X-ray Data Collection, Structure Determination and Refinement for 1-6. A colorless crystal of **1** with approximate dimensions 0.16 x 0.16 x 0.42 mm was found to have diffraction symmetry $\bar{1}$ and the systematic absences were consistent with the centrosymmetric space group P $\bar{1}$ which was determined to be correct by solution and subsequent refinement of the structure. There were two solvent molecules of THF present per dimeric formula unit. Several carbon atoms were disordered and were included in two components. At convergence, wR2 = 0.1270 and GOF = 1.104 for 731 variables refined against 20777 unique data (As a comparison for refinement on F, R1 = 0.0511 for those 18648 data with $F > 2.0\sigma(F)$).

A colorless crystal of **2** with approximate dimensions 0.23 x 0.23 x 0.33 mm was found to have diffraction symmetry 2/m and the systematic absences were consistent with the centrosymmetric space group C2/c which was determined to be correct by solution and subsequent refinement of the structure. At convergence, wR2 = 0.1442 and GOF = 1.087 for 370 variables refined against 9910 unique data (As a comparison for refinement on F, R1 = 0.0443 for those 9010 data with $F > 2.0\sigma(F)$).

A colorless crystal of **3** with approximate dimensions 0.20 x 0.20 x 0.53 mm was found to have diffraction symmetry 2/m and the systematic absences were consistent with the centrosymmetric space group C2/c which was determined to be correct by solution and subsequent refinement of the structure. At convergence, wR2 = 0.1123 and GOF = 1.071 for 412 variables refined against 9850 unique data (As a comparison for refinement on F, R1 = 0.0528 for those 7932 data with $F > 2.0\sigma(F)$).

A colorless crystal of **4** with approximate dimensions 0.17 x 0.26 x 0.33 mm^3 was was found to have diffraction symmetry *mmm* and the systematic absences were consistent

with the noncentrosymmetric space group $Pca2_1$ which was determined to be correct by solution and subsequent refinement of the structure. At convergence, wR2 = 0.2204 and GOF = 0.990 for 379 variables refined against 14289 unique data (As a comparison for refinement on F, R1 = 0.0810 for those 9949 data with $F > 2.0\sigma(F)$). Several peaks in the difference map were not assignable as atoms. The absolute structure of **3** was not able to be determined by refinement of Flack parameter.[14] The structure was refined using the TWIN command in SHELXTL.

A colorless crystal of **5** with approximate dimensions 0.20 x 0.23 x 0.27 mm^3 was found to have diffraction symmetry was *mmm* and the systematic absences were consistent with the noncentrosymmetric space group $Pca2_1$ which was determined to be correct by solution and subsequent refinement of the structure. At convergence, wR2 = 0.0836 and GOF = 1.093 for 702 variables refined against 18778 unique data (As a comparison for refinement on F, R1 = 0.0410 for those 16128 data with $F > 2.0\sigma(F)$). The absolute structure of **5** was assigned by refinement of Flack parameter.[i]

A colorless crystal of **6** with approximate dimensions 0.16 x 0.16 x 0.42 mm was found to have diffraction symmetry 2/m and the systematic absences were consistent with the centrosymmetric space group $P2_1/m$ which was determined to be correct by solution and subsequent refinement of the structure. At convergence, wR2 = 0.1553 and GOF = 1.069 for 208 variables refined against 5772 unique data (As a comparison for refinement on F, R1 = 0.0616 for those 3124 data with $F > 2.0\sigma(F)$).

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[i] Flack, H. D. *Acta. Cryst.* **1983**, *A39*, 876.

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

Identification code	maa62z	
Empirical formula	$C_{54}\ H_{126}\ Ce_2\ C_{14}\ O_{18}\ Zr_4 \bullet 2(C_4H_8O)$	
Formula weight	1994.68	
Temperature	158(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 12.4147(6) Å	α= 103.8160(10)°.
	b = 19.0034(9) Å	β= 93.9810(10)°.
	c = 19.4922(9) Å	γ = 92.8480(10)°.
Volume	4444.4(4) Å^3	
Z	2	
Density (calculated)	1.491 Mg/m^3	
Absorption coefficient	1.631 mm^{-1}	
F(000)	2036	
Crystal size	0.42 x 0.16 x 0.16 mm^3	
Theta range for data collection	1.08 to 28.34°.	
Index ranges	$-16 \le h \le 16$, $-24 \le k \le 25$, $-26 \le l \le 26$	
Reflections collected	46377	
Independent reflections	20777 [R(int) = 0.0774]	
Completeness to theta = 28.34°	93.6 %	
Absorption correction	Numerical	
Max. and min. transmission	0.7803 and 0.5475	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	20777 / 0 / 731	
Goodness-of-fit on F^2	1.104	
Final R indices [I > 2sigma(I)]	R1 = 0.0511, wR2 = 0.1221	
R indices (all data)	R1 = 0.0580, wR2 = 0.1270	
Extinction coefficient	0.00121(10)	
Largest diff. peak and hole	1.912 and -1.565 e.Å^{-3}	

