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Supporting Information

Dense inorganic–organic sodium–gadolinium sulfite–oxalate networks constructed from short bridging ligands: synthesis, structures and magnetic refrigeration behaviour

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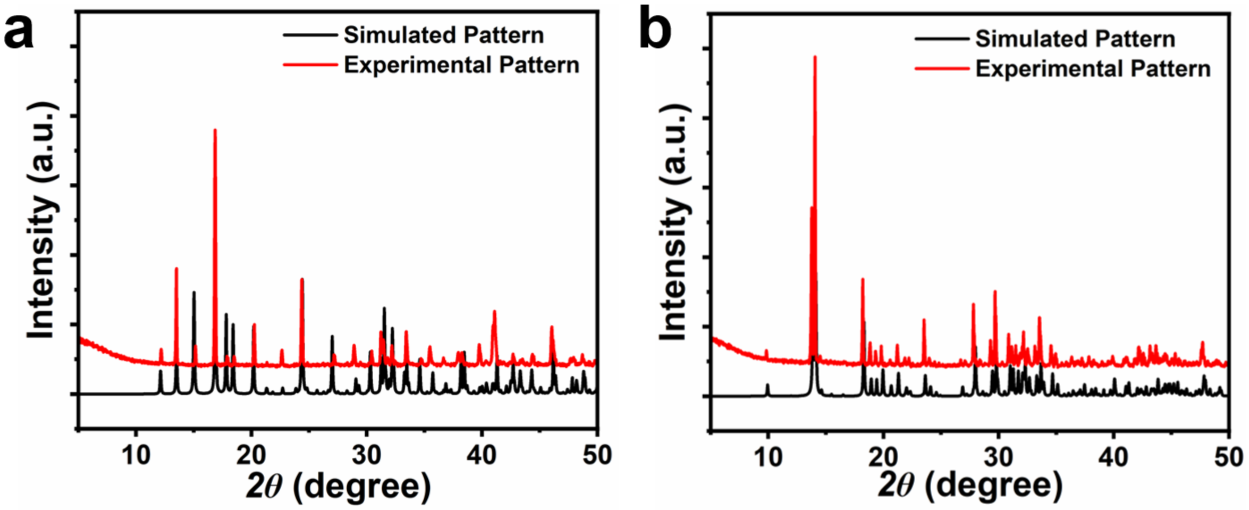

Fig. S1. PXRD pattern for **(a)** compound **$[NaGd(SO_3)(C_2O_4)(H_2O)_2]_\infty$, 1** and **(b)** **$[Na_3Gd(SO_3)_2(C_2O_4)(H_2O)]_\infty$, 2**.

FTIR

Compounds **1** and **2** were characterized by FTIR spectroscopy to ensure the presence of key functional groups within their crystal structures (Fig. S2). Both spectra show distinct absorption bands for the sulfite (SO_3^{2-}) anion at nearly 970, 930, 620, and 470 cm^{-1}. Additional bands at around 2450 cm^{-1} (C=O stretching), 1950 cm^{-1} (asymmetric C=C stretching), and 1070 cm^{-1} (C–O bending) support the presence of the oxalate ($C_2O_4^{2-}$) anion. Moreover, the broad features observed in the 3450–3500 cm^{-1} region are attributed to O–H stretching vibrations, which originate from water molecules.

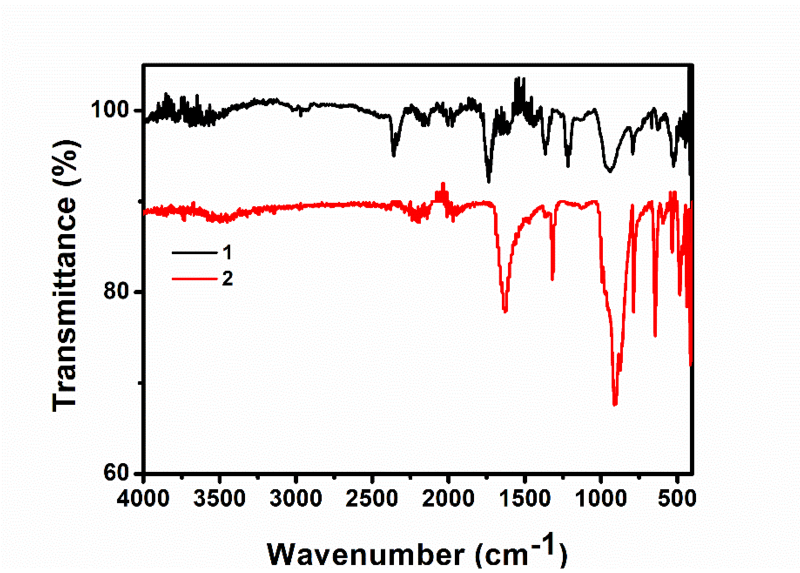

Fig. S2. FTIR spectra for compound **1** and **2**.

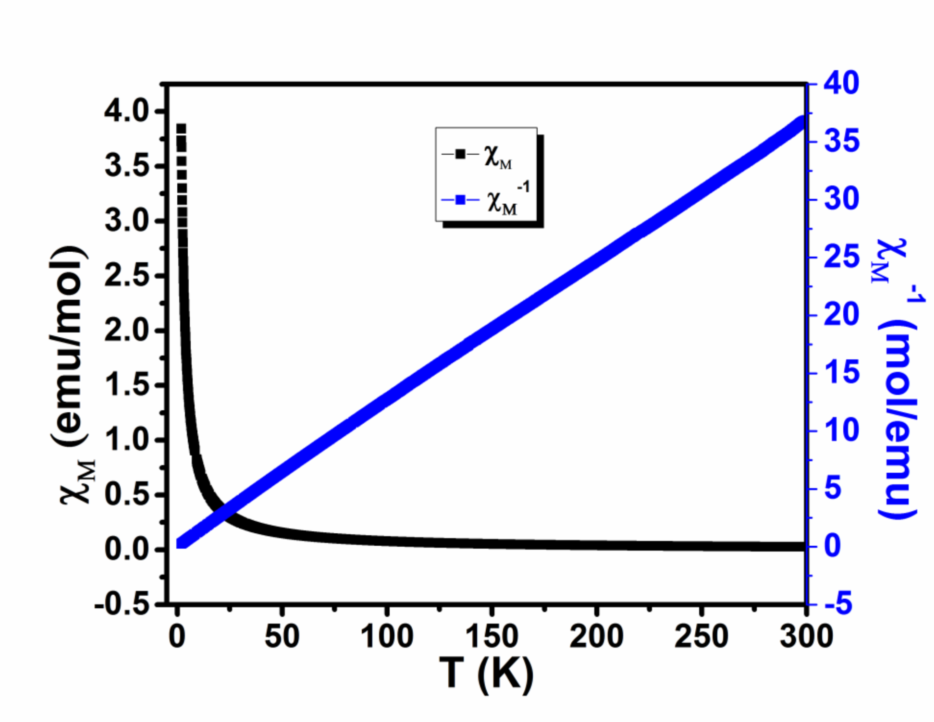

Fig. S3. Temperature dependence of the field DC magnetic susceptibility (χ_M) and (χ_M^{-1}) of compound **2** at 1000 Oe.

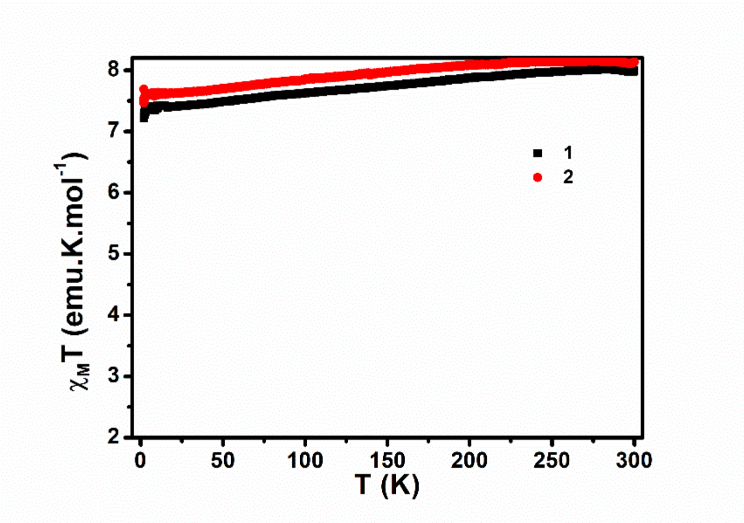

Fig. S4. Temperature dependence of the $\chi_M T$ curves of compounds **1** and **2** at 1000 Oe.

