SupplementaryInformation

Bi-Porous Metal-Organic Framework with Hydrophilic and Hydrophobic Channels: Selective Gas Sorption and Reversible Iodine Uptake Studies

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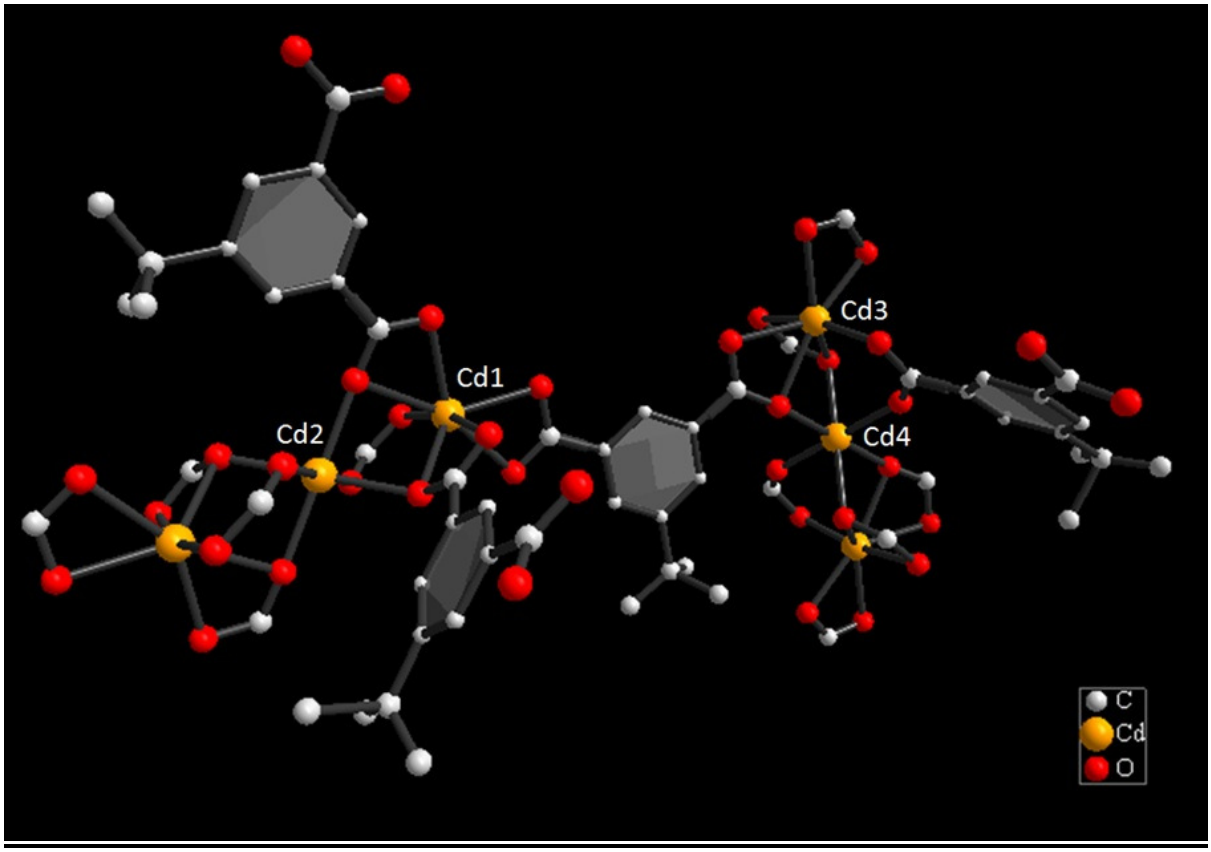


Figure S1. Asymmetric unit of the compound **1**.

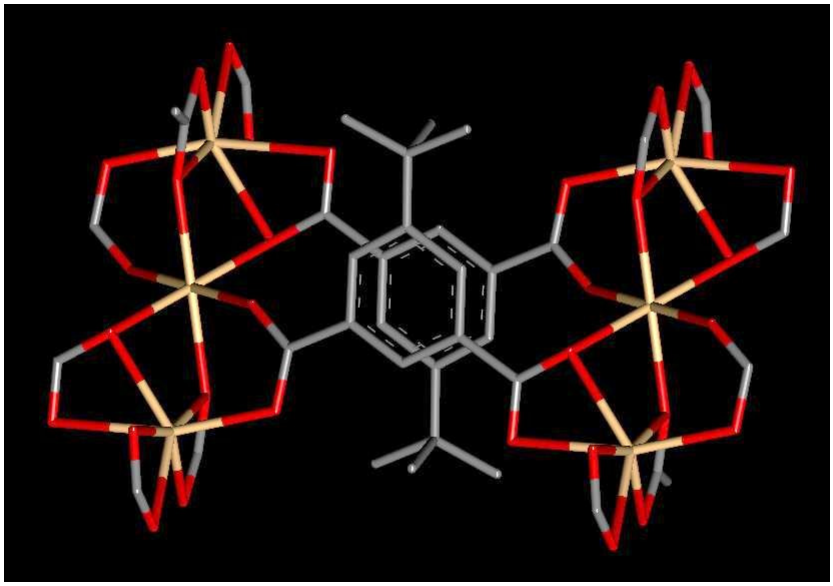
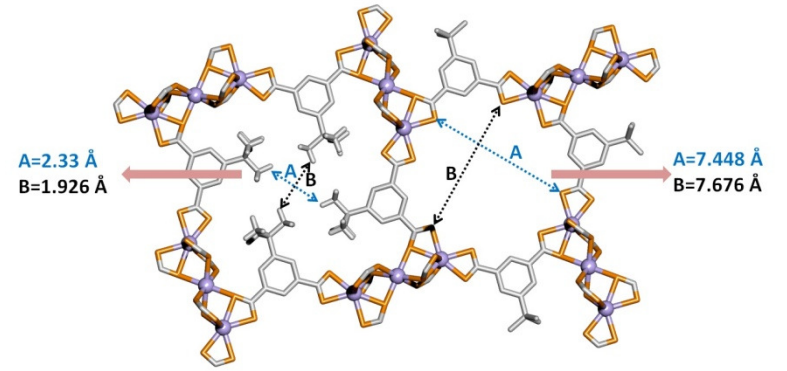


Figure S2. Strong π-π interaction between the two phenyl rings of 5tbip ligands in the compound **1** with the distance of 3.6 Å.



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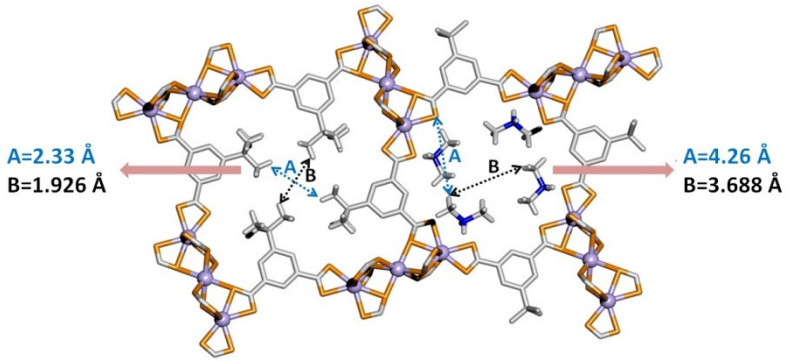

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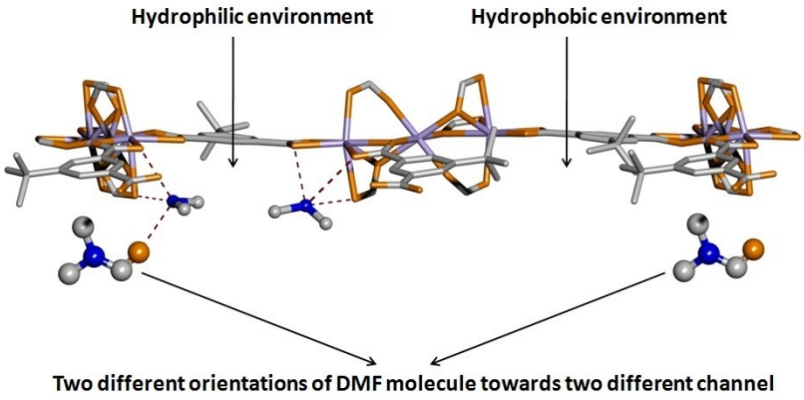

c

Figure S3. A) Diagram showing pore dimensions of channel A and B including van der Waal radii. B) Pore dimension including cations in hydrophilic channel. C) cross section of part of 1 showing hydrogen bonding and the two different orientations of DMF molecule towards two different channels.