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

	x	y	z	U(eq)	SOF
Ce(1)	9762(1)	3820(1)	26(1)	21(1)	1.00
Zr(1)	10538(1)	2544(1)	1000(1)	24(1)	1.00
Zr(2)	7909(1)	2791(1)	770(1)	23(1)	1.00
Cl(1)	11044(1)	5118(1)	657(1)	30(1)	1.00
Cl(2)	10752(1)	3372(1)	-1170(1)	40(1)	1.00
O(1)	9436(2)	3498(2)	1198(2)	21(1)	1.00
O(2)	9307(2)	2530(2)	58(2)	22(1)	1.00
O(3)	11301(2)	3317(2)	572(2)	28(1)	1.00
O(4)	7813(2)	3593(2)	190(2)	25(1)	1.00
O(5)	8974(3)	2137(2)	1237(2)	29(1)	1.00
O(6)	6887(3)	2050(2)	206(2)	35(1)	1.00
O(7)	7082(3)	3165(2)	1559(2)	37(1)	1.00
O(8)	11181(3)	1676(2)	546(2)	40(1)	1.00
O(9)	11276(3)	2729(2)	1931(2)	40(1)	1.00
C(1)	9641(4)	4126(3)	1806(2)	31(1)	1.00
C(2)	8913(4)	4724(3)	1723(3)	37(1)	1.00
C(3)	9467(5)	3912(3)	2493(3)	40(1)	1.00
C(4)	9263(4)	1985(3)	-615(2)	29(1)	1.00
C(5)	8455(5)	2174(3)	-1152(3)	38(1)	1.00
C(6)	8988(5)	1225(3)	-522(3)	39(1)	1.00
C(7)	12371(5)	3558(3)	436(3)	34(1)	0.85
C(7')	12490(20)	3323(16)	724(16)	23(5)	0.15
C(8)	12976(5)	3959(4)	1163(4)	57(2)	1.00
C(9)	12952(5)	2933(4)	42(4)	61(2)	1.00
C(10)	6754(4)	3812(4)	8(3)	43(1)	1.00
C(11)	6543(5)	3689(4)	-787(3)	47(1)	1.00
C(12)	6591(6)	4559(4)	416(4)	61(2)	1.00
C(13)	8614(5)	1598(3)	1598(3)	45(1)	1.00
C(14)	8651(7)	1922(4)	2384(3)	63(2)	1.00
C(15)	9220(8)	936(4)	1408(5)	77(3)	1.00
C(16)	6151(5)	1492(4)	-232(4)	48(1)	1.00

C(17)	5876(7)	929(4)	151(4)	68(2)	1.00
C(18)	5177(6)	1837(4)	-471(5)	70(2)	1.00
C(19)	6354(7)	3182(5)	2097(5)	24(2)	0.55
C(19')	6119(19)	3393(13)	1945(13)	83(6)	0.45
C(20)	5368(6)	2713(4)	1803(4)	59(2)	1.00
C(21)	6283(9)	3876(6)	2550(7)	79(4)	0.55
C(21')	5961(9)	4011(6)	2245(7)	52(3)	0.45
C(22)	11676(7)	1013(4)	294(5)	69(2)	1.00
C(23)	12031(7)	973(5)	-436(5)	76(2)	1.00
C(24)	12490(10)	880(6)	802(7)	118(4)	1.00
C(25)	11734(8)	2774(5)	2637(5)	47(2)	0.66
C(25')	12178(18)	2668(11)	2405(12)	51(4)	0.33
Ce(2)	5017(1)	1190(1)	4970(1)	20(1)	1.00
Zr(3)	6809(1)	2745(1)	5705(1)	21(1)	1.00
Zr(4)	4206(1)	2846(1)	6024(1)	21(1)	1.00
Cl(3)	5932(1)	-158(1)	4374(1)	27(1)	1.00
Cl(4)	3745(1)	887(1)	3749(1)	40(1)	1.00
O(10)	5202(2)	2546(2)	5041(2)	21(1)	1.00
O(11)	5543(2)	2094(2)	6142(2)	19(1)	1.00
O(12)	3484(2)	1847(2)	5466(2)	26(1)	1.00
O(13)	6925(2)	1687(2)	5080(2)	26(1)	1.00
O(14)	5733(3)	3509(2)	6258(2)	27(1)	1.00
O(15)	3322(3)	3529(2)	5698(2)	37(1)	1.00
O(16)	3680(3)	2921(2)	6938(2)	32(1)	1.00
O(17)	7500(3)	3340(2)	5159(2)	34(1)	1.00
O(18)	7914(3)	2811(2)	6456(2)	30(1)	1.00
C(26)	12441(8)	3455(6)	2898(5)	92(3)	1.00
C(27)	12362(11)	2097(6)	2605(7)	76(3)	0.66
C(27')	11916(11)	2145(6)	2813(7)	83(8)	0.33
C(28)	4900(4)	2745(3)	4380(3)	32(1)	1.00
C(29)	5595(3)	2375(2)	3801(2)	42(1)	1.00
C(30)	5008(3)	3566(2)	4471(2)	44(1)	1.00
C(31)	5668(3)	1766(2)	6748(2)	23(1)	1.00
C(32)	5992(4)	2337(3)	7429(2)	30(1)	1.00
C(33)	6502(4)	1201(3)	6616(3)	33(1)	1.00
C(34)	2398(4)	1498(3)	5297(3)	37(1)	1.00

