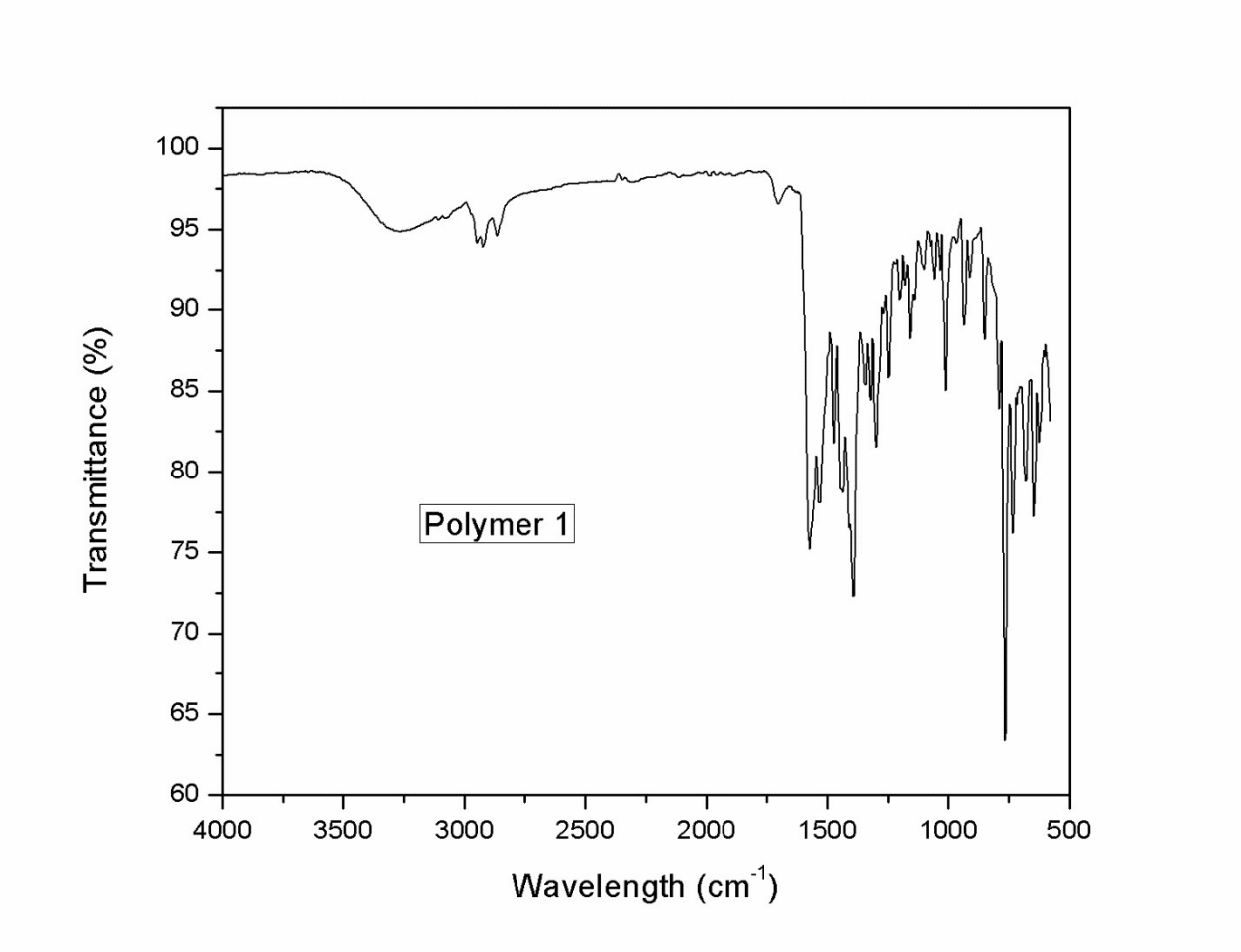


Figure S1. IR spectrum of **1**.

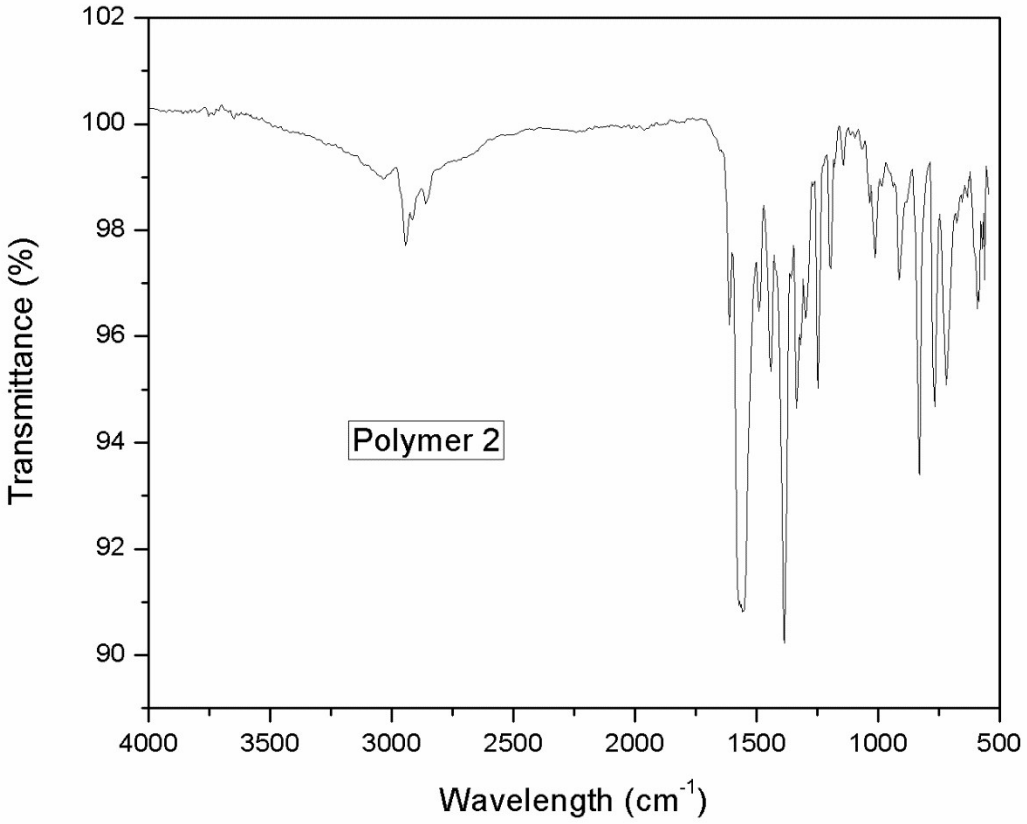


Figure S2. IR spectrum of **2**.

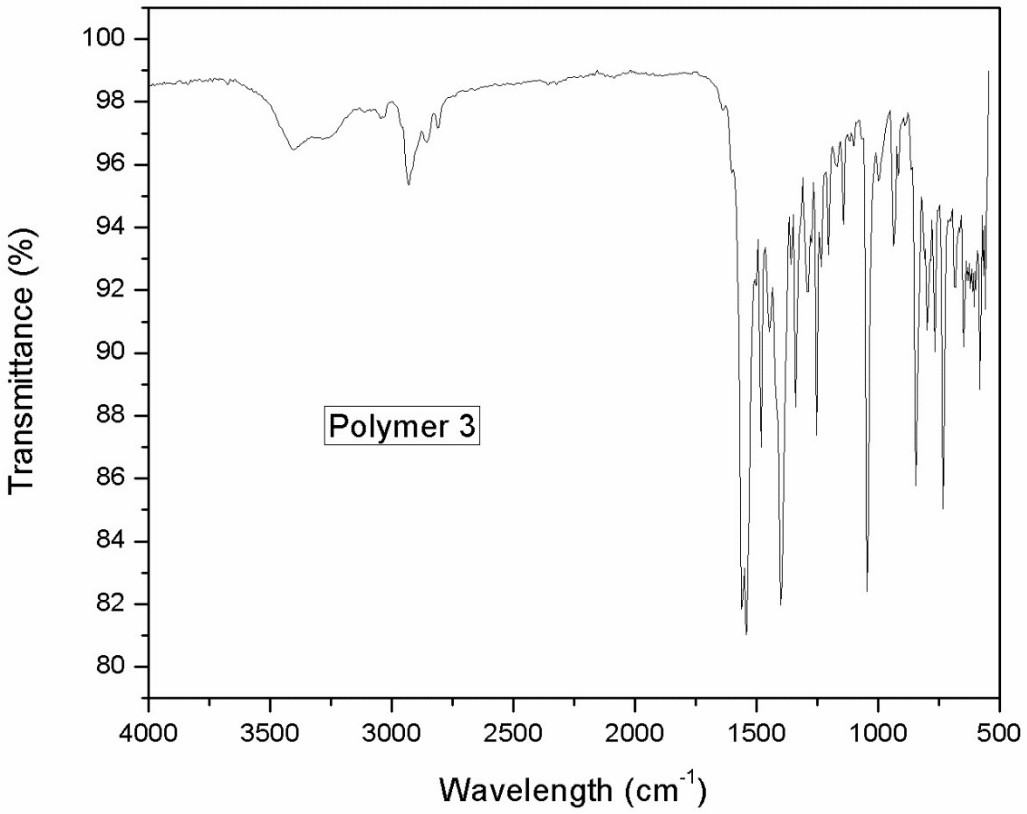


Figure S3. IR spectrum of **3**.

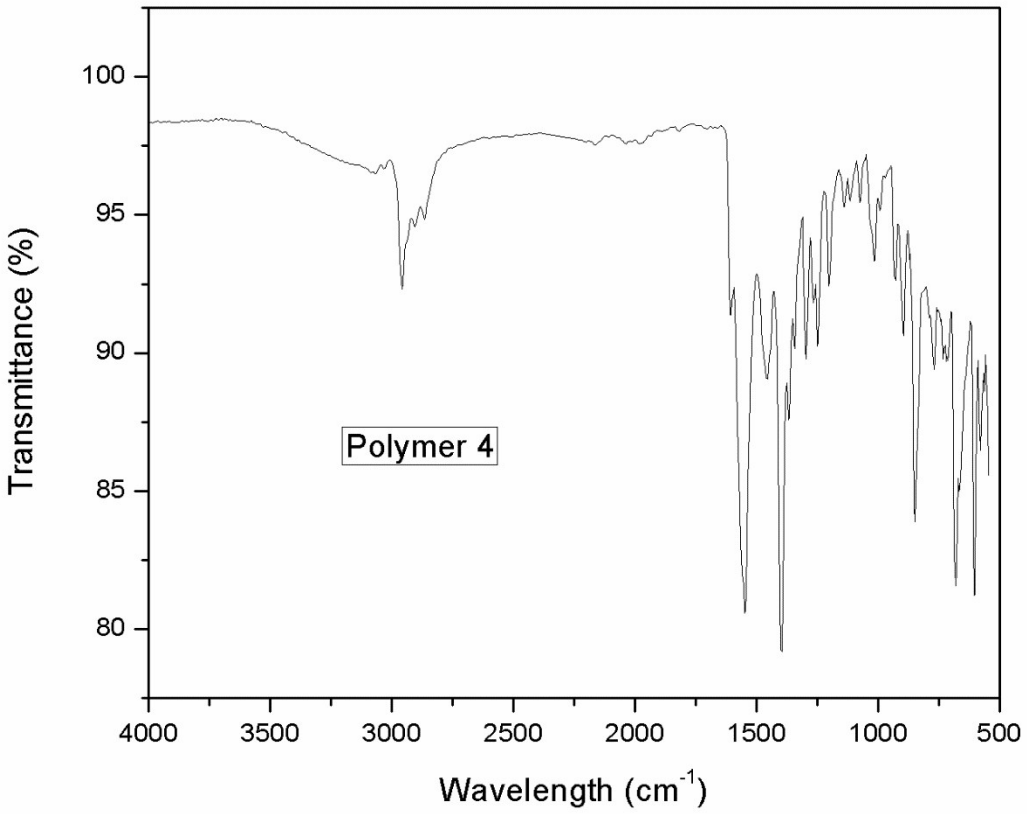


Figure S4. IR spectrum of **4**.

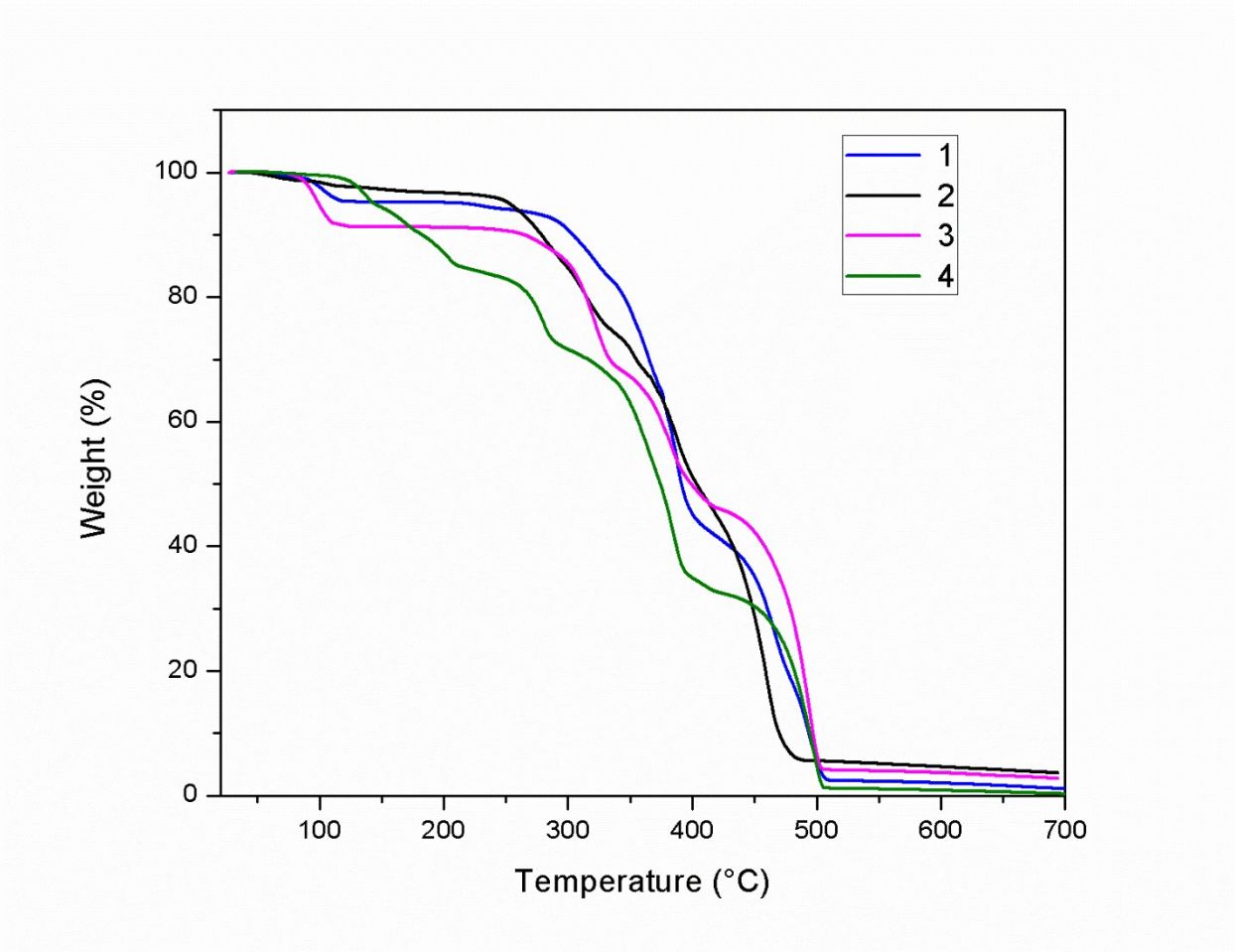


Figure S5. Thermogravimetric analyses for **1**-**4**.

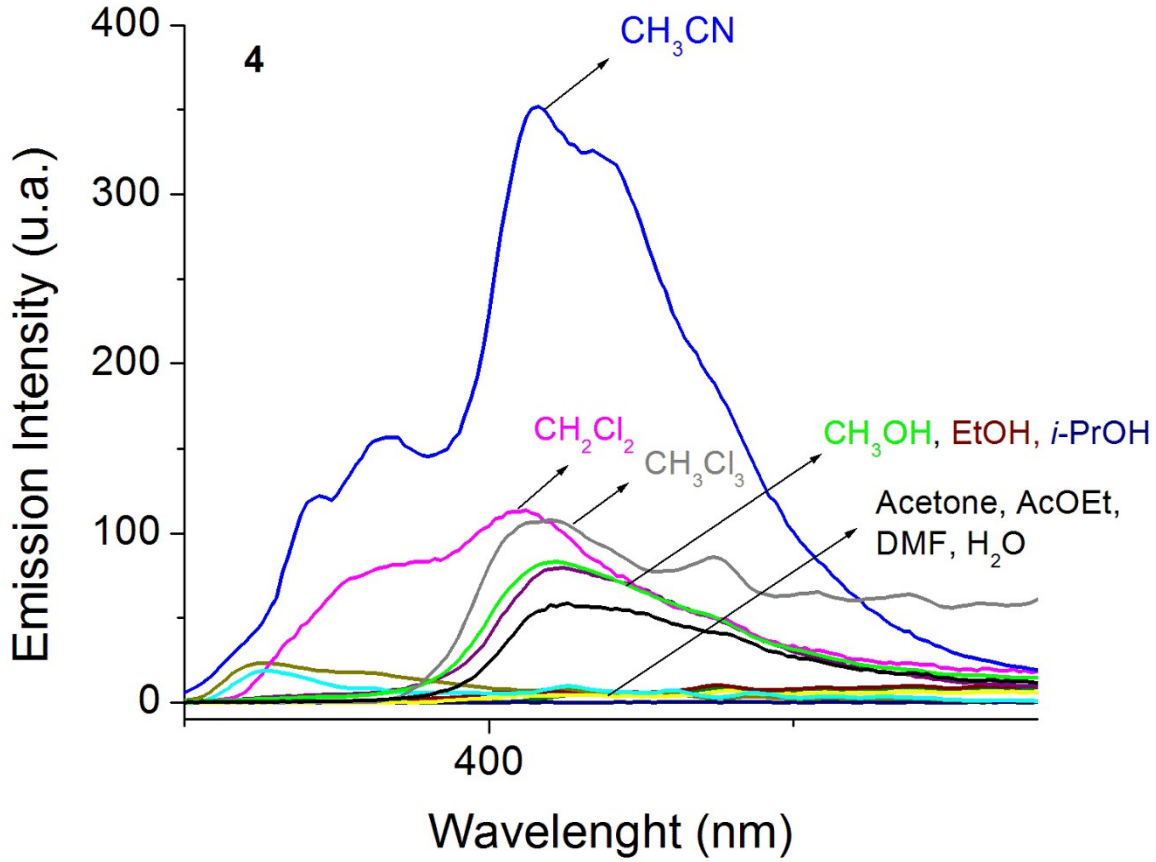


Figure S6. Emission spectra of **4** upon excitation at 345 nm at room temperature in different pure organic solvents and water.