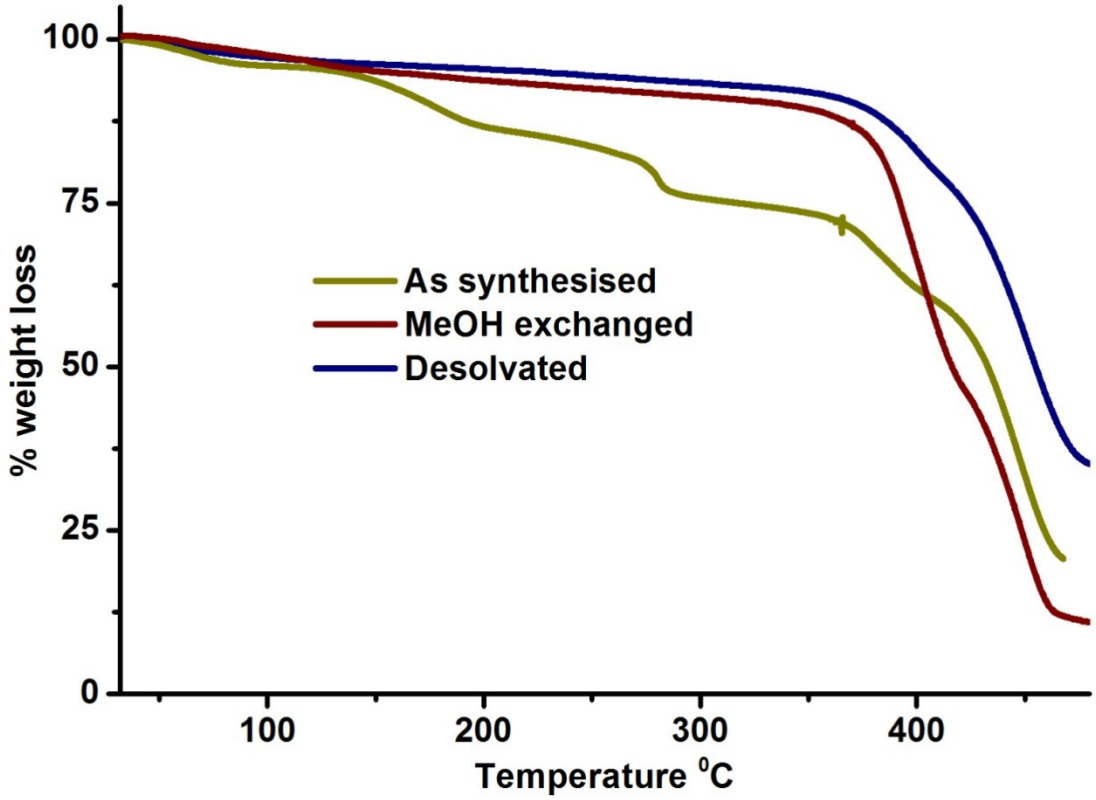

Figure S4. Thermogravimetric analysis of as synthesised compound **1** shows continuous weight loss due to trapped solvent molecules inside the pores and the solvent exchanged compound showed the stable phase at higher temperature.

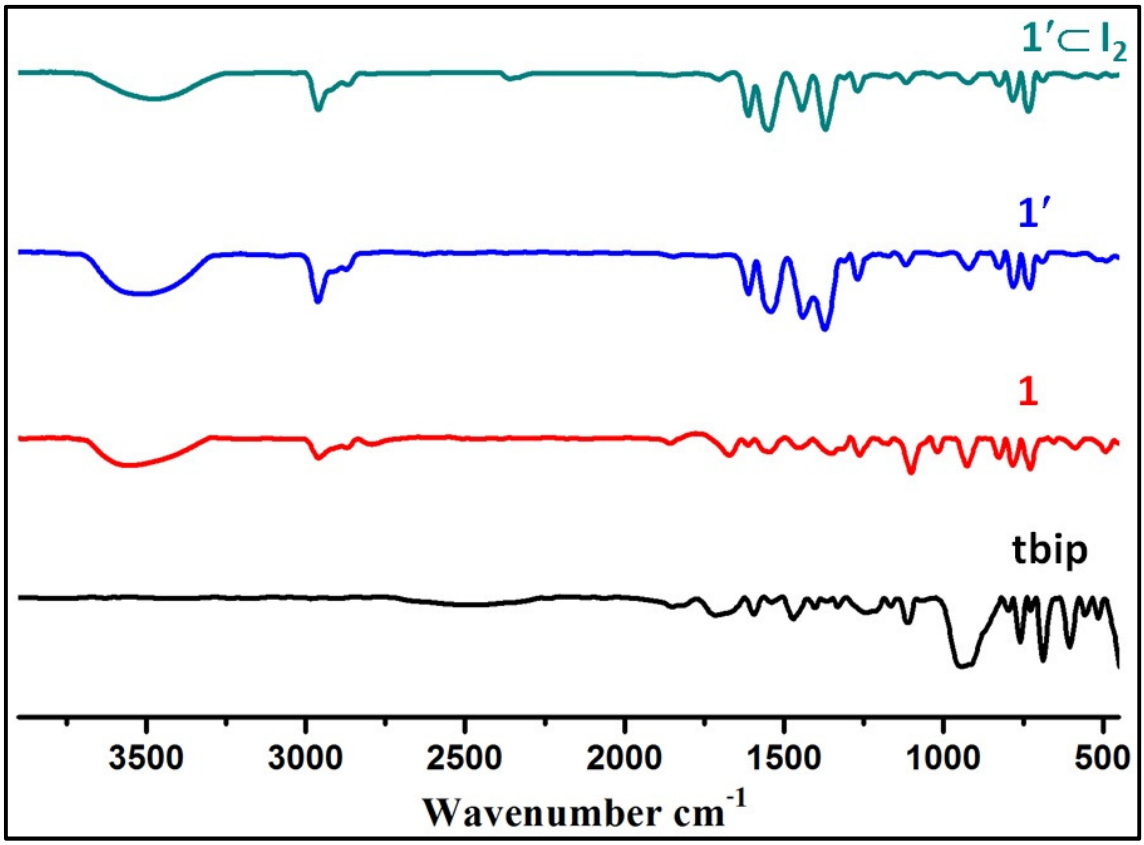

Figure S5. IR spectra of the different forms the compound **1**

Gas adsorption details:

Low pressure gas sorption measurements were performed using BelSorpmax (Bel Japan). All of the gases used were of 99.999% purity. As-synthesized compound was gently heated at 120 °C under vacuum for overnight to get guest free compounds. Prior to adsorption measurement the guest free sample **1′** was again degassed at 120 °C under vacuum for 2 hrs using BelPrepvacII and purged with N_2 on cooling. Isosteric heat of sorption was calculated using sorption data of CO_2 at two different temperatures viz. 273K and 298K by using BelSorpMax analysis tool.

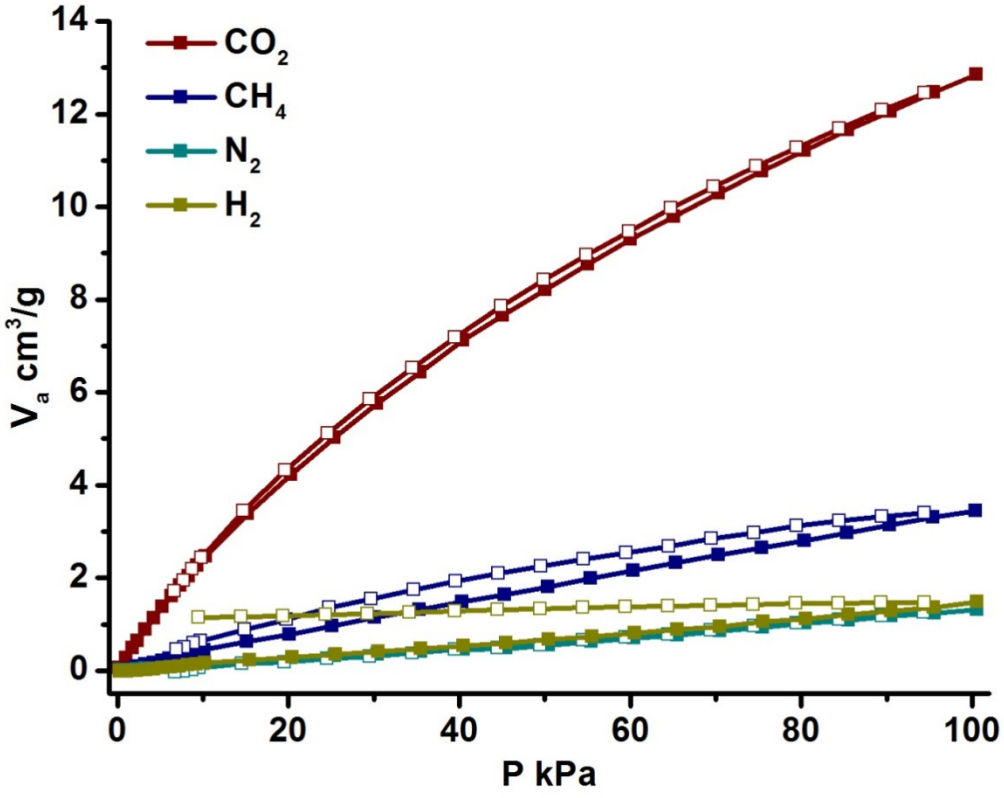

Figure S6. Sorption isotherms for compound **1′** at 273 K showing selective uptake of CO_2.

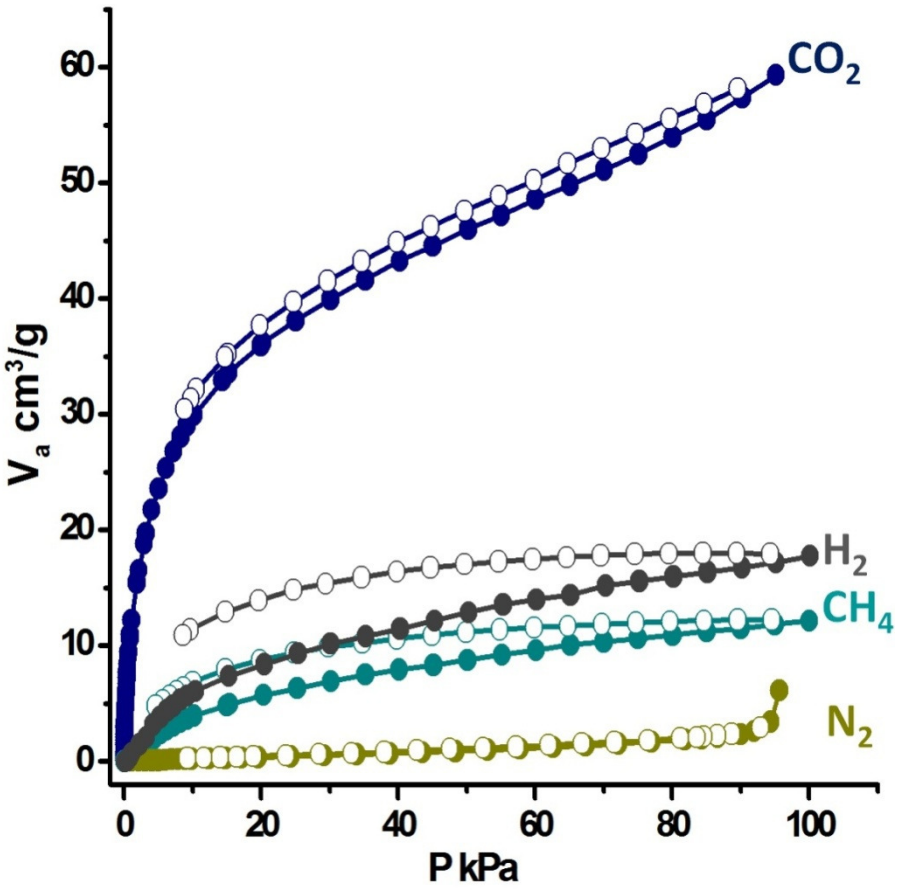

Figure S7. Low temperaturesorption isotherms for compound **1′;** CO_2 (195K), N_2 (77K), CH_4 (195K), H_2 (77K).

