Table S1. Crystal data and structure refinement for **Supermolecule.**

	Supermolecule
Empirical formula	$C_{84}H_{102}Ce_3N_5O_{89}S_8$
Formula weight	3275.49
Temperature (K)	173(2)
λ (Å)	0.71073
Crystal system	Monoclinic
Space group	*P* 21/c
Unit cell dimensions	a = 14.8361(5) Å b = 36.0691(12) Å, β= 101.9030(10)° c = 23.6851(9) Å
Volume (Å^3)	12402.0(8)
Z	4
Calc. density (gcm^{-3})	1.754
μ(mm^{-1})	1.341
F_{000}	6592
Crystal size (mm^3)	0.20 x 0.15 x 0.10
θ range for data collection	1.51 - 25.00°
Miller index ranges	-16≤h≤17, -30≤k≤42, -28≤l≤27
Reflections collected	106344
Independent reflections	21784 [$R_{(int)}$ = 0.0583]
Completeness to θ_{max}	99.8 %
Max. and min. transmission	0.8776 and 0.7753
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	21784 / 59 / 1855
Goodness-of-fit on F^2	1.028
Final *R* indices [I >2σ(I)]	R_1 = 0.0496, wR_2 = 0.1181
R indices (all data)	R_1 = 0.0689, wR_2 = 0.1282
Largest diff. peak and hole (e Å^{-3})	3.446 and -2.381

Table S2. Bond lengths [Å] and bond angles [º] for **Supermolecule**.