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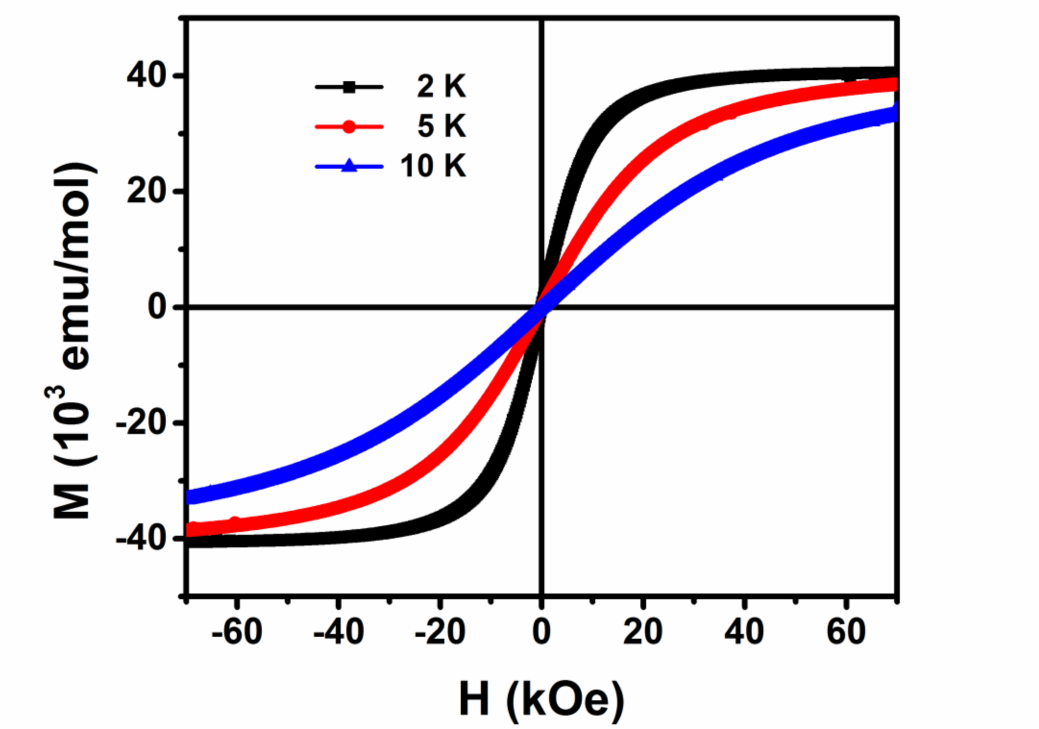

Fig. S5. Isothermal Magnetization vs. magnetic field (H) profile diagram at 2, 5 and 10 K for compound **2**.

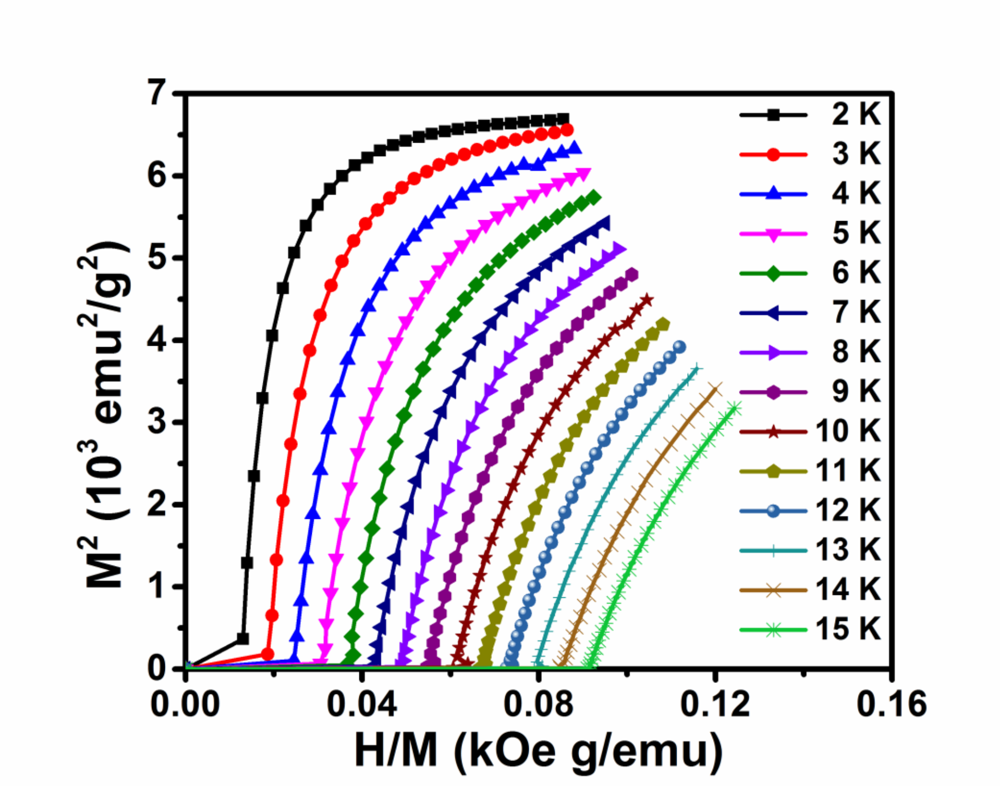

Fig. S6. The Arrott plots (M^2 vs H/M) for compound **2**.

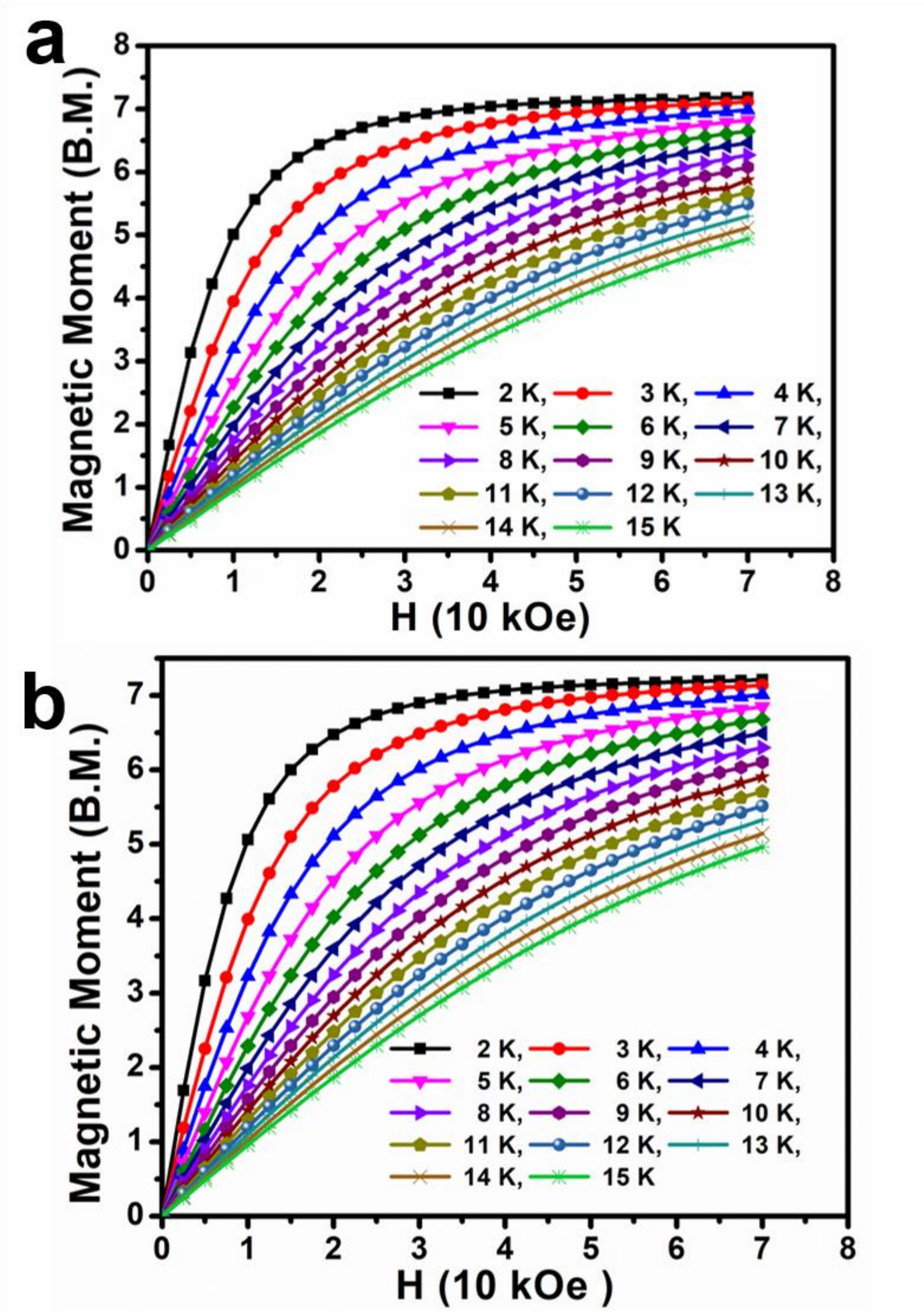

Fig. S7. First quadrant Isothermal Magnetization vs. magnetic field (H) profile diagram at 2, 5 and 10 K for compound **1** (a) and **2** (b).

