\#2}$)	–84.88(11)
	N(6)–N(5)–N(4)–N(3)	179.8(3)	N(5)–N(6)–C(3)–O(2)	–1.0(5)	O(5$^{\#3}$)–Ba(1)–O(4)–Ba(1$^{\#2}$)	141.04(9)
	N(5)–N(4)–N(3)–C(2)	3.5(5)	C(4)–N(6)–C(3)–O(2)	–180.0(3)	Ba(1$^{\#1}$)–Ba(1)–O(4)–Ba(1$^{\#2}$)	81.69(17)
	N(5)–N(4)–N(3)–C(1)	179.9(3)	N(5)–N(6)–C(3)–N(8)	179.3(3)	O(3$^{\#1}$ –Ba(1)–O(5)–Ba(1$^{\#3}$)	77.95(8)
	O(1)–C(1)–N(3)–N(4)	2.3(5)	C(4)–N(6)–C(3)–N(8)	0.3(4)	O(2)–Ba(1)–O(5)–Ba(1)$^{\#3}$	9.29(12)
	N(1)–C(1)–N(3)–N(4)	–178.6(3)	N(1)–N(2)–C(2)–N(3)	–0.4(4)	O(4)–Ba(1)–O(5)–Ba(1$^{\#3}$)	–72.08(8)

Table S4. (Continued)

O(1)–C(1)–N(3)–C(2)	179.5(3)	N(4)–N(3)–C(2)–N(2)	177.8(3)	O(6)–Ba(1)–O(5)–Ba(1$^{\#3}$)	–141.90(9)
N(1)–C(1)–N(3)–C(2)	–1.4(3)	C(1)–N(3)–C(2)–N(2)	1.1(4)	O(4$^{\#2}$)–Ba(1)–O(5)–Ba(1$^{\#3}$)	–119.84(9)
N(4)–N(5)–N(6)–C(4)	–2.8(5)	O(3$^{\#1}$)–Ba(1)–O(3)–Ba(1$^{\#1}$)	0.0	O(3)–Ba(1)–O(5)–Ba(1$^{\#3}$)	116.84(10)
N(4)–N(5)–N(6)–C(3)	178.6(3)	O(2)–Ba(1)–O(3)–Ba(1$^{\#1}$)	89.55(9)	N(8$^{\#1}$)–Ba(1)–O(5)–Ba(1$^{\#3}$)	149.72(9)
N(7)–C(4)–N(6)–N(5)	–179.3(3)	O(4)–Ba(1)–O(3)–Ba(1$^{\#1}$)	152.93(7)	O(5$^{\#3}$)–Ba(1)–O(5)–Ba(1$^{\#3}$)	0.0
N(7)–C(4)–N(6)–C(3)	–0.5(4)	O(6)–Ba(1)–O(3)–Ba(1$^{\#1}$)	–130.50(8)	Ba(1$^{\#2}$)–Ba(1)–O(5)–Ba(1$^{\#3}$)	–91.39(7)
O(1)–C(1)–N(1)–N(2)	–179.7(3)	O(4$^{\#2}$)–Ba(1)–O(3)–Ba(1$^{\#1}$)	176.84(9)	Ba(1$^{\#1}$)–Ba(1)–O(5)–Ba(1$^{\#3}$)	92.66(7)
N(3)–C(1)–N(1)–N(2)	1.1(3)	O(5)–Ba(1)–O(3)–Ba(1$^{\#1}$)	–40.11(14)		

Table S5. The selected hydrogen bond distances (Å) and angles (°) of ZTO and its salts