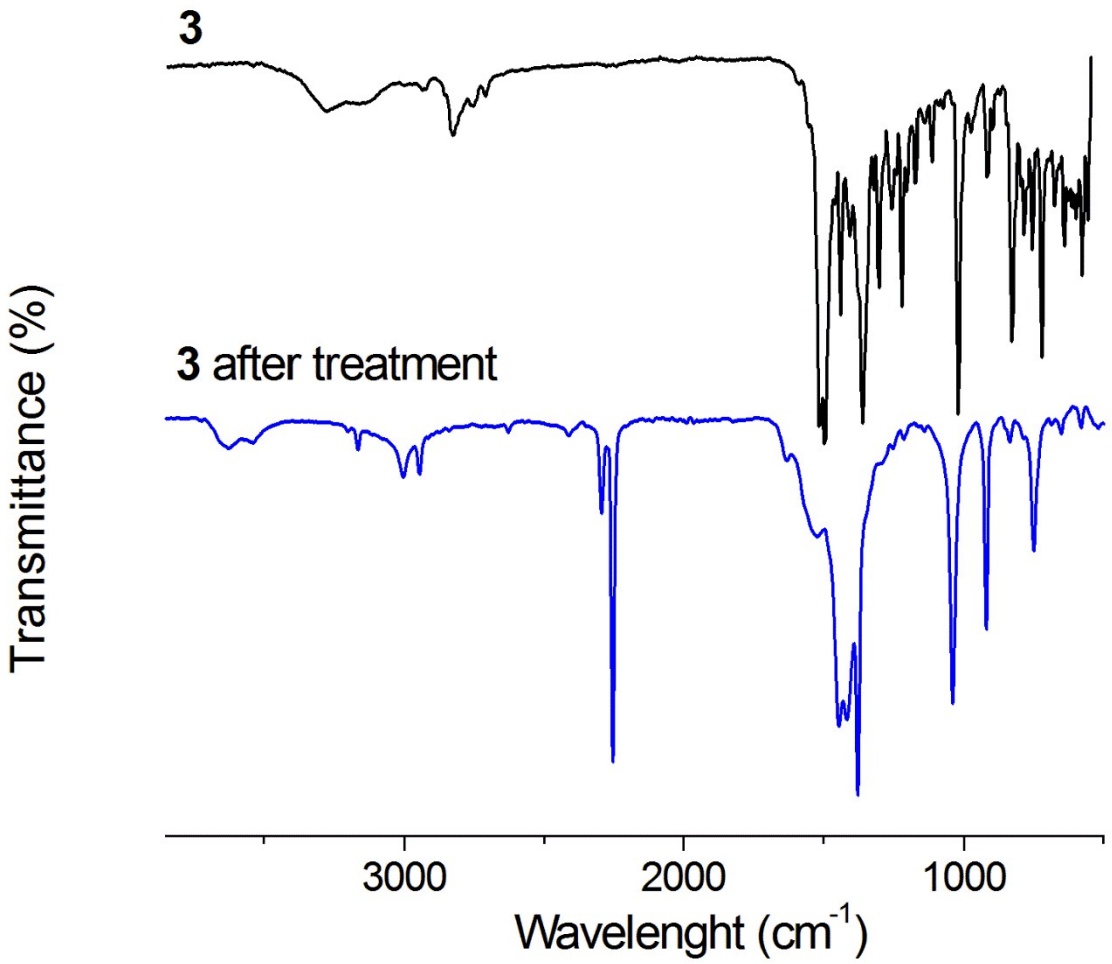
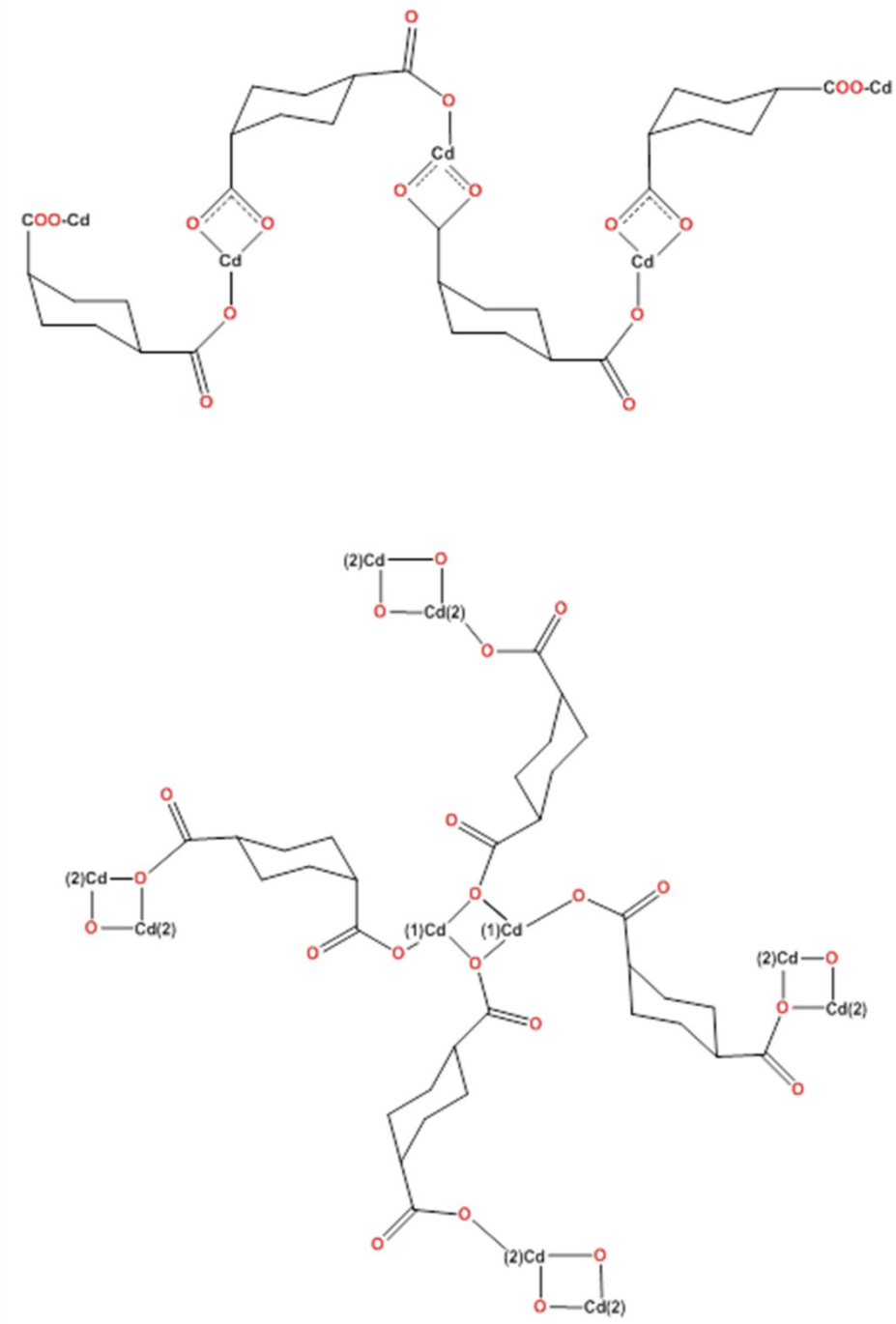
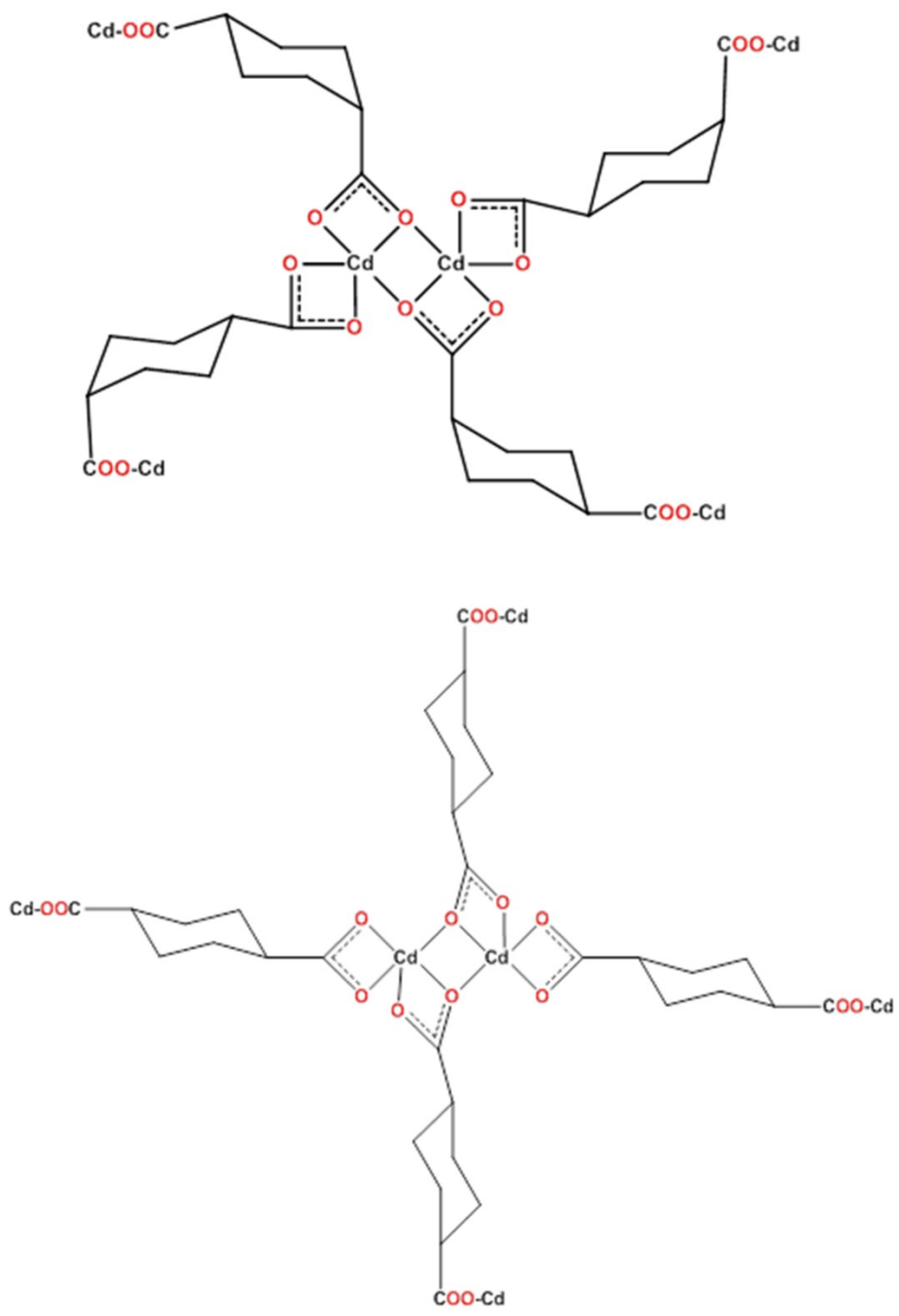


Figure S7. IR spectra of **3** before (black) and after treatment (blue) with CH_3CN.



Scheme S1. Coordination modes of 1,4-chdc in **1** and **2**.



Scheme S2. Coordination modes of 1,4-chdc in **3** and **4**.

Table S1. Crystallographic data for **1**.

Identification code	mo_091SMV15_0m	
Empirical formula	C18 H22 Cd N2 O6	
Formula weight	474.77	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 6.7908(3) Å	α= 90°.
	b = 18.9259(8) Å	β= 97.0738(11)°.
	c = 14.8220(7) Å	γ = 90°.
Volume	1890.45(15) $Å^3$	
Z	4	
Density (calculated)	1.668 Mg/m^3	
Absorption coefficient	1.192 mm^{-1}	
F(000)	960	
Crystal size	0.426 x 0.243 x 0.199 mm^3	
Theta range for data collection	2.152 to 26.371°.	
Index ranges	-8<=h<=7, -23<=k<=23, -18<=l<=18	
Reflections collected	16722	
Independent reflections	3867 [R(int) = 0.0169]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3867 / 558 / 380	
Goodness-of-fit on F^2	1.087	
Final R indices [I>2sigma(I)]	R1 = 0.0246, wR2 = 0.0660	
R indices (all data)	R1 = 0.0278, wR2 = 0.0684	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.684 and -0.480 $e.Å^{-3}$	

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for mo_091SMV15_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cd(1)	6806(1)	3521(1)	3438(1)	45(1)
O(1)	10047(3)	3389(1)	3126(1)	59(1)
N(1)	7007(3)	4693(1)	3949(1)	42(1)
N(2)	7796(3)	3560(1)	5033(1)	47(1)
C(1)	6621(4)	5244(1)	3388(2)	50(1)
C(2)	6649(4)	5935(1)	3687(2)	53(1)
C(3)	7112(3)	6064(1)	4595(2)	52(1)
C(4)	7529(3)	5506(1)	5179(2)	49(1)
C(5)	7473(3)	4819(1)	4845(2)	40(1)
C(6)	7871(3)	4193(1)	5441(2)	42(1)
C(7)	8270(3)	4249(2)	6381(2)	55(1)
C(8)	8567(4)	3645(2)	6899(2)	67(1)
C(9)	8486(4)	3006(2)	6481(2)	71(1)
C(10)	8105(4)	2981(2)	5543(2)	61(1)
C(11)	4585(19)	2317(5)	3685(13)	40(1)
O(2)	6394(12)	2284(6)	3574(4)	47(1)
O(3)	3802(19)	2912(5)	3831(6)	44(2)
C(12)	3390(15)	1644(5)	3772(6)	44(1)
C(13)	1807(11)	1714(5)	4414(5)	50(1)
C(14)	2683(8)	1729(3)	5419(4)	52(1)
C(15)	3905(8)	1061(2)	5652(3)	50(1)
C(16)	5514(9)	992(3)	5025(4)	52(1)
C(17)	4680(16)	989(5)	4019(5)	54(2)
C(18)	4651(9)	1062(2)	6673(3)	61(1)
O(4)	6346(8)	1297(2)	6900(3)	85(1)
O(5)	3547(8)	842(3)	7223(2)	92(1)
O(6)	179(10)	98(3)	6500(5)	138(2)
C(11A)	4560(30)	2391(9)	3640(20)	41(2)
O(2A)	6190(20)	2333(10)	3338(8)	45(2)
O(3A)	3720(30)	2980(10)	3639(11)	43(2)
C(12A)	3340(30)	1726(9)	3739(12)	46(2)

C(13A)	2140(19)	1797(9)	4555(8)	49(2)
C(14A)	3520(12)	1782(5)	5439(6)	44(2)
C(15A)	4871(12)	1117(4)	5542(5)	38(1)
C(16A)	6023(14)	1035(5)	4735(5)	41(2)
C(17A)	4640(30)	1061(9)	3826(8)	47(2)
C(18A)	6134(13)	1155(4)	6455(5)	47(1)
O(4A)	7974(9)	1200(4)	6487(4)	80(2)
O(5A)	5242(13)	1153(4)	7170(4)	65(2)
O(6A)	11606(10)	571(4)	7243(4)	73(2)

Bond lengths [Å] and angles [°] for mo_091SMV15_0m.