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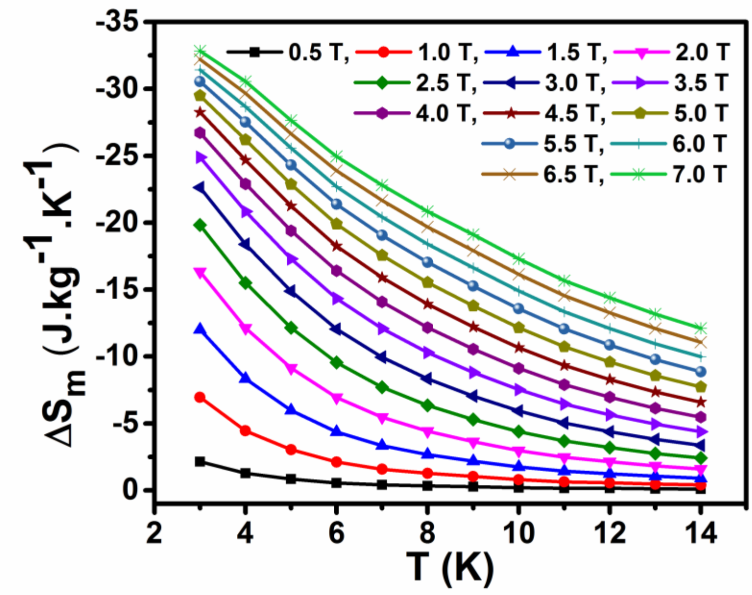

Fig. S8. Temperature-dependent change in magnetic entropy at an interval of 0.5 T applied field of compound **2**.

Thermogravimetric analysis (TGA)

The thermal stability of compounds **1** and **2** was evaluated by thermogravimetric analysis (TGA) using a TA instrument over the temperature range of 30–700 °C at a constant heating rate of 5 °C min^{-1} under a continuous N_2 atmosphere. Both compounds exhibit multi-step thermal decomposition profiles, indicating the sequential removal of coordinated water molecules followed by decomposition of the framework ligands (Fig. S9). For both materials, the first weight-loss step occurs between 280–310 °C, corresponding to the elimination of coordinated aqua ligands. The observed mass losses of 8.12% for compound **1** and 4.03% for compound **2** agree well with the calculated values of 8.0% and 3.92%, respectively, confirming the presence of lattice/coordinated water molecules as determined from single-crystal structural analysis. The second decomposition stage, observed in the temperature range of 425–600 °C, is attributed to the breakdown of the anhydrous framework accompanied by the evolution of SO_3 and CO_2 gases from the sulfite and oxalate ligands. This step results in weight losses of 18.12% (calc. 18.05%) for **1** and 15.98% (calc. 16.05%) for **2**, further supporting the proposed compositions. The decomposition was carried out under a N_2 atmosphere up to 700 °C, with a total treatment duration of 2 h. Upon complete decomposition, the remaining residual product were analyzed by PXRD. The final products consist of thermally stable inorganic phases, including Gd_2O_3, Gd_2O_2S, NaS, and Gd_2OS_2 for compound **1** (Fig. S10), and NaS, Gd_2OS_2, and Gd_2O_2S for compound **2** (Fig. S11). The formation of these oxide/sulfide species reflects the decomposition of sulfite-containing frameworks under an inert atmosphere. Both the compounds demonstrate good thermal stability up to ~280 °C, indicating that the coordination frameworks remain intact under moderate thermal conditions. The close agreement between experimental and calculated mass losses further confirms the structural integrity and compositional accuracy of the synthesized materials.

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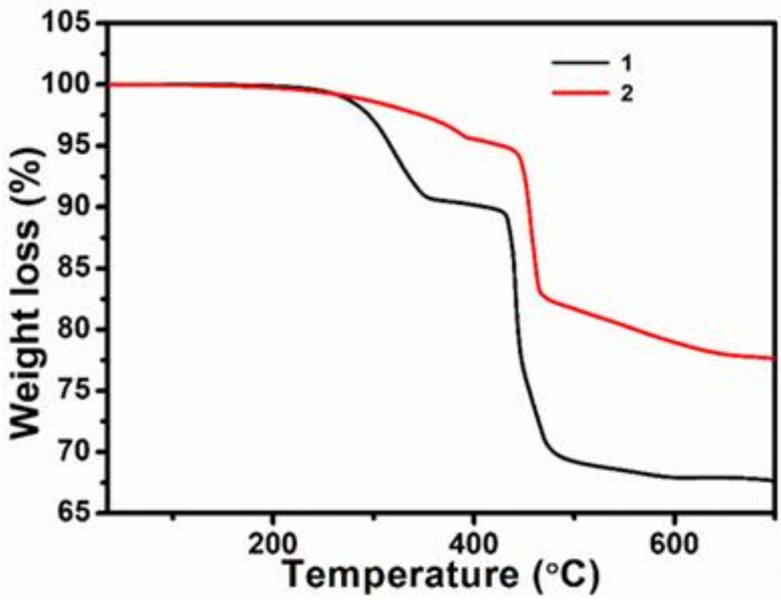

Fig. S9. TGA curves of **1** and **2**.

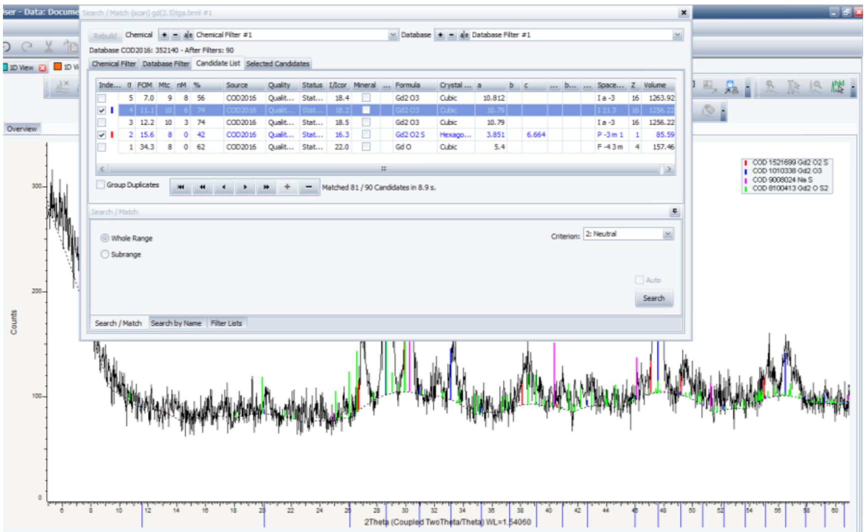

Fig. S10. Post calcination PXRD pattern analysis of **$[NaGd(SO_3)(C_2O_4)(H_2O)_2]_\infty$, 1** showing formation of Gd_2O_3(COD 1010338), Gd_2O_2S (COD 1521699), NaS (COD 9014900) and Gd_2OS_2(COD 8100413) mixtures.

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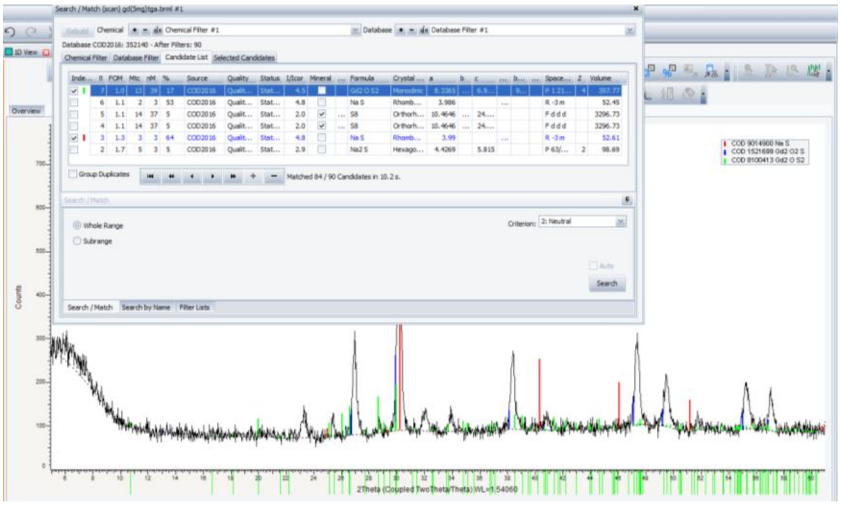

Fig. S11. Post calcination PXRD analysis of **[$Na_3Gd(SO_3)_2(C_2O_4)(H_2O)]_\infty$, 2** showing formation of NaS (COD 9014900), Gd_2OS_2(COD 8100413) and Gd_2O_2S (COD 1521699) mixtures.

