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Table S1. Crystal data and structure refinement for (1)

formula	$C_{27}H_{19}Cd_2NO_9$
M_w	726.23
T [K]	293(2)
λ (Mo_{Ka}) [Å]	0.71073
Crystal system	Triclinic
Space group	$P\bar{1}$ (No. 2)
a [Å]	8.582(4)
b [Å]	12.239(5)
c [Å]	12.439(5)
α [°]	99.029(4)
β [°]	91.210(4)
γ [°]	93.000(6)
V [Å^3]	1288(1)
Z	2
ρ_{calc} [g cm^{-3}]	1.873
μ [mm^{-1}]	1.707
F(000)	712
crystal size [mm]	0.64 × 0.46 × 0.38
θ range [°]	2.17 to 28.00
Index ranges	$0 \le h \le 11$, $-16 \le k \le 16$, $-16 \le l \le 16$
Reflections collected	6243
Independent reflections	6228
Absorption correction	psi-scan
Max. and min. transmission	0.5631 and 0.4079
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6228 / 0 / 353
Goodness-of-fit on F^2	1.064
R indices [$I > 2\sigma(I)$]	R_1 = 0.0434, wR_2 = 0.1057
R indices (all data)	R_1 = 0.0636, wR_2 = 0.1164
$\Delta\rho_{max}$ / $\Delta\rho_{min}$ [e Å^{-3}]	0.739 / -0.808

Table S2. Bond lengths [Å] and angles [°] for (1)