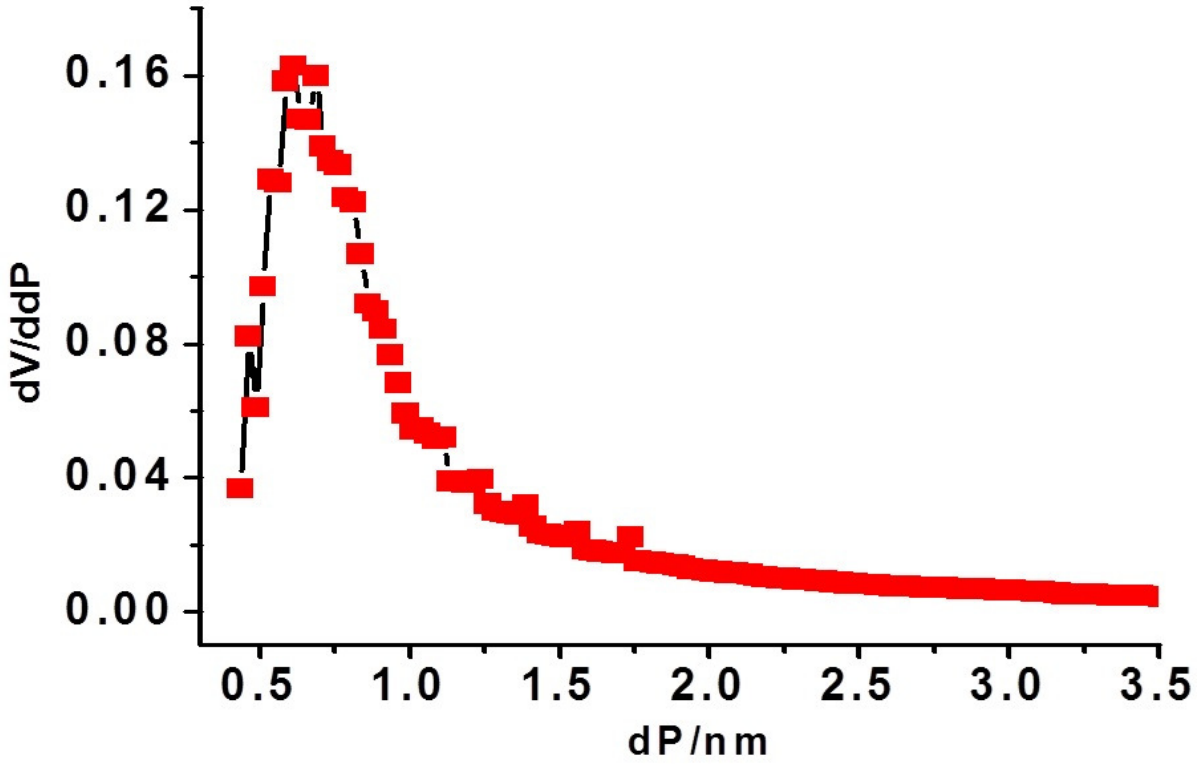

Figure S8. Pore size distribution plot of compound 1′ showing the average pore diameter of 0.6 nm.

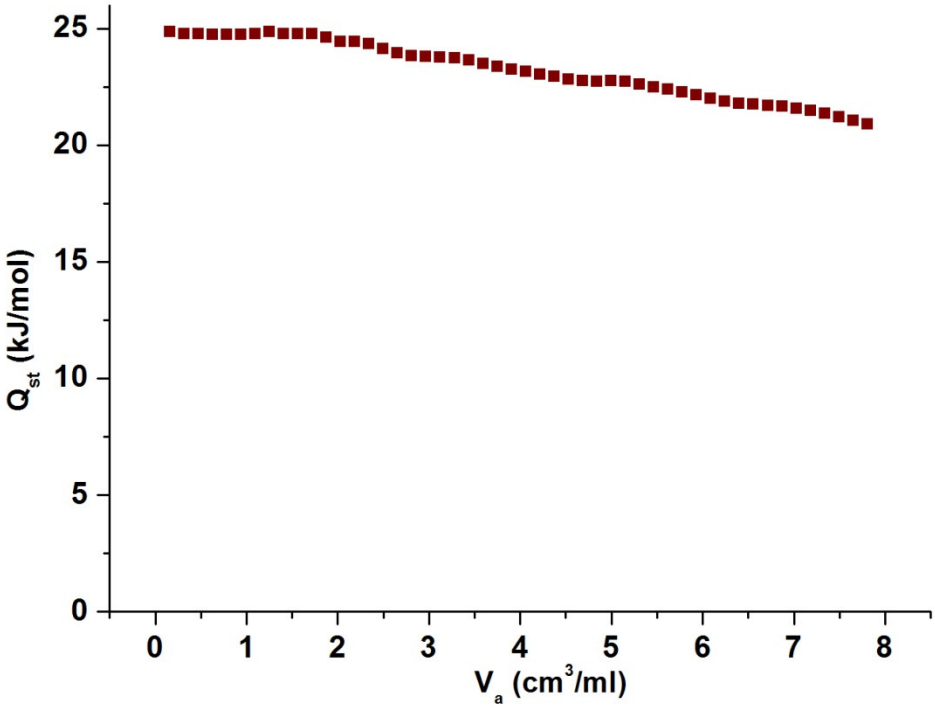

Figure S9. Heat of adsorption calculated from CO_2 sorption at 273 K and 298 K.

Details of Iodine inclusion study and electrical conductivity measurement:

The MOF sample, obtained after solution state iodine uptake study (performed using 3ml of 0.01 M iodine in cyclohexane and 50 mg of **1′**) was taken out of the mother liquor (supernatant pale yellow cyclohexane solution) by filtration, washed several times with fresh cyclohexane to remove any traces of free iodine on the surface of sample. This was followed by air-drying at room temperature, to allow sublimation of free iodine (if present) on the surface, to finally obtain a dark brown phase, **1′⊂nI$_2$**.

The dc electrical conductivity values of the compounds were measured by a conventional four-probe method using pressed pellets and evaluated by the equation, $\rho = \rho_o/f(w/s)$; Where, $\rho_o = 2\pi sV/I$; ρ is the resistivity, w is the thickness, s is probe spacing, V is the voltage across the two inner probes, I is the current through the two outer probes, $f(w/s)$ is the correction factor. (B. Dhara and N. Ballav, *RSC Adv.*, 2013, **3**, 4909–4913) Room temperature current–voltage characteristics for both the compounds are similar and seem to be Ohmic from the linear fits of the data points. The absolute dc conductivity values for the compounds **1'** and **1'⊂ nI$_2$** were in the range of ~1.714 X 10^{-8} $Scm^{-1}$and ~1.298 X 10^{-6} Scm^{-1}, respectively. This clearly confirmed about ~76 times enhancement of the conductivity value (σ) on iodine inclusion.

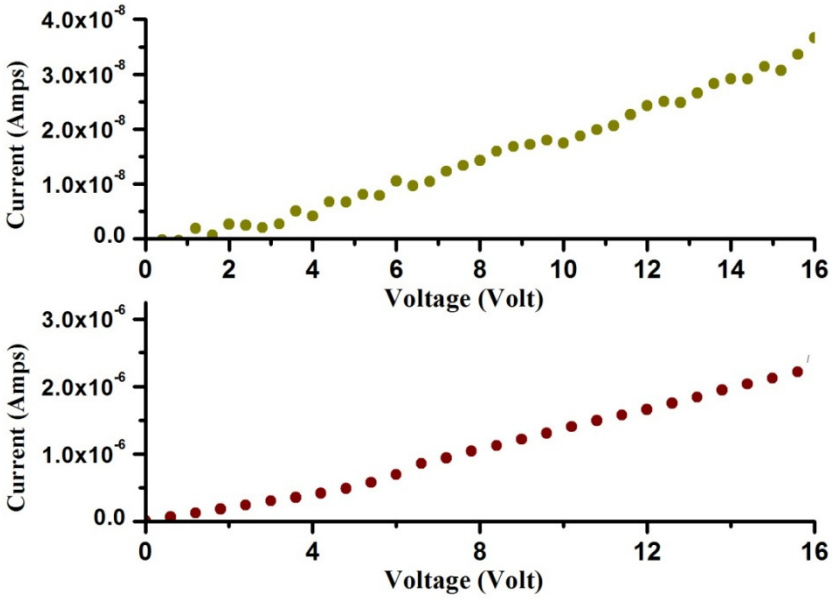

Figure S10: Room temperature current-voltage characteristics for compound **1'** and **1'⊂nI$_2$**.

Table S1. Crystal data and structure refinement for compound **1**.