Compound	D–H···A	d(D···H)	d(H···A)	∠DHA	d(D···A)
ZTO	N(2)–H(2)···O(1)	0.90	2.53	129	3.17
	N(2)–H(2)···N(1)	0.09	2.08	149	2.89
2	O(3)–H(3WC)···O(2)	0.86	1.92	167	2.76
	N(1)–H(1A)···N(7)	0.86	1.78	173	2.63
	O(3)–H(3WB)···N(2)	0.86	1.98	172	2.83
	O(4)–H(4WB)···O(2)	0.86	1.99	174	2.85
	O(4)–H(4WA)···O(3)	0.86	2.01	176	2.87
3	N(1)–H(1)···N(7)	1.05	1.66	176	2.70
	O(5)–H(05A)···O(1)	0.80	2.32	151	3.04
	O(5)–H(05B)···O(3)	0.82	2.12	158	2.89
	O(5)–H(05B)···N(12)	0.82	2.60	130	3.18
	O(6)–H(06A)···O(4)	0.89	2.07	153	2.89
	O(6)–H(06A)···N(13)	0.89	2.54	131	3.20
	O(6)–H(06B)···O(2)	0.82	2.10	155	2.86
	O(6)–H(06B)···N(5)	0.82	2.62	132	3.23
	N(15)–H(15)···N(9)	1.06	1.65	172	2.71
4	N(2)–H(2A)···N(2)	0.86	1.81	172	2.67
	C(1)–H(1A)···O(2)	0.93	2.42	166	2.33
5	N(8)–H(1N)···N(1)	0.95	1.80	176	2.75
	N(9)–H(2N)···O(2)	0.89	2.34	150	3.14
	N(9)–H(3N)···N(7)	0.91	2.20	160	3.08
	N(10)–H(10A)···O(1)	0.89	1.90	166	2.77
	N(10)–H(10B)···O(1)	0.89	1.96	163	2.83
	N(10)–H(10C)···N(2)	0.89	2.09	155	2.92
6	N(1) – H(1N) ···N(7)	0.98	1.76	177	2.75
	O(3) – H(3A) ···O(2)	0.87	2.19	147	2.97
	O(3) – H(3A) ···N(5)	0.87	2.51	141	3.23
	O(3) – H(3B) ···N(2)	0.86	2.01	165	2.85
	O(4) – H(4A) ···O(6)	0.82	1.93	174	2.74
	O(4) – H(4B) ···O(2)	0.87	1.92	174	2.79
	O(5) – H(5A) ···O(1)	0.90	1.83	178	2.73
	O(5) – H(5B) ···N(8)	0.87	1.99	169	2.85
	O(6) – H(6A) ···O(2)	0.90	1.80	166	2.68
	O(6) – H(6B) ···O(7)	0.82	1.93	158	2.71
	O(7) – H(7A) ···O(6)	0.88	1.91	164	2.76
	O(7) – H(7B) ···O(1)	0.92	1.97	171	2.88

Table S5 (continue)

7	O(3)–H(3A)···O(2)	0.99	1.71	174	2.70
	O(3)–H(3B)···N(7)	0.99	1.94	165	2.91
	O(4)–H(4A)···O(2)	0.84	1.92	161	2.73
	O(4)–H(4B)···N(7)	0.85	2.17	162	2.99
	O(5)–H(5A)···O(2)	0.85	1.89	167	2.72
	O(5)–H(5B)···N(7)	0.84	2.49	125	3.05
	O(5)–H(5B)···N(8)	0.84	2.08	158	2.87
	O(6)–H(6A)···O(1)	0.82	1.93	166	2.74
	O(6) –H(6B)···N(2)	0.84	2.07	136	2.74
8	O(3)–H(3A)···O(2)	0.99	1.69	175	2.68
	O(3)–H(3B)···N(7)	0.99	1.95	165	2.91
	O(4)–H(4A)···N(7)	0.83	2.16	148	2.89
	O(5)–H(5A)···O(1)	0.84	1.99	156	2.78
	O(5)–H(5B)···N(2)	0.85	2.10	135	2.77
	O(6)–H(6A)···O(2)	0.83	1.91	168	2.73
	O(6)–H(6B)···N(8)	0.84	2.17	149	2.91
9	O(3)–H(03A)···O(1)	0.84	1.83	169	2.65
	O(3)–H(03B)···N(1)	0.84	2.11	164	2.93
	O(4)–H(04A)···O(1)	0.85	1.94	150	2.71
	O(4)–H(04B)···N(1)	0.84	1.98	169	2.81
	O(5)–H(05A)···N(1)	0.83	2.58	135	3.22
	O(5)–H(05A)···N(2)	0.83	2.19	168	3.01
	O(5)–H(05B)···O(1)	0.84	1.98	156	2.77
	O(6)–H(06A)···O(2)	0.84	2.03	155	2.82
	O(6)–H(06B)···N(7)	0.84	2.07	149	2.82