Cd(1)–O(6)^{A}	2.251(3)	C(1)–C(9)	1.443(6)
Cd(1)–O(1)^{B}	2.307(4)	C(1)–C(11)	1.519(6)
Cd(1)–O(1W)	2.323(3)	C(2)–C(3)	1.443(6)
Cd(1)–O(4)	2.362(3)	C(3)–C(4)	1.396(6)
Cd(1)–O(5)	2.487(3)	C(3)–C(21)	1.513(6)
Cd(1)–O(2)^{B}	2.492(3)	C(4)–C(10)	1.432(6)
Cd(1)–C(21)^{B}	2.752(4)	C(5)–C(6)	1.364(7)
Cd(2)–N(1)	2.211(4)	C(5)–C(10)	1.445(7)
Cd(2)–O(6)	2.216(3)	C(6)–C(7)	1.429(8)
Cd(2)–O(7)^{C}	2.267(4)	C(7)–C(8)	1.378(7)
Cd(2)–O(5)	2.314(3)	C(8)–C(9)	1.448(6)
Cd(2)–O(2W)	2.495(4)	C(9)–C(10)	1.435(6)
O(1)–C(21)	1.274(6)	C(11)–C(12)	1.408(5)
O(1)–Cd(1)^{D}	2.307(4)	C(11)–C(19)	1.434(6)
O(2)–C(21)	1.273(6)	C(12)–C(13)	1.459(6)
O(2)–Cd(1)^{D}	2.492(3)	C(13)–C(14)	1.386(6)
O(2)–O(3)	2.604(4)	C(13)–C(22)	1.519(5)
O(3)–C(2)	1.382(5)	C(14)–C(20)	1.419(6)
O(4)–C(22)	1.276(5)	C(15)–C(16)	1.383(7)
O(5)–C(22)	1.298(5)	C(15)–C(20)	1.447(6)
O(6)–C(12)	1.353(5)	C(16)–C(17)	1.418(7)
O(6)–Cd(1)^{A}	2.251(3)	C(17)–C(18)	1.395(7)
O(7)–C(23)	1.330(6)	C(18)–C(19)	1.444(6)
O(7)–Cd(2)^{C}	2.267(4)	C(19)–C(20)	1.449(6)
O(7)–O(1W)	2.740(5)	C(23)–C(24)	1.422(7)
O(2W)–O(1)^{E}	2.908(6)	C(24)–C(25)	1.385(8)
N(1)–C(23)	1.361(6)	C(25)–C(26)	1.404(9)
N(1)–C(27)	1.368(6)	C(26)–C(27)	1.379(8)
C(1)–C(2)	1.396(6)		
O(6)^{A}–Cd(1)–O(1)^{B}	168.73(12)	O(3)–C(2)–C(1)	119.1(4)
O(6)^{A}–Cd(1)–O(1W)	98.92(12)	O(3)–C(2)–C(3)	120.2(4)
O(1b)–Cd(1)–O(1W)	85.56(14)	C(1)–C(2)–C(3)	120.7(4)
O(6)^{A}–Cd(1)–O(4)	82.53(11)	C(4)–C(3)–C(2)	119.9(4)
O(1)^{B}–Cd(1)–O(4)	101.02(13)	C(4)–C(3)–C(21)	119.2(4)
O(1W)–Cd(1)–O(4)	138.49(12)	C(2)–C(3)–C(21)	120.9(4)
O(6)^{A}–Cd(1)–O(5)	94.46(10)	C(3)–C(4)–C(10)	120.7(4)
O(1b)–Cd(1)–O(5)	96.28(13)	C(6)–C(5)–C(10)	121.2(5)
O(1W)–Cd(1)–O(5)	84.27(11)	C(5)–C(6)–C(7)	119.7(5)
O(4)–Cd(1)–O(5)	54.39(10)	C(8)–C(7)–C(6)	120.6(5)
O(6)^{A}–Cd(1)–O(2)^{B}	114.86(11)	C(7)–C(8)–C(9)	121.8(5)
O(1)^{B}–Cd(1)–O(2)^{B}	54.94(12)	C(10)–C(9)–C(1)	120.0(4)
O(1W)–Cd(1)–O(2)^{B}	125.87(12)	C(10)–C(9)–C(8)	116.7(4)
O(4)–Cd(1)–O(2)^{B}	88.94(11)	C(1)–C(9)–C(8)	123.2(4)
O(5)–Cd(1)–O(2)^{B}	130.17(11)	C(4)–C(10)–C(9)	119.1(4)
N(1)–Cd(2)–O(6)	133.04(13)	C(4)–C(10)–C(5)	121.0(5)
N(1)–Cd(2)–O(7)^{C}	115.31(15)	C(9)–C(10)–C(5)	119.9(4)
O(6)–Cd(2)–O(7)^{C}	105.01(13)	C(12)–C(11)–C(19)	120.5(4)
N(1)–Cd(2)–O(5)	120.60(13)	C(12)–C(11)–C(1)	116.6(4)
O(6)–Cd(2)–O(5)	79.13(11)	C(19)–C(11)–C(1)	122.9(4)
O(7)^{C}–Cd(2)–O(5)	91.97(13)	O(6)–C(12)–C(11)	119.4(4)
N(1)–Cd(2)–O(2W)	80.92(14)	O(6)–C(12)–C(13)	121.2(3)
O(6)–Cd(2)–O(2W)	77.70(12)	C(11)–C(12)–C(13)	119.4(4)
O(7)^{C}–Cd(2)–O(2W)	87.52(14)	C(14)–C(13)–C(12)	119.1(4)
O(5)–Cd(2)–O(2W)	155.84(12)	C(14)–C(13)–C(22)	118.3(4)
C(21)–O(1)–Cd(1)^{D}	96.1(3)	C(12)–C(13)–C(22)	122.5(4)
C(21)–O(2)–Cd(1)^{D}	87.7(3)	C(13)–C(14)–C(20)	122.3(4)
C(21)–O(2)–O(3)	90.9(3)	C(16)–C(15)–C(20)	121.8(4)

Cd(1)^{D}–O(2)–O(3)	169.41(17)	C(15)–C(16)–C(17)	119.3(4)
C(2)–O(3)–O(2)	87.2(2)	C(18)–C(17)–C(16)	121.4(4)
C(22)–O(4)–Cd(1)	96.4(3)	C(17)–C(18)–C(19)	120.8(4)
C(22)–O(5)–Cd(2)	129.7(3)	C(11)–C(19)–C(18)	122.7(4)
C(22)–O(5)–Cd(1)	90.1(2)	C(11)–C(19)–C(20)	119.3(4)
Cd(2)–O(5)–Cd(1)	139.56(14)	C(18)–C(19)–C(20)	118.0(4)
C(12)–O(6)–Cd(2)	121.2(2)	C(14)–C(20)–C(15)	122.6(4)
C(12)–O(6)–Cd(1)^{A}	109.3(2)	C(14)–C(20)–C(19)	118.7(4)
Cd(2)–O(6)–Cd(1)^{A}	117.17(12)	C(15)–C(20)–C(19)	118.7(4)
C(23)–O(7)–Cd(2)^{C}	131.3(3)	O(2)–C(21)–O(1)	121.2(4)
C(23)–O(7)–O(1W)	114.4(3)	O(2)–C(21)–C(3)	119.4(4)
Cd(2)^{C}–O(7)–O(1W)	114.06(16)	O(1)–C(21)–C(3)	119.3(4)
Cd(1)–O(1W)–O(7)	123.56(16)	O(4)–C(22)–O(5)	119.1(4)
Cd(2)–O(2W)–O(1)^{E}	117.59(16)	O(4)–C(22)–C(13)	118.7(4)
C(23)–N(1)–C(27)	120.2(4)	O(5)–C(22)–C(13)	122.2(4)
C(23)–N(1)–Cd(2)	111.9(3)	O(7)–C(23)–N(1)	115.2(4)
C(27)–N(1)–Cd(2)	127.7(4)	O(7)–C(23)–C(24)	124.9(5)
C(2)–C(1)–C(9)	119.5(4)	N(1)–C(23)–C(24)	119.9(5)
C(2)–C(1)–C(11)	121.0(4)	C(25)–C(24)–C(23)	118.5(5)
C(9)–C(1)–C(11)	119.2(4)	C(24)–C(25)–C(26)	121.2(5)
C(27)–C(26)–C(25)	117.6(6)	N(1)–C(27)–C(26)	122.4(6)