Identification code	Compound**1**	
Empirical formula	C58 H78 Cd3 N4 O18	
Formula weight	1456.44	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.8523(7) Å	α= 89.715(2)°.
	b = 19.5244(15) Å	β= 83.058(2)°.
	c = 19.6699(15) Å	γ = 87.776(2)°.
Volume	3753.1(5) $Å^3$	
Z	2	
Density (calculated)	1.289 Mg/m^3	
Absorption coefficient	0.902 mm^{-1}	
F(000)	1484	
Crystal size	0.18 x 0.15 x 0.12 mm^3	
Theta range for data collection	1.04 to 25.00°.	
Index ranges	-11<=h<=11, -23<=k<=23, 0<=l<=23	
Reflections collected	13119	
Independent reflections	13119 [R(int) = 0.0000]	
Completeness to theta = 25.00°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8995 and 0.8545	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13119 / 163 / 751	
Goodness-of-fit on F^2	1.221	
Final R indices [I>2sigma(I)]	R1 = 0.0993, wR2 = 0.2920	
R indices (all data)	R1 = 0.1223, wR2 = 0.3074	
Largest diff. peak and hole	5.116 and -1.478 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for compound **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cd(1)	9992(1)	1542(1)	768(1)	29(1)
Cd(2)	10637(1)	5739(1)	3443(1)	30(1)
Cd(3)	10000	0	0	27(1)
Cd(4)	10000	5000	5000	29(1)
C(1)	9839(12)	2223(6)	1960(6)	37(3)
C(2)	9857(11)	2587(5)	2638(5)	36(2)
C(3)	10055(11)	3293(5)	2663(5)	32(2)
C(4)	10094(10)	3599(5)	3299(5)	30(2)
C(5)	9971(11)	3201(5)	3902(5)	35(2)
C(6)	9807(13)	2508(6)	3874(6)	43(3)
C(7)	9707(13)	2204(6)	3237(6)	47(3)
C(8)	10334(10)	4344(5)	3326(6)	33(2)
C(9)	9744(18)	2076(6)	4524(6)	79(4)
C(10)	9840(20)	1321(7)	4426(10)	122(7)
C(11)	10920(20)	2221(14)	4916(13)	146(8)
C(12)	8460(20)	2274(13)	4970(13)	169(11)
C(13)	7524(10)	847(6)	837(5)	32(2)
C(14)	6261(9)	448(6)	894(5)	33(2)
C(15)	5000(11)	733(5)	789(5)	34(2)
C(16)	3872(10)	348(6)	849(5)	32(2)
C(17)	4013(12)	-341(6)	1035(6)	42(3)
C(18)	5207(10)	-651(6)	1179(6)	39(3)
C(19)	6375(10)	-251(6)	1082(5)	37(2)
C(20)	12488(12)	628(6)	736(5)	37(3)
C(21)	4070(20)	-1679(13)	1703(12)	135(5)
C(23)	5580(30)	-1809(12)	719(10)	174(8)
C(24)	6680(20)	-1667(13)	1583(13)	135(6)
C(25)	7948(11)	5827(5)	4120(6)	39(3)
C(26)	6571(11)	5891(5)	4534(6)	38(3)
C(27)	5405(10)	5777(5)	4240(6)	32(2)
C(28)	4121(11)	5838(5)	4628(6)	35(2)
C(29)	4048(12)	6040(6)	5324(6)	45(3)
C(30)	5186(11)	6185(6)	5621(6)	40(3)

C(31)	6511(12)	6080(6)	5214(6)	44(3)
C(32)	12802(12)	5712(6)	4355(6)	40(3)
C(33)	5020(20)	6414(9)	6379(9)	119(5)
C(34)	6330(20)	6446(14)	6684(14)	154(6)
C(35)	4220(20)	5864(12)	6773(14)	159(6)
C(36)	4000(20)	6994(12)	6513(15)	155(6)
C(37)	10668(11)	6934(6)	2740(5)	39(3)
C(38)	10486(11)	7595(5)	2381(5)	36(2)
C(39)	10341(14)	8196(6)	2757(6)	50(3)
C(40)	10242(11)	8851(5)	2464(5)	36(2)
C(41)	9575(10)	2358(5)	-1680(5)	30(2)
C(42)	9759(10)	1730(5)	-1388(5)	29(2)
C(43)	9839(11)	1141(5)	-1750(5)	37(2)
C(44)	9924(10)	1677(5)	-625(5)	32(2)
C(45)	10111(15)	9501(6)	2884(7)	54(3)
C(46)	11190(20)	10002(11)	2593(12)	126(8)
C(47)	8890(30)	9935(14)	2779(15)	188(17)
C(48)	10120(30)	9443(10)	3601(9)	117(7)
C(49)	8030(30)	6222(18)	1316(14)	208(17)
C(51)	6810(40)	2998(18)	138(19)	210(17)
C(52)	7310(50)	3702(16)	1060(30)	380(40)
C(53)	4980(30)	6923(12)	2971(13)	450(60)
C(54)	7020(30)	7535(19)	3420(20)	280(30)
C(55)	4750(50)	7650(18)	3980(16)	440(60)
C(56)	5310(50)	1040(20)	2670(20)	380(40)
C(57)	3320(30)	1680(20)	2341(19)	320(40)
C(58)	5560(30)	2117(13)	1935(11)	250(20)
N(1)	8140(20)	5927(13)	2006(10)	147(8)
N(2)	7480(40)	2994(17)	770(20)	290(20)
N(3)	5610(20)	7330(9)	3404(11)	164(11)
N(4)	4820(30)	1627(14)	2303(10)	217(16)
O(1)	9721(13)	1602(4)	1965(4)	72(3)
O(2)	9970(9)	2564(4)	1411(4)	47(2)
O(3)	10480(9)	4584(4)	3923(4)	45(2)
O(4)	10455(8)	4713(4)	2812(4)	37(2)
O(5)	7391(8)	1494(4)	747(4)	41(2)
O(6)	8691(7)	544(4)	885(4)	37(2)
O(7)	11616(8)	194(5)	649(4)	54(2)

O(8)	12247(9)	1272(5)	728(4)	53(2)
O(9)	7985(7)	5773(4)	3498(4)	41(2)
O(10)	9007(7)	5864(4)	4436(4)	33(2)
O(11)	11798(7)	5655(4)	4785(5)	52(2)
O(12)	12761(8)	5696(4)	3704(5)	52(2)
O(13)	10599(8)	6370(4)	2409(4)	44(2)
O(14)	10739(11)	6935(4)	3368(4)	61(3)
O(15)	9783(8)	2210(4)	-257(4)	39(2)
O(16)	10174(8)	1093(4)	-377(4)	39(2)
O(17)	5860(30)	6707(13)	2540(14)	225(13)
O(18)	5040(30)	2580(15)	1648(16)	247(16)
C(50)	7900(30)	5182(12)	2014(11)	136(10)
C(22)	5342(19)	-1404(7)	1391(8)	92(4)

Table S3. Bond lengths [Å] and angles [°] for compound **1**.

Cd(1)-O(8)	2.255(9)
Cd(1)-O(1)	2.339(9)
Cd(1)-O(2)	2.366(8)
Cd(1)-O(6)	2.369(8)
Cd(1)-O(16)	2.405(7)
Cd(1)-O(15)	2.422(7)
Cd(1)-O(5)	2.573(7)
Cd(1)-C(1)	2.687(11)
Cd(1)-Cd(3)	3.3742(7)
Cd(2)-O(12)	2.213(8)
Cd(2)-O(14)	2.344(8)
Cd(2)-O(13)	2.376(7)
Cd(2)-O(10)	2.381(7)
Cd(2)-O(4)	2.387(7)
Cd(2)-O(3)	2.444(8)
Cd(2)-O(9)	2.600(7)
Cd(2)-C(37)	2.704(11)
Cd(2)-Cd(4)	3.3788(7)
Cd(3)-O(7)	2.203(8)
Cd(3)-O(7)#1	2.203(8)
Cd(3)-O(16)#1	2.262(7)
Cd(3)-O(16)	2.262(7)
Cd(3)-O(6)	2.277(7)
Cd(3)-O(6)#1	2.277(7)
Cd(3)-Cd(1)#1	3.3743(7)
Cd(4)-O(11)	2.223(8)
Cd(4)-O(11)#2	2.223(8)
Cd(4)-O(3)	2.261(7)
Cd(4)-O(3)#2	2.261(7)
Cd(4)-O(10)#2	2.268(6)
Cd(4)-O(10)	2.268(6)
Cd(4)-Cd(2)#2	3.3788(7)
C(1)-O(1)	1.222(14)
C(1)-O(2)	1.262(13)
C(1)-C(2)	1.515(14)
C(2)-C(7)	1.388(15)

C(2)-C(3)	1.402(15)
C(3)-C(4)	1.394(14)
C(3)-H(3)	0.9300
C(4)-C(5)	1.411(15)
C(4)-C(8)	1.486(14)
C(5)-C(6)	1.372(16)
C(5)-H(5)	0.9300
C(6)-C(7)	1.405(15)
C(6)-C(9)	1.524(17)
C(7)-H(7)	0.9300
C(8)-O(4)	1.235(13)
C(8)-O(3)	1.292(13)
C(9)-C(10)	1.486(9)
C(9)-C(12)	1.487(10)
C(9)-C(11)	1.505(10)
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(11)-H(11A)	0.9600
C(11)-H(11B)	0.9600
C(11)-H(11C)	0.9600
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-O(5)	1.278(13)
C(13)-O(6)	1.286(11)
C(13)-C(14)	1.487(14)
C(14)-C(15)	1.380(14)
C(14)-C(19)	1.416(16)
C(15)-C(16)	1.359(15)
C(15)-H(15)	0.9300
C(16)-C(17)	1.399(16)
C(16)-C(20)#3	1.491(14)
C(17)-C(18)	1.362(15)
C(17)-H(17)	0.9300
C(18)-C(19)	1.409(15)
C(18)-C(22)	1.532(18)
C(19)-H(19)	0.9300

C(20)-O(7)	1.257(13)
C(20)-O(8)	1.271(14)
C(20)-C(16)#4	1.491(14)
C(21)-C(22)	1.449(16)
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(23)-C(22)	1.532(16)
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-C(22)	1.490(16)
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-O(9)	1.224(13)
C(25)-O(10)	1.283(12)
C(25)-C(26)	1.497(16)
C(26)-C(27)	1.373(14)
C(26)-C(31)	1.383(16)
C(27)-C(28)	1.398(15)
C(27)-H(27)	0.9300
C(28)-C(29)	1.418(16)
C(28)-C(32)#3	1.493(15)
C(29)-C(30)	1.366(16)
C(29)-H(29)	0.9300
C(30)-C(31)	1.454(16)
C(30)-C(33)	1.546(19)
C(31)-H(31)	0.9300
C(32)-O(11)	1.229(14)
C(32)-O(12)	1.288(14)
C(32)-C(28)#4	1.493(15)
C(33)-C(34)	1.486(10)
C(33)-C(36)	1.487(10)
C(33)-C(35)	1.512(10)
C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600