Cd(1)-O(5A)#1	2.134(7)
Cd(1)-O(2A)	2.29(2)
Cd(1)-O(4)#1	2.289(5)
Cd(1)-O(1)	2.3181(19)
Cd(1)-N(1)	2.3439(19)
Cd(1)-O(2)	2.368(11)
Cd(1)-N(2)	2.378(2)
Cd(1)-O(3A)	2.38(2)
Cd(1)-O(3)	2.473(13)
Cd(1)-C(11A)	2.664(17)
O(1)-H(1A)	0.771(16)
O(1)-H(1B)	0.863(17)
N(1)-C(1)	1.339(3)
N(1)-C(5)	1.348(3)
N(2)-C(10)	1.333(3)
N(2)-C(6)	1.340(3)
C(1)-C(2)	1.380(4)
C(1)-H(1)	0.9300
C(2)-C(3)	1.366(4)
C(2)-H(2)	0.9300
C(3)-C(4)	1.373(4)
C(3)-H(3)	0.9300
C(4)-C(5)	1.391(3)
C(4)-H(4)	0.9300
C(5)-C(6)	1.483(3)
C(6)-C(7)	1.391(3)
C(7)-C(8)	1.378(4)
C(7)-H(7)	0.9300
C(8)-C(9)	1.357(5)
C(8)-H(8)	0.9300
C(9)-C(10)	1.383(4)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-O(2)	1.261(8)

C(11)-O(3)	1.275(7)
C(11)-C(12)	1.523(7)
C(12)-C(13)	1.527(8)
C(12)-C(17)	1.537(7)
C(12)-H(12)	0.9800
C(13)-C(14)	1.535(7)
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(14)-C(15)	1.528(6)
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(15)-C(16)	1.525(7)
C(15)-C(18)	1.536(6)
C(15)-H(15)	0.9800
C(16)-C(17)	1.527(7)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-O(4)	1.241(8)
C(18)-O(5)	1.245(7)
O(4)-Cd(1)#2	2.289(5)
O(6)-H(6A)	0.831(16)
O(6)-H(6B)	0.861(19)
C(11A)-O(3A)	1.249(12)
C(11A)-O(2A)	1.250(12)
C(11A)-C(12A)	1.524(12)
C(12A)-C(17A)	1.534(12)
C(12A)-C(13A)	1.544(12)
C(12A)-H(12A)	0.9800
C(13A)-C(14A)	1.514(11)
C(13A)-H(13C)	0.9700
C(13A)-H(13D)	0.9700
C(14A)-C(15A)	1.555(10)
C(14A)-H(14C)	0.9700
C(14A)-H(14D)	0.9700

C(15A)-C(18A)	1.512(9)
C(15A)-C(16A)	1.516(9)
C(15A)-H(15A)	0.9800
C(16A)-C(17A)	1.545(11)
C(16A)-H(16C)	0.9700
C(16A)-H(16D)	0.9700
C(17A)-H(17C)	0.9700
C(17A)-H(17D)	0.9700
C(18A)-O(4A)	1.247(11)
C(18A)-O(5A)	1.283(11)
O(5A)-Cd(1)#2	2.134(7)
O(6A)-H(6C)	0.85(2)
O(6A)-H(6D)	0.969(17)

O(5A)#1-Cd(1)-O(2A)	99.2(3)
O(5A)#1-Cd(1)-O(1)	103.7(2)
O(2A)-Cd(1)-O(1)	92.9(4)
O(4)#1-Cd(1)-O(1)	80.42(16)
O(5A)#1-Cd(1)-N(1)	90.76(19)
O(2A)-Cd(1)-N(1)	162.6(3)
O(4)#1-Cd(1)-N(1)	100.05(13)
O(1)-Cd(1)-N(1)	98.47(7)
O(4)#1-Cd(1)-O(2)	103.4(2)
O(1)-Cd(1)-O(2)	92.0(2)
N(1)-Cd(1)-O(2)	155.63(18)
O(5A)#1-Cd(1)-N(2)	156.3(2)
O(2A)-Cd(1)-N(2)	97.0(3)
O(4)#1-Cd(1)-N(2)	166.55(14)
O(1)-Cd(1)-N(2)	92.44(7)
N(1)-Cd(1)-N(2)	69.55(7)
O(2)-Cd(1)-N(2)	88.18(17)
O(5A)#1-Cd(1)-O(3A)	83.4(4)
O(2A)-Cd(1)-O(3A)	55.2(5)
O(1)-Cd(1)-O(3A)	148.2(4)
N(1)-Cd(1)-O(3A)	112.6(4)
N(2)-Cd(1)-O(3A)	92.0(4)

O(4)#1-Cd(1)-O(3)	106.8(3)
O(1)-Cd(1)-O(3)	145.9(2)
N(1)-Cd(1)-O(3)	112.5(2)
O(2)-Cd(1)-O(3)	53.9(2)
N(2)-Cd(1)-O(3)	85.5(2)
O(5A)#1-Cd(1)-C(11A)	95.7(8)
O(2A)-Cd(1)-C(11A)	27.9(4)
O(1)-Cd(1)-C(11A)	120.5(4)
N(1)-Cd(1)-C(11A)	137.3(5)
N(2)-Cd(1)-C(11A)	90.6(8)
O(3A)-Cd(1)-C(11A)	28.0(3)
Cd(1)-O(1)-H(1A)	109(2)
Cd(1)-O(1)-H(1B)	137.4(19)
H(1A)-O(1)-H(1B)	113(3)
C(1)-N(1)-C(5)	118.6(2)
C(1)-N(1)-Cd(1)	122.48(15)
C(5)-N(1)-Cd(1)	118.89(15)
C(10)-N(2)-C(6)	118.9(2)
C(10)-N(2)-Cd(1)	122.92(18)
C(6)-N(2)-Cd(1)	117.86(15)
N(1)-C(1)-C(2)	123.0(2)
N(1)-C(1)-H(1)	118.5
C(2)-C(1)-H(1)	118.5
C(3)-C(2)-C(1)	118.6(2)
C(3)-C(2)-H(2)	120.7
C(1)-C(2)-H(2)	120.7
C(2)-C(3)-C(4)	119.2(2)
C(2)-C(3)-H(3)	120.4
C(4)-C(3)-H(3)	120.4
C(3)-C(4)-C(5)	120.1(2)
C(3)-C(4)-H(4)	120.0
C(5)-C(4)-H(4)	120.0
N(1)-C(5)-C(4)	120.6(2)
N(1)-C(5)-C(6)	116.7(2)
C(4)-C(5)-C(6)	122.8(2)
N(2)-C(6)-C(7)	120.8(2)

N(2)-C(6)-C(5)	116.87(19)
C(7)-C(6)-C(5)	122.3(2)
C(8)-C(7)-C(6)	119.4(3)
C(8)-C(7)-H(7)	120.3
C(6)-C(7)-H(7)	120.3
C(9)-C(8)-C(7)	119.4(3)
C(9)-C(8)-H(8)	120.3
C(7)-C(8)-H(8)	120.3
C(8)-C(9)-C(10)	118.7(3)
C(8)-C(9)-H(9)	120.6
C(10)-C(9)-H(9)	120.6
N(2)-C(10)-C(9)	122.6(3)
N(2)-C(10)-H(10)	118.7
C(9)-C(10)-H(10)	118.7
O(2)-C(11)-O(3)	119.9(9)
O(2)-C(11)-C(12)	120.5(7)
O(3)-C(11)-C(12)	119.1(8)
C(11)-O(2)-Cd(1)	95.1(6)
C(11)-O(3)-Cd(1)	89.9(7)
C(11)-C(12)-C(13)	113.8(7)
C(11)-C(12)-C(17)	113.6(7)
C(13)-C(12)-C(17)	110.2(7)
C(11)-C(12)-H(12)	106.2
C(13)-C(12)-H(12)	106.2
C(17)-C(12)-H(12)	106.2
C(12)-C(13)-C(14)	112.8(6)
C(12)-C(13)-H(13A)	109.0
C(14)-C(13)-H(13A)	109.0
C(12)-C(13)-H(13B)	109.0
C(14)-C(13)-H(13B)	109.0
H(13A)-C(13)-H(13B)	107.8
C(15)-C(14)-C(13)	109.8(5)
C(15)-C(14)-H(14A)	109.7
C(13)-C(14)-H(14A)	109.7
C(15)-C(14)-H(14B)	109.7
C(13)-C(14)-H(14B)	109.7

H(14A)-C(14)-H(14B)	108.2
C(16)-C(15)-C(14)	110.0(4)
C(16)-C(15)-C(18)	115.3(4)
C(14)-C(15)-C(18)	109.0(4)
C(16)-C(15)-H(15)	107.4
C(14)-C(15)-H(15)	107.4
C(18)-C(15)-H(15)	107.4
C(15)-C(16)-C(17)	112.8(5)
C(15)-C(16)-H(16A)	109.0
C(17)-C(16)-H(16A)	109.0
C(15)-C(16)-H(16B)	109.0
C(17)-C(16)-H(16B)	109.0
H(16A)-C(16)-H(16B)	107.8
C(16)-C(17)-C(12)	111.2(6)
C(16)-C(17)-H(17A)	109.4
C(12)-C(17)-H(17A)	109.4
C(16)-C(17)-H(17B)	109.4
C(12)-C(17)-H(17B)	109.4
H(17A)-C(17)-H(17B)	108.0
O(4)-C(18)-O(5)	123.8(6)
O(4)-C(18)-C(15)	116.7(6)
O(5)-C(18)-C(15)	119.5(5)
C(18)-O(4)-Cd(1)#2	109.4(5)
H(6A)-O(6)-H(6B)	109(3)
O(3A)-C(11A)-O(2A)	120.1(15)
O(3A)-C(11A)-C(12A)	119.0(14)
O(2A)-C(11A)-C(12A)	118.6(14)
O(3A)-C(11A)-Cd(1)	63.3(11)
O(2A)-C(11A)-Cd(1)	59.0(10)
C(12A)-C(11A)-Cd(1)	177.6(11)
C(11A)-O(2A)-Cd(1)	93.1(11)
C(11A)-O(3A)-Cd(1)	88.7(12)
C(11A)-C(12A)-C(17A)	111.9(12)
C(11A)-C(12A)-C(13A)	110.5(13)
C(17A)-C(12A)-C(13A)	111.1(12)
C(11A)-C(12A)-H(12A)	107.7

C(17A)-C(12A)-H(12A)	107.7
C(13A)-C(12A)-H(12A)	107.7
C(14A)-C(13A)-C(12A)	110.2(11)
C(14A)-C(13A)-H(13C)	109.6
C(12A)-C(13A)-H(13C)	109.6
C(14A)-C(13A)-H(13D)	109.6
C(12A)-C(13A)-H(13D)	109.6
H(13C)-C(13A)-H(13D)	108.1
C(13A)-C(14A)-C(15A)	113.3(8)
C(13A)-C(14A)-H(14C)	108.9
C(15A)-C(14A)-H(14C)	108.9
C(13A)-C(14A)-H(14D)	108.9
C(15A)-C(14A)-H(14D)	108.9
H(14C)-C(14A)-H(14D)	107.7
C(18A)-C(15A)-C(16A)	114.9(7)
C(18A)-C(15A)-C(14A)	108.2(6)
C(16A)-C(15A)-C(14A)	111.1(6)
C(18A)-C(15A)-H(15A)	107.5
C(16A)-C(15A)-H(15A)	107.5
C(14A)-C(15A)-H(15A)	107.5
C(15A)-C(16A)-C(17A)	111.6(9)
C(15A)-C(16A)-H(16C)	109.3
C(17A)-C(16A)-H(16C)	109.3
C(15A)-C(16A)-H(16D)	109.3
C(17A)-C(16A)-H(16D)	109.3
H(16C)-C(16A)-H(16D)	108.0
C(12A)-C(17A)-C(16A)	112.4(11)
C(12A)-C(17A)-H(17C)	109.1
C(16A)-C(17A)-H(17C)	109.1
C(12A)-C(17A)-H(17D)	109.1
C(16A)-C(17A)-H(17D)	109.1
H(17C)-C(17A)-H(17D)	107.8
O(4A)-C(18A)-O(5A)	122.8(8)
O(4A)-C(18A)-C(15A)	119.5(7)
O(5A)-C(18A)-C(15A)	117.7(8)
C(18A)-O(5A)-Cd(1)#2	119.5(7)

H(6C)-O(6A)-H(6D)	104(3)

Symmetry transformations used to generate equivalent atoms:

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

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_091SMV15_0m. 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)	46(1)	45(1)	45(1)	-8(1)	3(1)	1(1)
O(1)	43(1)	80(1)	53(1)	16(1)	1(1)	10(1)
N(1)	41(1)	47(1)	38(1)	-7(1)	3(1)	1(1)
N(2)	41(1)	53(1)	46(1)	2(1)	1(1)	-4(1)
C(1)	54(1)	53(1)	42(1)	-3(1)	4(1)	1(1)
C(2)	48(1)	48(1)	63(2)	1(1)	12(1)	1(1)
C(3)	44(1)	47(1)	68(2)	-15(1)	14(1)	-4(1)
C(4)	38(1)	60(2)	48(1)	-20(1)	6(1)	-7(1)
C(5)	25(1)	53(1)	42(1)	-8(1)	4(1)	-2(1)
C(6)	27(1)	60(1)	40(1)	-5(1)	3(1)	-4(1)
C(7)	41(1)	81(2)	42(1)	-6(1)	2(1)	-1(1)
C(8)	50(2)	106(3)	43(1)	8(2)	-1(1)	2(2)
C(9)	54(2)	90(2)	66(2)	31(2)	-2(1)	-1(2)
C(10)	56(2)	61(2)	64(2)	10(1)	-4(1)	-4(1)
C(11)	45(2)	44(3)	30(3)	-4(2)	-5(2)	4(2)
O(2)	46(2)	50(2)	45(3)	-2(3)	3(2)	5(2)
O(3)	43(2)	42(2)	43(4)	1(2)	-4(3)	6(2)
C(12)	52(2)	46(3)	32(2)	-2(2)	-10(2)	-8(2)
C(13)	56(3)	58(3)	35(2)	5(2)	-8(2)	-6(2)
C(14)	62(3)	50(2)	41(2)	4(2)	-5(2)	4(2)
C(15)	69(3)	39(2)	37(2)	-3(1)	-14(2)	-2(2)
C(16)	70(3)	36(2)	46(3)	-2(2)	-9(2)	4(2)
C(17)	74(3)	37(2)	46(3)	-7(2)	-6(3)	0(2)
C(18)	84(3)	46(2)	46(2)	-3(2)	-19(2)	7(2)
O(4)	105(3)	81(2)	58(3)	-5(2)	-37(2)	-8(2)
O(5)	124(4)	103(3)	45(2)	11(2)	-10(2)	0(3)
O(6)	134(5)	130(5)	140(5)	16(4)	-17(4)	-33(4)
C(11A)	45(3)	44(3)	31(4)	-3(3)	-3(3)	-4(3)
O(2A)	49(3)	51(3)	35(4)	0(4)	5(3)	8(3)
O(3A)	44(3)	47(4)	37(5)	7(3)	-1(4)	6(3)
C(12A)	54(3)	46(3)	35(3)	-1(3)	-6(3)	-1(3)

C(13A)	54(4)	52(4)	38(3)	3(3)	-1(3)	-11(3)
C(14A)	50(3)	49(3)	31(3)	0(2)	0(3)	-3(3)
C(15A)	52(3)	32(2)	29(2)	0(2)	0(2)	-4(3)
C(16A)	62(4)	31(3)	29(3)	0(2)	6(3)	1(3)
C(17A)	66(3)	41(3)	32(3)	-3(3)	-8(3)	-7(3)
C(18A)	76(3)	37(3)	25(3)	-5(2)	-9(3)	4(3)
O(4A)	69(3)	118(5)	46(3)	-10(3)	-18(2)	4(3)
O(5A)	96(4)	73(3)	25(3)	-6(2)	-2(3)	1(3)
O(6A)	89(4)	76(4)	57(3)	7(3)	24(3)	-2(3)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3})
for mo_091SMV15_0m.

	x	y	z	U(eq)
H(1A)	10240(40)	3646(15)	2742(18)	71
H(1B)	11120(40)	3189(16)	3374(18)	71
H(1)	6320	5157	2769	60
H(2)	6359	6305	3279	63
H(3)	7144	6525	4815	63
H(4)	7850	5588	5799	59
H(7)	8337	4691	6659	66
H(8)	8820	3675	7529	80
H(9)	8683	2592	6819	85
H(10)	8064	2543	5257	73
H(12)	2677	1553	3167	53
H(13A)	892	1320	4314	61
H(13B)	1060	2145	4271	61
H(14A)	3519	2142	5536	62
H(14B)	1620	1757	5799	62
H(15)	3011	656	5534	60
H(16A)	6245	558	5166	63
H(16B)	6437	1383	5138	63
H(17A)	3889	566	3886	64
H(17B)	5766	979	3652	64
H(6A)	1250(80)	260(30)	6740(70)	165
H(6B)	-550(100)	430(30)	6250(30)	165
H(12A)	2391	1677	3188	55
H(13C)	1405	2238	4508	58
H(13D)	1195	1412	4546	58
H(14C)	2734	1799	5942	52
H(14D)	4351	2201	5473	52
H(15A)	4004	704	5553	46
H(16C)	6725	588	4781	49
H(16D)	6998	1410	4745	49

H(17C)	5439	1048	3327	57
H(17D)	3794	647	3780	57
H(6C)	12560(80)	770(60)	7020(40)	87
H(6D)	10540(50)	580(20)	6740(30)	87

Torsion angles [°] for mo_091SMV15_0m.