Bond lengths		Bond angles			
Ce(1)-O(12)	2.508(4)	O(12)-Ce(1)-O(11)	71.63(13)	O(33)-Ce(2)-O(86)	55.2(4)
Ce(1)-O(11)	2.536(4)	O(12)-Ce(1)-O(8)	74.52(13)	O(35)-Ce(2)-O(86)	55.5(4)
Ce(1)-O(8)	2.546(4)	O(11)-Ce(1)-O(8)	142.22(14)	O(27B)-Ce(2)-O(86)	111.0(5)
Ce(1)-O(5)	2.552(4)	O(12)-Ce(1)-O(5)	78.73(13)	O(27A)-Ce(2)-O(86)	117.8(4)
Ce(1)-O(10)	2.553(4)	O(11)-Ce(1)-O(5)	68.06(13)	O(36)-Ce(2)-O(86)	66.0(4)
Ce(1)-O(9)	2.576(4)	O(8)-Ce(1)-O(5)	120.75(13)	O(29)-Ce(2)-O(86)	122.1(3)
Ce(1)-O(2)	2.591(4)	O(12)-Ce(1)-O(10)	135.24(14)	O(32)-Ce(2)-O(86)	67.1(4)
Ce(1)-O(3)	2.620(4)	O(11)-Ce(1)-O(10)	134.57(14)	O(30)-Ce(2)-O(86)	119.5(3)
Ce(1)-N(2)	2.674(5)	O(8)-Ce(1)-O(10)	65.58(14)	O(34)-Ce(2)-O(86)	106.3(4)
Ce(1)-N(1)	2.731(5)	O(5)-Ce(1)-O(10)	139.38(14)	N(3)-Ce(2)-O(86)	174.5(4)
Ce(2)-O(33)	2.461(6)	O(12)-Ce(1)-O(9)	133.89(13)	O(35)-Ce(2)-O(27A)	80.1(3)
Ce(2)-O(35)	2.464(6)	O(11)-Ce(1)-O(9)	123.63(14)	O(27B)-Ce(2)-O(27A)	24.3(3)
Ce(2)-O(27B)	2.487(13)	O(8)-Ce(1)-O(9)	92.10(14)	O(33)-Ce(2)-O(36)	87.8(2)
Ce(2)-O(27A)	2.491(7)	O(5)-Ce(1)-O(9)	70.81(15)	O(35)-Ce(2)-O(36)	72.7(2)
Ce(2)-O(36)	2.500(4)	O(10)-Ce(1)-O(9)	68.83(15)	O(27B)-Ce(2)-O(36)	118.2(4)
Ce(2)-O(29)	2.528(5)	O(12)-Ce(1)-O(2)	141.44(13)	O(27A)-Ce(2)-O(36)	142.4(2)
Ce(2)-O(32)	2.617(6)	O(11)-Ce(1)-O(2)	71.00(13)	O(27B)-Ce(2)-O(34)	140.3(3)
Ce(2)-O(30)	2.622(4)	O(8)-Ce(1)-O(2)	143.99(14)	O(27A)-Ce(2)-O(34)	134.54(18)
Ce(2)-O(34)	2.634(4)	O(5)-Ce(1)-O(2)	78.94(13)	O(36)-Ce(2)-O(34)	65.84(14)
Ce(2)-N(3)	2.730(5)	O(10)-Ce(1)-O(2)	80.00(14)	O(29)-Ce(2)-O(34)	73.35(15)
Ce(2)-O(86)	2.736(13)	O(9)-Ce(1)-O(2)	64.61(13)	O(32)-Ce(2)-O(34)	131.98(15)
Ce(3)-O(51)	2.454(4)	O(12)-Ce(1)-O(3)	65.38(13)	O(30)-Ce(2)-O(34)	89.36(15)
Ce(3)-O(53)	2.499(4)	O(11)-Ce(1)-O(3)	83.63(13)	O(33)-Ce(2)-N(3)	124.0(2)
Ce(3)-O(56)	2.500(4)	O(8)-Ce(1)-O(3)	67.22(13)	O(35)-Ce(2)-N(3)	125.9(2)
Ce(3)-O(55)	2.507(4)	O(5)-Ce(1)-O(3)	139.94(13)	O(27B)-Ce(2)-N(3)	72.9(3)
Ce(3)-O(54)	2.529(4)	O(10)-Ce(1)-O(3)	80.66(14)	O(27A)-Ce(2)-N(3)	67.43(18)
Ce(3)-O(52)	2.545(4)	O(9)-Ce(1)-O(3)	148.44(15)	O(36)-Ce(2)-N(3)	108.82(15)
Ce(3)-O(60)	2.554(4)	O(2)-Ce(1)-O(3)	118.87(12)	O(29)-Ce(2)-N(3)	60.11(15)
Ce(3)-O(57)	2.591(4)	O(12)-Ce(1)-N(2)	66.64(13)	O(32)-Ce(2)-N(3)	118.07(17)
Ce(3)-N(4)	2.681(4)	O(11)-Ce(1)-N(2)	117.69(14)	O(30)-Ce(2)-N(3)	58.46(15)
		O(8)-Ce(1)-N(2)	60.80(14)	O(34)-Ce(2)-N(3)	69.06(14)
		O(5)-Ce(1)-N(2)	60.15(13)	O(51)-Ce(3)-O(53)	72.67(16)
		O(10)-Ce(1)-N(2)	107.52(14)	O(51)-Ce(3)-O(56)	70.94(17)
		O(9)-Ce(1)-N(2)	68.34(14)	O(53)-Ce(3)-O(56)	135.18(17)
		O(2)-Ce(1)-N(2)	125.27(13)	O(51)-Ce(3)-O(55)	101.49(16)
		O(3)-Ce(1)-N(2)	115.84(14)	O(53)-Ce(3)-O(55)	142.66(16)
		O(12)-Ce(1)-N(1)	113.65(13)	O(56)-Ce(3)-O(55)	70.75(15)
		O(11)-Ce(1)-N(1)	68.61(14)	O(51)-Ce(3)-O(54)	144.33(16)
		O(8)-Ce(1)-N(1)	111.77(14)	O(53)-Ce(3)-O(54)	133.40(15)
		O(5)-Ce(1)-N(1)	127.35(13)	O(56)-Ce(3)-O(54)	73.92(18)
		O(10)-Ce(1)-N(1)	66.66(14)	O(55)-Ce(3)-O(54)	71.98(15)
		O(9)-Ce(1)-N(1)	112.30(14)	O(51)-Ce(3)-O(52)	70.28(14)
		O(2)-Ce(1)-N(1)	59.62(13)	O(53)-Ce(3)-O(52)	72.38(15)
		O(33)-Ce(2)-O(29)	72.2(2)	O(56)-Ce(3)-O(52)	117.22(16)

