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SUPPORTING INFORMATION

Novel mixed 1D-2D lanthanide coordination polymers based on p-sulfonatocalix[4]arene and 4,4'-bipyridine-N,N'-dioxide where p-sulfonatocalix[4]arene acts as a guest

Ahmad Husain and Clive L. Oliver*

Centre for Supramolecular Chemistry Research, Department of Chemistry, University of Cape Town, Rondebosch, 7701, South Africa
E-mail: Clive.Oliver@uct.ac.za (Dr. Clive L. Oliver)

***Corresponding author:**

Clive L. Oliver

Centre for Supramolecular Chemistry Research, Department of Chemistry, University of Cape Town, Rondebosch 7701, South Africa

E-mail: clive.oliver@uct.ac.za

Fax: +27 21 6505195

Phone: +27 21 6503830

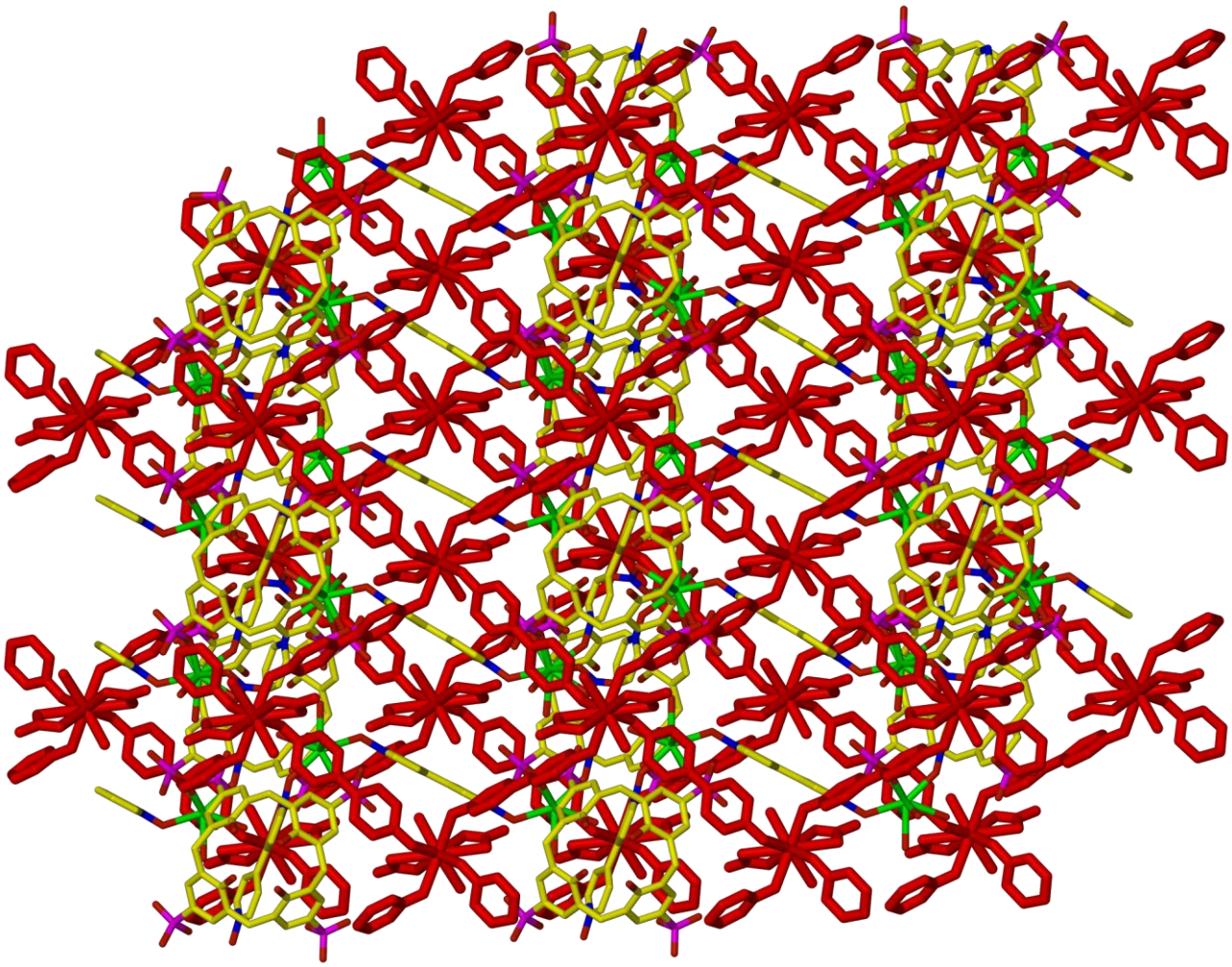

Figure S1. Displaying 1D-2D sandwich structure of **1.**

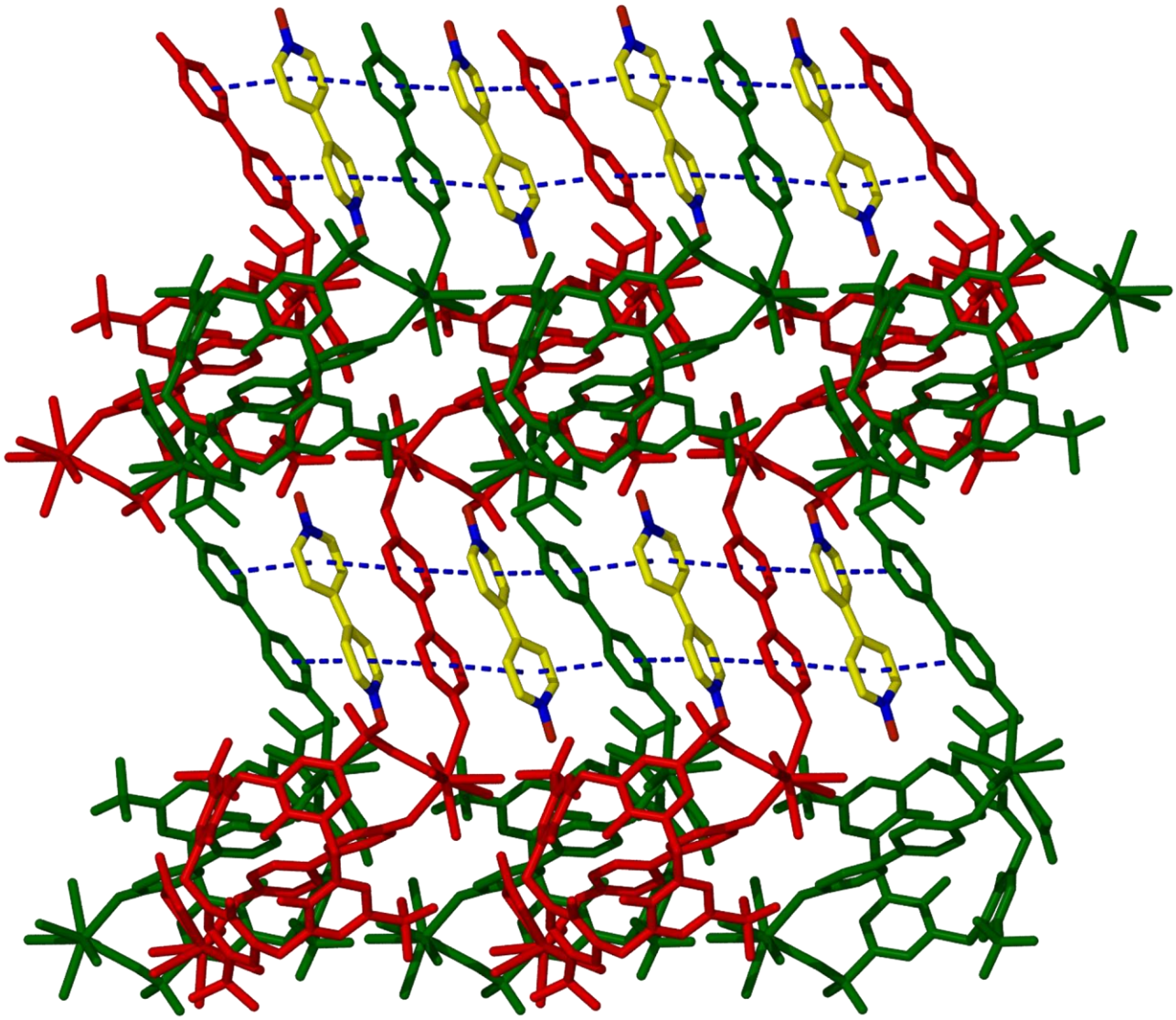

Figure S2. (a**)** Display of π···π interaction (3.874-4.218 Å) between lattice 4,4′-bpdo and ligated 4,4′-bpdo molecules from the 1D chains of **1**. Neighbouring chains are shown in red and green colour to distinguish the 1D strands, whilst the lattice 4,4'-bpdo molecules are displayed in different colours in order to distinguish them from the ligated 4,4'-bpdo molecules.