C(35)-H(35A)	0.9600
C(35)-H(35B)	0.9600
C(35)-H(35C)	0.9600
C(36)-H(36A)	0.9600
C(36)-H(36B)	0.9600
C(36)-H(36C)	0.9600
C(37)-O(14)	1.246(13)
C(37)-O(13)	1.289(13)
C(37)-C(38)	1.484(14)
C(38)-C(39)	1.384(15)
C(38)-C(41)#5	1.390(14)
C(39)-C(40)	1.404(15)
C(39)-H(39)	0.9300
C(40)-C(43)#5	1.417(15)
C(40)-C(45)	1.510(16)
C(41)-C(42)	1.368(13)
C(41)-C(38)#5	1.390(14)
C(41)-H(41)	0.9300
C(42)-C(43)	1.350(15)
C(42)-C(44)	1.530(13)
C(43)-C(40)#5	1.418(15)
C(43)-H(43)	0.9300
C(44)-O(15)	1.263(13)
C(44)-O(16)	1.265(12)
C(45)-C(48)	1.41(2)
C(45)-C(47)	1.48(2)
C(45)-C(46)	1.53(2)
C(46)-H(46A)	0.9600
C(46)-H(46B)	0.9600
C(46)-H(46C)	0.9600
C(47)-H(47A)	0.9600
C(47)-H(47B)	0.9600
C(47)-H(47C)	0.9600
C(48)-H(48A)	0.9600
C(48)-H(48B)	0.9600
C(48)-H(48C)	0.9600
C(49)-N(1)	1.486(17)
C(49)-H(49A)	0.9600

C(49)-H(49B)	0.9600
C(49)-H(49C)	0.9600
C(51)-N(2)	1.479(19)
C(51)-H(51A)	0.9600
C(51)-H(51B)	0.9600
C(51)-H(51C)	0.9600
C(52)-N(2)	1.488(19)
C(52)-H(52A)	0.9600
C(52)-H(52B)	0.9600
C(52)-H(52C)	0.9600
C(53)-O(17)	1.199(10)
C(53)-N(3)	1.385(10)
C(53)-H(53)	0.9300
C(54)-N(3)	1.461(10)
C(54)-H(54A)	0.9600
C(54)-H(54B)	0.9600
C(54)-H(54C)	0.9600
C(55)-N(3)	1.462(10)
C(55)-H(55A)	0.9600
C(55)-H(55B)	0.9600
C(55)-H(55C)	0.9600
C(56)-N(4)	1.457(10)
C(56)-H(56A)	0.9600
C(56)-H(56B)	0.9600
C(56)-H(56C)	0.9600
C(57)-N(4)	1.469(10)
C(57)-H(57A)	0.9600
C(57)-H(57B)	0.9600
C(57)-H(57C)	0.9600
C(58)-O(18)	1.194(10)
C(58)-N(4)	1.376(10)
C(58)-H(58)	0.9300
N(1)-C(50)	1.483(17)
N(1)-H(1A)	0.9000
N(1)-H(1B)	0.9000
N(2)-H(2A)	0.9000
N(2)-H(2B)	0.9000
C(50)-H(50A)	0.9600

C(50)-H(50B)	0.9600
C(50)-H(50C)	0.9600

O(8)-Cd(1)-O(1)	92.2(4)
O(8)-Cd(1)-O(2)	97.4(3)
O(1)-Cd(1)-O(2)	55.0(3)
O(8)-Cd(1)-O(6)	110.9(3)
O(1)-Cd(1)-O(6)	87.2(3)
O(2)-Cd(1)-O(6)	133.8(3)
O(8)-Cd(1)-O(16)	86.2(3)
O(1)-Cd(1)-O(16)	161.4(3)
O(2)-Cd(1)-O(16)	143.6(3)
O(6)-Cd(1)-O(16)	76.1(3)
O(8)-Cd(1)-O(15)	104.9(3)
O(1)-Cd(1)-O(15)	143.1(3)
O(2)-Cd(1)-O(15)	90.0(2)
O(6)-Cd(1)-O(15)	115.4(2)
O(16)-Cd(1)-O(15)	54.4(2)
O(8)-Cd(1)-O(5)	164.2(3)
O(1)-Cd(1)-O(5)	91.6(3)
O(2)-Cd(1)-O(5)	97.3(3)
O(6)-Cd(1)-O(5)	53.9(2)
O(16)-Cd(1)-O(5)	85.3(3)
O(15)-Cd(1)-O(5)	80.9(3)
O(8)-Cd(1)-C(1)	94.5(3)
O(1)-Cd(1)-C(1)	27.0(3)
O(2)-Cd(1)-C(1)	28.0(3)
O(6)-Cd(1)-C(1)	111.3(3)
O(16)-Cd(1)-C(1)	171.6(3)
O(15)-Cd(1)-C(1)	117.5(3)
O(5)-Cd(1)-C(1)	95.8(3)
O(8)-Cd(1)-Cd(3)	82.0(2)
O(1)-Cd(1)-Cd(3)	119.4(2)
O(2)-Cd(1)-Cd(3)	174.35(18)
O(6)-Cd(1)-Cd(3)	42.37(16)
O(16)-Cd(1)-Cd(3)	42.05(18)
O(15)-Cd(1)-Cd(3)	95.59(16)
O(5)-Cd(1)-Cd(3)	82.77(17)

C(1)-Cd(1)-Cd(3)	146.4(2)
O(12)-Cd(2)-O(14)	88.9(3)
O(12)-Cd(2)-O(13)	108.1(3)
O(14)-Cd(2)-O(13)	55.9(3)
O(12)-Cd(2)-O(10)	111.8(3)
O(14)-Cd(2)-O(10)	89.5(3)
O(13)-Cd(2)-O(10)	125.6(2)
O(12)-Cd(2)-O(4)	104.6(3)
O(14)-Cd(2)-O(4)	144.7(3)
O(13)-Cd(2)-O(4)	88.8(3)
O(10)-Cd(2)-O(4)	114.1(3)
O(12)-Cd(2)-O(3)	85.8(3)
O(14)-Cd(2)-O(3)	161.0(3)
O(13)-Cd(2)-O(3)	143.0(3)
O(10)-Cd(2)-O(3)	75.6(3)
O(4)-Cd(2)-O(3)	54.2(2)
O(12)-Cd(2)-O(9)	164.3(3)
O(14)-Cd(2)-O(9)	92.9(3)
O(13)-Cd(2)-O(9)	85.6(3)
O(10)-Cd(2)-O(9)	52.7(2)
O(4)-Cd(2)-O(9)	82.7(2)
O(3)-Cd(2)-O(9)	87.4(3)
O(12)-Cd(2)-C(37)	99.5(3)
O(14)-Cd(2)-C(37)	27.4(3)
O(13)-Cd(2)-C(37)	28.5(3)
O(10)-Cd(2)-C(37)	108.4(3)
O(4)-Cd(2)-C(37)	117.3(3)
O(3)-Cd(2)-C(37)	171.2(3)
O(9)-Cd(2)-C(37)	89.0(3)
O(12)-Cd(2)-Cd(4)	82.4(2)
O(14)-Cd(2)-Cd(4)	119.2(2)
O(13)-Cd(2)-Cd(4)	167.49(19)
O(10)-Cd(2)-Cd(4)	42.08(15)
O(4)-Cd(2)-Cd(4)	95.20(17)
O(3)-Cd(2)-Cd(4)	41.99(18)
O(9)-Cd(2)-Cd(4)	83.18(17)
C(37)-Cd(2)-Cd(4)	145.3(2)
O(7)-Cd(3)-O(7)#1	180.0(3)

O(7)-Cd(3)-O(16)#1	91.9(3)
O(7)#1-Cd(3)-O(16)#1	88.1(3)
O(7)-Cd(3)-O(16)	88.1(3)
O(7)#1-Cd(3)-O(16)	91.9(3)
O(16)#1-Cd(3)-O(16)	180.0
O(7)-Cd(3)-O(6)	81.2(3)
O(7)#1-Cd(3)-O(6)	98.8(3)
O(16)#1-Cd(3)-O(6)	99.2(3)
O(16)-Cd(3)-O(6)	80.8(3)
O(7)-Cd(3)-O(6)#1	98.8(3)
O(7)#1-Cd(3)-O(6)#1	81.2(3)
O(16)#1-Cd(3)-O(6)#1	80.8(3)
O(16)-Cd(3)-O(6)#1	99.2(3)
O(6)-Cd(3)-O(6)#1	179.999(1)
O(7)-Cd(3)-Cd(1)	61.4(2)
O(7)#1-Cd(3)-Cd(1)	118.6(2)
O(16)#1-Cd(3)-Cd(1)	134.59(18)
O(16)-Cd(3)-Cd(1)	45.41(18)
O(6)-Cd(3)-Cd(1)	44.5(2)
O(6)#1-Cd(3)-Cd(1)	135.5(2)
O(7)-Cd(3)-Cd(1)#1	118.6(2)
O(7)#1-Cd(3)-Cd(1)#1	61.4(2)
O(16)#1-Cd(3)-Cd(1)#1	45.41(18)
O(16)-Cd(3)-Cd(1)#1	134.59(18)
O(6)-Cd(3)-Cd(1)#1	135.5(2)
O(6)#1-Cd(3)-Cd(1)#1	44.5(2)
Cd(1)-Cd(3)-Cd(1)#1	180.0
O(11)-Cd(4)-O(11)#2	179.999(1)
O(11)-Cd(4)-O(3)	88.0(3)
O(11)#2-Cd(4)-O(3)	92.0(3)
O(11)-Cd(4)-O(3)#2	92.0(3)
O(11)#2-Cd(4)-O(3)#2	88.0(3)
O(3)-Cd(4)-O(3)#2	180.00(16)
O(11)-Cd(4)-O(10)#2	98.7(3)
O(11)#2-Cd(4)-O(10)#2	81.3(3)
O(3)-Cd(4)-O(10)#2	98.4(3)
O(3)#2-Cd(4)-O(10)#2	81.6(3)
O(11)-Cd(4)-O(10)	81.3(3)