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Table S1. Comparison table of change in Magnetic Entropy ($-\Delta S_m$) for Gd(III) Molecular MCE Compounds.

Compounds	**$-\Delta S_m$ (J K^{-1} kg^{-1})**	**ΔH (T)**	**T (K)**	**References**
$[Gd(OH)CO_3]_n$	66.4	7	1.8	[1]
$\{[Gd_2(CO_3)(ox)_2(H_2O)_2]\cdot 3H_2O\}_n$	58.5	7	2	[2]
$[Gd_4(SO_4)_4(\mu_3\text{-}OH)_4(H_2O)_4]_n$	51.29	7	2	[3]
$[Gd(HCOO)(SO_4)(H_2O)]_n$	49.91	7	2	[4]
$[Gd(C_2O_4)(H_2O)_3Cl]$	48.0	7	2.2	[5]
$[Gd(HCOO)(OAc)_2(H_2O)_2]_n$	45.9	7	1.8	[6]
$GdPO_4$	44.79	9	2	[7]
$[NaGd(SO_3)(C_2O_4)(H_2O)_2]$	**41.58**	**7**	**3**	**This work**
$Li_3K_9Gd_3(BO_3)_7$	39.3	7	2	[8]
$[Gd_{28}(IN)_{25}(C_2O_4)_6(HCOO)(\mu_3\text{-}OH)_{36}(\mu_2\text{-}OH)_2(H_2O)_{36}]$	37.5	7	2	[9]
$[Na_3Gd(SO_3)_2(C_2O_4)(H_2O)]$	**32.84**	**7**	**3**	**This work**
[Gd(BTC)(DMF)]	32	5	1.8	[10]
$[Gd(BTC)(H_2O)]\cdot 4H_2O$	38	5	1.8	[10]
$Gd_{17.33}(BO_3)_4(B_2O_5)_2O_{16}$	26.5	7	4.4	[11]
$\{[Gd_2(FUM)_3(H_2O)_4]\cdot 3H_2O\}_n$	21	5	2.5	[12]

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Table S2. Complete list of bond lengths [Å] and bond angles [◦] for compounds **1-2**#

Bond lengths	[Å]	Bond lengths	[Å]	Bond lengths	[Å]
		[NaGd(SO$_3$)(C$_2$O$_4$)(H$_2$O)$_2$]$_\infty$, 1			
Gd1-O1	2.304(3)	Gd1-O2W^{d}	2.670(3)	Na1-O6^{c}	2.631(3)
Gd1-O2^{b}	2.409(3)	S1-O1	1.526(3)	Na1-O7^{f}	2.400(3)
Gd1-O3^{a}	2.302(3)	S1-O2	1.524(3)	Na1-O2W	2.489(4)
Gd1-O4	2.529(3)	S1-O3	1.520(3)	O4-C2	1.246(5)
Gd1-O5	2.483(3)	Na1-O1^{a}	2.899(3)	O6-C1	1.252(6)
Gd1-O6^{c}	2.506(3)	Na1-O3^{a}	2.709(3)	O7-C2	1.258(5)
Gd1-O7^{c}	2.500(3)	Na1-O4^{a}	2.401(3)	O5-C1	1.251(5)
Gd1-O1W	2.415(3)	Na1-O5	2.297(3)	C2-C1	1.544(6)
Bond angles	[°]	Bond angles	[°]	Bond angles	[°]
O3^{a}-Gd1-O1	144.53(12)	O4-Gd1-Na1	99.17(7)	O5-Na1-Gd1^{a}	138.15(10)
O3^{a}-Gd1-O2^{b}	85.33(12)	O2W^{d}-Gd1-Na1	116.48(8)	O7^{f}-Na1-Gd1^{a}	39.88(8)
O1-Gd1-O2^{b}	86.09(11)	O3^{a}-Gd1-Na1^{e}	164.78(8)	O4^{a}-Na1-Gd1^{a}	40.60(8)
O3^{a}-Gd1-O1W	81.48(12)	O1-Gd1-Na1^{e}	49.44(8)	O2W-Na1-Gd1^{a}	123.93(10)
O1-Gd1-O1W	83.62(11)	O2^{b}-Gd1-Na1^{e}	104.40(8)	O6^{c}-Na1-Gd1^{a}	127.82(9)
O2^{b}-Gd1-O1W	140.56(11)	O1W-Gd1-Na1^{e}	97.36(9)	O3^{a}-Na1-Gd1^{a}	84.73(8)
O3^{a}-Gd1-O5	76.55(11)	O5-Gd1-Na1^{e}	96.04(7)	O1^{a}-Na1-Gd1^{a}	37.09(6)
O1-Gd1-O5	130.63(10)	O7^{c}-Gd1-Na1^{e}	38.01(7)	Gd1-Na1-Gd1^{a}	121.71(5)
O2^{b}-Gd1-O5	67.88(10)	O6^{c}-Gd1-Na1^{e}	98.19(8)	Na1-O2W-Gd1^{g}	134.38(15)
O1W-Gd1-O5	142.12(10)	O4-Gd1-Na1^{e}	38.18(8)	Na1-O2W-H2WA	111(4)
O3^{a}-Gd1-O7^{c}	128.96(11)	O2W^{d}-Gd1-Na1^{e}	121.37(8)	Gd1^{g}-O2W-H2WA	99(4)
O1-Gd1-O7^{c}	75.50(11)	Na1-Gd1-Na1^{e}	121.71(5)	Na1-O2W-H2WB	107(4)
O2^{b}-Gd1-O7^{c}	140.33(10)	O3-S1-O2	104.76(18)	Gd1^{g}-O2W-H2WB	98(4)
O1W-Gd1-O7^{c}	72.56(11)	O3-S1-O1	102.5(2)	H2WA-O2W-H2WB	104(7)
O5-Gd1-O7^{c}	98.13(10)	O2-S1-O1	104.58(19)	C2-O4-Na1^{e}	144.6(3)
O3^{a}-Gd1-O6^{c}	66.77(11)	O5-Na1-O7^{f}	167.60(14)	C2-O4-Gd1	113.3(3)
O1-Gd1-O6^{c}	138.63(11)	O5-Na1-O4^{a}	114.64(13)	Na1^{e}-O4-Gd1	101.22(12)
O2^{b}-Gd1-O6^{c}	131.90(10)	O7^{f}-Na1-O4^{a}	71.26(11)	C1-O6-Gd1^{h}	120.6(3)
O1W-Gd1-O6^{c}	75.15(11)	O5-Na1-O2W	91.21(12)	C1-O6-Na1^{h}	126.9(3)
O5-Gd1-O6^{c}	67.95(10)	O7^{f}-Na1-O2W	97.81(12)	Gd1^{h}-O6-Na1^{h}	93.75(11)
O7^{c}-Gd1-O6^{c}	64.47(10)	O4^{a}-Na1-O2W	104.95(13)	S1-O1-Gd1	144.97(19)
O3^{a}-Gd1-O4	140.13(11)	O5-Na1-O6^{c}	68.48(11)	S1-O1-Na1^{e}	98.51(16)
O1-Gd1-O4	68.14(10)	O7^{f}-Na1-O6^{c}	103.19(12)	Gd1-O1-Na1^{e}	93.47(11)
O2^{b}-Gd1-O4	72.99(10)	O4^{a}-Na1-O6^{c}	166.30(13)	S1-O2-Gd1^{b}	143.96(19)
O1W-Gd1-O4	135.50(11)	O2W-Na1-O6^{c}	88.07(12)	S1-O3-Gd1^{e}	152.11(19)
O5-Gd1-O4	64.46(10)	O5-Na1-O3^{a}	72.17(11)	S1-O3-Na1^{e}	107.01(17)
O7^{c}-Gd1-O4	67.60(10)	O7^{f}-Na1-O3^{a}	95.78(12)	Gd1^{e}-O3-Na1^{e}	96.60(12)
O6^{c}-Gd1-O4	103.71(10)	O4^{a}-Na1-O3^{a}	107.96(12)	Gd1-O1W-H1WA	131(5)
O3^{a}-Gd1-O2W^{d}	72.68(11)	O2W-Na1-O3^{a}	146.92(13)	Gd1-O1W-H1WB	127(7)
O1-Gd1-O2W^{d}	72.02(11)	O6^{c}-Na1-O3^{a}	59.45(10)	H1WA-O1W-H1WB	102(8)
O2^{b}-Gd1-O2W^{d}	70.42(10)	O5-Na1-O1^{a}	105.88(11)	C2-O7-Na1^{i}	123.0(3)
O1W-Gd1-O2W^{d}	70.19(11)	O7^{f}-Na1-O1^{a}	66.70(10)	C2-O7-Gd1^{h}	120.5(3)
O5-Gd1-O2W^{d}	129.38(11)	O4^{a}-Na1-O1^{a}	60.68(10)	Na1^{i}-O7-Gd1^{h}	102.11(12)
O7^{c}-Gd1-O2W^{d}	132.46(10)	O2W-Na1-O1^{a}	161.02(12)	C1-O5-Na1	140.5(3)
O6^{c}-Gd1-O2W^{d}	129.52(10)	O6^{c}-Na1-O1^{a}	105.67(11)	C1-O5-Gd1	114.7(3)
O4-Gd1-O2W^{d}	126.75(10)	O3^{a}-Na1-O1^{a}	50.00(10)	Na1-O5-Gd1	103.34(12)
O3^{a}-Gd1-Na1	45.85(9)	O5-Na1-Gd1	40.10(8)	O4-C2-O7	125.9(4)
O1-Gd1-Na1	167.09(8)	O7^{f}-Na1-Gd1	127.65(10)	O4-C2-C1	117.6(4)
O2^{b}-Gd1-Na1	87.88(8)	O4^{a}-Na1-Gd1	131.78(10)	O7-C2-C1	116.5(4)
O1W-Gd1-Na1	108.11(8)	O2W-Na1-Gd1	113.55(10)	O5-C1-O6	126.9(4)
O5-Gd1-Na1	36.55(7)	O6^{c}-Na1-Gd1	41.78(7)	O5-C1-C2	116.3(4)
O7^{c}-Gd1-Na1	102.40(7)	O3^{a}-Na1-Gd1	37.54(7)	O6-C1-C2	116.8(4)