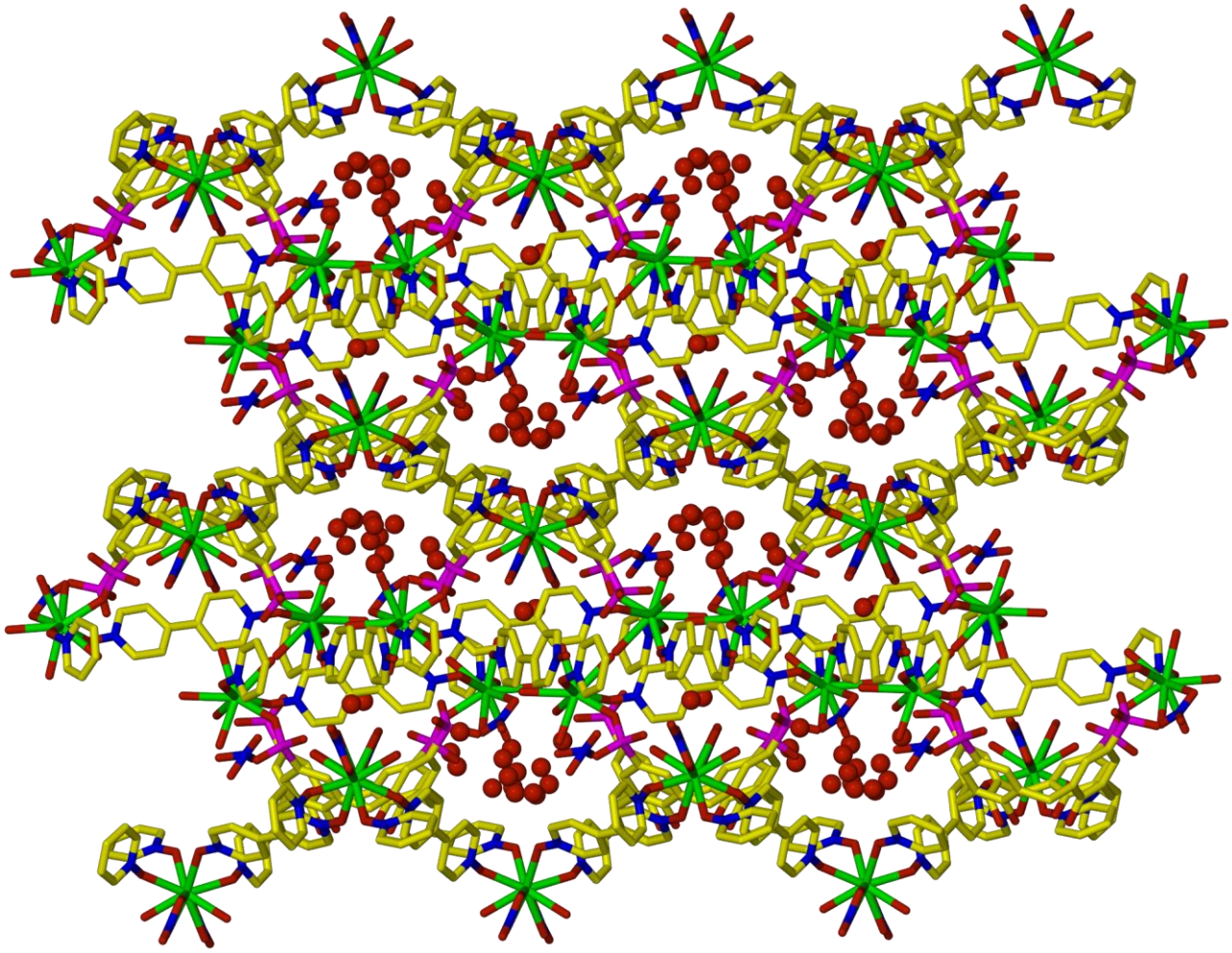

Figure S3. Display of hydrated channels in the crystal lattice as viewed down the *c*-axis. Red balls represent the oxygen atoms of the lattice water molecules.