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Table S6. Thermal decomposition peak temperature of ZTO and its salts

Compound	β / ℃ min^{-1}	endothermic stage		exothermic stage			
		T_{o1}/ ℃	T_{p1}/ ℃	T_{o2}/ ℃	T_{p2}/ ℃	T_{o3}/ ℃	T_{p3}/ ℃
ZTO	2	–	–	278.98	282.40	–	–
	5	–	–	287.44	288.75	–	–
	10	–	–	293.86	295.80	–	–
	20	–	–	300.41	304.61	–	–
1	2	228.08	240.70	246.14	256.17	266.19	273.27
	5	241.19	251.67	257.81	268.97	276.91	284.35
	10	249.98	261.39	275.09	294.76	329.88	340.62
	20	260.91	273.27	289.44	312.12	339.66	351.79
2	2	86.91	123.45	209.59	214.58	234.66	245.41
	5	88.70	132.10	216.88	224.78	365.16	257.23
	10	91.58	143.88	222.02	233.00	381.42	268.13
	20	125.85	153.66	230.94	244.09	394.58	279.20
3	2	130.35	135.10	259.33	269.25	–	–
	5	136.80	145.29	274.26	278.09	–	–
	10	140.12	149.39	279.70	284.23	–	–
	20	146.86	162.29	285.34	291.09	–	–
4	2	200.21	206.03	218.31	222.96	–	–
	5	210.02	218.34	229.19	233.99	–	–
	10	220.31	227.14	237.67	242.09	–	–
	20	229.01	237.92	247.05	252.43	–	–
5	2	141.69	148.08	276.29	278.06	–	–
	5	153.41	159.29	284.30	285.97	–	–
	10	161.83	169.64	290.42	292.78	–	–
	20	166.09	179.29	294.70	299.01	–	–
6	2	106.67	122.58	142.81	190.82	269.87	270.84
	5	114.74	134.38	154.80	207.06	281.44	288.73
	10	120.47	143.73	167.89	219.40	287.66	300.19
	20	127.28	156.74	197.82	235.61	299.90	311.03
7	2	115.96	128.65	177.87	208.57	307.46	329.04
	5	118.56	138.04	187.54	226.15	318.38	344.38
	10	122.39	145.64	199.51	237.68	326.07	355.77
	20	125.77	156.77	218.36	257.88	341.78	368.02
8	2	125.74	143.62	257.75	274.94	–	–
	5	134.94	152.94	265.90	286.99	374.55	378.18
	10	136.66	159.79	275.04	297.54	400.43	405.82
	20	147.46	172.33	292.51	307.18	445.42	454.17

Table S6 (continue)

9	2	81.84	94.28	228.55	241.15	264.18	281.90
	5	83.52	99.88	232.91	248.77	275.67	293.38
	10	89.49	109.37	243.50	260.44	286.63	302.57
	20	94.92	117.86	247.91	272.93	297.24	313.44

[*] *β*: heating rates; T_e: extrapolated onset temperature in the DSC curve; *T*p: maximum peak temperature in the DSC curve; 1, 2 and 3 represents the decomposition stage of title compounds.