O6^{c}-Gd1-Na1	44.47(8)	O1^{a}-Na1-Gd1	85.23(7)		
		$[Na_3Gd(SO_3)_2(C_2O_4)(H_2O)]_\infty$, 2			
Gd1-O1	2.291(3)	S2-O5	1.530(3)	O4-Na2^{j}	2.35(3)
Gd1-O4	2.355(3)	S2-O4	1.533(3)	O4-Na1^{o}	2.424(3)
Gd1-O3^{j}	2.376(3)	O6-Na2^{j}	2.52(4)	O5-Na3	2.376(3)
Gd1-O6^{k}	2.426(3)	O6-Na1^{p}	2.638(3)	O5-Na1^{o}	2.825(4)
Gd1-O7	2.447(3)	O8-C2	1.248(5)	C2-O9	1.259(5)
Gd1-O10^{l}	2.510(3)	O8-Na1^{o}	2.526(3)	C2-C1	1.545(6)
Gd1-O9^{l}	2.510(3)	O8-Na2^{j}	2.739(18)	C1-O10	1.249(5)
Gd1-O5^{k}	2.530(3)	O2-Na2	2.26(3)	O9-Na2^{o}	2.33(2)
Gd1-O8	2.543(3)	O2-Na1	2.334(4)	O9-Na1^{j}	2.580(3)
S1-O2	1.517(3)	O3-Na3^{j}	2.594(3)	O10-Na3^{q}	2.517(3)
S1-O1	1.527(3)	O7-C1	1.256(5)	Na1-O1W	2.319(14)
S1-O3	1.544(3)	O7-Na3^{k}	2.539(3)	Na2-O1W^{s}	2.86(2)
S2-O6	1.520(3)	O1-Na3^{m}	2.521(4)	O4-Na2A^{k}	2.46(3)
Na3-O1WA^{o}	2.769(11)	O6-Na2A^{j}	2.37(3)	O2-Na2A	2.31(3)
O2-Na3^{m}	2.515(3)	Na1-O1WA	2.396(14)	O9-Na2A^{n}	2.52(2)
Na1-O1WA	2.396(14)	O3-Na2A	2.57(3)	O3-Na2	2.58(2)
Na3-O1WA^{o}	2.769(11)	O4-Na2A^{o}	2.99(2)	O4-Na2^{j}	2.397(4)
O1-Gd1-O4	148.33(11)	C1-O7-Gd1	121.4(3)	O2^{n}-Na3-Gd1^{n}	93.80(9)
O1-Gd1-O3^{j}	81.54(12)	C1-O7-Na3^{k}	131.4(3)	O10^{w}-Na3-Gd1^{n}	43.55(7)
O4-Gd1-O3^{j}	85.38(11)	Gd1-O7-Na3^{k}	101.63(12)	O1^{n}-Na3-Gd1^{n}	38.57(8)
O1-Gd1-O6^{k}	133.83(11)	S1-O1-Gd1	149.8(2)	O7^{t}-Na3-Gd1^{n}	133.25(10)
O4-Gd1-O6^{k}	71.86(11)	S1-O1-Na3^{m}	99.06(16)	O3^{t}-Na3-Gd1^{n}	40.63(7)
O3^{j}-Gd1-O6^{k}	138.97(11)	Gd1-O1-Na3^{m}	98.11(12)	S1^{n}-Na3-Gd1^{n}	65.45(4)
O1-Gd1-O7	73.13(11)	S2-O4-Gd1	141.30(18)	O5-Na3-Na1^{n}	92.36(10)
O4-Gd1-O7	133.89(10)	S2-O4-Na2^{j}	98.65(16)	O2^{n}-Na3-Na1^{n}	36.29(8)
O3^{j}-Gd1-O7	83.73(11)	Gd1-O4-Na2^{j}	98.26(12)	O10^{w}-Na3-Na1^{n}	104.05(9)
O6^{k}-Gd1-O7	88.08(11)	S2-O4-Na1^{o}	109.98(16)	O1^{n}-Na3-Na1^{n}	88.35(10)
O1-Gd1-O10^{l}	72.35(11)	Gd1-O4-Na1^{o}	103.78(12)	O7^{t}-Na3-Na1^{n}	99.52(10)
O4-Gd1-O10^{l}	75.99(10)	Na2^{j}-O4-Na1^{o}	92.41(13)	O3^{t}-Na3-Na1^{n}	160.40(10)
O3^{j}-Gd1-O10^{l}	66.87(10)	S2-O5-Na3	125.47(19)	S1^{n}-Na3-Na1^{n}	60.08(5)
O6^{k}-Gd1-O10^{l}	134.50(11)	S2-O5-Gd1^{t}	97.65(15)	Gd1^{n}-Na3-Na1^{n}	119.84(6)
O7-Gd1-O10^{l}	137.19(10)	Na3-O5-Gd1^{t}	103.90(13)	O5-Na3-Na2^{n}	57.59(9)
O1-Gd1-O9^{l}	92.66(11)	S2-O5-Na1^{o}	92.97(15)	O2^{n}-Na3-Na2^{n}	34.46(8)
O4-Gd1-O9^{l}	74.28(10)	Na3-O5-Na1^{o}	126.77(14)	O10^{w}-Na3-Na2^{n}	131.66(10)
O3^{j}-Gd1-O9^{l}	130.41(10)	Gd1^{t}-O5-Na1^{o}	105.63(12)	O1^{n}-Na3-Na2^{n}	66.46(9)
O6^{k}-Gd1-O9^{l}	76.23(10)	O8-C2-O9	126.9(4)	O7^{t}-Na3-Na2^{n}	120.21(10)
O7-Gd1-O9^{l}	141.48(10)	O8-C2-C1	116.5(4)	O3^{t}-Na3-Na2^{n}	117.11(10)
O10^{l}-Gd1-O9^{l}	64.50(10)	O9-C2-C1	116.6(4)	S1^{n}-Na3-Na2^{n}	49.63(4)
O1-Gd1-O5^{k}	76.49(11)	O10-C1-O(7)	125.6(4)	Gd1^{n}-Na3-Na2^{n}	102.47(5)
O4-Gd1-O5^{k}	123.98(11)	O10-C1-C2	116.9(4)	Na1^{n}-Na3-Na2^{n}	58.32(5)
O3^{j}-Gd1-O5^{k}	149.36(11)	O7-C1-C2	117.5(4)	O5-Na3-Gd1^{t}	39.45(8)
O6^{k}-Gd1-O5^{k}	57.38(10)	C2-O9-Na2^{o}	115.9(3)	O2^{n}-Na3-Gd1^{t}	127.25(9)
O7-Gd1-O5^{k}	69.67(11)	C2-O9-Gd1^{s}	120.0(3)	O10^{w}-Na3-Gd1^{t}	129.40(10)
O10^{l}-Gd1-O5^{k}	124.30(10)	Na2^{o}-O9-Gd1^{s}	98.13(12)	O1^{n}-Na3-Gd1^{t}	139.79(11)
O9^{l}-Gd1-O5^{k}	72.26(10)	C2-O9-Na1^{j}	114.9(3)	O7^{t}-Na3-Gd1^{t}	38.32(7)
O1-Gd1-O8	131.35(11)	Na2^{o}-O9-Na1^{j}	88.03(12)	O3^{t}-Na3-Gd1^{t}	84.27(8)
O4-Gd1-O8	69.00(10)	Gd1^{s}-O9-Na1^{j}	114.01(12)	S1^{n}-Na3-Gd1^{t}	145.30(6)
O3^{j}-Gd1-O8	70.47(10)	C1-O10-Gd1^{s}	120.8(3)	Gd1^{n}-Na3-Gd1^{t}	124.46(5)
O6^{k}-Gd1-O8	69.62(10)	C1-O10-Na3^{q}	132.5(3)	Na1^{n}-Na3-Gd1^{t}	114.72(6)
O7-Gd1-O8	65.11(10)	Gd1^{s}-O10-Na3^{q}	92.75(11)	Na2^{n}-Na3-Gd1^{t}	96.99(5)
O10^{l}-Gd1-O8	126.00(10)	O2-Na1-O1W	86.69(19)	O2-Na2-O4^{u}	130.77(14)
O9^{l}-Gd1-O8	135.76(10)	O2-Na1-O4^{v}	161.11(14)	O2-Na2-O9^{v}	115.86(14)