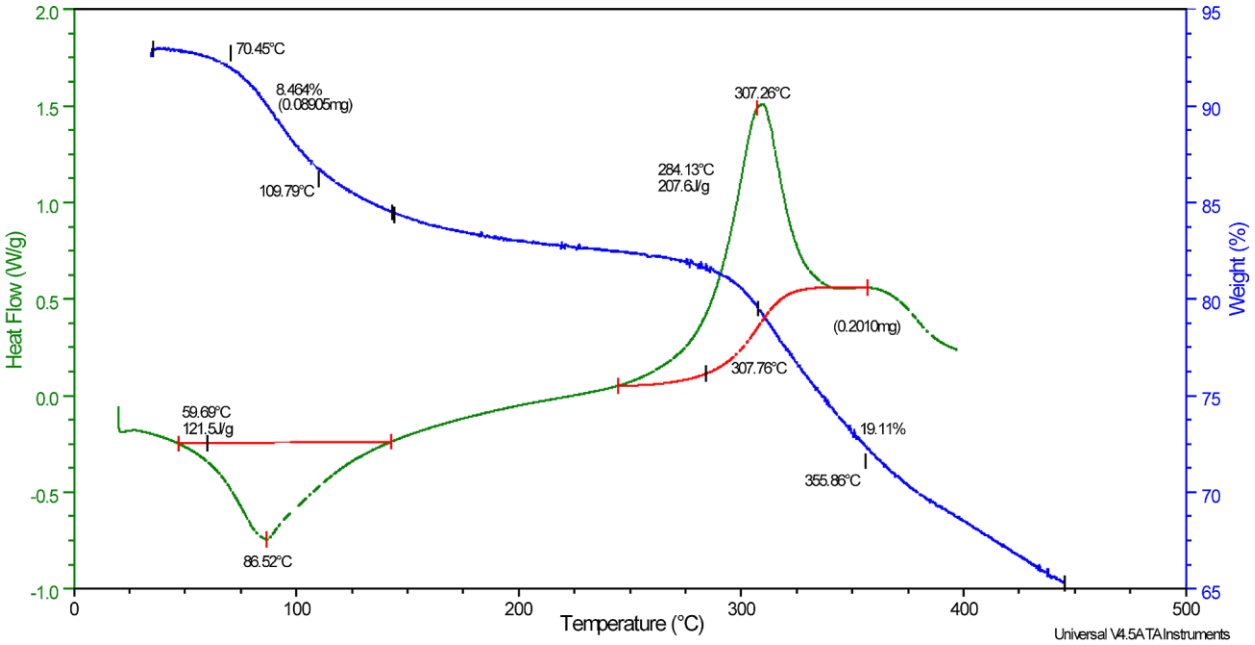

Figure S4. TGA and DSC curve for compound **1.**

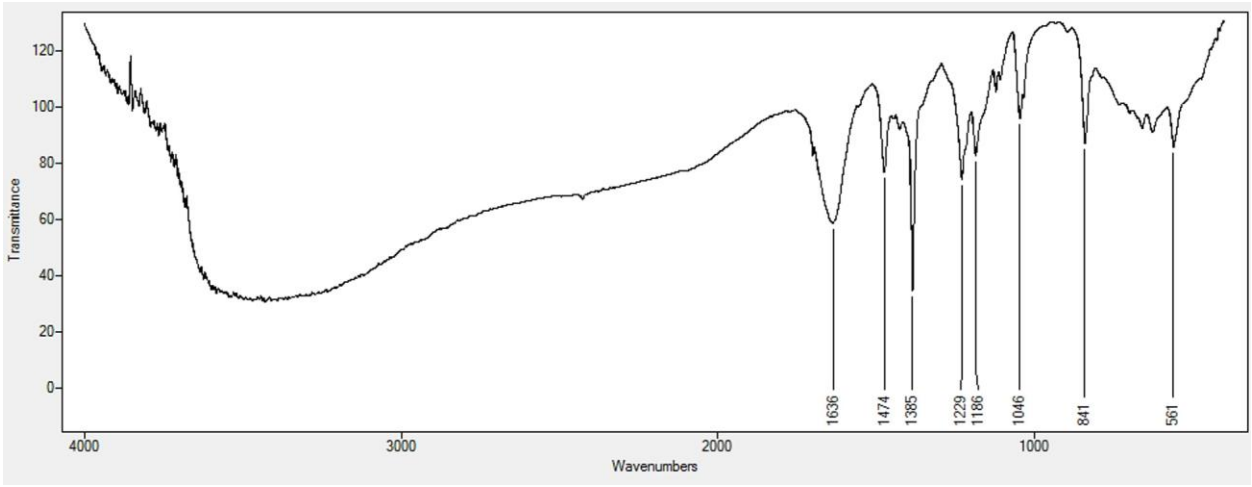

Figure S5. IR spectrum of compound **1.**

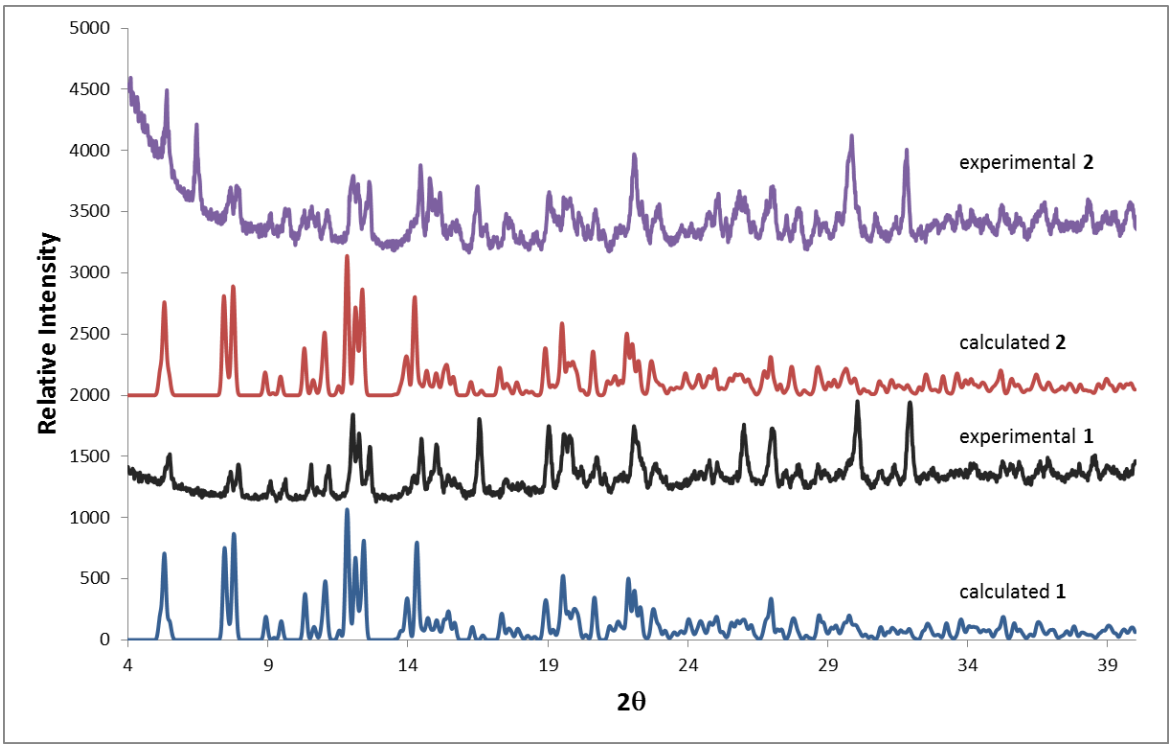

Figure S6. PXRD patterns of **1** and **2** compared with their respective calculated patterns

Table S1. Bond lengths [Å] for **1** and **2**.

$C_{78}H_{105}N_{14}O_{61}S_4Sm_3$ (**1**)		$C_{78}H_{105}N_{14}O_{61}S_4Nd_3$ (**2**)	
Sm(2)-O(19)	2.303(3)	Nd(1)-O(4)	2.446(4)
Sm(2)-O(13)	2.353(3)	Nd(1)-O(1)	2.447(4)
Sm(2)-O(14)	2.405(4)	Nd(1)-O(2)	2.464(4)
Sm(2)-O(20)	2.421(3)	Nd(1)-O(3)	2.489(4)
Sm(2)-O(17)	2.422(4)	Nd(1)-O(12)	2.509(4)
Sm(2)-O(16)	2.459(4)	Nd(1)-O(11)	2.533(4)
Sm(2)-O(18)	2.472(4)	Nd(1)-O(8)	2.620(4)
Sm(2)-O(15)	2.491(3)	Nd(1)-O(7)	2.628(4)
Sm(3)-O(36)	2.342(3)	Nd(1)-O(5)	2.667(4)
Sm(3)-O(44)	2.379(4)	Nd(1)-O(9)	2.692(4)
Sm(3)-O(27)	2.392(4)	Nd(2)-O(21)	2.364(4)
Sm(3)-O(41)	2.423(4)	Nd(2)-O(13)	2.417(4)