C(5)-N(1)-C(1)-C(2)	-1.0(3)
Cd(1)-N(1)-C(1)-C(2)	177.03(18)
N(1)-C(1)-C(2)-C(3)	0.7(4)
C(1)-C(2)-C(3)-C(4)	-0.1(4)
C(2)-C(3)-C(4)-C(5)	-0.2(3)
C(1)-N(1)-C(5)-C(4)	0.6(3)
Cd(1)-N(1)-C(5)-C(4)	-177.43(15)
C(1)-N(1)-C(5)-C(6)	179.47(19)
Cd(1)-N(1)-C(5)-C(6)	1.4(2)
C(3)-C(4)-C(5)-N(1)	-0.1(3)
C(3)-C(4)-C(5)-C(6)	-178.8(2)
C(10)-N(2)-C(6)-C(7)	0.2(3)
Cd(1)-N(2)-C(6)-C(7)	174.38(16)
C(10)-N(2)-C(6)-C(5)	-178.7(2)
Cd(1)-N(2)-C(6)-C(5)	-4.5(2)
N(1)-C(5)-C(6)-N(2)	2.1(3)
C(4)-C(5)-C(6)-N(2)	-179.1(2)
N(1)-C(5)-C(6)-C(7)	-176.8(2)
C(4)-C(5)-C(6)-C(7)	2.0(3)
N(2)-C(6)-C(7)-C(8)	-0.9(3)
C(5)-C(6)-C(7)-C(8)	178.0(2)
C(6)-C(7)-C(8)-C(9)	0.7(4)
C(7)-C(8)-C(9)-C(10)	0.0(4)
C(6)-N(2)-C(10)-C(9)	0.5(4)
Cd(1)-N(2)-C(10)-C(9)	-173.3(2)
C(8)-C(9)-C(10)-N(2)	-0.6(4)
O(3)-C(11)-O(2)-Cd(1)	-11.1(15)
C(12)-C(11)-O(2)-Cd(1)	176.9(13)
O(2)-C(11)-O(3)-Cd(1)	10.6(14)
C(12)-C(11)-O(3)-Cd(1)	-177.3(14)
O(2)-C(11)-C(12)-C(13)	145.9(13)
O(3)-C(11)-C(12)-C(13)	-26.1(17)
O(2)-C(11)-C(12)-C(17)	18.7(18)
O(3)-C(11)-C(12)-C(17)	-153.3(12)

C(11)-C(12)-C(13)-C(14)	-73.6(11)
C(17)-C(12)-C(13)-C(14)	55.3(9)
C(12)-C(13)-C(14)-C(15)	-57.5(7)
C(13)-C(14)-C(15)-C(16)	56.4(6)
C(13)-C(14)-C(15)-C(18)	-176.2(5)
C(14)-C(15)-C(16)-C(17)	-56.7(6)
C(18)-C(15)-C(16)-C(17)	179.6(5)
C(15)-C(16)-C(17)-C(12)	55.0(8)
C(11)-C(12)-C(17)-C(16)	76.2(11)
C(13)-C(12)-C(17)-C(16)	-52.9(10)
C(16)-C(15)-C(18)-O(4)	28.9(6)
C(14)-C(15)-C(18)-O(4)	-95.3(6)
C(16)-C(15)-C(18)-O(5)	-152.0(5)
C(14)-C(15)-C(18)-O(5)	83.7(6)
O(5)-C(18)-O(4)-Cd(1)#2	-12.1(6)
C(15)-C(18)-O(4)-Cd(1)#2	166.9(3)
O(3A)-C(11A)-O(2A)-Cd(1)	18(3)
C(12A)-C(11A)-O(2A)-Cd(1)	-180(2)
O(2A)-C(11A)-O(3A)-Cd(1)	-17(3)
C(12A)-C(11A)-O(3A)-Cd(1)	-179(2)
O(3A)-C(11A)-C(12A)-C(17A)	-174(2)
O(2A)-C(11A)-C(12A)-C(17A)	23(3)
O(3A)-C(11A)-C(12A)-C(13A)	-49(3)
O(2A)-C(11A)-C(12A)-C(13A)	148(2)
C(11A)-C(12A)-C(13A)-C(14A)	-69.7(18)
C(17A)-C(12A)-C(13A)-C(14A)	55.1(16)
C(12A)-C(13A)-C(14A)-C(15A)	-55.2(13)
C(13A)-C(14A)-C(15A)-C(18A)	-178.6(8)
C(13A)-C(14A)-C(15A)-C(16A)	54.4(10)
C(18A)-C(15A)-C(16A)-C(17A)	-175.3(8)
C(14A)-C(15A)-C(16A)-C(17A)	-52.1(10)
C(11A)-C(12A)-C(17A)-C(16A)	69(2)
C(13A)-C(12A)-C(17A)-C(16A)	-55.0(17)
C(15A)-C(16A)-C(17A)-C(12A)	54.0(13)
C(16A)-C(15A)-C(18A)-O(4A)	8.2(10)
C(14A)-C(15A)-C(18A)-O(4A)	-116.6(8)

C(16A)-C(15A)-C(18A)-O(5A)	-173.1(7)
C(14A)-C(15A)-C(18A)-O(5A)	62.1(9)
O(4A)-C(18A)-O(5A)-Cd(1)#2	15.0(10)
C(15A)-C(18A)-O(5A)-Cd(1)#2	-163.7(5)

Symmetry transformations used to generate equivalent atoms:

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

Hydrogen bonds for mo_091SMV15_0m [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1A)...O(5)#3	0.771(16)	2.65(3)	3.215(6)	132(3)
O(1)-H(1A)...O(4A)#1	0.771(16)	2.28(3)	2.765(5)	122(3)
O(1)-H(1A)...O(6A)#1	0.771(16)	1.94(2)	2.655(7)	153(3)
O(1)-H(1B)...O(3)#4	0.863(17)	1.93(2)	2.784(12)	168(3)
O(1)-H(1B)...O(3A)#4	0.863(17)	1.81(3)	2.63(2)	160(3)
O(6)-H(6A)...O(5)	0.831(16)	1.968(17)	2.786(7)	168(6)
O(6A)-H(6C)...O(5A)#4	0.85(2)	1.946(19)	2.718(11)	150(5)
O(6A)-H(6D)...O(4A)	0.969(17)	2.102(17)	2.842(9)	131.9(18)

Symmetry transformations used to generate equivalent atoms:

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

#4 x+1,y,z

Table S2. Crystallographic data for **2**.

Crystal data and structure refinement for mo_211GOI15_0m.		
Identification code	mo_211GOI15_0m	
Empirical formula	C40 H48 Cd2 N4 O10	
Formula weight	969.62	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.9591(4) Å	α= 89.2412(6)°.
	b = 11.3715(4) Å	β= 73.2173(5)°.
	c = 16.5949(5) Å	γ = 84.5276(6)°.
Volume	1970.75(12) $Å^3$	
Z	2	
Density (calculated)	1.634 Mg/m^3	
Absorption coefficient	1.142 mm^{-1}	
F(000)	984	
Crystal size	0.291 x 0.084 x 0.080 mm^3	
Theta range for data collection	1.282 to 27.446°.	
Index ranges	-14<=h<=14, -14<=k<=14, -21<=l<=21	
Reflections collected	40494	
Independent reflections	8998 [R(int) = 0.0323]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8998 / 6 / 525	
Goodness-of-fit on F^2	1.066	
Final R indices [I>2sigma(I)]	R1 = 0.0224, wR2 = 0.0529	
R indices (all data)	R1 = 0.0252, wR2 = 0.0544	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.187 and -1.091 $e.Å^{-3}$	

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for mo_211GOI15_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cd(1)	3682(1)	4273(1)	4780(1)	14(1)
Cd(2)	3602(1)	913(1)	9768(1)	13(1)
O(1)	4799(1)	2602(1)	4158(1)	18(1)
O(2)	3462(1)	1293(1)	4827(1)	22(1)
O(3)	2850(1)	992(1)	1928(1)	23(1)
O(4)	4498(1)	312(1)	849(1)	15(1)
O(5)	2236(1)	3132(1)	5709(1)	19(1)
O(6)	4642(1)	2421(1)	9193(1)	18(1)
O(7)	3293(1)	3892(1)	9929(1)	24(1)
O(8)	3114(1)	3912(2)	6898(1)	26(1)
O(9)	4525(1)	4742(1)	5853(1)	15(1)
O(10)	1996(1)	2127(1)	10737(1)	20(1)
N(1)	2363(2)	6068(2)	5003(1)	18(1)
N(2)	2284(2)	4326(1)	3946(1)	16(1)
N(3)	2195(2)	1101(1)	8885(1)	16(1)
N(4)	2441(2)	-693(1)	9921(1)	16(1)
C(1)	2428(2)	6906(2)	5548(1)	23(1)
C(2)	1510(2)	7858(2)	5791(1)	24(1)
C(3)	456(2)	7958(2)	5478(1)	19(1)
C(4)	410(2)	7104(2)	4894(1)	17(1)
C(5)	1375(2)	6175(2)	4667(1)	15(1)
C(6)	1379(2)	5242(2)	4034(1)	15(1)
C(7)	518(2)	5314(2)	3563(1)	18(1)
C(8)	581(2)	4427(2)	2971(1)	20(1)
C(9)	1512(2)	3483(2)	2897(1)	20(1)
C(10)	2331(2)	3466(2)	3391(1)	19(1)
C(11)	-600(2)	8936(2)	5776(1)	23(1)
C(12)	-310(2)	4483(2)	2430(2)	34(1)
C(13)	4472(2)	1555(2)	4303(1)	17(1)
C(14)	5414(2)	544(2)	3816(1)	18(1)
C(15)	6256(2)	922(2)	2960(1)	19(1)

C(16)	5484(2)	1175(2)	2335(1)	17(1)
C(17)	4739(2)	125(2)	2237(1)	17(1)
C(18)	3923(2)	-259(2)	3096(1)	18(1)
C(19)	4732(2)	-532(2)	3698(1)	20(1)
C(20)	3948(2)	501(2)	1641(1)	15(1)
C(21)	2092(2)	2014(2)	8381(1)	19(1)
C(22)	1228(2)	2113(2)	7918(1)	21(1)
C(23)	397(2)	1240(2)	7971(1)	18(1)
C(24)	497(2)	294(2)	8497(1)	18(1)
C(25)	1408(2)	245(2)	8940(1)	15(1)
C(26)	1588(2)	-774(2)	9484(1)	15(1)
C(27)	944(2)	-1777(2)	9518(1)	18(1)
C(28)	1191(2)	-2729(2)	10000(1)	20(1)
C(29)	2071(2)	-2628(2)	10446(1)	20(1)
C(30)	2673(2)	-1603(2)	10395(1)	18(1)
C(31)	-547(2)	1306(2)	7465(1)	26(1)
C(32)	550(2)	-3834(2)	10022(2)	28(1)
C(33)	4294(2)	3509(2)	9383(1)	16(1)
C(34)	5216(2)	4400(2)	8917(1)	16(1)
C(35)	4487(2)	5547(2)	8734(1)	19(1)
C(36)	3799(2)	5340(2)	8077(1)	18(1)
C(37)	4743(2)	4832(2)	7252(1)	16(1)
C(38)	5539(2)	3709(2)	7417(1)	17(1)
C(39)	6182(2)	3904(2)	8099(1)	17(1)
C(40)	4058(2)	4478(2)	6630(1)	16(1)

Bond lengths [Å] and angles [°] for mo_211GOI15_0m.

Cd(1)-O(1)	2.2478(13)
Cd(1)-O(9)	2.3188(13)
Cd(1)-O(9)#1	2.3269(13)
Cd(1)-N(2)	2.3399(16)
Cd(1)-O(5)	2.3453(15)
Cd(1)-N(1)	2.3533(16)
Cd(2)-O(6)	2.2028(14)
Cd(2)-N(4)	2.2931(16)
Cd(2)-O(4)#2	2.3463(13)
Cd(2)-O(10)	2.3557(14)
Cd(2)-O(4)#3	2.3623(13)
Cd(2)-N(3)	2.4088(16)
O(1)-C(13)	1.277(2)
O(2)-C(13)	1.253(2)
O(3)-C(20)	1.240(2)
O(4)-C(20)	1.289(2)
O(4)-Cd(2)#4	2.3463(13)
O(4)-Cd(2)#3	2.3623(13)
O(5)-H(5A)	0.861(17)
O(5)-H(5B)	0.866(17)
O(6)-C(33)	1.275(2)
O(7)-C(33)	1.248(2)
O(8)-C(40)	1.239(2)
O(9)-C(40)	1.286(2)
O(9)-Cd(1)#1	2.3268(13)
O(10)-H(10A)	0.831(16)
O(10)-H(10B)	0.851(17)
N(1)-C(1)	1.343(3)
N(1)-C(5)	1.349(2)
N(2)-C(10)	1.338(2)
N(2)-C(6)	1.346(2)
N(3)-C(21)	1.342(3)
N(3)-C(25)	1.346(2)
N(4)-C(30)	1.342(3)

N(4)-C(26)	1.349(2)
C(1)-C(2)	1.384(3)
C(1)-H(1)	0.9500
C(2)-C(3)	1.392(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.395(3)
C(3)-C(11)	1.503(3)
C(4)-C(5)	1.394(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.502(3)
C(6)-C(7)	1.385(3)
C(7)-C(8)	1.401(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.389(3)
C(8)-C(12)	1.503(3)
C(9)-C(10)	1.379(3)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.536(3)
C(14)-C(19)	1.535(3)
C(14)-C(15)	1.536(3)
C(14)-H(14)	1.0000
C(15)-C(16)	1.526(3)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.545(3)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(20)	1.525(3)
C(17)-C(18)	1.532(3)

C(17)-H(17)	1.0000
C(18)-C(19)	1.528(3)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(21)-C(22)	1.378(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.396(3)
C(22)-H(22)	0.9500
C(23)-C(24)	1.392(3)
C(23)-C(31)	1.505(3)
C(24)-C(25)	1.397(3)
C(24)-H(24)	0.9500
C(25)-C(26)	1.492(3)
C(26)-C(27)	1.390(3)
C(27)-C(28)	1.390(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.388(3)
C(28)-C(32)	1.493(3)
C(29)-C(30)	1.383(3)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.539(3)
C(34)-C(39)	1.535(3)
C(34)-C(35)	1.537(3)
C(34)-H(34)	1.0000
C(35)-C(36)	1.525(3)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900

C(36)-C(37)	1.538(3)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-C(40)	1.519(3)
C(37)-C(38)	1.544(3)
C(37)-H(37)	1.0000
C(38)-C(39)	1.525(3)
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900

O(1)-Cd(1)-O(9)	106.99(5)
O(1)-Cd(1)-O(9)#1	87.89(5)
O(9)-Cd(1)-O(9)#1	73.97(5)
O(1)-Cd(1)-N(2)	93.01(5)
O(9)-Cd(1)-N(2)	159.65(5)
O(9)#1-Cd(1)-N(2)	111.40(5)
O(1)-Cd(1)-O(5)	89.28(5)
O(9)-Cd(1)-O(5)	90.27(5)
O(9)#1-Cd(1)-O(5)	162.38(5)
N(2)-Cd(1)-O(5)	86.12(5)
O(1)-Cd(1)-N(1)	161.08(6)
O(9)-Cd(1)-N(1)	90.79(5)
O(9)#1-Cd(1)-N(1)	90.96(5)
N(2)-Cd(1)-N(1)	69.87(6)
O(5)-Cd(1)-N(1)	97.23(5)
O(6)-Cd(2)-N(4)	160.70(6)
O(6)-Cd(2)-O(4)#2	104.64(5)
N(4)-Cd(2)-O(4)#2	92.82(5)
O(6)-Cd(2)-O(10)	93.06(5)
N(4)-Cd(2)-O(10)	95.20(5)
O(4)#2-Cd(2)-O(10)	89.77(5)
O(6)-Cd(2)-O(4)#3	87.41(5)
N(4)-Cd(2)-O(4)#3	90.11(5)
O(4)#2-Cd(2)-O(4)#3	72.57(5)

O(10)-Cd(2)-O(4)#3	161.82(5)
O(6)-Cd(2)-N(3)	93.42(5)
N(4)-Cd(2)-N(3)	69.88(6)
O(4)#2-Cd(2)-N(3)	161.61(5)
O(10)-Cd(2)-N(3)	85.78(5)
O(4)#3-Cd(2)-N(3)	112.35(5)
C(13)-O(1)-Cd(1)	126.41(12)
C(20)-O(4)-Cd(2)#4	124.99(12)
C(20)-O(4)-Cd(2)#3	127.00(12)
Cd(2)#4-O(4)-Cd(2)#3	107.43(5)
Cd(1)-O(5)-H(5A)	93(2)
Cd(1)-O(5)-H(5B)	92(2)
H(5A)-O(5)-H(5B)	108(2)
C(33)-O(6)-Cd(2)	126.16(12)
C(40)-O(9)-Cd(1)	124.64(12)
C(40)-O(9)-Cd(1)#1	129.33(12)
Cd(1)-O(9)-Cd(1)#1	106.03(5)
Cd(2)-O(10)-H(10A)	94(2)
Cd(2)-O(10)-H(10B)	94(2)
H(10A)-O(10)-H(10B)	112(2)
C(1)-N(1)-C(5)	118.39(17)
C(1)-N(1)-Cd(1)	122.93(14)
C(5)-N(1)-Cd(1)	117.87(12)
C(10)-N(2)-C(6)	118.40(17)
C(10)-N(2)-Cd(1)	122.50(13)
C(6)-N(2)-Cd(1)	119.09(12)
C(21)-N(3)-C(25)	118.04(17)
C(21)-N(3)-Cd(2)	125.20(13)
C(25)-N(3)-Cd(2)	116.67(13)
C(30)-N(4)-C(26)	119.09(17)
C(30)-N(4)-Cd(2)	120.39(13)
C(26)-N(4)-Cd(2)	120.33(13)
N(1)-C(1)-C(2)	122.72(19)
N(1)-C(1)-H(1)	118.6
C(2)-C(1)-H(1)	118.6
C(1)-C(2)-C(3)	119.71(19)

C(1)-C(2)-H(2)	120.1
C(3)-C(2)-H(2)	120.1
C(2)-C(3)-C(4)	117.39(18)
C(2)-C(3)-C(11)	120.84(18)
C(4)-C(3)-C(11)	121.75(18)
C(5)-C(4)-C(3)	119.99(18)
C(5)-C(4)-H(4)	120.0
C(3)-C(4)-H(4)	120.0
N(1)-C(5)-C(4)	121.73(17)
N(1)-C(5)-C(6)	116.19(16)
C(4)-C(5)-C(6)	122.08(17)
N(2)-C(6)-C(7)	121.60(17)
N(2)-C(6)-C(5)	115.79(17)
C(7)-C(6)-C(5)	122.61(17)
C(6)-C(7)-C(8)	120.12(18)
C(6)-C(7)-H(7)	119.9
C(8)-C(7)-H(7)	119.9
C(9)-C(8)-C(7)	117.30(18)
C(9)-C(8)-C(12)	120.71(19)
C(7)-C(8)-C(12)	121.99(19)
C(10)-C(9)-C(8)	119.37(18)
C(10)-C(9)-H(9)	120.3
C(8)-C(9)-H(9)	120.3
N(2)-C(10)-C(9)	123.19(18)
N(2)-C(10)-H(10)	118.4
C(9)-C(10)-H(10)	118.4
C(3)-C(11)-H(11A)	109.5
C(3)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(3)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(8)-C(12)-H(12A)	109.5
C(8)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(8)-C(12)-H(12C)	109.5