	O(35)-Ce(2)-O(29)	147.9(2)	O(55)-Ce(3)-O(52)	71.06(15)
	O(27B)-Ce(2)-O(29)	97.4(4)	O(54)-Ce(3)-O(52)	133.95(15)
	O(27A)-Ce(2)-O(29)	74.2(2)	O(51)-Ce(3)-O(60)	135.18(14)
	O(36)-Ce(2)-O(29)	138.61(15)	O(53)-Ce(3)-O(60)	77.78(17)
	O(33)-Ce(2)-O(32)	67.53(19)	O(56)-Ce(3)-O(60)	146.95(16)
	O(35)-Ce(2)-O(32)	79.18(19)	O(55)-Ce(3)-O(60)	82.43(15)
	O(27B)-Ce(2)-O(32)	76.9(4)	O(54)-Ce(3)-O(60)	79.76(16)
	O(27A)-Ce(2)-O(32)	63.14(19)	O(52)-Ce(3)-O(60)	69.07(13)
	O(36)-Ce(2)-O(32)	133.09(16)	O(51)-Ce(3)-O(57)	86.29(14)
	O(29)-Ce(2)-O(32)	72.22(17)	O(53)-Ce(3)-O(57)	80.10(15)
	O(33)-Ce(2)-O(30)	154.4(2)	O(56)-Ce(3)-O(57)	72.34(15)
	O(35)-Ce(2)-O(30)	74.09(19)	O(55)-Ce(3)-O(57)	137.08(14)
	O(27B)-Ce(2)-O(30)	60.6(4)	O(54)-Ce(3)-O(57)	77.42(14)
	O(27A)-Ce(2)-O(30)	79.0(2)	O(52)-Ce(3)-O(57)	147.97(14)
	O(36)-Ce(2)-O(30)	68.97(16)	O(60)-Ce(3)-O(57)	121.01(12)
	O(29)-Ce(2)-O(30)	118.38(14)	O(51)-Ce(3)-N(4)	129.16(15)
	O(32)-Ce(2)-O(30)	136.70(17)	O(53)-Ce(3)-N(4)	65.24(14)
	O(33)-Ce(2)-O(34)	70.71(17)	O(56)-Ce(3)-N(4)	123.74(16)
	O(35)-Ce(2)-O(34)	138.5(2)	O(55)-Ce(3)-N(4)	129.26(15)
	O(33)-Ce(2)-O(35)	110.1(3)	O(54)-Ce(3)-N(4)	68.16(15)
	O(33)-Ce(2)-O(27B)	144.4(4)	O(52)-Ce(3)-N(4)	119.04(14)
	O(35)-Ce(2)-O(27B)	61.4(4)	O(60)-Ce(3)-N(4)	60.90(13)
	O(33)-Ce(2)-O(27A)	126.5(2)	O(57)-Ce(3)-N(4)	60.14(13)

Table S3. Hydrogen bond parameters in compound **Supermolecule**.

Donor–H---Acceptor	H---A (Å)	D---A (Å)	D–H---A (º)
O(1)–H(1) ---O(68)	1.72	2.544(7)	165
O(4)–H(4) ---O(80)	1.81	2.631(10)	165
O(7)–H(7) ---O(77)	1.67	2.494(8)	168
O(9)–H(9A)---O(42)#1	2.36(6)	3.133(6)	156(8)
O(9)–H(9A)---O(20)#2	2.43(7)	3.071(7)	135(6)
O(10)–H(10A)---O(21)#2	2.25(7)	3.080(6)	166(6)
O(10)–H(10B)---O(67)	1.91(7)	2.764(6)	172(9)
Intra O(11)–H(11A)---O(12)	2.58(10)	2.952(6)	108(6)
Intra O(11)–H(11A)---O(13)	1.91(5)	2.744(6)	171(7)
O(11)–H(11B)---O(43)#3	1.90(3)	2.744(6)	176(11)
Intra O(15)–H(15)---O(18)	2.03	2.786(6)	149
Intra O(16)–H(16)---O(15)	2.05	2.831(6)	155
O(16)–H(16)---O(23)#1	2.50	2.958(6)	116
Intra O(17)–H(17)---O(16)	2.37	2.918(6)	124
O(17)–H(17)---O(69)#4	2.01	2.677(7)	135
Intra O(18)–H(18)---O(17)	2.03	2.790(6)	151
O(33)–H(33A)---O(67)#5	1.96(7)	2.763(7)	159(7)
O(33)–H(33B)---O(73)#5	2.24(7)	2.829(10)	127(6)
O(33)–H(33B)---O(48)#6	2.53(8)	3.137(8)	130(6)
Intra O(34)–H(34A)---O(36)	2.36(6)	2.792(6)	112(6)