Please do not adjust margins

O5^{k}-Gd1-O8	109.33(10)	O1W-Na1-O4^{v}	112.07(19)	O4^{u}-Na2-O9^{v}	81.41(12)
O1-Gd1-S2^{k}	105.48(9)	O2-Na1-O8^{v}	100.09(12)	O2-Na2-O6^{u}	162.44(16)
O4-Gd1-S2^{k}	98.05(8)	O1W-Na1-O8^{v}	136.41(15)	O4^{u}-Na2-O6^{u}	59.58(11)
O3^{j}-Gd1-S2^{k}	156.28(8)	O4^{v}-Na1-O8^{v}	68.24(11)	O9^{v}-Na2-O6^{u}	77.63(12)
O6^{k}-Gd1-S2^{k}	28.36(8)	O2-Na1-O9^{u}	87.56(12)	O2-Na2-O3	59.86(11)
O7-Gd1-S2^{k}	76.98(8)	O1W-Na1-O9^{u}	134.10(15)	O4^{u}-Na2-O3	80.37(11)
O10^{l}-Gd1-S2^{k}	136.79(7)	O4^{v}-Na1-O9^{u}	77.81(11)	O9^{v}-Na2-O3	146.62(15)
O9^{l}-Gd1-S2^{k}	72.63(7)	O8^{v}-Na1-O9^{u}	89.40(12)	O6^{u}-Na2-O3	115.61(13)
O5^{k}-Gd1-S2^{k}	29.03(8)	O2-Na1-O6^{p}	123.15(13)	O2-Na2-O8^{u}	73.24(12)
O8-Gd1-S2^{k}	88.75(7)	O1W-Na1-O6^{p}	73.64(14)	O4^{u}-Na2-O8^{u}	62.54(11)
O1-Gd1-Na2^{j}	125.09(9)	O4^{v}-Na1-O6^{p}	67.19(11)	O9^{v}-Na2-O8^{u}	84.46(12)
O4-Gd1-Na2^{j}	41.30(8)	O8^{v}-Na1-O6^{p}	66.65(11)	O6^{u}-Na2-O8^{u}	121.15(12)
O3^{j}-Gd1-Na2^{j}	45.58(9)	O9^{u}-Na1-O6^{p}	142.80(12)	O3-Na2-O8^{u}	62.32(10)
O6^{k}-Gd1-Na2^{j}	100.60(8)	O2-Na1-O5^{v}	130.35(13)	O2-Na2-O1W^{s}	96.14(14)
O7-Gd1-Na2^{j}	107.80(8)	O1W-Na1-O5^{v}	83.40(18)	O4^{u}-Na2-O1W^{s}	95.53(14)
O10^{l}-Gd1-Na2^{j}	73.54(8)	O4^{v}-Na1-O5^{v}	53.76(10)	O9^{v}-Na2-O1W^{s}	140.30(14)
O9^{l}-Gd1-Na2^{j}	109.55(8)	O8^{v}-Na1-O5^{v}	120.05(12)	O6^{u}-Na2-O1W^{s}	67.20(13)
O5^{k}-Gd1-Na2^{j}	157.45(9)	O9^{u}-Na1-O5^{v}	66.53(10)	O3-Na2-O1W^{s}	69.41(12)
O8-Gd1-Na2^{j}	52.94(8)	O6^{p}-Na1-O5^{v}	100.24(12)	O8^{u}-Na2-O1W^{s}	129.21(12)
S2^{k}-Gd1-Na2^{j}	128.73(4)	O2-Na1-S2^{v}	153.12(11)	O2-Na2-S1	29.36(8)
O1-Gd1-Na3^{m}	43.32(9)	O1W-Na1-S2^{v}	99.82(18)	O4^{u}-Na2-S1	108.63(10)
O4-Gd1-Na3^{m}	109.63(8)	O4^{v}-Na1-S2^{v}	26.04(7)	O9^{v}-Na2-S1	139.39(12)
O3^{j}-Gd1-Na3^{m}	45.31(8)	O8^{v}-Na1-S2^{v}	93.06(9)	O6^{u}-Na2-S1	141.93(12)
O6^{k}-Gd1-Na3^{m}	175.67(8)	O9^{u}-Na1-S2^{v}	69.11(8)	O3-Na2-S1	30.84(7)
O7-Gd1-Na3^{m}	93.50(8)	O6^{p}-Na1-S2^{v}	83.58(9)	O8^{u}-Na2-S1	67.70(8)
O10^{l}-Gd1-Na3^{m}	43.71(8)	O5^{v}-Na1-S2^{v}	27.76(7)	O1W^{s}-Na2-S1	79.25(10)
O9^{l}-Gd1-Na3^{m}	100.13(8)	O2-Na1-Na2^{r}	117.75(11)	O2-Na2-S2^{u}	159.22(12)
O5^{k}-Gd1-Na3^{m}	119.48(8)	O1W-Na1-Na2^{r}	153.00(19)	O4^{u}-Na2-S2^{u}	29.98(8)
O8-Gd1-Na3^{m}	114.70(7)	O4^{v}-Na1-Na2^{r}	43.47(9)	O9^{v}-Na2-S2^{u}	75.44(9)
S2^{k}-Gd1-Na3^{m}	148.48(4)	O8^{v}-Na1-Na2^{r}	54.83(8)	O6^{u}-Na2-S2^{u}	29.79(8)
Na2^{j}-Gd1-Na3^{m}	82.77(5)	O9^{u}-Na1-Na2^{r}	44.17(8)	O3-Na2-S2^{u}	100.78(9)
O2-S1-O1	102.71(19)	O6^{p}-Na1-Na2^{r}	99.22(9)	O8^{u}-Na2-S2^{u}	91.52(9)
O2-S1-O3	105.47(18)	O5^{v}-Na1-Na2^{r}	72.12(8)	O1W^{s}-Na2-S2^{u}	82.44(11)
O1-S1-O3	102.14(18)	S2^{v}-Na1-Na2^{r}	53.20(5)	S1-Na2-S2^{u}	131.61(7)
O2-S1-Na2	47.67(13)	O2-Na1-Na2^{l}	140.67(11)	O2-Na2-S2^{m}	86.40(10)
O1-S1-Na2	103.15(15)	O1W-Na1-Na2^{l}	55.09(16)	O4^{u}-Na2-S2^{m}	141.26(10)
O3-S1-Na2	58.58(13)	O4^{v}-Na1-Na2^{l}	58.13(9)	O9^{v}-Na2-S2^{m}	70.63(9)
O2-S1-Na3^{m}	52.01(13)	O8^{v}-Na1-Na2^{l}	102.20(9)	O6^{u}-Na2-S2^{m}	87.95(10)
O1-S1-Na3^{m}	52.32(13)	O9^{u}-Na1-Na2^{l}	124.44(10)	O3-Na2-S2^{m}	136.47(10)
O3-S1-Na3^{m}	123.27(14)	O6^{p}-Na1-Na2^{l}	43.44(8)	O8^{u}-Na2-S2^{m}	136.85(10)
Na2-S1-Na3^{m}	77.63(6)	O5^{v}-Na1-Na2^{l}	60.65(8)	O1W^{s}-Na2-S2^{m}	89.74(11)
O6-S2-O(5)	102.63(18)	S2^{v}-Na1-Na2^{l}	56.30(5)	S1-Na2-S2^{m}	110.06(7)
O6-S2-O4	103.77(19)	Na2^{r}-Na1-Na2^{l}	101.58(5)	S2^{u}-Na2-S2^{m}	114.26(7)
O5-S2-O4	103.14(18)	O2-Na1-Na2	35.38(9)	O2-Na2-Na1^{r}	113.27(12)
O6-S2-Na2^{j}	52.82(14)	O1W-Na1-Na2	114.18(18)	O4^{u}-Na2-Na1^{r}	44.12(9)
O5-S2-Na2^{j}	105.69(14)	O4^{v}-Na1-Na2	129.61(10)	O9^{v}-Na2-Na1^{r}	47.80(9)
O4-S2-Na2^{j}	51.37(13)	O8^{v}-Na1-Na2	64.88(8)	O6^{u}-Na2-Na1^{r}	84.01(10)
O6-S2-Gd1^{t}	49.34(12)	O9^{u}-Na1-Na2	84.18(9)	O3-Na2-Na1^{r}	101.03(10)
O5-S2-Gd1^{t}	53.32(12)	O6^{p}-Na1-Na2	108.29(10)	O8^{u}-Na2-Na1^{r}	45.54(8)
O4-S2-Gd1^{t}	113.28(12)	O5^{v}-Na1-Na2	149.63(10)	O1W^{s}-Na2-Na1^{r}	139.41(12)
Na2^{j}-S2-Gd1^{t}	74.53(4)	S2^{v}-Na1-Na2	145.84(7)	S1-Na2-Na1^{r}	113.23(8)
O6-S2-Na2^{n}	173.48(15)	Na2^{r}-Na1-Na2	92.82(7)	S2^{u}-Na2-Na1^{r}	60.05(5)
O5-S2-Na2^{n}	78.08(13)	Na2^{l}-Na1-Na2	149.70(7)	S2^{m}-Na2-Na1^{r}	118.24(7)
O4-S2-Na2^{n}	69.85(13)	O2-Na1-Gd1^{v}	139.31(11)	O2-Na2-Na1^{s}	115.62(12)
Na2^{j}-S2-Na2^{n}	120.69(5)	O1W-Na1-Gd1^{v}	110.32(14)	O4^{u}-Na2-Na1^{s}	104.21(10)