H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
O(2)-C(13)-O(1)	124.94(17)
O(2)-C(13)-C(14)	117.99(17)
O(1)-C(13)-C(14)	117.04(17)
C(19)-C(14)-C(15)	109.89(16)
C(19)-C(14)-C(13)	112.09(16)
C(15)-C(14)-C(13)	113.11(16)
C(19)-C(14)-H(14)	107.1
C(15)-C(14)-H(14)	107.1
C(13)-C(14)-H(14)	107.1
C(16)-C(15)-C(14)	111.65(16)
C(16)-C(15)-H(15A)	109.3
C(14)-C(15)-H(15A)	109.3
C(16)-C(15)-H(15B)	109.3
C(14)-C(15)-H(15B)	109.3
H(15A)-C(15)-H(15B)	108.0
C(15)-C(16)-C(17)	112.20(16)
C(15)-C(16)-H(16A)	109.2
C(17)-C(16)-H(16A)	109.2
C(15)-C(16)-H(16B)	109.2
C(17)-C(16)-H(16B)	109.2
H(16A)-C(16)-H(16B)	107.9
C(20)-C(17)-C(18)	112.89(16)
C(20)-C(17)-C(16)	107.60(16)
C(18)-C(17)-C(16)	110.75(15)
C(20)-C(17)-H(17)	108.5
C(18)-C(17)-H(17)	108.5
C(16)-C(17)-H(17)	108.5
C(19)-C(18)-C(17)	111.36(16)
C(19)-C(18)-H(18A)	109.4
C(17)-C(18)-H(18A)	109.4
C(19)-C(18)-H(18B)	109.4
C(17)-C(18)-H(18B)	109.4
H(18A)-C(18)-H(18B)	108.0
C(18)-C(19)-C(14)	111.01(16)

C(18)-C(19)-H(19A)	109.4
C(14)-C(19)-H(19A)	109.4
C(18)-C(19)-H(19B)	109.4
C(14)-C(19)-H(19B)	109.4
H(19A)-C(19)-H(19B)	108.0
O(3)-C(20)-O(4)	123.61(18)
O(3)-C(20)-C(17)	119.72(17)
O(4)-C(20)-C(17)	116.64(16)
N(3)-C(21)-C(22)	123.24(19)
N(3)-C(21)-H(21)	118.4
C(22)-C(21)-H(21)	118.4
C(21)-C(22)-C(23)	119.65(19)
C(21)-C(22)-H(22)	120.2
C(23)-C(22)-H(22)	120.2
C(24)-C(23)-C(22)	117.19(18)
C(24)-C(23)-C(31)	121.52(18)
C(22)-C(23)-C(31)	121.28(19)
C(23)-C(24)-C(25)	120.04(18)
C(23)-C(24)-H(24)	120.0
C(25)-C(24)-H(24)	120.0
N(3)-C(25)-C(24)	121.84(18)
N(3)-C(25)-C(26)	116.13(17)
C(24)-C(25)-C(26)	122.01(17)
N(4)-C(26)-C(27)	121.39(18)
N(4)-C(26)-C(25)	116.75(17)
C(27)-C(26)-C(25)	121.82(17)
C(26)-C(27)-C(28)	119.81(18)
C(26)-C(27)-H(27)	120.1
C(28)-C(27)-H(27)	120.1
C(29)-C(28)-C(27)	117.93(18)
C(29)-C(28)-C(32)	121.13(19)
C(27)-C(28)-C(32)	120.93(19)
C(30)-C(29)-C(28)	119.75(19)
C(30)-C(29)-H(29)	120.1
C(28)-C(29)-H(29)	120.1
N(4)-C(30)-C(29)	122.03(18)

N(4)-C(30)-H(30)	119.0
C(29)-C(30)-H(30)	119.0
C(23)-C(31)-H(31A)	109.5
C(23)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(23)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(28)-C(32)-H(32A)	109.5
C(28)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(28)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
O(7)-C(33)-O(6)	125.07(18)
O(7)-C(33)-C(34)	118.42(17)
O(6)-C(33)-C(34)	116.48(16)
C(39)-C(34)-C(35)	109.67(16)
C(39)-C(34)-C(33)	113.77(16)
C(35)-C(34)-C(33)	111.61(16)
C(39)-C(34)-H(34)	107.1
C(35)-C(34)-H(34)	107.1
C(33)-C(34)-H(34)	107.1
C(36)-C(35)-C(34)	111.29(16)
C(36)-C(35)-H(35A)	109.4
C(34)-C(35)-H(35A)	109.4
C(36)-C(35)-H(35B)	109.4
C(34)-C(35)-H(35B)	109.4
H(35A)-C(35)-H(35B)	108.0
C(35)-C(36)-C(37)	111.23(16)
C(35)-C(36)-H(36A)	109.4
C(37)-C(36)-H(36A)	109.4
C(35)-C(36)-H(36B)	109.4
C(37)-C(36)-H(36B)	109.4
H(36A)-C(36)-H(36B)	108.0
C(40)-C(37)-C(36)	111.96(16)

C(40)-C(37)-C(38)	106.53(15)
C(36)-C(37)-C(38)	111.01(15)
C(40)-C(37)-H(37)	109.1
C(36)-C(37)-H(37)	109.1
C(38)-C(37)-H(37)	109.1
C(39)-C(38)-C(37)	112.34(16)
C(39)-C(38)-H(38A)	109.1
C(37)-C(38)-H(38A)	109.1
C(39)-C(38)-H(38B)	109.1
C(37)-C(38)-H(38B)	109.1
H(38A)-C(38)-H(38B)	107.9
C(38)-C(39)-C(34)	111.89(16)
C(38)-C(39)-H(39A)	109.2
C(34)-C(39)-H(39A)	109.2
C(38)-C(39)-H(39B)	109.2
C(34)-C(39)-H(39B)	109.2
H(39A)-C(39)-H(39B)	107.9
O(8)-C(40)-O(9)	124.05(18)
O(8)-C(40)-C(37)	117.94(17)
O(9)-C(40)-C(37)	117.95(16)

Symmetry transformations used to generate equivalent atoms:

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

#4 x,y,z-1

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_211GOI15_0m. 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)	13(1)	17(1)	11(1)	-2(1)	-4(1)	0(1)
Cd(2)	13(1)	16(1)	11(1)	-1(1)	-4(1)	-3(1)
O(1)	19(1)	18(1)	18(1)	-4(1)	-4(1)	0(1)
O(2)	24(1)	22(1)	17(1)	-3(1)	-2(1)	-1(1)
O(3)	22(1)	31(1)	14(1)	-1(1)	-2(1)	8(1)
O(4)	16(1)	19(1)	10(1)	-2(1)	-4(1)	-1(1)
O(5)	18(1)	23(1)	15(1)	-4(1)	-4(1)	-2(1)
O(6)	20(1)	16(1)	18(1)	1(1)	-4(1)	-3(1)
O(7)	26(1)	21(1)	20(1)	-1(1)	1(1)	0(1)
O(8)	26(1)	40(1)	14(1)	2(1)	-6(1)	-17(1)
O(9)	17(1)	20(1)	9(1)	1(1)	-4(1)	-3(1)
O(10)	20(1)	24(1)	15(1)	-1(1)	-4(1)	-1(1)
N(1)	17(1)	20(1)	18(1)	-4(1)	-6(1)	-1(1)
N(2)	15(1)	19(1)	14(1)	-2(1)	-4(1)	-1(1)
N(3)	16(1)	19(1)	14(1)	-1(1)	-4(1)	-2(1)
N(4)	15(1)	19(1)	15(1)	-1(1)	-4(1)	-3(1)
C(1)	21(1)	27(1)	24(1)	-8(1)	-11(1)	-1(1)
C(2)	24(1)	24(1)	25(1)	-10(1)	-9(1)	-2(1)
C(3)	19(1)	19(1)	18(1)	-2(1)	-3(1)	-1(1)
C(4)	15(1)	19(1)	16(1)	-1(1)	-4(1)	-2(1)
C(5)	16(1)	17(1)	12(1)	-1(1)	-3(1)	-3(1)
C(6)	15(1)	17(1)	11(1)	0(1)	-2(1)	-2(1)
C(7)	18(1)	20(1)	17(1)	-2(1)	-6(1)	1(1)
C(8)	21(1)	23(1)	17(1)	-2(1)	-8(1)	0(1)
C(9)	22(1)	20(1)	17(1)	-5(1)	-5(1)	0(1)
C(10)	17(1)	19(1)	19(1)	-5(1)	-4(1)	1(1)
C(11)	23(1)	20(1)	26(1)	-7(1)	-7(1)	3(1)
C(12)	40(1)	34(1)	33(1)	-11(1)	-25(1)	8(1)
C(13)	20(1)	20(1)	12(1)	-4(1)	-9(1)	3(1)
C(14)	19(1)	20(1)	14(1)	-4(1)	-8(1)	5(1)
C(15)	16(1)	26(1)	16(1)	-5(1)	-5(1)	1(1)

C(16)	17(1)	22(1)	12(1)	-3(1)	-3(1)	-2(1)
C(17)	19(1)	20(1)	11(1)	-3(1)	-5(1)	2(1)
C(18)	23(1)	19(1)	13(1)	0(1)	-6(1)	-2(1)
C(19)	31(1)	17(1)	14(1)	-1(1)	-8(1)	2(1)
C(20)	17(1)	16(1)	12(1)	-2(1)	-4(1)	-3(1)
C(21)	18(1)	20(1)	19(1)	1(1)	-4(1)	-4(1)
C(22)	22(1)	21(1)	18(1)	4(1)	-5(1)	-2(1)
C(23)	17(1)	23(1)	15(1)	-2(1)	-5(1)	0(1)
C(24)	16(1)	21(1)	16(1)	-2(1)	-4(1)	-3(1)
C(25)	14(1)	17(1)	12(1)	-3(1)	-1(1)	-1(1)
C(26)	13(1)	19(1)	13(1)	-3(1)	-2(1)	-1(1)
C(27)	19(1)	21(1)	17(1)	-2(1)	-7(1)	-3(1)
C(28)	21(1)	19(1)	21(1)	-1(1)	-6(1)	-4(1)
C(29)	22(1)	17(1)	21(1)	2(1)	-7(1)	-1(1)
C(30)	17(1)	21(1)	17(1)	1(1)	-6(1)	-1(1)
C(31)	27(1)	30(1)	24(1)	4(1)	-15(1)	-4(1)
C(32)	38(1)	20(1)	34(1)	4(1)	-18(1)	-11(1)
C(33)	20(1)	18(1)	11(1)	1(1)	-8(1)	-3(1)
C(34)	22(1)	17(1)	12(1)	0(1)	-7(1)	-4(1)
C(35)	29(1)	16(1)	14(1)	-1(1)	-8(1)	-2(1)
C(36)	22(1)	19(1)	13(1)	-2(1)	-7(1)	0(1)
C(37)	19(1)	20(1)	10(1)	1(1)	-5(1)	-4(1)
C(38)	17(1)	21(1)	11(1)	-2(1)	-3(1)	-1(1)
C(39)	16(1)	21(1)	14(1)	2(1)	-4(1)	-4(1)
C(40)	17(1)	18(1)	13(1)	0(1)	-4(1)	-2(1)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3})
for mo_211GOI15_0m.

	x	y	z	U(eq)
H(5A)	2520(30)	3270(30)	6126(15)	54(10)
H(5B)	2640(30)	2477(19)	5470(17)	49(9)
H(10A)	2210(30)	1860(20)	11151(14)	46(9)
H(10B)	2330(30)	2760(20)	10560(20)	65(11)
H(1)	3133	6842	5776	28
H(2)	1599	8440	6170	29
H(4)	-279	7155	4652	20
H(7)	-116	5967	3641	22
H(9)	1583	2854	2510	24
H(10)	2959	2813	3336	23
H(11A)	-235	9698	5710	35
H(11B)	-1048	8823	6371	35
H(11C)	-1205	8924	5443	35
H(12A)	61	4908	1912	50
H(12B)	-1136	4899	2738	50
H(12C)	-438	3680	2286	50
H(14)	5998	284	4162	21
H(15A)	6657	1640	3038	23
H(15B)	6950	288	2728	23
H(16A)	6071	1352	1780	21
H(16B)	4871	1882	2529	21
H(17)	5371	-554	1972	20
H(18A)	3240	378	3342	22
H(18B)	3509	-970	3022	22
H(19A)	5376	-1207	3473	24
H(19B)	4175	-759	4251	24
H(21)	2643	2623	8342	23
H(22)	1197	2773	7565	25
H(24)	-54	-317	8555	21
H(27)	338	-1812	9212	22

H(29)	2260	-3260	10784	24
H(30)	3270	-1542	10706	22
H(31A)	-84	1271	6864	38
H(31B)	-1099	2050	7597	38
H(31C)	-1073	641	7607	38
H(32A)	37	-3775	9625	43
H(32B)	-9	-3943	10592	43
H(32C)	1199	-4511	9864	43
H(34)	5718	4612	9301	19
H(35A)	3854	5855	9260	23
H(35B)	5097	6148	8528	23
H(36A)	3358	6097	7962	21
H(36B)	3143	4785	8301	21
H(37)	5334	5440	6991	19
H(38A)	4973	3066	7588	20
H(38B)	6204	3457	6888	20
H(39A)	6842	4462	7894	21
H(39B)	6616	3145	8216	21

Torsion angles [°] for mo_211GOI15_0m.

C(5)-N(1)-C(1)-C(2)	1.4(3)
Cd(1)-N(1)-C(1)-C(2)	-168.03(17)
N(1)-C(1)-C(2)-C(3)	1.2(4)
C(1)-C(2)-C(3)-C(4)	-2.8(3)
C(1)-C(2)-C(3)-C(11)	175.7(2)
C(2)-C(3)-C(4)-C(5)	2.0(3)
C(11)-C(3)-C(4)-C(5)	-176.54(19)
C(1)-N(1)-C(5)-C(4)	-2.2(3)
Cd(1)-N(1)-C(5)-C(4)	167.73(14)
C(1)-N(1)-C(5)-C(6)	177.48(18)
Cd(1)-N(1)-C(5)-C(6)	-12.6(2)
C(3)-C(4)-C(5)-N(1)	0.5(3)
C(3)-C(4)-C(5)-C(6)	-179.17(18)
C(10)-N(2)-C(6)-C(7)	-0.6(3)
Cd(1)-N(2)-C(6)-C(7)	-179.42(14)
C(10)-N(2)-C(6)-C(5)	179.86(17)
Cd(1)-N(2)-C(6)-C(5)	1.1(2)
N(1)-C(5)-C(6)-N(2)	7.6(2)
C(4)-C(5)-C(6)-N(2)	-172.67(18)
N(1)-C(5)-C(6)-C(7)	-171.89(18)
C(4)-C(5)-C(6)-C(7)	7.8(3)
N(2)-C(6)-C(7)-C(8)	-0.6(3)
C(5)-C(6)-C(7)-C(8)	178.89(18)
C(6)-C(7)-C(8)-C(9)	1.3(3)
C(6)-C(7)-C(8)-C(12)	-178.4(2)
C(7)-C(8)-C(9)-C(10)	-0.9(3)
C(12)-C(8)-C(9)-C(10)	178.8(2)
C(6)-N(2)-C(10)-C(9)	1.1(3)
Cd(1)-N(2)-C(10)-C(9)	179.83(15)
C(8)-C(9)-C(10)-N(2)	-0.3(3)
Cd(1)-O(1)-C(13)-O(2)	-0.4(3)
Cd(1)-O(1)-C(13)-C(14)	-178.32(12)
O(2)-C(13)-C(14)-C(19)	29.2(2)
O(1)-C(13)-C(14)-C(19)	-152.69(17)

O(2)-C(13)-C(14)-C(15)	154.16(17)
O(1)-C(13)-C(14)-C(15)	-27.8(2)
C(19)-C(14)-C(15)-C(16)	56.1(2)
C(13)-C(14)-C(15)-C(16)	-70.0(2)
C(14)-C(15)-C(16)-C(17)	-54.3(2)
C(15)-C(16)-C(17)-C(20)	176.82(15)
C(15)-C(16)-C(17)-C(18)	53.0(2)
C(20)-C(17)-C(18)-C(19)	-175.34(16)
C(16)-C(17)-C(18)-C(19)	-54.6(2)
C(17)-C(18)-C(19)-C(14)	57.9(2)
C(15)-C(14)-C(19)-C(18)	-57.8(2)
C(13)-C(14)-C(19)-C(18)	68.9(2)
Cd(2)#4-O(4)-C(20)-O(3)	2.6(3)
Cd(2)#3-O(4)-C(20)-O(3)	-167.56(14)
Cd(2)#4-O(4)-C(20)-C(17)	-175.21(12)
Cd(2)#3-O(4)-C(20)-C(17)	14.7(2)
C(18)-C(17)-C(20)-O(3)	33.3(2)
C(16)-C(17)-C(20)-O(3)	-89.2(2)
C(18)-C(17)-C(20)-O(4)	-148.85(17)
C(16)-C(17)-C(20)-O(4)	88.64(19)
C(25)-N(3)-C(21)-C(22)	-0.3(3)
Cd(2)-N(3)-C(21)-C(22)	-176.63(15)
N(3)-C(21)-C(22)-C(23)	0.7(3)
C(21)-C(22)-C(23)-C(24)	-0.3(3)
C(21)-C(22)-C(23)-C(31)	-179.08(19)
C(22)-C(23)-C(24)-C(25)	-0.5(3)
C(31)-C(23)-C(24)-C(25)	178.32(18)
C(21)-N(3)-C(25)-C(24)	-0.5(3)
Cd(2)-N(3)-C(25)-C(24)	176.14(14)
C(21)-N(3)-C(25)-C(26)	177.93(16)
Cd(2)-N(3)-C(25)-C(26)	-5.4(2)
C(23)-C(24)-C(25)-N(3)	0.9(3)
C(23)-C(24)-C(25)-C(26)	-177.45(17)
C(30)-N(4)-C(26)-C(27)	0.2(3)
Cd(2)-N(4)-C(26)-C(27)	175.06(14)
C(30)-N(4)-C(26)-C(25)	-177.55(16)

Cd(2)-N(4)-C(26)-C(25)	-2.7(2)
N(3)-C(25)-C(26)-N(4)	5.4(2)
C(24)-C(25)-C(26)-N(4)	-176.15(17)
N(3)-C(25)-C(26)-C(27)	-172.31(17)
C(24)-C(25)-C(26)-C(27)	6.1(3)
N(4)-C(26)-C(27)-C(28)	-0.9(3)
C(25)-C(26)-C(27)-C(28)	176.71(17)
C(26)-C(27)-C(28)-C(29)	0.9(3)
C(26)-C(27)-C(28)-C(32)	-177.72(19)
C(27)-C(28)-C(29)-C(30)	-0.3(3)
C(32)-C(28)-C(29)-C(30)	178.4(2)
C(26)-N(4)-C(30)-C(29)	0.5(3)
Cd(2)-N(4)-C(30)-C(29)	-174.38(15)
C(28)-C(29)-C(30)-N(4)	-0.4(3)
Cd(2)-O(6)-C(33)-O(7)	-0.3(3)
Cd(2)-O(6)-C(33)-C(34)	177.45(12)
O(7)-C(33)-C(34)-C(39)	-162.78(17)
O(6)-C(33)-C(34)-C(39)	19.3(2)
O(7)-C(33)-C(34)-C(35)	-38.0(2)
O(6)-C(33)-C(34)-C(35)	144.05(17)
C(39)-C(34)-C(35)-C(36)	58.0(2)
C(33)-C(34)-C(35)-C(36)	-69.0(2)
C(34)-C(35)-C(36)-C(37)	-57.7(2)
C(35)-C(36)-C(37)-C(40)	172.87(16)
C(35)-C(36)-C(37)-C(38)	54.0(2)
C(40)-C(37)-C(38)-C(39)	-174.43(15)
C(36)-C(37)-C(38)-C(39)	-52.3(2)
C(37)-C(38)-C(39)-C(34)	54.0(2)
C(35)-C(34)-C(39)-C(38)	-56.0(2)
C(33)-C(34)-C(39)-C(38)	69.8(2)
Cd(1)-O(9)-C(40)-O(8)	1.9(3)
Cd(1)#1-O(9)-C(40)-O(8)	-177.42(14)
Cd(1)-O(9)-C(40)-C(37)	178.90(12)
Cd(1)#1-O(9)-C(40)-C(37)	-0.4(2)
C(36)-C(37)-C(40)-O(8)	-45.4(2)
C(38)-C(37)-C(40)-O(8)	76.1(2)

C(36)-C(37)-C(40)-O(9)	137.37(18)
C(38)-C(37)-C(40)-O(9)	-101.11(19)

Symmetry transformations used to generate equivalent atoms:

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

#4 x,y,z-1

Table S3. Crystallographic data for **3**.