Sm(3)-O(40)	2.458(4)	Nd(2)-O(35)	2.428(4)
Sm(3)-O(43)	2.460(4)	Nd(2)-O(15)	2.453(4)
Sm(3)-O(42)	2.538(4)	Nd(2)-O(16)	2.488(4)
Sm(3)-O(38)	2.554(4)	Nd(2)-O(14)	2.488(4)
Sm(3)-O(37)	2.651(4)	Nd(2)-O(17)	2.573(4)
Sm(1)-O(3)	2.414(4)	Nd(2)-O(18)	2.581(4)
Sm(1)-O(1)	2.416(4)	Nd(2)-O(19)	2.668(4)
Sm(1)-O(2)	2.450(4)	Nd(3)-O(22)	2.334(4)
Sm(1)-O(4)	2.453(4)	Nd(3)-O(28)	2.394(4)
Sm(1)-O(5)	2.486(4)	Nd(3)-O(24)	2.425(4)
Sm(1)-O(6)	2.507(4)	Nd(3)-O(29)	2.442(4)
Sm(1)-O(7)	2.586(4)	Nd(3)-O(27)	2.461(4)
Sm(1)-O(11)	2.604(4)	Nd(3)-O(23)	2.488(4)
Sm(1)-O(10)	2.660(4)	Nd(3)-O(26)	2.503(4)
Sm(1)-O(8)	2.675(4)	Nd(3)-O(25)	2.521(4)

Table S2. Bond angles [°] for **1** and **2**.

$C_{78}H_{105}N_{14}O_{61}S_4Sm_3$ (**1**)		$C_{78}H_{105}N_{14}O_{61}S_4Nd_3$ (**2**)	
O(19)-Sm(2)-O(13)	152.75(13)	O(4)-Nd(1)-O(1)	75.17(14)
O(19)-Sm(2)-O(14)	93.36(14)	O(4)-Nd(1)-O(2)	142.02(15)
O(13)-Sm(2)-O(14)	91.07(14)	O(1)-Nd(1)-O(2)	74.96(15)
O(19)-Sm(2)-O(20)	78.13(13)	O(4)-Nd(1)-O(3)	73.81(14)
O(13)-Sm(2)-O(20)	81.19(13)	O(1)-Nd(1)-O(3)	73.90(13)
O(14)-Sm(2)-O(20)	139.82(12)	O(2)-Nd(1)-O(3)	75.78(14)
O(19)-Sm(2)-O(17)	103.47(15)	O(4)-Nd(1)-O(12)	67.75(14)
O(13)-Sm(2)-O(17)	87.60(14)	O(1)-Nd(1)-O(12)	141.87(14)
O(14)-Sm(2)-O(17)	145.21(12)	O(2)-Nd(1)-O(12)	132.69(15)

O(20)-Sm(2)-O(17)	74.22(12)	O(3)-Nd(1)-O(12)	87.28(14)
O(19)-Sm(2)-O(16)	64.99(13)	O(4)-Nd(1)-O(11)	133.98(14)
O(13)-Sm(2)-O(16)	142.25(12)	O(1)-Nd(1)-O(11)	87.72(14)
O(14)-Sm(2)-O(16)	84.87(14)	O(2)-Nd(1)-O(11)	67.10(15)
O(20)-Sm(2)-O(16)	124.11(13)	O(3)-Nd(1)-O(11)	141.79(14)
O(17)-Sm(2)-O(16)	75.41(14)	O(12)-Nd(1)-O(11)	124.63(14)
O(19)-Sm(2)-O(18)	80.96(14)	O(4)-Nd(1)-O(8)	77.63(14)
O(13)-Sm(2)-O(18)	75.45(13)	O(1)-Nd(1)-O(8)	115.32(14)
O(14)-Sm(2)-O(18)	69.59(12)	O(2)-Nd(1)-O(8)	137.16(14)
O(20)-Sm(2)-O(18)	70.30(12)	O(3)-Nd(1)-O(8)	146.39(14)
O(17)-Sm(2)-O(18)	142.48(12)	O(12)-Nd(1)-O(8)	65.48(15)
O(16)-Sm(2)-O(18)	136.04(13)	O(11)-Nd(1)-O(8)	71.77(14)
O(19)-Sm(2)-O(15)	134.31(12)	O(4)-Nd(1)-O(7)	138.46(14)
O(13)-Sm(2)-O(15)	72.57(12)	O(1)-Nd(1)-O(7)	145.89(14)
O(14)-Sm(2)-O(15)	73.39(12)	O(2)-Nd(1)-O(7)	75.85(15)
O(20)-Sm(2)-O(15)	138.45(12)	O(3)-Nd(1)-O(7)	115.13(14)
O(17)-Sm(2)-O(15)	73.07(13)	O(12)-Nd(1)-O(7)	72.15(14)
O(16)-Sm(2)-O(15)	70.30(12)	O(11)-Nd(1)-O(7)	64.74(15)
O(18)-Sm(2)-O(15)	129.82(13)	O(8)-Nd(1)-O(7)	76.34(14)
O(36)-Sm(3)-O(44)	145.52(15)	O(4)-Nd(1)-O(5)	118.63(13)
O(36)-Sm(3)-O(27)	80.78(13)	O(1)-Nd(1)-O(5)	130.90(14)
O(44)-Sm(3)-O(27)	95.63(14)	O(2)-Nd(1)-O(5)	67.62(14)
O(36)-Sm(3)-O(41)	72.44(13)	O(3)-Nd(1)-O(5)	67.08(12)
O(44)-Sm(3)-O(41)	88.16(15)	O(12)-Nd(1)-O(5)	65.09(14)
O(27)-Sm(3)-O(41)	136.39(13)	O(11)-Nd(1)-O(5)	104.98(14)
O(36)-Sm(3)-O(40)	126.53(13)	O(8)-Nd(1)-O(5)	113.70(13)
O(44)-Sm(3)-O(40)	71.29(13)	O(7)-Nd(1)-O(5)	48.27(13)