Gd1^{t}-S2-Na2^{n}	131.18(5)	O4^{v}-Na1-Gd1^{v}	37.46(8)	O9^{v}-Na2-Na1^{s}	101.03(10)
O6-S2-Na1^{o}	108.71(14)	O8^{v}-Na1-Gd1^{v}	42.23(7)	O6^{u}-Na2-Na1^{s}	48.10(9)
O5-S2-Na1^{o}	59.27(13)	O9^{u}-Na1-Gd1^{v}	103.35(9)	O3-Na2-Na1^{s}	110.43(11)
O4-S2-Na1^{o}	43.98(12)	O6^{p}-Na1-Gd1^{v}	39.93(7)	O8^{u}-Na2-Na1^{s}	165.04(10)
Na2^{j}-S2-Na1^{o}	66.75(6)	O5^{v}-Na1-Gd1^{v}	89.20(8)	O1W^{s}-Na2-Na1^{s}	41.07(9)
Gd1^{t}-S2-Na1^{o}	83.52(4)	S2^{v}-Na1-Gd1^{v}	62.54(4)	S1-Na2-Na1^{s}	113.51(8)
Na2^{n}-S2-Na1^{o}	65.93(6)	Na2^{r}-Na1-Gd1^{v}	59.35(4)	S2^{u}-Na2-Na1^{s}	76.63(6)
S2-O6-Gd1^{t}	102.30(16)	Na2^{l}-Na1-Gd1^{v}	61.33(4)	S2^{m}-Na2-Na1^{s}	57.77(5)
S2-O6-Na2^{j}	97.39(17)	Na2-Na1-Gd1^{v}	105.93(6)	Na1^{r}-Na2-Na1^{s}	130.30(6)
Gd1^{t}-O6-Na2^{j}	100.15(13)	O5-Na3-O2^{n}	89.66(12)	Na1-O1W-Na2^{l}	83.84(18)
S2-O6-Na1^{p}	159.58(19)	O5-Na3-O10^{w}	163.59(14)	Na1-O1W-H1WA	127(4)
Gd1^{t}-O6-Na1^{p}	95.84(11)	O2^{n}-Na3-O10^{w}	103.28(12)	Na2^{l}-O1W-H1WA	72(5)
Na2^{j}-O6-Na1^{p}	88.46(12)	O5-Na3-O1^{n}	112.21(13)	Na1-O1W-H1WB	124(4)
C2-O8-Na1^{o}	135.2(3)	O2^{n}-Na3-O1^{n}	56.28(11)	Na2^{l}-O1W-H1WB	95(5)
C2-O8-Gd1	118.4(3)	O10^{w}-Na3-O1^{n}	68.60(11)	H1WA-O1W-H1WB	
Na1^{o}-O8-Gd1	95.87(11)	O5-Na3-O7^{t}	70.60(11)	Na2^{l}-O1W-H1WB	95(5)
C2-O8-Na2^{j}	129.6(3)	O2^{n}-Na3-O7^{t}	132.09(13)	H1WA-O1W-H1WB	
Na1^{o}-O8-Na2^{j}	79.63(10)	O10^{w}-Na3-O7^{t}	106.37(12)	Na2^{l}-O1W-H1WB	95(5)
Gd1-O8-Na2^{j}	82.53(9)	O1^{n}-Na3-O7^{t}	171.63(13)	H1WA-O1W-H1WB	105(3)
S1-O2-Na2	102.97(17)	O5-Na3-O3^{t}	100.48(13)		
S1-O2-Na1	132.51(19)	O2^{n}-Na3-O3^{t}	128.23(13)		
Na2-O2-Na1	108.35(15)	O10^{w}-Na3-O3^{t}	63.60(11)		
S1-O2-Na3^{m}	99.64(16)	O1^{n}-Na3-O3^{t}	73.15(11)		
Na2-O2-Na3^{m}	107.01(14)	O7^{t}-Na3-O3^{t}	98.70(12)		
Na1-O2-Na3^{m}	104.11(13)	O5-Na3-S1^{n}	106.30(10)		
S1-O3-Gd1^{u}	143.76(19)	O2^{n}-Na3-S1^{n}	28.35(8)		
S1-O3-Na2	90.58(15)	O10^{w}-Na3-S1^{n}	82.13(9)		
Gd1^{u}-O3-Na2	93.12(12)	O1^{n}-Na3-S1^{n}	28.61(8)		
S1-O3-Na3^{k}	108.08(17)	O7^{t}-Na3-S1^{n}	159.53(11)		
Gd1^{u}-O3-Na3^{k}	94.07(11)	O3^{t}-Na3-S1^{n}	101.75(9)		
Na2-O3-Na3^{k}	135.63(15)	O5-Na3-Gd1^{n}	126.70(11)		

[#]Symmetry transformations used to generate equivalent atoms:

a) x+1,y,z; b) -x+1,-y+1,-z+1; c) x,-y+1/2,z+1/2; d) -x+2,y+1/2,-z+3/2; e) x-1,y,z; f) x+1,-y+1/2,z+1/2; g) -x+2,y-1/2,-z+3/2; h) x,-y+1/2,z-1/2; i) x-1,-y+1/2,z-1/2; j) -x+1,y-1/2,-z+1/2; k) -x,y+1/2,-z+1/2; l) x,-y+3/2,z+1/2; m) x+1,y,z; n) x-1,y,z; o) x-1,-y+3/2,z-1/2; p) -x+1,-y+1,-z+1; q) x+1,-y+3/2,z-1/2; r) -x+2,-y+2,-z+1; s) x,-y+3/2,z-1/2; t) -x,y-1/2,-z+1/2; u) -x+1,y+1/2,-z+1/2; v) x+1,-y+3/2,z+1/2; w) x-1,-y+3/2,z+1/2