Crystal data and structure refinement for mo_035GOI16_0m.

Identification code	mo_035GOI16_0m	
Empirical formula	C21 H28 Cd N2 O6	
Formula weight	516.85	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 10.5501(5) Å	α= 90°.
	b = 15.2993(7) Å	β= 93.3664(9)°.
	c = 13.2627(6) Å	γ = 90°.
Volume	2137.03(17) $Å^3$	
Z	4	
Density (calculated)	1.606 Mg/m^3	
Absorption coefficient	1.062 mm^{-1}	
F(000)	1056	
Crystal size	0.313 x 0.236 x 0.146 mm^3	
Theta range for data collection	1.934 to 27.444°.	
Index ranges	-13<=h<=13, -19<=k<=19, -17<=l<=17	
Reflections collected	23168	
Independent reflections	4877 [R(int) = 0.0235]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4877 / 5 / 283	
Goodness-of-fit on F^2	1.035	
Final R indices [I>2sigma(I)]	R1 = 0.0181, wR2 = 0.0430	
R indices (all data)	R1 = 0.0196, wR2 = 0.0438	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.419 and -0.245 $e.Å^{-3}$	

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)
for mo_035GOI16_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cd(01)	1423(1)	5677(1)	10377(1)	10(1)
O(1)	224(1)	5158(1)	9010(1)	14(1)
O(2)	2080(1)	5589(1)	8525(1)	16(1)
O(3)	814(1)	7895(1)	4906(1)	16(1)
O(4)	692(1)	8188(1)	6518(1)	19(1)
O(5)	1478(1)	6673(1)	3520(1)	27(1)
O(6)	3987(1)	6321(1)	3633(1)	36(1)
N(1)	3497(1)	6128(1)	10805(1)	13(1)
N(2)	2672(1)	4461(1)	10865(1)	13(1)
C(1)	3857(1)	6964(1)	10774(1)	16(1)
C(2)	5080(1)	7256(1)	11038(1)	16(1)
C(3)	5965(1)	6621(1)	11337(1)	17(1)
C(4)	5615(1)	5749(1)	11360(1)	16(1)
C(5)	4362(1)	5518(1)	11092(1)	12(1)
C(6)	3915(1)	4596(1)	11103(1)	12(1)
C(7)	4726(1)	3900(1)	11355(1)	15(1)
C(8)	4237(1)	3058(1)	11366(1)	17(1)
C(9)	2953(1)	2915(1)	11125(1)	16(1)
C(10)	2211(1)	3644(1)	10872(1)	14(1)
C(11)	5399(2)	8212(1)	10976(1)	21(1)
C(12)	2370(2)	2016(1)	11122(1)	22(1)
C(13)	547(1)	5059(1)	7234(1)	13(1)
C(14)	-714(1)	5521(1)	6938(1)	14(1)
C(15)	-521(1)	6507(1)	6813(1)	14(1)
C(16)	403(1)	6683(1)	5987(1)	14(1)
C(17)	1687(1)	6233(1)	6258(1)	14(1)
C(18)	1528(1)	5254(1)	6457(1)	15(1)
C(19)	1003(1)	5290(1)	8315(1)	11(1)
C(20)	632(1)	7650(1)	5802(1)	13(1)
C(21)	4081(2)	5417(1)	3773(1)	29(1)

Bond lengths [Å] and angles [°] for mo_035GOI16_0m.

Cd(01)-O(1)	2.2911(10)
Cd(01)-N(1)	2.3328(12)
Cd(01)-O(1)#1	2.3413(10)
Cd(01)-N(2)	2.3476(12)
Cd(01)-O(3)#2	2.3522(10)
Cd(01)-O(4)#2	2.4573(11)
Cd(01)-O(2)	2.5948(11)
O(1)-C(19)	1.2857(17)
O(1)-Cd(01)#1	2.3413(10)
O(2)-C(19)	1.2411(18)
O(3)-C(20)	1.2714(17)
O(3)-Cd(01)#3	2.3522(10)
O(4)-C(20)	1.2553(18)
O(4)-Cd(01)#3	2.4573(11)
O(5)-H(5A)	0.849(10)
O(5)-H(5B)	0.847(10)
O(6)-C(21)	1.398(2)
O(6)-H(6A)	0.856(16)
N(1)-C(1)	1.3348(19)
N(1)-C(5)	1.3451(18)
N(2)-C(10)	1.3415(18)
N(2)-C(6)	1.3468(18)
C(1)-C(2)	1.391(2)
C(1)-H(1)	0.9500
C(2)-C(3)	1.389(2)
C(2)-C(11)	1.504(2)
C(3)-C(4)	1.385(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.393(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.489(2)
C(6)-C(7)	1.393(2)
C(7)-C(8)	1.389(2)
C(7)-H(7)	0.9500

C(8)-C(9)	1.391(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.392(2)
C(9)-C(12)	1.507(2)
C(10)-H(10)	0.9500
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(19)	1.5264(19)
C(13)-C(18)	1.5322(19)
C(13)-C(14)	1.538(2)
C(13)-H(13)	1.0000
C(14)-C(15)	1.5323(19)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.5329(19)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(20)	1.5216(19)
C(16)-C(17)	1.543(2)
C(16)-H(16)	1.0000
C(17)-C(18)	1.5319(19)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800

O(1)-Cd(01)-N(1)	139.58(4)
O(1)-Cd(01)-O(1)#1	72.51(4)
N(1)-Cd(01)-O(1)#1	141.47(4)

O(1)-Cd(01)-N(2)	102.63(4)
N(1)-Cd(01)-N(2)	70.40(4)
O(1)#1-Cd(01)-N(2)	83.58(4)
O(1)-Cd(01)-O(3)#2	88.97(4)
N(1)-Cd(01)-O(3)#2	91.53(4)
O(1)#1-Cd(01)-O(3)#2	113.74(4)
N(2)-Cd(01)-O(3)#2	161.66(4)
O(1)-Cd(01)-O(4)#2	123.61(4)
N(1)-Cd(01)-O(4)#2	87.98(4)
O(1)#1-Cd(01)-O(4)#2	84.58(4)
N(2)-Cd(01)-O(4)#2	125.56(4)
O(3)#2-Cd(01)-O(4)#2	54.27(3)
O(1)-Cd(01)-O(2)	53.00(3)
N(1)-Cd(01)-O(2)	86.94(4)
O(1)#1-Cd(01)-O(2)	123.07(3)
N(2)-Cd(01)-O(2)	92.48(4)
O(3)#2-Cd(01)-O(2)	83.14(3)
O(4)#2-Cd(01)-O(2)	136.92(3)
C(19)-O(1)-Cd(01)	99.62(8)
C(19)-O(1)-Cd(01)#1	148.53(9)
Cd(01)-O(1)-Cd(01)#1	107.49(4)
C(19)-O(2)-Cd(01)	86.56(8)
C(20)-O(3)-Cd(01)#3	94.56(9)
C(20)-O(4)-Cd(01)#3	90.10(9)
H(5A)-O(5)-H(5B)	108.1(17)
C(21)-O(6)-H(6A)	106.8(17)
C(1)-N(1)-C(5)	118.97(13)
C(1)-N(1)-Cd(01)	122.73(10)
C(5)-N(1)-Cd(01)	118.30(9)
C(10)-N(2)-C(6)	119.25(13)
C(10)-N(2)-Cd(01)	122.85(10)
C(6)-N(2)-Cd(01)	117.83(9)
N(1)-C(1)-C(2)	124.15(14)
N(1)-C(1)-H(1)	117.9
C(2)-C(1)-H(1)	117.9
C(3)-C(2)-C(1)	116.45(14)

C(3)-C(2)-C(11)	123.16(14)
C(1)-C(2)-C(11)	120.38(14)
C(4)-C(3)-C(2)	120.26(14)
C(4)-C(3)-H(3)	119.9
C(2)-C(3)-H(3)	119.9
C(3)-C(4)-C(5)	119.29(14)
C(3)-C(4)-H(4)	120.4
C(5)-C(4)-H(4)	120.4
N(1)-C(5)-C(4)	120.87(13)
N(1)-C(5)-C(6)	116.81(13)
C(4)-C(5)-C(6)	122.32(13)
N(2)-C(6)-C(7)	121.03(13)
N(2)-C(6)-C(5)	116.56(12)
C(7)-C(6)-C(5)	122.40(13)
C(8)-C(7)-C(6)	119.25(14)
C(8)-C(7)-H(7)	120.4
C(6)-C(7)-H(7)	120.4
C(7)-C(8)-C(9)	119.98(14)
C(7)-C(8)-H(8)	120.0
C(9)-C(8)-H(8)	120.0
C(8)-C(9)-C(10)	117.16(14)
C(8)-C(9)-C(12)	122.41(14)
C(10)-C(9)-C(12)	120.43(14)
N(2)-C(10)-C(9)	123.31(14)
N(2)-C(10)-H(10)	118.3
C(9)-C(10)-H(10)	118.3
C(2)-C(11)-H(11A)	109.5
C(2)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(2)-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
C(19)-C(13)-C(18)	113.50(12)
C(19)-C(13)-C(14)	110.72(11)
C(18)-C(13)-C(14)	110.29(12)
C(19)-C(13)-H(13)	107.3
C(18)-C(13)-H(13)	107.3
C(14)-C(13)-H(13)	107.3
C(15)-C(14)-C(13)	111.23(12)
C(15)-C(14)-H(14A)	109.4
C(13)-C(14)-H(14A)	109.4
C(15)-C(14)-H(14B)	109.4
C(13)-C(14)-H(14B)	109.4
H(14A)-C(14)-H(14B)	108.0
C(14)-C(15)-C(16)	110.12(12)
C(14)-C(15)-H(15A)	109.6
C(16)-C(15)-H(15A)	109.6
C(14)-C(15)-H(15B)	109.6
C(16)-C(15)-H(15B)	109.6
H(15A)-C(15)-H(15B)	108.1
C(20)-C(16)-C(15)	113.50(12)
C(20)-C(16)-C(17)	109.00(12)
C(15)-C(16)-C(17)	110.01(11)
C(20)-C(16)-H(16)	108.1
C(15)-C(16)-H(16)	108.1
C(17)-C(16)-H(16)	108.1
C(18)-C(17)-C(16)	111.83(12)
C(18)-C(17)-H(17A)	109.2
C(16)-C(17)-H(17A)	109.2
C(18)-C(17)-H(17B)	109.2
C(16)-C(17)-H(17B)	109.2
H(17A)-C(17)-H(17B)	107.9
C(17)-C(18)-C(13)	113.06(11)
C(17)-C(18)-H(18A)	109.0
C(13)-C(18)-H(18A)	109.0
C(17)-C(18)-H(18B)	109.0

C(13)-C(18)-H(18B)	109.0
H(18A)-C(18)-H(18B)	107.8
O(2)-C(19)-O(1)	120.77(13)
O(2)-C(19)-C(13)	122.01(12)
O(1)-C(19)-C(13)	117.21(12)
O(4)-C(20)-O(3)	120.66(13)
O(4)-C(20)-C(16)	121.18(13)
O(3)-C(20)-C(16)	118.09(13)
O(6)-C(21)-H(21A)	109.5
O(6)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
O(6)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5

Symmetry transformations used to generate equivalent atoms:

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

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_035GOI16_0m. 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(01)	10(1)	8(1)	12(1)	1(1)	-1(1)	0(1)
O(1)	16(1)	14(1)	12(1)	0(1)	2(1)	-3(1)
O(2)	12(1)	18(1)	17(1)	0(1)	0(1)	0(1)
O(3)	21(1)	12(1)	14(1)	3(1)	1(1)	-2(1)
O(4)	29(1)	13(1)	16(1)	0(1)	2(1)	-1(1)
O(5)	41(1)	22(1)	18(1)	-4(1)	-2(1)	7(1)
O(6)	32(1)	22(1)	53(1)	2(1)	-5(1)	-6(1)
N(1)	13(1)	11(1)	15(1)	-1(1)	-1(1)	0(1)
N(2)	13(1)	12(1)	13(1)	0(1)	1(1)	0(1)
C(1)	15(1)	13(1)	20(1)	0(1)	-1(1)	2(1)
C(2)	17(1)	15(1)	14(1)	-1(1)	1(1)	-2(1)
C(3)	14(1)	19(1)	18(1)	-1(1)	0(1)	-4(1)
C(4)	14(1)	17(1)	16(1)	1(1)	-1(1)	2(1)
C(5)	13(1)	14(1)	10(1)	-1(1)	1(1)	1(1)
C(6)	14(1)	14(1)	10(1)	-1(1)	1(1)	-1(1)
C(7)	14(1)	17(1)	14(1)	-1(1)	0(1)	1(1)
C(8)	18(1)	14(1)	17(1)	1(1)	-1(1)	4(1)
C(9)	19(1)	12(1)	16(1)	1(1)	1(1)	1(1)
C(10)	13(1)	14(1)	16(1)	0(1)	1(1)	-1(1)
C(11)	21(1)	15(1)	26(1)	0(1)	-2(1)	-5(1)
C(12)	23(1)	12(1)	30(1)	2(1)	-2(1)	-1(1)
C(13)	16(1)	9(1)	12(1)	1(1)	1(1)	-2(1)
C(14)	14(1)	16(1)	13(1)	2(1)	-2(1)	-3(1)
C(15)	12(1)	15(1)	16(1)	3(1)	1(1)	2(1)
C(16)	16(1)	11(1)	14(1)	1(1)	0(1)	0(1)
C(17)	15(1)	12(1)	16(1)	2(1)	4(1)	1(1)
C(18)	20(1)	11(1)	14(1)	0(1)	4(1)	2(1)
C(19)	14(1)	6(1)	12(1)	2(1)	1(1)	3(1)
C(20)	10(1)	12(1)	17(1)	2(1)	-1(1)	2(1)
C(21)	30(1)	24(1)	32(1)	0(1)	-3(1)	-2(1)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3)
for mo_035GOI16_0m.

	x	y	z	U(eq)
H(5A)	1231(19)	6803(13)	2917(8)	33
H(5B)	1280(20)	7089(11)	3900(12)	33
H(6A)	3196(16)	6447(16)	3609(19)	54
H(1)	3239	7386	10557	19
H(3)	6814	6786	11526	20
H(4)	6222	5314	11555	19
H(7)	5602	4002	11518	18
H(8)	4781	2579	11538	20
H(10)	1334	3559	10696	17
H(11A)	5313	8403	10270	31
H(11B)	6273	8307	11244	31
H(11C)	4817	8550	11374	31
H(12A)	2100	1852	10428	33
H(12B)	1632	2018	11537	33
H(12C)	2997	1594	11397	33
H(13)	381	4415	7214	15
H(14A)	-1081	5273	6296	17
H(14B)	-1322	5416	7466	17
H(15A)	-180	6761	7459	17
H(15B)	-1347	6790	6630	17
H(16)	38	6420	5343	17
H(17A)	2254	6315	5697	17
H(17B)	2093	6513	6868	17
H(18A)	2357	5007	6700	18
H(18B)	1265	4960	5813	18
H(21A)	3708	5257	4407	43
H(21B)	4977	5244	3802	43
H(21C)	3624	5118	3209	43

Torsion angles [°] for mo_035GOI16_0m.