Intra O(34)–H(34A)---O(37)	1.94(7)	2.796(6)	175(9)
O(34)–H(34B)---O(19)#7	1.88(5)	2.726(6)	172(5)
Intra O(39)–H(39)---O(42)	2.00	2.799(6)	158
Intra O(40)–H(40)---O(39)	2.25	2.880(6)	132
O(40)–H(40)---O(34)#8	2.19	2.716(6)	121
Intra O(41)–H(41)---O(40)	1.89	2.691(6)	158
Intra O(42)–H(42)---O(41)	2.20	2.764(6)	125
O(42)–H(42)---O(20)#9	2.07	2.699(6)	131
O(52)–H(52A)---O(23)#10	2.00(6)	2.846(6)	173(12)
Intra O(52)–H(52B)---O(50)	2.06(6)	2.800(6)	144(6)
O(53)–H(53A)---O(74A)#10	1.99(8)	2.726(8)	148(10)
O(53)–H(53B)---O(25A)#11	1.91(4)	2.741(8)	170(13)
O(54)–H(54A)---O(14)#11	2.00(4)	2.850(6)	179(12)
O(54)–H(54B)---O(45)#10	1.88(7)	2.735(6)	173(10)
O(55)–H(55A)---O(62)#3	1.91(6)	2.744(8)	178(11)
O(55)–H(55B)---O(66)	2.02(6)	2.848(7)	166(7)
O(56)–H(56C)---O(63)#3	1.97(7)	2.732(11)	148(6)
O(56)–H(56D)---O(72)	1.87(6)	2.710(8)	173(7)
O(58)–H(58)---O(21)#11	1.82	2.628(6)	160
O(59)–H(59)---O(24)#10	2.02	2.659(6)	132
O(64)–H(64A)---O(65)#12	1.82(6)	2.624(6)	159(6)
O(64)–H(64B)---O(81)	1.79(5)	2.634(11)	175(9)
O(65)–H(65A)---O(6)#13	1.95(5)	2.789(6)	169(9)
O(65)–H(65B)---O(66)#14	1.99(7)	2.841(7)	171(9)
O(66)–H(66A)---O(23)#10	1.98(5)	2.822(6)	174(9)
O(66)–H(66B)---O(44)#10	1.88(7)	2.718(6)	165(6)
O(68)–H(68A)---O(46)#15	1.92(4)	2.763(7)	171(5)
O(68)–H(68B)---O(38)#15	1.97(6)	2.796(7)	166(8)
O(69)–H(69A)---O(22)#12	2.06(9)	2.881(8)	162(9)
O(70)–H(70C)---O(68)	2.19(6)	2.978(8)	152(6)
O(70)–H(70D)---O(79)#12	2.02(7)	2.869(11)	164(7)
O(71)–H(71A)---O(73)	1.85(10)	2.704(9)	171(11)
O(73)–H(73A)---O(72)#3	1.93(8)	2.779(9)	169(11)
O(75)–H(75A)---O(72)	2.18(6)	2.811(10)	131(7)
O(75)–H(75B)---O(49)	2.48(9)	2.986(9)	118(8)
O(75)–H(75B)---O(51)	2.54(9)	3.299(9)	148(9)
O(78)–H(78A)---O(43)#3	2.02(7)	2.799(8)	155(7)
O(78)–H(78B)---O(36)#3	2.43(7)	3.215(8)	156(7)
O(78)–H(78B)---O(38)#3	2.21(7)	2.863(10)	135(6)
O(79)–H(79A)---O(31)#16	1.93(7)	2.753(10)	162(9)
Intra C(20)–H(20)---O(13)	2.55	2.923(7)	104
Intra C(21)–H(21A)---O(15)	2.42	2.837(6)	105
Intra C(23)–H(23)---O(22)	2.51	2.902(7)	104
Intra C(30)–H(30)---O(26A)	2.49	2.911(10)	107
Intra C(35)–H(35A)---O(17)	2.33	2.764(7)	106
C(37)–H(37)---O(7)#7	2.46	3.367(7)	159