O(27)-Sm(3)-O(40)	147.99(13)	O(4)-Nd(1)-O(9)	69.05(13)
O(41)-Sm(3)-O(40)	73.82(13)	O(1)-Nd(1)-O(9)	67.53(14)
O(36)-Sm(3)-O(43)	76.94(13)	O(2)-Nd(1)-O(9)	118.81(14)
O(44)-Sm(3)-O(43)	69.72(13)	O(3)-Nd(1)-O(9)	131.62(13)
O(27)-Sm(3)-O(43)	70.14(13)	O(12)-Nd(1)-O(9)	105.56(14)
O(41)-Sm(3)-O(43)	70.66(13)	O(11)-Nd(1)-O(9)	64.93(14)
O(40)-Sm(3)-O(43)	127.13(13)	O(8)-Nd(1)-O(9)	48.02(13)
O(36)-Sm(3)-O(42)	136.42(14)	O(7)-Nd(1)-O(9)	113.21(13)
O(44)-Sm(3)-O(42)	74.72(15)	O(5)-Nd(1)-O(9)	160.27(12)
O(27)-Sm(3)-O(42)	78.39(14)	O(21)-Nd(2)-O(13)	145.91(15)
O(41)-Sm(3)-O(42)	143.35(14)	O(21)-Nd(2)-O(35)	80.40(14)
O(40)-Sm(3)-O(42)	70.07(14)	O(13)-Nd(2)-O(35)	95.45(15)
O(43)-Sm(3)-O(42)	128.95(13)	O(21)-Nd(2)-O(15)	72.75(15)
O(36)-Sm(3)-O(38)	71.97(12)	O(13)-Nd(2)-O(15)	88.27(17)
O(44)-Sm(3)-O(38)	136.23(12)	O(35)-Nd(2)-O(15)	135.83(14)
O(27)-Sm(3)-O(38)	117.80(12)	O(21)-Nd(2)-O(16)	77.31(14)
O(41)-Sm(3)-O(38)	86.00(13)	O(13)-Nd(2)-O(16)	69.63(14)
O(40)-Sm(3)-O(38)	65.42(12)	O(35)-Nd(2)-O(16)	69.79(14)
O(43)-Sm(3)-O(38)	145.58(13)	O(15)-Nd(2)-O(16)	70.50(14)
O(42)-Sm(3)-O(38)	84.71(13)	O(21)-Nd(2)-O(14)	126.52(14)
O(36)-Sm(3)-O(37)	70.16(13)	O(13)-Nd(2)-O(14)	71.44(14)
O(44)-Sm(3)-O(37)	140.74(15)	O(35)-Nd(2)-O(14)	148.37(14)
O(27)-Sm(3)-O(37)	69.78(12)	O(15)-Nd(2)-O(14)	73.94(14)
O(41)-Sm(3)-O(37)	127.96(13)	O(16)-Nd(2)-O(14)	127.09(14)
O(40)-Sm(3)-O(37)	101.55(12)	O(21)-Nd(2)-O(17)	136.35(15)
O(43)-Sm(3)-O(37)	131.16(12)	O(13)-Nd(2)-O(17)	74.16(16)
O(42)-Sm(3)-O(37)	66.81(13)	O(35)-Nd(2)-O(17)	78.52(15)

O(38)-Sm(3)-O(37)	48.68(11)	O(15)-Nd(2)-O(17)	143.57(16)
O(3)-Sm(1)-O(1)	75.42(13)	O(16)-Nd(2)-O(17)	128.34(15)
O(3)-Sm(1)-O(2)	142.89(14)	O(14)-Nd(2)-O(17)	70.29(15)
O(1)-Sm(1)-O(2)	75.12(13)	O(21)-Nd(2)-O(18)	72.19(14)
O(3)-Sm(1)-O(4)	74.01(13)	O(13)-Nd(2)-O(18)	136.14(14)
O(1)-Sm(1)-O(4)	73.39(12)	O(35)-Nd(2)-O(18)	117.63(13)
O(2)-Sm(1)-O(4)	76.32(12)	O(15)-Nd(2)-O(18)	86.83(14)
O(3)-Sm(1)-O(5)	67.87(13)	O(16)-Nd(2)-O(18)	146.30(14)
O(1)-Sm(1)-O(5)	142.14(13)	O(14)-Nd(2)-O(18)	65.33(13)
O(2)-Sm(1)-O(5)	132.48(13)	O(17)-Nd(2)-O(18)	84.58(15)
O(4)-Sm(1)-O(5)	87.61(13)	O(21)-Nd(2)-O(19)	70.01(13)
O(3)-Sm(1)-O(6)	133.87(12)	O(13)-Nd(2)-O(19)	140.32(15)
O(1)-Sm(1)-O(6)	88.02(13)	O(35)-Nd(2)-O(19)	69.85(13)
O(2)-Sm(1)-O(6)	66.61(12)	O(15)-Nd(2)-O(19)	128.36(14)
O(4)-Sm(1)-O(6)	141.78(12)	O(16)-Nd(2)-O(19)	131.22(14)
O(5)-Sm(1)-O(6)	124.27(13)	O(14)-Nd(2)-O(19)	101.55(13)
O(3)-Sm(1)-O(7)	77.62(14)	O(17)-Nd(2)-O(19)	66.95(15)
O(1)-Sm(1)-O(7)	116.11(13)	O(18)-Nd(2)-O(19)	48.42(12)
O(2)-Sm(1)-O(7)	136.43(13)	O(22)-Nd(3)-O(28)	152.05(14)
O(4)-Sm(1)-O(7)	146.48(12)	O(22)-Nd(3)-O(24)	93.70(15)
O(5)-Sm(1)-O(7)	65.13(13)	O(28)-Nd(3)-O(24)	90.78(15)
O(6)-Sm(1)-O(7)	71.71(13)	O(22)-Nd(3)-O(29)	77.79(15)
O(3)-Sm(1)-O(11)	138.04(13)	O(28)-Nd(3)-O(29)	81.03(14)
O(1)-Sm(1)-O(11)	146.03(13)	O(24)-Nd(3)-O(29)	139.76(13)
O(2)-Sm(1)-O(11)	75.62(14)	O(22)-Nd(3)-O(27)	103.29(15)
O(4)-Sm(1)-O(11)	115.49(12)	O(28)-Nd(3)-O(27)	87.97(15)
O(5)-Sm(1)-O(11)	71.72(13)	O(24)-Nd(3)-O(27)	145.49(14)