C(5)-N(1)-C(1)-C(2)	-1.1(2)
Cd(01)-N(1)-C(1)-C(2)	178.96(11)
N(1)-C(1)-C(2)-C(3)	0.9(2)
N(1)-C(1)-C(2)-C(11)	179.79(14)
C(1)-C(2)-C(3)-C(4)	0.1(2)
C(11)-C(2)-C(3)-C(4)	-178.76(14)
C(2)-C(3)-C(4)-C(5)	-0.8(2)
C(1)-N(1)-C(5)-C(4)	0.3(2)
Cd(01)-N(1)-C(5)-C(4)	-179.79(10)
C(1)-N(1)-C(5)-C(6)	-179.33(13)
Cd(01)-N(1)-C(5)-C(6)	0.60(16)
C(3)-C(4)-C(5)-N(1)	0.7(2)
C(3)-C(4)-C(5)-C(6)	-179.76(13)
C(10)-N(2)-C(6)-C(7)	0.0(2)
Cd(01)-N(2)-C(6)-C(7)	-177.10(10)
C(10)-N(2)-C(6)-C(5)	-179.28(12)
Cd(01)-N(2)-C(6)-C(5)	3.61(16)
N(1)-C(5)-C(6)-N(2)	-2.81(19)
C(4)-C(5)-C(6)-N(2)	177.59(13)
N(1)-C(5)-C(6)-C(7)	177.92(13)
C(4)-C(5)-C(6)-C(7)	-1.7(2)
N(2)-C(6)-C(7)-C(8)	-0.4(2)
C(5)-C(6)-C(7)-C(8)	178.86(13)
C(6)-C(7)-C(8)-C(9)	0.1(2)
C(7)-C(8)-C(9)-C(10)	0.5(2)
C(7)-C(8)-C(9)-C(12)	179.85(14)
C(6)-N(2)-C(10)-C(9)	0.7(2)
Cd(01)-N(2)-C(10)-C(9)	177.63(11)
C(8)-C(9)-C(10)-N(2)	-0.9(2)
C(12)-C(9)-C(10)-N(2)	179.73(14)
C(19)-C(13)-C(14)-C(15)	70.53(15)
C(18)-C(13)-C(14)-C(15)	-55.94(15)
C(13)-C(14)-C(15)-C(16)	59.88(15)
C(14)-C(15)-C(16)-C(20)	179.10(12)

C(14)-C(15)-C(16)-C(17)	-58.48(15)
C(20)-C(16)-C(17)-C(18)	179.88(12)
C(15)-C(16)-C(17)-C(18)	54.83(15)
C(16)-C(17)-C(18)-C(13)	-52.49(16)
C(19)-C(13)-C(18)-C(17)	-72.56(16)
C(14)-C(13)-C(18)-C(17)	52.33(16)
Cd(01)-O(2)-C(19)-O(1)	-2.23(12)
Cd(01)-O(2)-C(19)-C(13)	178.04(12)
Cd(01)-O(1)-C(19)-O(2)	2.55(14)
Cd(01)#1-O(1)-C(19)-O(2)	-146.82(13)
Cd(01)-O(1)-C(19)-C(13)	-177.70(10)
Cd(01)#1-O(1)-C(19)-C(13)	32.9(2)
C(18)-C(13)-C(19)-O(2)	-1.40(19)
C(14)-C(13)-C(19)-O(2)	-126.06(14)
C(18)-C(13)-C(19)-O(1)	178.86(12)
C(14)-C(13)-C(19)-O(1)	54.19(16)
Cd(01)#3-O(4)-C(20)-O(3)	-6.41(14)
Cd(01)#3-O(4)-C(20)-C(16)	170.63(12)
Cd(01)#3-O(3)-C(20)-O(4)	6.72(14)
Cd(01)#3-O(3)-C(20)-C(16)	-170.41(11)
C(15)-C(16)-C(20)-O(4)	37.05(19)
C(17)-C(16)-C(20)-O(4)	-85.93(16)
C(15)-C(16)-C(20)-O(3)	-145.83(13)
C(17)-C(16)-C(20)-O(3)	91.19(15)

Symmetry transformations used to generate equivalent atoms:

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

Hydrogen bonds for mo_035GOI16_0m [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(5A)...O(4)#3	0.849(10)	1.909(10)	2.7423(16)	167(2)
O(5)-H(5B)...O(3)	0.847(10)	1.902(10)	2.7418(16)	171.4(19)
O(6)-H(6A)...O(5)	0.856(16)	1.842(17)	2.697(2)	177(3)

Symmetry transformations used to generate equivalent atoms:

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

Table S4. Crystallographic data for **4**.

Crystal data and structure refinement for mo_092SMV15_0m.

Identification code	mo_092SMV15_0m	
Empirical formula	C27 H38 Cd N2 O5	
Formula weight	582.99	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.3522(6) Å	α= 71.9869(10)°.
	b = 11.1636(6) Å	β= 70.4676(10)°.
	c = 12.9507(7) Å	γ = 82.4361(11)°.
Volume	1340.75(13) $Å^3$	
Z	2	
Density (calculated)	1.444 Mg/m^3	
Absorption coefficient	0.853 mm^{-1}	
F(000)	604	
Crystal size	0.359 x 0.152 x 0.113 mm^3	
Theta range for data collection	1.919 to 26.372°.	
Index ranges	-12<=h<=12, -13<=k<=13, -16<=l<=16	
Reflections collected	26684	
Independent reflections	5462 [R(int) = 0.0172]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5462 / 438 / 423	
Goodness-of-fit on F^2	1.071	
Final R indices [I>2sigma(I)]	R1 = 0.0254, wR2 = 0.0724	
R indices (all data)	R1 = 0.0264, wR2 = 0.0734	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.901 and -1.036 $e.Å^{-3}$	

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for mo_092SMV15_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cd(1)	5744(1)	8797(1)	4154(1)	27(1)
C(27)	3723(6)	10840(11)	1322(6)	138(2)
O(5)	5177(6)	11047(7)	465(4)	132(2)
C(27A)	4068(17)	11800(20)	1116(18)	136(2)
O(5A)	2792(14)	12676(15)	1114(12)	135(2)
O(1)	3850(2)	10046(2)	4680(2)	40(1)
O(2)	3164(2)	8336(2)	4580(2)	62(1)
O(3)	6396(2)	9975(2)	2168(2)	46(1)
O(4)	8042(2)	9231(2)	2915(1)	50(1)
N(1)	6511(2)	6960(2)	5304(2)	32(1)
N(2)	5937(2)	7073(2)	3417(2)	36(1)
C(1)	6860(3)	6957(2)	6209(2)	40(1)
C(2)	7511(3)	5944(2)	6796(2)	42(1)
C(3)	7783(2)	4843(2)	6470(2)	34(1)
C(4)	7353(2)	4822(2)	5562(2)	33(1)
C(5)	6757(2)	5894(2)	4981(2)	29(1)
C(6)	6443(2)	5964(2)	3916(2)	29(1)
C(7)	6734(2)	4970(2)	3427(2)	34(1)
C(8)	6553(2)	5122(2)	2376(2)	35(1)
C(9)	6006(3)	6277(2)	1889(2)	46(1)
C(10)	5704(3)	7208(2)	2432(2)	48(1)
C(11)	8586(8)	3744(6)	7052(6)	41(1)
C(12)	9674(7)	4246(6)	7381(7)	58(1)
C(13)	7577(7)	2960(8)	8112(6)	71(2)
C(14)	9359(11)	2940(9)	6274(8)	56(2)
C(11A)	8519(13)	3673(9)	7053(10)	49(2)
C(12A)	9137(14)	3947(11)	7868(10)	63(2)
C(13A)	7502(10)	2570(10)	7746(10)	61(2)
C(14A)	9637(16)	3199(14)	6110(12)	53(2)
C(15)	7002(6)	4112(5)	1737(5)	46(1)
C(16)	7002(10)	2782(7)	2537(8)	63(2)

C(17)	6031(8)	4114(7)	1057(6)	58(1)
C(18)	8428(6)	4432(9)	923(8)	72(2)
C(15A)	7076(18)	4082(13)	1770(14)	55(2)
C(16A)	6620(20)	2797(19)	2672(19)	57(3)
C(17A)	6520(20)	4260(20)	782(14)	64(3)
C(18A)	8663(14)	4050(18)	1344(18)	64(3)
C(19)	2897(2)	9390(2)	4739(2)	33(1)
C(20)	1440(2)	9952(2)	4988(2)	35(1)
C(21)	1049(2)	10402(2)	3886(2)	38(1)
C(22)	-404(2)	10978(2)	4090(2)	36(1)
C(23)	7652(2)	9779(2)	2073(2)	36(1)
C(24)	8699(2)	10191(2)	884(2)	36(1)
C(25)	8876(3)	9162(3)	295(2)	49(1)
C(26)	9919(3)	9519(3)	-908(2)	47(1)

Bond lengths [Å] and angles [°] for mo_092SMV15_0m.

Cd(1)-O(1)	2.2862(16)
Cd(1)-N(1)	2.3514(18)
Cd(1)-N(2)	2.3586(19)
Cd(1)-O(4)	2.3957(18)
Cd(1)-O(3)	2.4045(18)
Cd(1)-O(1)#1	2.4288(16)
Cd(1)-O(2)	2.628(2)
Cd(1)-C(23)	2.747(2)
C(27)-O(5)	1.5383(9)
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
O(5)-H(5)	0.8200
C(27A)-O(5A)	1.5394(9)
C(27A)-H(27D)	0.9600
C(27A)-H(27E)	0.9600
C(27A)-H(27F)	0.9600
O(5A)-H(5A)	0.8200
O(1)-C(19)	1.274(3)
O(1)-Cd(1)#1	2.4287(16)
O(2)-C(19)	1.236(3)
O(3)-C(23)	1.260(3)
O(4)-C(23)	1.243(3)
N(1)-C(1)	1.336(3)
N(1)-C(5)	1.346(3)
N(2)-C(10)	1.336(3)
N(2)-C(6)	1.337(3)
C(1)-C(2)	1.386(3)
C(1)-H(1)	0.9300
C(2)-C(3)	1.385(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.397(3)
C(3)-C(11)	1.530(5)
C(3)-C(11A)	1.539(7)

C(4)-C(5)	1.393(3)
C(4)-H(4)	0.9300
C(5)-C(6)	1.497(3)
C(6)-C(7)	1.394(3)
C(7)-C(8)	1.392(3)
C(7)-H(7)	0.9300
C(8)-C(9)	1.387(3)
C(8)-C(15)	1.534(4)
C(8)-C(15A)	1.539(8)
C(9)-C(10)	1.376(4)
C(9)-H(9)	0.9300
C(10)-H(10)	0.9300
C(11)-C(13)	1.510(8)
C(11)-C(14)	1.515(8)
C(11)-C(12)	1.549(7)
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(11A)-C(12A)	1.524(11)
C(11A)-C(14A)	1.551(12)
C(11A)-C(13A)	1.567(11)
C(12A)-H(12D)	0.9600
C(12A)-H(12E)	0.9600
C(12A)-H(12F)	0.9600
C(13A)-H(13D)	0.9600
C(13A)-H(13E)	0.9600
C(13A)-H(13F)	0.9600
C(14A)-H(14D)	0.9600
C(14A)-H(14E)	0.9600
C(14A)-H(14F)	0.9600

C(15)-C(18)	1.512(7)
C(15)-C(16)	1.526(7)
C(15)-C(17)	1.541(6)
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(15A)-C(17A)	1.521(13)
C(15A)-C(18A)	1.548(13)
C(15A)-C(16A)	1.555(13)
C(16A)-H(16D)	0.9600
C(16A)-H(16E)	0.9600
C(16A)-H(16F)	0.9600
C(17A)-H(17D)	0.9600
C(17A)-H(17E)	0.9600
C(17A)-H(17F)	0.9600
C(18A)-H(18D)	0.9600
C(18A)-H(18E)	0.9600
C(18A)-H(18F)	0.9600
C(19)-C(20)	1.525(3)
C(20)-C(22)#2	1.524(3)
C(20)-C(21)	1.530(3)
C(20)-H(20)	0.9800
C(21)-C(22)	1.526(3)
C(21)-H(21A)	0.9700
C(21)-H(21B)	0.9700
C(22)-C(20)#2	1.524(3)
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(23)-C(24)	1.528(3)
C(24)-C(26)#3	1.521(3)

C(24)-C(25)	1.526(4)
C(24)-H(24)	0.9800
C(25)-C(26)	1.535(3)
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(26)-C(24)#3	1.521(3)
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700

O(1)-Cd(1)-N(1)	128.05(6)
O(1)-Cd(1)-N(2)	128.24(6)
N(1)-Cd(1)-N(2)	68.92(6)
O(1)-Cd(1)-O(4)	133.44(7)
N(1)-Cd(1)-O(4)	90.88(6)
N(2)-Cd(1)-O(4)	85.64(7)
O(1)-Cd(1)-O(3)	94.69(6)
N(1)-Cd(1)-O(3)	137.17(6)
N(2)-Cd(1)-O(3)	83.13(7)
O(4)-Cd(1)-O(3)	54.09(6)
O(1)-Cd(1)-O(1)#1	71.32(6)
N(1)-Cd(1)-O(1)#1	87.96(6)
N(2)-Cd(1)-O(1)#1	155.89(6)
O(4)-Cd(1)-O(1)#1	88.09(6)
O(3)-Cd(1)-O(1)#1	111.61(6)
O(1)-Cd(1)-O(2)	52.02(6)
N(1)-Cd(1)-O(2)	102.59(7)
N(2)-Cd(1)-O(2)	77.83(6)
O(4)-Cd(1)-O(2)	153.04(7)
O(3)-Cd(1)-O(2)	102.35(7)
O(1)#1-Cd(1)-O(2)	115.30(6)
O(1)-Cd(1)-C(23)	116.61(7)
N(1)-Cd(1)-C(23)	114.04(7)
N(2)-Cd(1)-C(23)	82.41(7)
O(4)-Cd(1)-C(23)	26.87(7)
O(3)-Cd(1)-C(23)	27.28(7)
O(1)#1-Cd(1)-C(23)	101.90(6)

O(2)-Cd(1)-C(23)	128.13(8)
O(5)-C(27)-H(27A)	109.5
O(5)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
O(5)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(27)-O(5)-H(5)	109.5
O(5A)-C(27A)-H(27D)	109.5
O(5A)-C(27A)-H(27E)	109.5
H(27D)-C(27A)-H(27E)	109.5
O(5A)-C(27A)-H(27F)	109.5
H(27D)-C(27A)-H(27F)	109.5
H(27E)-C(27A)-H(27F)	109.5
C(27A)-O(5A)-H(5A)	109.5
C(19)-O(1)-Cd(1)	101.42(13)
C(19)-O(1)-Cd(1)#1	136.74(14)
Cd(1)-O(1)-Cd(1)#1	108.68(6)
C(19)-O(2)-Cd(1)	86.20(14)
C(23)-O(3)-Cd(1)	91.70(14)
C(23)-O(4)-Cd(1)	92.53(14)
C(1)-N(1)-C(5)	117.61(19)
C(1)-N(1)-Cd(1)	122.47(15)
C(5)-N(1)-Cd(1)	119.50(14)
C(10)-N(2)-C(6)	118.2(2)
C(10)-N(2)-Cd(1)	121.60(16)
C(6)-N(2)-Cd(1)	119.71(14)
N(1)-C(1)-C(2)	123.7(2)
N(1)-C(1)-H(1)	118.1
C(2)-C(1)-H(1)	118.1
C(3)-C(2)-C(1)	119.5(2)
C(3)-C(2)-H(2)	120.3
C(1)-C(2)-H(2)	120.3
C(2)-C(3)-C(4)	116.8(2)
C(2)-C(3)-C(11)	120.3(3)
C(4)-C(3)-C(11)	122.8(3)

C(2)-C(3)-C(11A)	123.5(5)
C(4)-C(3)-C(11A)	119.7(5)
C(5)-C(4)-C(3)	120.5(2)
C(5)-C(4)-H(4)	119.7
C(3)-C(4)-H(4)	119.7
N(1)-C(5)-C(4)	121.70(19)
N(1)-C(5)-C(6)	115.94(18)
C(4)-C(5)-C(6)	122.23(19)
N(2)-C(6)-C(7)	121.44(19)
N(2)-C(6)-C(5)	115.70(18)
C(7)-C(6)-C(5)	122.74(19)
C(8)-C(7)-C(6)	120.6(2)
C(8)-C(7)-H(7)	119.7
C(6)-C(7)-H(7)	119.7
C(9)-C(8)-C(7)	116.5(2)
C(9)-C(8)-C(15)	120.6(3)
C(7)-C(8)-C(15)	122.8(3)
C(9)-C(8)-C(15A)	123.6(7)
C(7)-C(8)-C(15A)	119.6(7)
C(10)-C(9)-C(8)	120.0(2)
C(10)-C(9)-H(9)	120.0
C(8)-C(9)-H(9)	120.0
N(2)-C(10)-C(9)	123.2(2)
N(2)-C(10)-H(10)	118.4
C(9)-C(10)-H(10)	118.4
C(13)-C(11)-C(14)	110.2(6)
C(13)-C(11)-C(3)	107.9(5)
C(14)-C(11)-C(3)	112.1(6)
C(13)-C(11)-C(12)	110.0(5)
C(14)-C(11)-C(12)	106.4(6)
C(3)-C(11)-C(12)	110.3(5)
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5

H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(11)-C(14)-H(14A)	109.5
C(11)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(11)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(12A)-C(11A)-C(3)	112.1(8)
C(12A)-C(11A)-C(14A)	111.0(11)
C(3)-C(11A)-C(14A)	108.3(10)
C(12A)-C(11A)-C(13A)	108.2(8)
C(3)-C(11A)-C(13A)	110.8(8)
C(14A)-C(11A)-C(13A)	106.3(9)
C(11A)-C(12A)-H(12D)	109.5
C(11A)-C(12A)-H(12E)	109.5
H(12D)-C(12A)-H(12E)	109.5
C(11A)-C(12A)-H(12F)	109.5
H(12D)-C(12A)-H(12F)	109.5
H(12E)-C(12A)-H(12F)	109.5
C(11A)-C(13A)-H(13D)	109.5
C(11A)-C(13A)-H(13E)	109.5
H(13D)-C(13A)-H(13E)	109.5
C(11A)-C(13A)-H(13F)	109.5
H(13D)-C(13A)-H(13F)	109.5
H(13E)-C(13A)-H(13F)	109.5
C(11A)-C(14A)-H(14D)	109.5
C(11A)-C(14A)-H(14E)	109.5
H(14D)-C(14A)-H(14E)	109.5
C(11A)-C(14A)-H(14F)	109.5
H(14D)-C(14A)-H(14F)	109.5