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Table S7. Thermal Kinetic parameters obtained by the data in Table 6

Compound	parameters	endothermic stage	exothermic stage	
		T_{p1}/ ℃	T_{p2}/ ℃	T_{p3}/ ℃
ZTO	E_K/kJ mol^{-1}	–	263.612	–
	r_K	–	0.991	–
	A/s^{-1}	–	1.552×10^{22}	–
	E_O/kJ mol^{-1}	–	259.633	–
	r_K	–	0.991	–
	E_a/kJ mol^{-1}	–	261.622	–
1	E_K/kJ mol^{-1}	157.109	89.724	56.618
	r_K	0.998	0.982	0.922
	A/s^{-1}	2.518×10^{13}	1.793×10^{6}	5.585×10^{2}
	E_O/kJ mol^{-1}	157.778	94.117	63.060
	r_K	0.998	0.985	0.942
	E_a/kJ mol^{-1}	157.444	91.921	59.839
2	E_K/kJ mol^{-1}	97.141	156.220	152.570
	r_K	0.993	0.997	0.999
	A/s^{-1}	2.213×10^{10}	1.546×10^{14}	6.152×10^{12}
	E_O/kJ mol^{-1}	98.869	156.486	153.537
	r_K	0.994	0.997	0.999
	E_a/kJ mol^{-1}	98.005	156.353	153.054
3	E_K/kJ mol^{-1}	120.220	260.361	–
	r_K	0.981	0.999	–
	A/s^{-1}	8.543×10^{12}	2.667×10^{22}	–
	E_O/kJ mol^{-1}	120.987	256.338	–
	r_K	0.983	0.999	–
	E_a/kJ mol^{-1}	120.604	258.349	–
4	E_K/kJ mol^{-1}	139.866	163.231	–
	r_K	0.999	0.999	–
	A/s^{-1}	3.822×10^{12}	3.288×10^{14}	–
	E_O/kJ mol^{-1}	140.812	162.330	–
	r_K	0.999	0.999	–
	E_a/kJ mol^{-1}	140.339	163.266	–
5	E_K/kJ mol^{-1}	108.706	276.923	–
	r_K	0.999	0.999	–
	A/s^{-1}	9.450×10^{10}	3.863×10^{23}	–
	E_O/kJ mol^{-1}	110.265	272.212	–
	r_K	0.999	0.999	–
	E_a/kJ mol^{-1}	109.485	274.567	–

*E_K & E_O: the apparent activation energy calculated by Kissinger's method and Ozawa–Doyle's method, respectively; A: the pre–exponential factor; r_K & r_O: linear correlation coefficient determined by Kissinger's method and Ozawa–Doyle's method, respectively.

Table S7. (continued)

Compound	parameters	endothermic stage	exothermic stage	
		T_{p1}/ ℃	T_{p2}/ ℃	T_{p1}/ ℃
6	E_K/kJ mol^{-1}	89.151	93.600	141.205
	r_K	0.997	0.998	0.996
	A/s^{-1}	1.938×10^{9}	9.150×10^{7}	8.160×10^{10}
	E_O/kJ mol^{-1}	91.277	96.666	143.178
	r_K	0.997	0.999	0.997
	E_a/kJ mol^{-1}	90.214	95.132	142.191
7	E_K/kJ mol^{-1}	111.374	92.335	179.732
	r_K	0.995	0.994	0.999
	A/s^{-1}	1.053×10^{12}	2.648×10^{7}	8.467×10^{12}
	E_O/kJ mol^{-1}	112.467	95.792	180.716
	r_K	0.995	0.995	0.999
	E_a/kJ mol^{-1}	111.921	94.064	180.224
8	E_K/kJ mol^{-1}	117.493	178.111	–
	r_K	0.989	0.999	–
	A/s^{-1}	1.862×10^{12}	2.303×10^{14}	–
	E_O/kJ mol^{-1}	118.547	178.277	–
	r_K	0.991	0.999	–
	E_a/kJ mol^{-1}	118.020	178.194	–
9	E_K/kJ mol^{-1}	105.189	154.449	188.886
	r_K	0.985	0.985	0.999
	A/s^{-1}	3.808×10^{12}	1.493×10^{12}	1.468×10^{14}
	E_O/kJ mol^{-1}	106.004	155.248	188.635
	r_K	0.987	0.986	0.999
	E_a/kJ mol^{-1}	105.597	154.849	188.635

*E_K & E_O: the apparent activation energy calculated by Kissinger's method and Ozawa–Doyle's method, respectively; A: the pre–exponential factor; r_K & r_O: linear correlation coefficient determined by Kissinger's method and Ozawa–Doyle's method, respectively.

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