O(6)-Sm(1)-O(11)	64.61(13)	O(29)-Nd(3)-O(27)	73.96(14)
O(7)-Sm(1)-O(11)	75.64(13)	O(22)-Nd(3)-O(23)	65.06(14)
O(3)-Sm(1)-O(10)	118.68(12)	O(28)-Nd(3)-O(23)	142.86(14)
O(1)-Sm(1)-O(10)	130.46(13)	O(24)-Nd(3)-O(23)	85.64(15)
O(2)-Sm(1)-O(10)	67.53(12)	O(29)-Nd(3)-O(23)	123.49(14)
O(4)-Sm(1)-O(10)	67.17(12)	O(27)-Nd(3)-O(23)	75.06(15)
O(5)-Sm(1)-O(10)	65.01(12)	O(22)-Nd(3)-O(26)	80.84(14)
O(6)-Sm(1)-O(10)	104.93(12)	O(28)-Nd(3)-O(26)	74.92(15)
O(7)-Sm(1)-O(10)	113.35(13)	O(24)-Nd(3)-O(26)	69.68(13)
O(19)-Sm(2)-O(13)	152.75(13)	O(29)-Nd(3)-O(26)	70.14(13)
O(19)-Sm(2)-O(14)	93.36(14)	O(27)-Nd(3)-O(26)	142.08(14)
O(13)-Sm(2)-O(14)	91.07(14)	O(23)-Nd(3)-O(26)	136.43(14)
O(19)-Sm(2)-O(20)	78.13(13)	O(22)-Nd(3)-O(25)	134.91(14)
O(13)-Sm(2)-O(20)	81.19(13)	O(28)-Nd(3)-O(25)	72.69(13)
O(14)-Sm(2)-O(20)	139.82(12)	O(24)-Nd(3)-O(25)	73.77(14)
O(19)-Sm(2)-O(17)	103.47(15)	O(29)-Nd(3)-O(25)	138.01(13)
O(13)-Sm(2)-O(17)	87.60(14)	O(27)-Nd(3)-O(25)	72.96(14)
O(14)-Sm(2)-O(17)	145.21(12)	O(23)-Nd(3)-O(25)	70.82(13)
O(20)-Sm(2)-O(17)	74.22(12)	O(26)-Nd(3)-O(25)	130.03(13)

Table S3. Hydrogen bond parameters for $C_{78}H_{105}N_{14}O_{61}S_4Sm_3$ (**1**) [Å and °].

D–H···A	d(H···A)	d(D···A)	<(DHA)
O(6)-HA···O(22)	2.05	2.735(5)	133.9
O(43)-H(43B)···O(45)#7	1.92	2.635(5)	135.7
O(40)-H(40B)···O(46)#8	1.94	2.700(6)	143.7
O(15)-H(15B)···O(45)#5	1.88	2.668(5)	147.4
O(41)-H(41A)···O(25)#8	1.97	2.878(7)	176.4

O(41)-H(41B)···O(56)	1.87	2.700(7)	150.5
O(17)-H(17B)···O(21)	1.88	2.722(5)	159.5
O(5)-HC···O(28)#9	2.13	2.734(5)	124.9
O(5)-HB···O(55B)#10	2.1	2.872(12)	145.3
O(5)-HB···O(55A)#10	1.89	2.719(13)	155.1
O(14)-H(14)···O(29)#11	1.85	2.707(5)	163.8
O(16)-H(16A)···O(39)#12	2.13	2.771(5)	129.4
O(18)-H(18B)···O(46)	1.95	2.639(5)	133.7
O(42)-H(42B)···O(26)	1.88	2.740(6)	156.9
O(35)-H(35)···O(32)	1.87	2.656(7)	154.4
O(32)-H(32)···O(33)	1.83	2.663(6)	172.1
O(34)-H(34)···O(35)	1.78	2.574(6)	157.1
O(53)-H(5AA)···O(24)	1.96(6)	2.743(7)	154(12)
O(53)-H(6AA)···O(52)	1.83(2)	2.672(8)	172(13)
O(51)-H(8AA)···O(31)#13	2.09(6)	2.892(6)	158(14)
O(54)-H(2AA)···O(45)#10	1.96	2.829(7)	177.2
O(56)-H(0BA)···O(46)#8	2.16(10)	2.865(8)	141(14)
O(57)-H(1BA)···O(61A)#8	2.18(10)	2.883(16)	139(14)
O(50)-H(3AA)···O(47)	2.04	2.872(10)	159.1
O(50)-H(4AA)···O(59)#10	2.15	2.768(14)	128.1

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z #2 -x+2,-y,-z-1 #3 -x+1,-y,-z-1
#4 -x+2,-y,-z #5 -x+2,-y+1,-z #6 -x+1,-y+1,-z+2
#7 x,y,z+1 #8 -x+1,-y+1,-z+1 #9 x,y,z-1 #10 -x+1,-y+1,-z
#11 -x+2,-y+1,-z+1 #12 x+1,y,z #13 x-1,y,z

Table S4. Hydrogen bond parameters for $C_{78}H_{105}N_{14}O_{61}S_4Nd_3$ (**2**) [Å and °].