Intra C(39)–H(39A)---O(19)	2.51	2.893(8)	104
Intra C(42)–H(42A)---O(15)	2.55	2.961(7)	105
C(46)–H(46)---O(61A)#4	2.54	3.28(2)	135
Intra C(51)–H(51)---O(36)	2.51	2.903(7)	105
C(55)–H(55)---O(70)#5	2.49	3.428(9)	172
Intra C(60)–H(60)---O(48)	2.48	2.872(8)	105
Intra C(63)–H(63A)---O(40)	2.33	2.752(7)	105
C(63)–H(63B)---O(63)#3	2.50	3.453(11)	160
Intra C(65)–H(65)---O(51)	2.43	2.845(7)	106
C(70)–H(70A)---O(61A)#17	2.53	3.499(16)	165
Intra C(72)–H(72)---O(45)	2.54	2.927(7)	105
C(74)–H(74)---O(64)#5	2.53	3.409(7)	154
Intra C(77)–H(77B)---O(42)	2.37	2.788(7)	104
C(80)–H(80)---O(24)#11	2.53	3.407(7)	155

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z #2 x,1/2-y,1/2+z #3 1-x,-y,-z #4 -1+x,y,-1+z #5 x,y,-1+z
#6 1-x,-y,-1-z #7 x,1/2-y,-1/2+z #8 -x,-y,-1-z #9 -x,-1/2+y,-1/2-z #10 x,-1/2-y,-1/2+z
#11 1-x,-1/2+y,-1/2-z #12 1-x,-y,1-z #13 1+x,y,z #14 1-x,1/2+y,-1/2-z #15 x,y,1+z
#16 1+x,y,1+z #17 1-x,-1/2+y,1/2-z

Table S4 Analysis of Cg---Cg (centoroid---centoroid) Interactions for **Supermolecule**.

Cg(I)-Cg(J)	Symmetry transformations	Cg---Cg (Å)	Torsion angle (º)
Cg(1)---Cg(10)	[1-X,-Y,-Z]	4.642(4)	37.9(3)
Cg(1)---Cg(12)	[1-X,-Y,-Z]	4.402(4)	31.2(3)
Cg(2)---Cg(5)	[X,Y,Z]	3.657(3)	12.1(3)
Cg(2)---Cg(12)	[-X,-Y,-Z]	4.265(4)	9.1(3)
Cg(3)---Cg(7)	[X,Y,Z]	3.682(3)	3.9(3)
Cg(3)---Cg(10)	[-X,-Y,-1-Z]	4.025(4)	2.8(3)
Cg(4)---Cg(5)	[1-X,-1/2+Y,-1/2-Z]	4.620(3)	12.8(3)
Cg(4)---Cg(7)	[1-X,-1/2+Y,-1/2-Z]	4.790(3)	17.6(3)
Cg(5)---Cg(6)	[X,Y,Z]	4.746(3)	77.8(3)
Cg(5)---Cg(7)	[X,Y,Z]	5.860(3)	30.4(2)
Cg(5)---Cg(8)	[X,Y,Z]	4.696(3)	80.6(3)
Cg(6)---Cg(4)	[1-X,1/2+Y,-1/2-Z]	4.858(3)	86.3(3)
Cg(6)---Cg(6)	[-X,-Y,-Z]	3.532(3)	0
Cg(6)---Cg(7)	[X,Y,Z]	4.662(3)	81.2(3)
Cg(7)---Cg(8)	[X,Y,Z]	4.790(3)	77.4(3)
Cg(8)---Cg(11)	[-X,1/2+Y,-1/2-Z]	3.597(4)	5.1(3)
Cg(9)---Cg(1)	[1-X,-Y,-Z]	5.278(4)	65.1(3)
Cg(9)---Cg(9)	[-X,-Y,-1-Z]	3.693(4)	0
Cg(9)---Cg(10)	[X,Y,Z]	4.719(4)	77.5(3)
Cg(9)---Cg(12)	[X,Y,Z]	4.681(4)	78.0(3)
Cg(10)---Cg(11)	[X,Y,Z]	4.933(4)	69.8(3)
Cg(11)---Cg(1)	[1-X,-Y,-Z]	4.948(4)	78.3(3)
Cg(11)---Cg(12)	[X,Y,Z]	4.883(4)	74.2(3)
Cg1~N(1)-C(6), Cg2~N(2)-C(13), Cg3~N(3)-C(48), Cg4~N(4)-C(83), Cg5~C(15)-C(20), Cg6~C(22)-C(27), Cg7~C(29)-C(34), Cg8~C(36)-C(41), Cg9~C(50)-C(55), Cg10~C(57)-C(62), Cg11~C(64)-C(69), Cg12~C(71)-C(76)			