Symmetry transformations used to generate equivalent atoms: ^{A} –*x*, –*y*+2, –*z*+2; ^{B} *x*, *y*+1, *z*; ^{C} –*x*–1, –*y*+2, –*z*+2; ^{D} *x*, *y*–1, *z*; ^{E} –*x*–1, –*y*+1, –*z*+2.

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Table S3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for (1)

	x	*y*	*z*	U_{eq}
Cd(1)	–670(1)	12386(1)	10104(1)	39(1)
Cd(2)	–3180(1)	9038(1)	9967(1)	44(1)
O(1)	–2606(4)	3166(3)	9211(3)	64(1)
O(2)	–251(4)	3964(3)	9078(3)	50(1)
O(3)	32(4)	5836(2)	8334(2)	44(1)
O(4)	382(4)	11211(2)	8642(3)	48(1)
O(5)	–1561(4)	10424(2)	9449(2)	44(1)
O(6)	–1462(3)	8043(2)	8999(2)	37(1)
O(7)	–4925(4)	10710(3)	11253(3)	62(1)
O(1W)	–2486(4)	12272(3)	11446(3)	61(1)
O(2W)	–4325(5)	7110(3)	9887(3)	72(1)
N(1)	–3918(5)	9142(3)	11670(3)	49(1)
C(1)	–2116(5)	6334(3)	7285(3)	37(1)
C(2)	–1482(5)	5618(3)	7925(3)	37(1)
C(3)	–2408(5)	4685(3)	8193(3)	40(1)
C(4)	–3958(6)	4497(4)	7818(4)	51(1)
C(5)	–6272(6)	5061(4)	6821(5)	61(1)
C(6)	–6944(7)	5767(5)	6226(5)	63(2)
C(7)	–6017(7)	6656(4)	5900(5)	62(1)
C(8)	–4464(6)	6834(4)	6218(4)	52(1)
C(9)	–3709(5)	6130(3)	6880(3)	41(1)
C(10)	–4647(6)	5221(4)	7169(4)	48(1)
C(11)	–1215(5)	7389(3)	7105(3)	37(1)
C(12)	–1060(5)	8250(3)	8001(3)	34(1)
C(13)	–420(5)	9340(3)	7845(3)	37(1)
C(14)	228(5)	9465(4)	6856(3)	42(1)
C(15)	887(6)	8709(4)	4932(4)	47(1)
C(16)	803(6)	7855(4)	4057(4)	55(1)
C(17)	11(7)	6834(4)	4166(4)	57(1)
C(18)	–654(6)	6664(4)	5144(4)	48(1)
C(19)	–577(5)	7534(3)	6077(3)	39(1)
C(20)	207(5)	8585(4)	5964(3)	42(1)
C(21)	–1713(6)	3891(3)	8864(4)	43(1)
C(22)	–531(5)	10366(3)	8696(3)	37(1)
C(23)	–4853(6)	9999(4)	11957(4)	50(1)
C(24)	–5656(6)	10087(5)	12953(4)	63(1)
C(25)	–5392(8)	9324(6)	13640(5)	75(2)
C(26)	–4365(8)	8474(6)	13364(5)	74(2)
C(27)	–3653(7)	8414(5)	12375(5)	64(1)

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for (1)