H(14E)-C(14A)-H(14F)	109.5
C(18)-C(15)-C(16)	110.3(5)
C(18)-C(15)-C(8)	106.6(4)
C(16)-C(15)-C(8)	112.8(6)
C(18)-C(15)-C(17)	109.6(5)
C(16)-C(15)-C(17)	106.4(5)
C(8)-C(15)-C(17)	111.2(4)
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17A)-C(15A)-C(8)	112.4(12)
C(17A)-C(15A)-C(18A)	110.3(11)
C(8)-C(15A)-C(18A)	109.3(11)
C(17A)-C(15A)-C(16A)	109.6(14)
C(8)-C(15A)-C(16A)	107.7(14)
C(18A)-C(15A)-C(16A)	107.4(12)
C(15A)-C(16A)-H(16D)	109.5
C(15A)-C(16A)-H(16E)	109.5
H(16D)-C(16A)-H(16E)	109.5
C(15A)-C(16A)-H(16F)	109.5
H(16D)-C(16A)-H(16F)	109.5

H(16E)-C(16A)-H(16F)	109.5
C(15A)-C(17A)-H(17D)	109.5
C(15A)-C(17A)-H(17E)	109.5
H(17D)-C(17A)-H(17E)	109.5
C(15A)-C(17A)-H(17F)	109.5
H(17D)-C(17A)-H(17F)	109.5
H(17E)-C(17A)-H(17F)	109.5
C(15A)-C(18A)-H(18D)	109.5
C(15A)-C(18A)-H(18E)	109.5
H(18D)-C(18A)-H(18E)	109.5
C(15A)-C(18A)-H(18F)	109.5
H(18D)-C(18A)-H(18F)	109.5
H(18E)-C(18A)-H(18F)	109.5
O(2)-C(19)-O(1)	120.3(2)
O(2)-C(19)-C(20)	121.7(2)
O(1)-C(19)-C(20)	118.07(19)
C(22)#2-C(20)-C(19)	112.22(19)
C(22)#2-C(20)-C(21)	110.41(18)
C(19)-C(20)-C(21)	109.52(18)
C(22)#2-C(20)-H(20)	108.2
C(19)-C(20)-H(20)	108.2
C(21)-C(20)-H(20)	108.2
C(22)-C(21)-C(20)	111.62(19)
C(22)-C(21)-H(21A)	109.3
C(20)-C(21)-H(21A)	109.3
C(22)-C(21)-H(21B)	109.3
C(20)-C(21)-H(21B)	109.3
H(21A)-C(21)-H(21B)	108.0
C(20)#2-C(22)-C(21)	110.96(19)
C(20)#2-C(22)-H(22A)	109.4
C(21)-C(22)-H(22A)	109.4
C(20)#2-C(22)-H(22B)	109.4
C(21)-C(22)-H(22B)	109.4
H(22A)-C(22)-H(22B)	108.0
O(4)-C(23)-O(3)	121.4(2)
O(4)-C(23)-C(24)	120.1(2)

O(3)-C(23)-C(24)	118.5(2)
O(4)-C(23)-Cd(1)	60.60(12)
O(3)-C(23)-Cd(1)	61.03(12)
C(24)-C(23)-Cd(1)	173.64(16)
C(26)#3-C(24)-C(25)	110.0(2)
C(26)#3-C(24)-C(23)	113.07(19)
C(25)-C(24)-C(23)	109.01(19)
C(26)#3-C(24)-H(24)	108.2
C(25)-C(24)-H(24)	108.2
C(23)-C(24)-H(24)	108.2
C(24)-C(25)-C(26)	111.6(2)
C(24)-C(25)-H(25A)	109.3
C(26)-C(25)-H(25A)	109.3
C(24)-C(25)-H(25B)	109.3
C(26)-C(25)-H(25B)	109.3
H(25A)-C(25)-H(25B)	108.0
C(24)#3-C(26)-C(25)	111.6(2)
C(24)#3-C(26)-H(26A)	109.3
C(25)-C(26)-H(26A)	109.3
C(24)#3-C(26)-H(26B)	109.3
C(25)-C(26)-H(26B)	109.3
H(26A)-C(26)-H(26B)	108.0

Symmetry transformations used to generate equivalent atoms:

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

Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_092SMV15_0m. 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)	22(1)	30(1)	30(1)	-13(1)	-5(1)	4(1)
C(27)	136(4)	184(5)	94(3)	-32(3)	-47(3)	11(4)
O(5)	130(4)	183(5)	87(3)	-32(3)	-50(3)	12(3)
C(27A)	135(4)	182(5)	91(3)	-32(3)	-46(3)	12(4)
O(5A)	137(4)	179(5)	88(3)	-34(4)	-43(3)	13(4)
O(1)	22(1)	57(1)	50(1)	-30(1)	-9(1)	1(1)
O(2)	39(1)	55(1)	102(2)	-46(1)	-19(1)	14(1)
O(3)	34(1)	50(1)	46(1)	-12(1)	-3(1)	4(1)
O(4)	42(1)	72(1)	28(1)	-9(1)	-6(1)	-9(1)
N(1)	34(1)	32(1)	31(1)	-13(1)	-9(1)	2(1)
N(2)	38(1)	34(1)	42(1)	-16(1)	-19(1)	6(1)
C(1)	52(1)	38(1)	36(1)	-17(1)	-15(1)	2(1)
C(2)	53(1)	48(1)	35(1)	-18(1)	-20(1)	2(1)
C(3)	34(1)	39(1)	30(1)	-9(1)	-10(1)	0(1)
C(4)	35(1)	32(1)	34(1)	-13(1)	-11(1)	3(1)
C(5)	25(1)	33(1)	28(1)	-12(1)	-5(1)	-1(1)
C(6)	23(1)	33(1)	31(1)	-13(1)	-7(1)	1(1)
C(7)	35(1)	33(1)	36(1)	-14(1)	-13(1)	5(1)
C(8)	32(1)	42(1)	36(1)	-18(1)	-10(1)	-1(1)
C(9)	60(2)	49(1)	41(1)	-16(1)	-29(1)	2(1)
C(10)	63(2)	40(1)	54(2)	-17(1)	-38(1)	11(1)
C(11)	43(2)	43(2)	40(2)	-8(1)	-23(1)	6(1)
C(12)	53(3)	62(3)	69(3)	-20(3)	-35(2)	5(2)
C(13)	58(2)	70(3)	58(2)	13(2)	-15(2)	5(2)
C(14)	65(4)	49(3)	53(3)	-15(3)	-26(2)	15(3)
C(11A)	45(2)	49(2)	46(2)	-5(2)	-18(2)	9(2)
C(12A)	67(4)	65(4)	60(3)	-11(3)	-32(3)	7(3)
C(13A)	54(3)	55(3)	60(4)	1(3)	-17(3)	3(3)
C(14A)	50(4)	42(4)	53(3)	-2(3)	-12(3)	6(3)
C(15)	46(2)	57(2)	48(2)	-36(1)	-15(1)	6(1)
C(16)	73(4)	56(2)	64(3)	-35(2)	-15(3)	14(2)

C(17)	56(3)	77(3)	57(3)	-41(2)	-20(2)	0(2)
C(18)	52(2)	97(4)	69(3)	-46(3)	-3(2)	-2(2)
C(15A)	53(3)	61(3)	55(3)	-35(2)	-9(2)	4(2)
C(16A)	53(5)	58(3)	61(4)	-36(3)	-4(4)	7(3)
C(17A)	63(5)	77(5)	60(4)	-38(4)	-15(4)	4(4)
C(18A)	53(3)	70(5)	68(5)	-37(4)	-5(3)	4(3)
C(19)	22(1)	43(1)	38(1)	-19(1)	-10(1)	6(1)
C(20)	20(1)	43(1)	45(1)	-20(1)	-10(1)	5(1)
C(21)	24(1)	50(1)	39(1)	-14(1)	-7(1)	1(1)
C(22)	27(1)	45(1)	38(1)	-13(1)	-13(1)	6(1)
C(23)	38(1)	38(1)	30(1)	-15(1)	-1(1)	-2(1)
C(24)	34(1)	41(1)	26(1)	-9(1)	-3(1)	2(1)
C(25)	44(1)	64(2)	39(1)	-25(1)	2(1)	-16(1)
C(26)	43(1)	67(2)	33(1)	-24(1)	0(1)	-14(1)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3)
for mo_092SMV15_0m.

	x	y	z	U(eq)
H(27A)	3685	11051	1996	207
H(27B)	3499	9973	1523	207
H(27C)	3077	11367	981	207
H(5)	5737	10905	814	198
H(27D)	4833	12273	1008	205
H(27E)	4276	11411	508	205
H(27F)	3891	11152	1834	205
H(5A)	2280	12396	885	202
H(1)	6655	7676	6459	48
H(2)	7762	6002	7404	51
H(4)	7465	4086	5344	40
H(7)	7053	4198	3806	41
H(9)	5843	6422	1195	56
H(10)	5320	7968	2098	57
H(12A)	10264	4801	6712	86
H(12B)	10209	3550	7700	86
H(12C)	9224	4696	7935	86
H(13A)	6898	2663	7903	106
H(13B)	7138	3465	8622	106
H(13C)	8053	2253	8486	106
H(14A)	8718	2523	6122	83
H(14B)	9928	2322	6637	83
H(14C)	9923	3465	5568	83
H(12D)	9563	4750	7522	95
H(12E)	9812	3301	8028	95
H(12F)	8427	3963	8567	95
H(13D)	7161	2335	7234	92
H(13E)	6749	2842	8307	92
H(13F)	7972	1859	8121	92
H(14D)	9214	2966	5647	80

H(14E)	10122	2479	6459	80
H(14F)	10269	3857	5641	80
H(16A)	7204	2182	2105	95
H(16B)	6117	2625	3103	95
H(16C)	7686	2701	2907	95
H(17A)	6101	4894	462	87
H(17B)	5105	4025	1561	87
H(17C)	6283	3425	725	87
H(18A)	8766	3804	523	107
H(18B)	9026	4456	1345	107
H(18C)	8399	5241	383	107
H(16D)	5637	2762	2912	86
H(16E)	6914	2714	3320	86
H(16F)	7022	2123	2341	86
H(17D)	6853	5027	204	96
H(17E)	5536	4304	1053	96
H(17F)	6820	3561	466	96
H(18D)	8992	3452	910	95
H(18E)	9002	3808	1987	95
H(18F)	8980	4872	869	95
H(20)	1419	10686	5258	42
H(21A)	1691	11025	3323	46
H(21B)	1114	9695	3584	46
H(22A)	-449	11734	4322	44
H(22B)	-634	11215	3384	44
H(24)	8334	10956	438	43
H(25A)	7998	9021	242	59
H(25B)	9181	8383	751	59
H(26A)	10034	8829	-1242	57
H(26B)	9570	10251	-1386	57

Torsion angles [°] for mo_092SMV15_0m.

C(5)-N(1)-C(1)-C(2)	2.9(4)
Cd(1)-N(1)-C(1)-C(2)	-169.7(2)
N(1)-C(1)-C(2)-C(3)	-2.4(4)
C(1)-C(2)-C(3)-C(4)	-1.1(4)
C(1)-C(2)-C(3)-C(11)	175.9(4)
C(1)-C(2)-C(3)-C(11A)	179.1(6)
C(2)-C(3)-C(4)-C(5)	3.8(3)
C(11)-C(3)-C(4)-C(5)	-173.1(4)
C(11A)-C(3)-C(4)-C(5)	-176.3(6)
C(1)-N(1)-C(5)-C(4)	0.0(3)
Cd(1)-N(1)-C(5)-C(4)	172.83(16)
C(1)-N(1)-C(5)-C(6)	-175.85(19)
Cd(1)-N(1)-C(5)-C(6)	-3.1(2)
C(3)-C(4)-C(5)-N(1)	-3.5(3)
C(3)-C(4)-C(5)-C(6)	172.2(2)
C(10)-N(2)-C(6)-C(7)	0.5(3)
Cd(1)-N(2)-C(6)-C(7)	-171.82(16)
C(10)-N(2)-C(6)-C(5)	176.6(2)
Cd(1)-N(2)-C(6)-C(5)	4.3(2)
N(1)-C(5)-C(6)-N(2)	-0.8(3)
C(4)-C(5)-C(6)-N(2)	-176.7(2)
N(1)-C(5)-C(6)-C(7)	175.2(2)
C(4)-C(5)-C(6)-C(7)	-0.6(3)
N(2)-C(6)-C(7)-C(8)	2.4(3)
C(5)-C(6)-C(7)-C(8)	-173.4(2)
C(6)-C(7)-C(8)-C(9)	-3.3(3)
C(6)-C(7)-C(8)-C(15)	173.2(4)
C(6)-C(7)-C(8)-C(15A)	171.2(8)
C(7)-C(8)-C(9)-C(10)	1.5(4)
C(15)-C(8)-C(9)-C(10)	-175.1(4)
C(15A)-C(8)-C(9)-C(10)	-172.7(8)
C(6)-N(2)-C(10)-C(9)	-2.4(4)
Cd(1)-N(2)-C(10)-C(9)	169.8(2)
C(8)-C(9)-C(10)-N(2)	1.4(5)

C(2)-C(3)-C(11)-C(13)	86.1(6)
C(4)-C(3)-C(11)-C(13)	-97.1(6)
C(2)-C(3)-C(11)-C(14)	-152.3(6)
C(4)-C(3)-C(11)-C(14)	24.5(8)
C(2)-C(3)-C(11)-C(12)	-34.0(7)
C(4)-C(3)-C(11)-C(12)	142.8(5)
C(2)-C(3)-C(11A)-C(12A)	-10.6(12)
C(4)-C(3)-C(11A)-C(12A)	169.6(7)
C(2)-C(3)-C(11A)-C(14A)	-133.4(9)
C(4)-C(3)-C(11A)-C(14A)	46.8(12)
C(2)-C(3)-C(11A)-C(13A)	110.4(8)
C(4)-C(3)-C(11A)-C(13A)	-69.4(10)
C(9)-C(8)-C(15)-C(18)	82.8(6)
C(7)-C(8)-C(15)-C(18)	-93.6(6)
C(9)-C(8)-C(15)-C(16)	-156.0(5)
C(7)-C(8)-C(15)-C(16)	27.7(7)
C(9)-C(8)-C(15)-C(17)	-36.6(7)
C(7)-C(8)-C(15)-C(17)	147.1(5)
C(9)-C(8)-C(15A)-C(17A)	-18.8(16)
C(7)-C(8)-C(15A)-C(17A)	167.2(11)
C(9)-C(8)-C(15A)-C(18A)	104.0(12)
C(7)-C(8)-C(15A)-C(18A)	-70.0(14)
C(9)-C(8)-C(15A)-C(16A)	-139.6(12)
C(7)-C(8)-C(15A)-C(16A)	46.3(16)
Cd(1)-O(2)-C(19)-O(1)	-2.9(2)
Cd(1)-O(2)-C(19)-C(20)	176.0(2)
Cd(1)-O(1)-C(19)-O(2)	3.4(3)
Cd(1)#1-O(1)-C(19)-O(2)	-130.3(2)
Cd(1)-O(1)-C(19)-C(20)	-175.58(16)
Cd(1)#1-O(1)-C(19)-C(20)	50.7(3)
O(2)-C(19)-C(20)-C(22)#2	47.8(3)
O(1)-C(19)-C(20)-C(22)#2	-133.3(2)
O(2)-C(19)-C(20)-C(21)	-75.2(3)
O(1)-C(19)-C(20)-C(21)	103.8(2)
C(22)#2-C(20)-C(21)-C(22)	56.1(3)
C(19)-C(20)-C(21)-C(22)	-179.87(19)

C(20)-C(21)-C(22)-C(20)#2	-56.4(3)
Cd(1)-O(4)-C(23)-O(3)	5.2(2)
Cd(1)-O(4)-C(23)-C(24)	-172.71(19)
Cd(1)-O(3)-C(23)-O(4)	-5.2(2)
Cd(1)-O(3)-C(23)-C(24)	172.77(18)
O(4)-C(23)-C(24)-C(26)#3	-28.9(3)
O(3)-C(23)-C(24)-C(26)#3	153.1(2)
O(4)-C(23)-C(24)-C(25)	93.8(3)
O(3)-C(23)-C(24)-C(25)	-84.2(3)
C(26)#3-C(24)-C(25)-C(26)	-55.5(3)
C(23)-C(24)-C(25)-C(26)	-180.0(2)
C(24)-C(25)-C(26)-C(24)#3	56.4(3)

Symmetry transformations used to generate equivalent atoms:

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

Hydrogen bonds for mo_092SMV15_0m [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(5)...O(3)	0.82	2.03	2.779(5)	152.3

Symmetry transformations used to generate equivalent atoms:

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

Table S5. Elemental analysis results for **1**.

Document: 16-02-2016 (VarioMICRO) from: 16/02/2016 19:02:41

Análisis Elemental por Combustión "CCIQS UAEM-UNAM"
Muestra: 6-2,2-Cd 13/Ago/ Analizó: Alejandra Núñez
Teóricos: 5.9%N 45.5%C 4.6%H No.reg. 39

Text report

No.	Name	Weight [mg]	N [%]	C [%]	H [%]
14	6-2,2-Cd 13/Ago/15	1.8610	5.92	45.40	4.70

Name: eassuperuser, Access: VarioMICRO superuser 16/02/2016 19:34:44

varioMICRO V2.0.11 (1497134)2011-06-27, CHNS Mode, Ser. No.: 15113027
Elementar Analysensysteme GmbH