Figure S1 TGA and DSC of **supermolecule**.

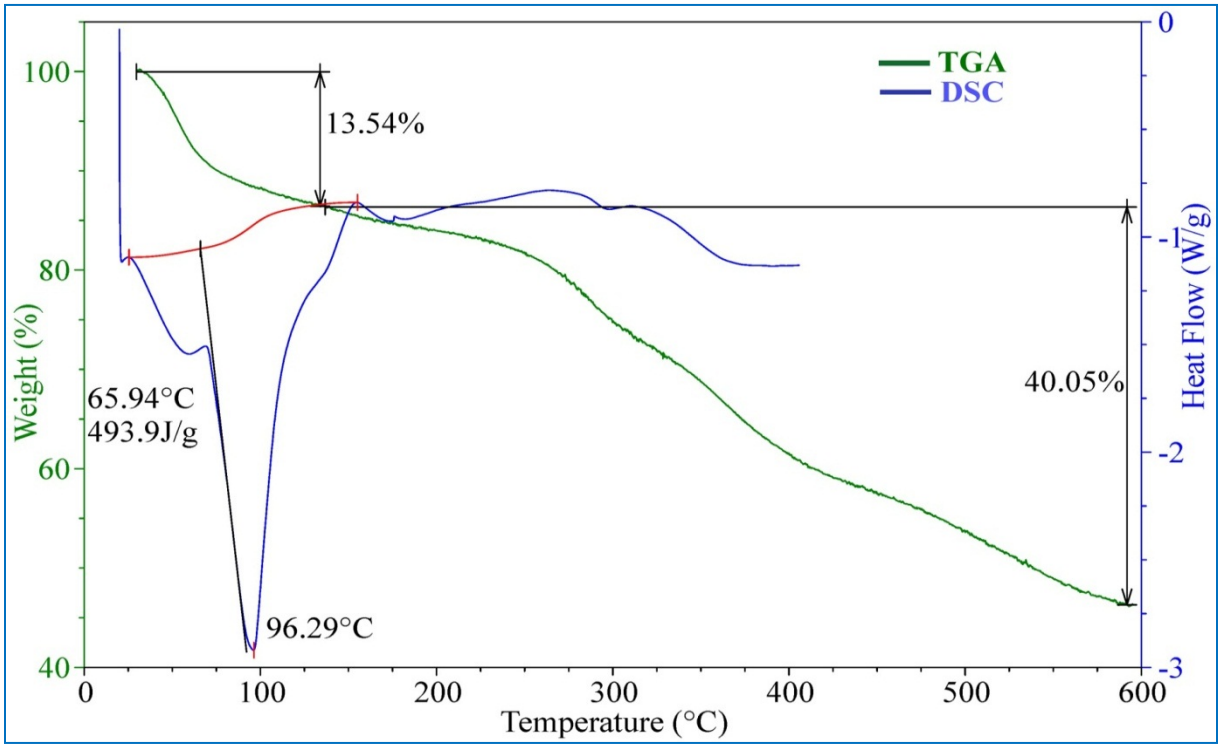

Figure S2 Hot stage microscope photographs of supermolecule.