	U11	U22	U33	U23	U13	U12
Cd(1)	44(1)	31(1)	44(1)	5(1)	–4(1)	2(1)
Cd(2)	44(1)	38(1)	50(1)	6(1)	8(1)	1(1)
O(1)	53(2)	59(2)	89(3)	41(2)	5(2)	2(2)
O(2)	54(2)	36(2)	60(2)	12(1)	–10(2)	2(1)
O(3)	41(2)	39(2)	53(2)	13(1)	–11(1)	–3(1)
O(4)	60(2)	30(2)	52(2)	0(1)	7(2)	–11(1)
O(5)	47(2)	36(2)	48(2)	3(1)	5(1)	–3(1)
O(6)	43(2)	32(1)	35(1)	5(1)	2(1)	4(1)
O(7)	53(2)	53(2)	80(3)	18(2)	–13(2)	–5(2)
O(1W)	61(2)	53(2)	62(2)	–4(2)	13(2)	–15(2)
O(2W)	72(3)	53(2)	87(3)	2(2)	26(2)	–7(2)
N(1)	50(2)	48(2)	49(2)	9(2)	7(2)	–1(2)
C(1)	45(2)	29(2)	35(2)	2(2)	0(2)	–2(2)
C(2)	38(2)	31(2)	40(2)	2(2)	–5(2)	–4(2)
C(3)	45(2)	29(2)	46(2)	7(2)	–3(2)	1(2)
C(4)	48(3)	40(2)	64(3)	14(2)	–8(2)	–6(2)
C(5)	49(3)	45(3)	86(4)	9(3)	–16(3)	–8(2)
C(6)	55(3)	57(3)	74(4)	2(3)	–25(3)	2(3)
C(7)	69(4)	46(3)	68(3)	6(2)	–24(3)	3(3)
C(8)	59(3)	44(3)	52(3)	8(2)	–15(2)	3(2)
C(9)	47(2)	32(2)	43(2)	–1(2)	–8(2)	1(2)
C(10)	46(3)	38(2)	58(3)	6(2)	–11(2)	–1(2)
C(11)	44(2)	28(2)	39(2)	7(2)	–4(2)	–1(2)
C(12)	35(2)	32(2)	34(2)	6(2)	–4(2)	0(2)
C(13)	44(2)	29(2)	36(2)	2(2)	–4(2)	2(2)
C(14)	50(3)	35(2)	40(2)	7(2)	–1(2)	–4(2)
C(15)	58(3)	45(3)	39(2)	9(2)	5(2)	0(2)
C(16)	66(3)	59(3)	40(2)	12(2)	11(2)	6(2)
C(17)	72(4)	51(3)	43(3)	–5(2)	3(2)	6(3)
C(18)	59(3)	39(2)	42(2)	0(2)	–3(2)	–1(2)
C(19)	45(2)	33(2)	38(2)	4(2)	–5(2)	1(2)
C(20)	47(3)	38(2)	41(2)	9(2)	–1(2)	2(2)
C(21)	50(3)	31(2)	49(2)	7(2)	–1(2)	3(2)
C(22)	44(2)	31(2)	36(2)	6(2)	–4(2)	–1(2)
C(23)	40(3)	47(3)	59(3)	1(2)	–6(2)	–5(2)
C(24)	52(3)	70(4)	59(3)	–10(3)	10(2)	1(3)
C(25)	72(4)	98(5)	51(3)	7(3)	10(3)	–16(4)
C(26)	82(4)	80(4)	64(4)	28(3)	6(3)	–11(3)
C(27)	72(4)	60(3)	64(3)	21(3)	2(3)	2(3)

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Table S5. Hydrogen coordinates (× 10^4) and isotropic displacement parameters (Å^2 × 10^3) for (1)

	x	*y*	*z*	U_{eq}
H(3)	414	5419	8745	80
H(1WA)	–3025	11671	11455	80
H(1WB)	–2608	12830	11932	80
H(2WA)	–4016	6594	9415	80
H(2WB)	–5023	6969	10329	80
H(4A)	–4573	3880	8005	80
H(5A)	–6877	4450	7028	80
H(6A)	–8036	5663	6031	80
H(7A)	–6472	7138	5458	80
H(8A)	–3861	7432	5985	80
H(14A)	699	10173	6768	80
H(15A)	1405	9404	4850	80
H(16A)	1258	7955	3378	80
H(17A)	–31	6239	3561	80
H(18A)	–1198	5968	5189	80
H(24A)	–6378	10654	13140	80
H(25A)	–5911	9373	14321	80
H(26A)	–4172	7954	13848	80
H(27A)	–2932	7849	12174	80