O(11)#2-Cd(4)-O(10)	98.7(3)
O(3)-Cd(4)-O(10)	81.6(3)
O(3)#2-Cd(4)-O(10)	98.4(3)
O(10)#2-Cd(4)-O(10)	179.999(2)
O(11)-Cd(4)-Cd(2)#2	119.3(2)
O(11)#2-Cd(4)-Cd(2)#2	60.7(2)
O(3)-Cd(4)-Cd(2)#2	133.7(2)
O(3)#2-Cd(4)-Cd(2)#2	46.3(2)
O(10)#2-Cd(4)-Cd(2)#2	44.72(18)
O(10)-Cd(4)-Cd(2)#2	135.29(18)
O(11)-Cd(4)-Cd(2)	60.7(2)
O(11)#2-Cd(4)-Cd(2)	119.3(2)
O(3)-Cd(4)-Cd(2)	46.3(2)
O(3)#2-Cd(4)-Cd(2)	133.7(2)
O(10)#2-Cd(4)-Cd(2)	135.28(18)
O(10)-Cd(4)-Cd(2)	44.71(18)
Cd(2)#2-Cd(4)-Cd(2)	180.0
O(1)-C(1)-O(2)	122.0(10)
O(1)-C(1)-C(2)	118.5(10)
O(2)-C(1)-C(2)	119.5(10)
O(1)-C(1)-Cd(1)	60.4(6)
O(2)-C(1)-Cd(1)	61.7(5)
C(2)-C(1)-Cd(1)	175.8(7)
C(7)-C(2)-C(3)	120.3(10)
C(7)-C(2)-C(1)	118.6(10)
C(3)-C(2)-C(1)	121.1(10)
C(4)-C(3)-C(2)	118.6(10)
C(4)-C(3)-H(3)	120.7
C(2)-C(3)-H(3)	120.7
C(3)-C(4)-C(5)	120.5(9)
C(3)-C(4)-C(8)	118.8(10)
C(5)-C(4)-C(8)	120.6(9)
C(6)-C(5)-C(4)	120.6(9)
C(6)-C(5)-H(5)	119.7
C(4)-C(5)-H(5)	119.7
C(5)-C(6)-C(7)	118.9(10)
C(5)-C(6)-C(9)	120.3(10)
C(7)-C(6)-C(9)	120.8(10)

C(2)-C(7)-C(6)	120.9(11)
C(2)-C(7)-H(7)	119.5
C(6)-C(7)-H(7)	119.5
O(4)-C(8)-O(3)	121.2(10)
O(4)-C(8)-C(4)	123.0(9)
O(3)-C(8)-C(4)	115.7(10)
C(10)-C(9)-C(12)	109.9(15)
C(10)-C(9)-C(11)	104.2(15)
C(12)-C(9)-C(11)	107.3(16)
C(10)-C(9)-C(6)	116.2(12)
C(12)-C(9)-C(6)	108.3(14)
C(11)-C(9)-C(6)	110.7(15)
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
O(5)-C(13)-O(6)	122.4(10)
O(5)-C(13)-C(14)	117.3(9)
O(6)-C(13)-C(14)	120.2(10)
C(15)-C(14)-C(19)	119.5(10)
C(15)-C(14)-C(13)	122.9(10)
C(19)-C(14)-C(13)	117.5(9)
C(16)-C(15)-C(14)	120.8(10)
C(16)-C(15)-H(15)	119.6

C(14)-C(15)-H(15)	119.6
C(15)-C(16)-C(17)	118.5(10)
C(15)-C(16)-C(20)#3	123.1(10)
C(17)-C(16)-C(20)#3	118.5(10)
C(18)-C(17)-C(16)	124.2(11)
C(18)-C(17)-H(17)	117.9
C(16)-C(17)-H(17)	117.9
C(17)-C(18)-C(19)	116.3(11)
C(17)-C(18)-C(22)	123.6(12)
C(19)-C(18)-C(22)	120.0(11)
C(18)-C(19)-C(14)	120.5(10)
C(18)-C(19)-H(19)	119.7
C(14)-C(19)-H(19)	119.7
O(7)-C(20)-O(8)	123.8(10)
O(7)-C(20)-C(16)#4	116.1(10)
O(8)-C(20)-C(16)#4	120.1(10)
C(22)-C(21)-H(21A)	109.5
C(22)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(22)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
O(9)-C(25)-O(10)	124.4(11)
O(9)-C(25)-C(26)	117.6(10)
O(10)-C(25)-C(26)	117.9(10)
C(27)-C(26)-C(31)	121.3(11)

C(27)-C(26)-C(25)	120.6(10)
C(31)-C(26)-C(25)	118.1(10)
C(26)-C(27)-C(28)	120.4(11)
C(26)-C(27)-H(27)	119.8
C(28)-C(27)-H(27)	119.8
C(27)-C(28)-C(29)	118.6(10)
C(27)-C(28)-C(32)#3	124.1(10)
C(29)-C(28)-C(32)#3	117.3(10)
C(30)-C(29)-C(28)	122.2(11)
C(30)-C(29)-H(29)	118.9
C(28)-C(29)-H(29)	118.9
C(29)-C(30)-C(31)	117.7(11)
C(29)-C(30)-C(33)	119.2(12)
C(31)-C(30)-C(33)	123.1(11)
C(26)-C(31)-C(30)	119.6(10)
C(26)-C(31)-H(31)	120.2
C(30)-C(31)-H(31)	120.2
O(11)-C(32)-O(12)	124.1(11)
O(11)-C(32)-C(28)#4	116.0(10)
O(12)-C(32)-C(28)#4	119.8(11)
C(34)-C(33)-C(36)	118.0(17)
C(34)-C(33)-C(35)	105.7(16)
C(36)-C(33)-C(35)	98.5(17)
C(34)-C(33)-C(30)	114.6(18)
C(36)-C(33)-C(30)	112.0(16)
C(35)-C(33)-C(30)	105.7(15)
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5

C(33)-C(36)-H(36A)	109.5
C(33)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(33)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
O(14)-C(37)-O(13)	121.5(10)
O(14)-C(37)-C(38)	119.3(10)
O(13)-C(37)-C(38)	118.8(9)
O(14)-C(37)-Cd(2)	60.0(6)
O(13)-C(37)-Cd(2)	61.5(5)
C(38)-C(37)-Cd(2)	172.4(8)
C(39)-C(38)-C(41)#5	117.7(9)
C(39)-C(38)-C(37)	119.2(10)
C(41)#5-C(38)-C(37)	123.1(10)
C(38)-C(39)-C(40)	123.9(10)
C(38)-C(39)-H(39)	118.1
C(40)-C(39)-H(39)	118.1
C(39)-C(40)-C(43)#5	115.0(10)
C(39)-C(40)-C(45)	122.9(10)
C(43)#5-C(40)-C(45)	121.9(9)
C(42)-C(41)-C(38)#5	119.6(10)
C(42)-C(41)-H(41)	120.2
C(38)#5-C(41)-H(41)	120.2
C(43)-C(42)-C(41)	122.6(9)
C(43)-C(42)-C(44)	117.5(9)
C(41)-C(42)-C(44)	119.9(9)
C(42)-C(43)-C(40)#5	120.9(9)
C(42)-C(43)-H(43)	119.5
C(40)#5-C(43)-H(43)	119.5
O(15)-C(44)-O(16)	121.6(9)
O(15)-C(44)-C(42)	119.8(9)
O(16)-C(44)-C(42)	118.6(9)
C(48)-C(45)-C(47)	106.3(17)
C(48)-C(45)-C(40)	118.1(12)
C(47)-C(45)-C(40)	113.3(13)
C(48)-C(45)-C(46)	109.7(16)
C(47)-C(45)-C(46)	97(2)

C(40)-C(45)-C(46)	110.1(12)
C(45)-C(46)-H(46A)	109.5
C(45)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(45)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
C(45)-C(47)-H(47A)	109.5
C(45)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(45)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(45)-C(48)-H(48A)	109.5
C(45)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(45)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
N(1)-C(49)-H(49A)	109.5
N(1)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
N(1)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
N(2)-C(51)-H(51A)	109.5
N(2)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
N(2)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
N(2)-C(52)-H(52A)	109.5
N(2)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
N(2)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
O(17)-C(53)-N(3)	107(3)

O(17)-C(53)-H(53)	126.5
N(3)-C(53)-H(53)	126.5
N(3)-C(54)-H(54A)	109.5
N(3)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
N(3)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
N(3)-C(55)-H(55A)	109.5
N(3)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
N(3)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
N(4)-C(56)-H(56A)	109.5
N(4)-C(56)-H(56B)	109.5
H(56A)-C(56)-H(56B)	109.5
N(4)-C(56)-H(56C)	109.5
H(56A)-C(56)-H(56C)	109.5
H(56B)-C(56)-H(56C)	109.5
N(4)-C(57)-H(57A)	109.5
N(4)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5
N(4)-C(57)-H(57C)	109.5
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5
O(18)-C(58)-N(4)	123(4)
O(18)-C(58)-H(58)	118.5
N(4)-C(58)-H(58)	118.5
C(50)-N(1)-C(49)	110.9(19)
C(50)-N(1)-H(1A)	109.5
C(49)-N(1)-H(1A)	109.5
C(50)-N(1)-H(1B)	109.5
C(49)-N(1)-H(1B)	109.5
H(1A)-N(1)-H(1B)	108.1
C(51)-N(2)-C(52)	107(2)
C(51)-N(2)-H(2A)	110.3
C(52)-N(2)-H(2A)	110.3