Table S3. Hydrogen bonding table for $(CN_3H_6)[Na_2Gd_3(SO_3)_6]$, **1** and **2**.[#]

D–H···A	Symmetry of A	D–H	H···A	D–A	∠D–H···A
		$[NaGd(SO_3)(C_2O_4)(H_2O)_2]_\infty$, 1			
O1W–H1WA···O7	1-x,-y,1-z	0.82(5)	2.07(6)	2.863(4)	163(5)
O1W–H1WB···O6	2-x,-y,1-z	0.82(7)	2.00(7)	2.813(5)	171(8)
O2W–H2WA···O1	1-x,-y,-z	0.82(5)	2.12(6)	2.886(5)	156(6)
O2W–H2WB···O2	1+x,y,z	0.81(4)	2.09(3)	2.874(5)	164(5)
		$[Na_3Gd(SO_3)_2(C_2O_4)(H_2O)]_\infty$, 2			
O1W–H1WA···O10	1-x,-y,-z	0.817(19)	2.101(19)	2.905(5)	168(5)
O1W–H1WB···O1	x,1/2-y,-1/2+z	0.82(6)	2.59(7)	3.299(7)	147(6)
O1W–H1WB···O7	x,1/2-y,-1/2+z	0.82(6)	2.41(6)	3.023(6)	133(6)

[#]Where 'D' is donor and 'A' is acceptor, the bond lengths are in (Å) and angles are in (°).

Table S4. Atomic coordinates (×10[4]) and equivalent isotropic displacement parameters (Å×10[3]) for **1-2** U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	X	y	Z	U(eq)		x	Y	Z	U(eq)
				$[NaGd(SO_3)(C_2O_4)(H_2O)_2]_\infty$, 1					
Gd1	7595.5(3)	4172.4(2)	7221.3(2)	6.94(9)	O5	9497(4)	2628(2)	6461(3)	11.1(3)
S1	2628.8(13)	5416.6(8)	6999.1(11)	8.4(2)	O6	9561(4)	1610(2)	4420(3)	11.1(3)
Na1	12571(2)	2809.8(14)	7747.2(19)	13.7(4)	O7	5517(4)	1638(2)	4207(3)	11.1(3)
O1	4323(4)	4679(2)	6611(3)	12.9(6)	O1W	7328(5)	5391(2)	9266(4)	13.6(6)
O2	1946(4)	5887.4(19)	5479(4)	11.2(6)	O2W	12274(5)	1073(2)	8876(4)	13.7(6)
O3	923(4)	4696(2)	7397(4)	17.2(7)	C1	8681(6)	2132(3)	5388(5)	8.3(5)
O4	5457(4)	2709(2)	6180(3)	11.1(3)	C2	6346(6)	2170(3)	5246(5)	8.3(5)
				$[Na_3Gd(SO_3)_2(C_2O_4)(H_2O)]_\infty$, 2					
Gd1	2314.0(2)	7853.2(2)	2335.2(2)	5.73(8)	O5	-2082(3)	5601(3)	2865(2)	14.9(6)
S1	5801.5(11)	9699.7(11)	3693.6(8)	9.3(2)	O6	37(3)	4055(3)	3448(2)	14.6(6)
S2	-416.0(11)	5656.7(11)	3409.6(8)	10.1(2)	O7	3292(3)	8667(3)	795(2)	12.0(6)
Na1	8466.4(19)	8364.0(19)	5906.4(13)	15.6(4)	O8	1109(3)	6644(3)	578(2)	9.2(5)
Na2	8850(20)	9190(20)	3195(16)	16(3)	O9	1403(3)	6174(3)	-1083(2)	9.8(6)
Na2A	8680(30)	8980(30)	2980(17)	15(3)	O10	3306(3)	8437(3)	-933(2)	10.8(6)
Na3	-4117.6(19)	6260.5(18)	3666.5(15)	17.1(4)	O10	3306(3)	8437(3)	-933(2)	11(1)
O1	4717(3)	8667(3)	2976(2)	16.2(6)	O1W	6774(14)	6660(15)	6299(9)	16(2)
O2	7102(3)	8701(3)	4167(2)	12.9(6)	O1WA	6551(15)	6553(15)	5865(9)	19(2)
O3	6379(3)	10659(3)	2874(2)	14.0(6)	C1	2872(4)	8086(4)	-106(3)	9.3(6)
O4	327(3)	6306(3)	2545(2)	11.9(6)	C2	1683(4)	6858(4)	-212(3)	9.3(6)

Table S5. Anisotropic displacement parameters (Å[2]×10[3]) for complex **1-2**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12		U11	U22	U33	U23	U13	U12
							$[NaGd(SO_3)(C_2O_4)(H_2O)_2]_\infty$, 1						
Gd1	3.97(12)	10.61(13)	6.36(14)	0.10(6)	1.83(8)	0.37(5)	O5	8.3(7)	14.6(7)	10.4(8)	-2.9(5)	1.7(6)	0.0(5)
S1	6.0(4)	10.3(5)	8.9(5)	1.1(3)	1.2(4)	-0.5(3)	O6	8.3(7)	14.6(7)	10.4(8)	-2.9(5)	1.7(6)	0.0(5)
Na1	3.5(8)	26.7(10)	10.9(9)	-0.9(6)	0.6(6)	1.1(5)	O7	8.3(7)	14.6(7)	10.4(8)	-2.9(5)	1.7(6)	0.0(5)
O1	5.1(13)	20.1(15)	13.6(15)	0.7(11)	2.5(11)	4.4(10)	O1W	9.4(15)	18.1(16)	13.5(16)	-5.5(12)	2.3(12)	1.4(11)
O2	10.1(14)	18.1(15)	5.5(15)	3.8(10)	1.8(12)	0.4(10)	O2W	9.7(15)	22.0(15)	9.4(16)	-1.0(12)	-0.1(13)	0.2(11)
O3	8.1(15)	25.2(16)	18.2(17)	9.8(12)	0.6(12)	-3.7(11)	C1	9.0(13)	8.2(12)	8.0(14)	2.3(9)	3.4(11)	-0.2(9)
O4	8.3(7)	14.6(7)	10.4(8)	-2.9(5)	1.7(6)	0.0(5)	C2	9.0(13)	8.2(12)	8.0(14)	2.3(9)	3.4(11)	-0.2(9)
							$[Na_3Gd(SO_3)_2(C_2O_4)(H_2O)]_\infty$, 2						
Gd1	5.13(11)	6.89(11)	4.88(11)	-0.02(7)	0.37(7)	-0.23(6)	O5	11.4(15)	11.9(14)	21.5(16)	-3.3(12)	3.6(13)	0.3(11)
S1	9.0(5)	10.7(5)	8.1(5)	0.8(4)	1.4(4)	-1.1(4)	O6	11.5(15)	11.4(14)	17.2(15)	1.2(12)	-5.7(12)	-1.2(11)
S2	12.7(5)	10.1(5)	8.0(4)	-1.5(4)	3.2(4)	-3.7(4)	O7	12.8(14)	15.6(15)	7.9(13)	-1.0(11)	2.7(11)	-4.0(11)
Na1	13.5(8)	17.2(8)	14.4(8)	1.1(7)	-1.4(7)	-1.8(7)	O8	10.4(14)	10.5(13)	6.6(13)	-0.6(11)	1.6(11)	0.1(11)
Na2	8(5)	16(6)	27(8)	10(5)	7(5)	4(4)	O9	12.6(14)	10.9(14)	5.5(13)	-0.3(11)	1.1(11)	0.1(11)
Na2A	13(5)	18(5)	15(6)	2(3)	2(4)	-2(3)	O10	11.1(14)	14.1(14)	6.2(13)	0.9(11)	-0.6(11)	-1.3(11)
Na3	10.9(8)	13.6(8)	27.9(10)	1.9(7)	7.0(7)	2.1(6)	O1W	12(5)	12(4)	25(6)	-1(5)	7(5)	1(3)
O1	9.0(14)	16.6(15)	19.5(16)	3.5(12)	-5.1(12)	-5.7(11)	O1WA	17(5)	10(4)	30(7)	0(5)	8(5)	-1(3)
O2	11.2(15)	16.7(15)	9.2(14)	2.2(12)	-1.7(11)	0.8(11)	C1	6.9(13)	11.0(14)	9.0(14)	0.2(10)	-0.6(11)	2.2(11)
O3	16.4(15)	13.8(15)	10.7(14)	4.3(11)	0.5(12)	-5.4(12)	C2	6.9(13)	11.0(14)	9.0(14)	0.2(10)	-0.6(11)	2.2(11)
O4	11.0(14)	15.1(15)	9.2(13)	0.5(11)	1.5(11)	-5.6(11)							