D–H····A	d(H····A)	d(D····A)	<(DHA)

C(1)-H(1)···O(50)#3	2.63	3.261(8)	124.1
C(2)-H(2)···O(55)#7	2.61	3.554(12)	173.2
C(4)-H(4)···O(55)#8	2.57	3.510(10)	170.6
C(5)-H(5)···O(2)	2.35	3.154(7)	141.9
C(5)-H(5)···O(11)	2.58	3.122(7)	116.4
C(6)-H(6)···O(57A)#9	2.59	3.540(12)	172.9
C(10)-H(10)···O(47)#10	2.43	3.203(9)	137.9
C(12)-H(12)···O(61B)#9	2.66	3.567(16)	161
C(15)-H(15)···O(4)	2.23	3.035(7)	142.5
C(15)-H(15)···O(12)	2.54	3.073(7)	115.8
C(16)-H(16)···O(56)#11	2.35	3.179(9)	146
C(16)-H(16)···O(58B)#12	2.65	3.372(16)	133.2
C(21)-H(21)···O(58A)#12	2.64	3.397(15)	137.2
C(21)-H(21)···O(58B)#12	2.63	3.128(16)	113.2
C(22)-H(22)···O(58B)#12	2.28	2.971(17)	129.1
C(26)-H(26)···O(19)	2.38	3.119(8)	133.9
C(30)-H(30)···O(34)#12	2.35	3.244(9)	156.9
C(31)-H(31)···O(38)#8	2.34	3.284(7)	175.6
C(32)-H(32)···O(18)#12	2.49	3.335(7)	147.9
C(36)-H(36)···O(6)#8	2.48	3.357(8)	154
C(37)-H(37)···O(47)#12	2.5	3.377(10)	152.9
C(39)-H(39)···O(47)#13	2.52	3.391(10)	152.9
C(39)-H(39)···O(48)#13	2.59	3.290(9)	130.5
C(40)-H(40)···O(30)	2.58	3.399(7)	143.9
C(41)-H(41A)···O(9)#14	2.52	3.421(7)	157.5
C(43)-H(43A)···O(27)	2.64	3.481(7)	148.3
C(56)-H(56)···O(19)	2.35	3.240(7)	155.9

C(58)-H(58)···O(5)	2.49	3.380(7)	156.1
C(69)-H(69)···O(31)#12	2.25	3.192(8)	173.6
C(70)-H(70)···O(8)#5	2.55	3.169(7)	123
C(72)-H(72)···O(60B)#12	2.54	3.491(18)	177.5
C(73)-H(73)···O(54)#12	2.41	3.356(9)	170.9
C(74)-H(74)···O(37)#5	2.21	3.147(7)	170.3
C(75)-H(75)···O(7)#5	2.63	3.150(8)	114.6
C(75)-H(75)···O(8)#5	2.57	3.500(8)	167.3
C(77)-H(77)···O(60B)#12	2.59	3.497(18)	159.7
O(24)-H(24A)···S(4)#8	2.97(4)	3.801(4)	161(9)
O(24)-H(24A)···O(38)#8	1.86(2)	2.725(6)	174(9)
O(12)-H(12A)···O(37)	1.94(5)	2.739(6)	153(11)
O(11)-H(11B)···O(31)#11	1.88(3)	2.726(6)	168(9)
O(12)-H(12B)···O(58A)#12	2.10(6)	2.875(12)	149(9)
O(12)-H(12B)···O(58B)#12	1.86(3)	2.720(15)	174(11)
O(25)-H(25B)···O(46)#13	1.93	2.681(6)	142.5
O(24)-H(24B)···O(51)#10	1.87(6)	2.662(6)	148(11)
O(17)-H(17A)···O(54)#12	2.17(6)	2.937(8)	144(9)
O(17)-H(17B)···S(3)	2.97(9)	3.532(5)	124(8)
O(17)-H(17B)···O(36)	1.99(7)	2.745(7)	143(10)
O(50)-H(50A)···O(33)	1.93(4)	2.749(7)	159(10)
O(50)-H(50B)···O(57A)#12	1.98(6)	2.727(11)	145(9)
O(50)-H(50B)···O(57B)#12	1.85(3)	2.707(14)	171(10)
O(52)-H(52A)···O(40)#15	2.23(8)	2.910(7)	136(10)
O(52)-H(52B)···O(17)	2.20(6)	2.988(7)	150(9)
O(51)-H(51A)···O(6)#12	2.20(8)	2.921(7)	138(10)
O(51)-H(51B)···O(46)#14	1.98(3)	2.840(8)	163(9)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y,-z+2 #2 -x+2,-y,-z+1 #3 -x+1,-y,-z+1
#4 -x+1,-y,-z+2 #5 -x+1,-y+1,-z+2 #6 -x+2,-y+1,-z
#7 x,y-1,z+1 #8 -x+2,-y+1,-z+1 #9 x,y-1,z
#10 x+1,y,z #11 x,y,z+1 #12 -x+1,-y+1,-z+1
#13 x+1,y,z-1 #14 x,y,z-1 #15 x-1,y,z