C(51)-N(2)-H(2B)	110.3
C(52)-N(2)-H(2B)	110.3
H(2A)-N(2)-H(2B)	108.6
C(53)-N(3)-C(54)	134(2)
C(53)-N(3)-C(55)	117(2)
C(54)-N(3)-C(55)	109(2)
C(58)-N(4)-C(56)	129(2)
C(58)-N(4)-C(57)	118(2)
C(56)-N(4)-C(57)	113(2)
C(1)-O(1)-Cd(1)	92.6(7)
C(1)-O(2)-Cd(1)	90.3(6)
C(8)-O(3)-Cd(4)	161.7(8)
C(8)-O(3)-Cd(2)	90.0(6)
Cd(4)-O(3)-Cd(2)	91.7(3)
C(8)-O(4)-Cd(2)	94.1(6)
C(13)-O(5)-Cd(1)	87.3(6)
C(13)-O(6)-Cd(3)	124.2(6)
C(13)-O(6)-Cd(1)	96.4(6)
Cd(3)-O(6)-Cd(1)	93.1(3)
C(20)-O(7)-Cd(3)	140.7(7)
C(20)-O(8)-Cd(1)	112.1(7)
C(25)-O(9)-Cd(2)	87.1(7)
C(25)-O(10)-Cd(4)	126.5(6)
C(25)-O(10)-Cd(2)	95.8(7)
Cd(4)-O(10)-Cd(2)	93.2(2)
C(32)-O(11)-Cd(4)	139.4(8)
C(32)-O(12)-Cd(2)	112.0(7)
C(37)-O(13)-Cd(2)	90.0(6)
C(37)-O(14)-Cd(2)	92.6(7)
C(44)-O(15)-Cd(1)	91.5(6)
C(44)-O(16)-Cd(3)	163.5(7)
C(44)-O(16)-Cd(1)	92.3(6)
Cd(3)-O(16)-Cd(1)	92.5(3)
N(1)-C(50)-H(50A)	109.5
N(1)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
N(1)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5

H(50B)-C(50)-H(50C)	109.5
C(21)-C(22)-C(24)	121.2(17)
C(21)-C(22)-C(23)	101.2(16)
C(24)-C(22)-C(23)	90.6(15)
C(21)-C(22)-C(18)	113.5(16)
C(24)-C(22)-C(18)	118.2(16)
C(23)-C(22)-C(18)	105.4(14)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z #2 -x+2,-y+1,-z+1 #3 x-1,y,z

#4 x+1,y,z #5 -x+2,-y+1,-z

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for compound **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cd(1)	41(1)	24(1)	24(1)	-6(1)	-8(1)	-2(1)
Cd(2)	43(1)	23(1)	24(1)	4(1)	-9(1)	-1(1)
Cd(3)	37(1)	21(1)	26(1)	-2(1)	-8(1)	2(1)
Cd(4)	40(1)	26(1)	22(1)	-2(1)	-8(1)	-3(1)
C(1)	52(6)	30(6)	32(6)	-9(5)	-13(5)	-3(5)
C(2)	48(6)	26(6)	34(6)	-9(5)	-8(5)	1(5)
C(3)	49(6)	30(6)	17(5)	-4(4)	-7(4)	0(5)
C(4)	33(5)	26(5)	31(6)	-2(4)	-6(4)	-3(4)
C(5)	54(6)	33(6)	17(5)	-10(4)	-7(4)	5(5)
C(6)	63(7)	30(6)	34(6)	-2(5)	-5(5)	-1(5)
C(7)	82(9)	30(6)	30(6)	-2(5)	-10(6)	-13(6)
C(8)	36(5)	21(5)	41(6)	-13(5)	-3(5)	2(4)
C(9)	168(13)	39(8)	24(7)	-1(6)	13(7)	-8(9)
C(10)	199(17)	89(12)	76(11)	17(10)	-14(12)	7(12)
C(11)	146(8)	146(8)	146(8)	0(1)	-18(1)	-6(1)
C(12)	190(18)	147(17)	154(17)	62(14)	31(15)	24(14)
C(13)	29(5)	43(7)	26(5)	-2(5)	-14(4)	0(5)
C(14)	22(5)	52(7)	24(5)	-7(5)	0(4)	-2(5)
C(15)	49(6)	29(6)	23(5)	-5(4)	-3(4)	0(5)
C(16)	35(5)	41(6)	23(5)	-3(5)	-11(4)	-4(5)
C(17)	46(6)	40(7)	41(7)	-8(5)	-11(5)	-6(5)
C(18)	33(5)	44(7)	38(6)	11(5)	2(5)	-9(5)
C(19)	32(5)	45(7)	35(6)	-2(5)	-5(4)	-3(5)
C(20)	54(7)	32(6)	28(6)	-9(5)	-17(5)	-7(5)
C(21)	135(5)	134(6)	135(6)	0(1)	-16(1)	-5(1)
C(23)	310(19)	73(12)	130(14)	-34(10)	5(16)	16(14)
C(24)	135(6)	135(6)	135(6)	0(1)	-17(1)	-5(1)
C(25)	49(6)	23(6)	45(7)	-6(5)	-12(5)	6(5)
C(26)	48(6)	26(6)	39(7)	2(5)	-9(5)	0(5)
C(27)	42(6)	18(5)	37(6)	6(4)	-13(5)	-6(4)
C(28)	49(6)	18(5)	40(6)	6(5)	-7(5)	-2(4)
C(29)	47(7)	41(7)	45(7)	5(6)	-1(5)	3(5)
C(30)	47(6)	31(6)	43(7)	-4(5)	-12(5)	2(5)

C(31)	44(6)	40(7)	49(7)	5(6)	-10(5)	-1(5)
C(32)	50(7)	28(6)	42(7)	3(5)	-8(5)	2(5)
C(33)	231(14)	68(10)	72(11)	-32(7)	-71(10)	-12(5)
C(34)	153(6)	154(6)	153(6)	0(1)	-19(1)	-6(1)
C(35)	159(6)	158(6)	159(6)	0(1)	-19(1)	-7(1)
C(36)	154(6)	155(6)	155(6)	-1(1)	-19(1)	-5(1)
C(37)	50(6)	41(7)	28(6)	5(5)	-17(5)	2(5)
C(38)	47(6)	29(6)	34(6)	8(5)	-12(5)	-4(5)
C(39)	97(10)	29(6)	21(6)	-2(5)	2(6)	22(6)
C(40)	50(6)	31(6)	27(6)	4(5)	-9(5)	6(5)
C(41)	43(6)	23(5)	25(5)	8(4)	-7(4)	-10(4)
C(42)	35(5)	29(6)	26(5)	5(4)	-14(4)	-3(4)
C(43)	56(7)	21(5)	33(6)	4(5)	-5(5)	-6(5)
C(44)	40(6)	34(6)	23(5)	13(5)	-2(4)	-5(5)
C(45)	88(10)	35(7)	40(7)	0(6)	-11(7)	-3(7)
C(46)	146(15)	103(13)	126(14)	-55(12)	16(12)	-60(12)
C(47)	240(30)	160(20)	180(30)	-130(20)	-130(20)	130(20)
C(48)	217(17)	69(11)	63(10)	-10(9)	-9(11)	-10(12)
C(49)	190(30)	310(50)	140(30)	50(30)	-80(20)	-50(30)
C(51)	200(40)	190(40)	240(50)	40(30)	-20(30)	20(30)
C(52)	340(60)	60(20)	720(140)	-100(40)	-20(70)	-60(30)
C(53)	450(60)	450(60)	440(60)	10(20)	-60(20)	-20(20)
C(54)	170(30)	300(50)	410(60)	260(50)	-190(40)	-150(30)
C(55)	590(110)	320(70)	300(60)	180(50)	280(70)	300(70)
C(56)	390(40)	380(40)	370(50)	0(20)	-40(20)	20(20)
C(57)	110(20)	610(100)	250(50)	-290(60)	-40(30)	20(40)
C(58)	150(30)	400(60)	180(30)	-220(40)	20(20)	0(40)
N(1)	132(16)	180(20)	138(19)	-30(17)	-63(14)	-31(16)
N(2)	260(40)	270(50)	320(50)	70(40)	-20(40)	130(40)
N(3)	320(40)	60(11)	125(17)	62(12)	-60(20)	-20(16)
N(4)	330(40)	220(30)	82(16)	-100(20)	70(20)	-70(30)
O(1)	163(11)	24(5)	33(5)	-5(4)	-17(5)	-19(5)
O(2)	86(6)	34(4)	22(4)	-5(3)	-8(4)	-5(4)
O(3)	76(6)	32(4)	28(4)	-10(3)	-9(4)	-6(4)
O(4)	58(5)	23(4)	31(4)	2(3)	-5(3)	-2(3)
O(5)	47(2)	35(4)	41(4)	-6(4)	-6(3)	-13(3)
O(6)	41(4)	41(4)	28(4)	-11(3)	-4(3)	2(3)
O(7)	43(4)	69(6)	54(5)	18(5)	-21(4)	-15(4)

O(8)	59(5)	67(6)	38(5)	-16(4)	-19(4)	-21(4)
O(9)	44(1)	48(5)	29(4)	-2(3)	3(3)	-4(3)
O(10)	39(4)	29(4)	34(4)	8(3)	-8(3)	-4(3)
O(11)	29(4)	52(5)	75(6)	-26(5)	-1(4)	-5(4)
O(12)	53(5)	43(5)	60(6)	-3(4)	0(4)	-14(4)
O(13)	69(5)	30(4)	31(4)	3(3)	-9(4)	3(4)
O(14)	123(8)	35(5)	27(5)	5(4)	-24(5)	-9(5)
O(15)	63(5)	21(4)	33(4)	-6(3)	-13(4)	-1(3)
O(16)	64(5)	30(4)	25(4)	-2(3)	-16(3)	9(4)
O(17)	230(20)	220(20)	230(20)	150(20)	-40(20)	51(19)
O(18)	190(20)	200(20)	340(40)	-140(30)	0(20)	76(19)
C(50)	180(30)	140(20)	91(17)	-6(16)	-40(16)	50(20)
C(22)	152(8)	40(8)	85(10)	10(7)	-20(7)	6(7)

Gas Sorption Data:

CO_2,195K				CH_4,195K				N_2,77K			
Adsorption				Adorption		Desorption		Adsorption		Desorption	
P	V_a	P	V_a	P	V_a	P	V_a	P	V_a	P	V_a
0.00206	0.0624	10.154	29.955	0.0976	0.0187	94.591	12.235	0.4502	0.0524	92.907	2.9463
0.00495	0.1864	14.342	32.939	0.2557	0.1024	89.627	12.235	0.6612	0.0541	88.698	2.3663
0.00775	0.3143	15.242	33.632	0.6488	0.3163	84.679	12.185	0.8552	0.055	86.609	2.2387
0.0104	0.4387	19.918	35.974	1.0499	0.5496	79.714	12.087	1.0491	0.0554	84.641	2.1605
0.01358	0.5759	20.211	36.192	2.2452	1.1155	74.734	11.984	2.0936	0.0925	83.598	2.0845
0.01645	0.7187	25.059	38.139	3.1201	1.4606	69.773	11.853	3.0591	0.0928	81.142	2.0296
0.01952	0.8612	30.138	39.988	4.3164	1.9552	64.788	11.72	4.0204	0.0928	76.396	1.8036
0.02271	0.9988	35.185	41.651	5.3175	2.4368	59.824	11.579	4.9818	0.114	71.593	1.6575
0.02627	1.1363	40.227	43.267	6.1516	2.7366	54.843	11.387	5.9473	0.1372	66.782	1.5425
0.03314	1.4098	45.05	44.555	7.1364	3.0539	49.875	11.187	6.8964	0.1639	61.98	1.4155
0.0373	1.5492	50.236	46.065	8.1455	3.3719	44.935	10.926	7.87	0.1852	57.177	1.2851
0.04533	1.8185	55.075	47.253	9.1547	3.673	39.779	10.585	8.8232	0.2065	52.382	1.1766
0.05282	2.0935	60.064	48.616	10.192	3.933	34.786	10.235	9.7887	0.2029	47.543	1.0811
0.06112	2.3587	65.115	49.829	14.945	4.8227	29.81	9.9088	12.347	0.2508	42.76	0.9606
0.06987	2.6327	70.077	51.138	15.344	4.9562	24.797	9.3908	14.763	0.2848	37.978	0.8244
0.0795	2.9069	75.111	52.512	20.3	5.7285	19.787	8.7424	17.15	0.329	33.175	0.7233
0.08527	3.0436	80.068	54.002	25.24	6.3432	14.782	7.9445	19.557	0.3661	28.389	0.6272
0.09559	3.3135	85.091	55.498	30.184	6.9474	9.9889	6.8535	24.352	0.4314	23.59	0.5384
0.1074	3.5777	90.219	57.43	35.193	7.5189	8.6094	6.3723	29.142	0.5179	18.808	0.4388
0.1395	4.1861	95.18	59.352	40.133	7.9283	7.6369	6.0661	33.97	0.5818	16.396	0.39
0.1705	4.7305			45.134	8.3358	6.644	5.7072	38.748	0.6639	14.009	0.3411
0.2022	5.2682	**Desorption**		50.127	8.7418	5.6186	5.2541	43.579	0.7745	11.61	0.3117
0.2585	6.0447	89.629	58.16	55.149	9.2103	4.6257	4.7997	48.337	0.8807	9.2143	0.2747
0.3168	6.7264	84.659	56.851	60.146	9.6233			53.01	0.9885		
0.3655	7.2735	79.669	55.571	65.167	10.078			57.78	1.091		
0.4062	7.7293	74.663	54.263	70.05	10.338			62.587	1.2418		
0.4821	8.4167	69.649	52.997	75.018	10.642			67.402	1.3625		
0.5545	9.0285	64.724	51.68	80.056	10.918			72.188	1.5253		
0.6081	9.473	59.816	50.23	85.073	11.239			77.003	1.6859		
0.7845	10.683	54.733	48.907	90.042	11.491			81.826	1.8653		
0.8243	10.976	49.722	47.576	95.027	11.836			84.332	1.9949		
1.0361	12.197	44.79	46.235	100.07	12.181			86.67	2.107		
1.8122	15.44	39.796	44.887					90.026	2.3451		
2.1054	16.543	34.619	43.255					91.97	2.603		
2.8794	18.844	29.629	41.532					94.389	3.4207		
3.1319	19.767	24.651	39.728					95.668	6.1573		
3.9995	21.732	19.784	37.702								
5.026	23.612	15.038	35.224								
6.0565	25.344	14.712	34.971								
7.1849	26.816	10.505	32.171								

8.2235	28.082	9.7551	31.358								
9.136	29.045	8.7897	30.451								

H_2,77K				CO_2,273K				CH_4,273K	
Adsorption		Desorption		Adsorption		Desorption		Adsorption	
P	Va	P	Va	P	Va	P	Va	P	Va
0.1138	-0.01	94.369	17.927	0.1911	0.05609	94.474	12.456	0.2475	0.00308
0.3644	0.0815	89.421	18.019	0.9693	0.2653	89.461	12.082	0.664	0.01451
0.5382	0.2063	84.473	18.025	1.7656	0.4921	84.48	11.688	1.0602	0.03393
0.7362	0.325	79.509	17.981	2.3556	0.6466	79.5	11.28	2.2388	0.08023
0.8817	0.5356	74.532	17.923	3.2834	0.8874	74.726	10.886	3.2479	0.1261
1.0958	0.7086	69.564	17.801	4.2763	1.1357	69.778	10.438	4.2244	0.1656
2.2013	1.4402	64.592	17.665	5.2814	1.3745	64.797	9.9687	5.2416	0.205
3.2145	2.1083	59.627	17.485	6.2865	1.608	59.829	9.4696	6.1083	0.2559
4.1911	3.1797	54.651	17.288	7.2957	1.833	54.861	8.9557	7.1093	0.2975
5.2287	3.8072	49.671	17.047	8.2967	2.0432	49.892	8.4214	8.1143	0.3379
6.246	4.4093	44.702	16.777	9.3058	2.2629	44.919	7.8646	9.1193	0.3902
7.133	4.8004	39.779	16.411	10.311	2.4593	39.52	7.1805	10.112	0.4488
8.2601	5.3357	34.627	15.905	15.235	3.3884	34.527	6.5299	15.097	0.6244
9.1675	5.6757	29.411	15.367	20.26	4.228	29.534	5.8537	20.109	0.788
10.352	6.0697	24.65	14.844	25.351	5.0281	24.582	5.12	25.078	0.9651
15.259	7.356	19.629	13.914	30.352	5.7557	19.621	4.319	30.086	1.1421
20.447	8.3911	14.75	12.926	35.41	6.4396	14.698	3.437	35.331	1.3149
25.37	9.3346	9.5948	11.398	40.411	7.1212	9.7819	2.4324	40.34	1.4807
30.131	10.186	8.5653	10.908	45.033	7.6583	8.6995	2.1956	45.345	1.6441
35.27	10.823			50.022	8.2129	7.7066	1.9471	50.35	1.8126
40.3	11.468			55.031	8.7686	6.6934	1.7093	55.346	1.9925
45.309	12.154			60.061	9.2934			60.351	2.1658
50.293	12.87			65.082	9.7937			65.36	2.3304
55.306	13.562			70.344	10.299			70.369	2.4893
60.181	13.984			75.377	10.765			75.386	2.6416
65.165	14.377			80.431	11.217			80.391	2.8086
70.288	15.192			85.453	11.652			85.391	2.9732
75.191	15.573			90.438	12.064			90.404	3.1332
80.176	15.97			95.52	12.475			95.421	3.3059
85.177	16.366			100.52	12.853			100.43	3.442
90.182	16.764								
95.182	17.188								
100.15	17.771								

		N_2,273K				H_2,273K			
Desorption		Adsorption		Desorption		Adsorption		Desorption	
P	Va	P	Va	P	Va	P	va	P	Va
94.445	3.3953	0.2347	0.0047	94.376	1.2525	0.284	-0.01493	94.423	1.4755
89.468	3.324	0.6478	0.0096	89.448	1.1805	0.7012	-0.00455	89.413	1.4729
84.504	3.2269	1.0528	0.0079	84.459	1.0999	1.0826	-0.02103	84.427	1.4587
79.512	3.1252	2.2562	0.0259	79.454	1.0294	2.2889	1.22E-04	79.429	1.4506
74.535	2.9647	3.2694	0.0433	74.469	0.9644	3.2983	0.01106	74.394	1.4252
69.531	2.8454	4.2583	0.0481	69.46	0.873	4.2873	0.02743	69.412	1.4085
64.55	2.681	5.2634	0.0507	64.447	0.7848	5.2682	0.06097	64.418	1.3873
59.558	2.5486	6.2563	0.0792	59.466	0.7218	6.2654	0.07109	59.461	1.3716
54.573	2.402	7.2655	0.0896	54.465	0.6508	7.2707	0.0909	54.443	1.3629
49.585	2.2476	8.2543	0.1107	49.5	0.5483	8.2597	0.1129	49.449	1.3372
44.6	2.0898	9.2879	0.1288	44.491	0.4836	9.2528	0.1372	44.467	1.3146
39.608	1.9275	10.256	0.1662	39.49	0.4526	10.246	0.1615	39.481	1.2919
34.64	1.7404	15.473	0.2308	34.505	0.374	15.484	0.2246	34.198	1.259
29.671	1.5477	20.458	0.2833	29.528	0.297	20.482	0.2867	29.269	1.2277
24.789	1.3625	25.455	0.3171	24.507	0.2525	25.488	0.3497	24.336	1.2017
19.776	1.1031	30.472	0.345	19.542	0.1818	30.486	0.4105	19.399	1.1808
14.893	0.8907	35.469	0.4118	14.525	0.1448	35.497	0.469	14.458	1.1651
9.7419	0.6487	40.462	0.4578	9.5483	0.0516	40.495	0.5339	9.4848	1.1451
8.9118	0.5904	45.468	0.4809	8.7589	0.0172				
7.8539	0.5029	50.477	0.5461	7.7497	-0.02				
6.9058	0.4518	55.466	0.63	6.7405	-0.03				
		60.483	0.6995						
		65.492	0.7674						
		70.489	0.8582						
		75.495	0.9399						
		80.516	1.0265						
		85.521	1.0881						
		90.502	1.1809						
		95.572	1.2386						
		100.57	1.3187						