C(35)	1933(3)	1428(3)	5981(3)	52(2)	1.00
C(36)	1710(3)	1914(3)	4878(3)	56(2)	1.00
C(37)	7975(5)	1494(4)	4861(3)	27(1)	0.75
C(37')	7712(5)	1207(4)	4625(3)	44(5)	0.25
C(38)	8409(4)	927(3)	5208(3)	42(1)	1.00
C(39)	7928(6)	1266(4)	4072(4)	47(2)	0.75
C(39')	8538(6)	1819(4)	4445(4)	48(5)	0.25
C(40)	6097(5)	4238(3)	6633(3)	41(1)	1.00
C(41)	5836(5)	4774(3)	6201(3)	62(2)	1.00
C(42)	5725(5)	4409(3)	7354(3)	71(2)	1.00
C(43)	2728(6)	4133(4)	5628(4)	35(2)	0.70
C(43')	2243(6)	3868(4)	5660(4)	47(4)	0.30
C(44)	2114(6)	3983(4)	4925(3)	56(2)	0.70
C(44')	1772(6)	3775(4)	4950(3)	53(5)	0.30
C(45)	2068(6)	4309(4)	6301(3)	61(3)	0.70
C(45')	2325(6)	4539(4)	6204(3)	44(4)	0.30
C(46)	3032(5)	2996(3)	7523(3)	42(1)	1.00
C(47)	3098(4)	2344(3)	7839(3)	60(2)	1.00
C(48)	3368(4)	3709(3)	8062(3)	63(2)	1.00
C(49)	8160(5)	3839(4)	4914(4)	57(2)	1.00
C(50)	8944(5)	4273(4)	5506(3)	67(2)	1.00
C(51)	8687(5)	3443(4)	4272(3)	135(6)	1.00
C(52)	8746(4)	2927(3)	7020(3)	33(1)	1.00
C(53)	8762(4)	3701(4)	7458(3)	76(3)	1.00
C(54)	9805(4)	2724(4)	6723(3)	81(3)	1.00
O(19)	595(13)	307(9)	3243(9)	214(6)	1.00
C(55)	-503(16)	-199(11)	3023(11)	165(6)	1.00
C(56)	-298(14)	-847(10)	2564(10)	149(6)	1.00
C(57)	893(15)	-856(10)	2586(10)	81(4)	0.55
C(57')	381(19)	-569(13)	2162(13)	86(6)	0.45
C(58)	1225(14)	-36(10)	2548(10)	76(4)	0.55
C(58')	1270(20)	-210(15)	2830(15)	90(7)	0.45
O(20)	4704(12)	363(7)	7747(7)	184(5)	1.00
C(61)	5211(15)	-296(11)	8050(10)	168(7)	1.00
C(62)	4038(11)	-796(8)	7870(8)	118(4)	1.00
C(63)	3251(13)	-309(10)	7857(9)	141(5)	1.00

C(64)	3590(20)	332(13)	7749(12)	200(9)	1.00

Table 3. Bond lengths [Å] and angles [°] for (1).

Ce(1)-O(3)	2.466(3)
Ce(1)-O(4)	2.493(3)
Ce(1)-O(2)	2.506(3)
Ce(1)-O(1)	2.556(3)
Ce(1)-Cl(2)	2.6875(12)
Ce(1)-Cl(1)	2.8313(11)
Ce(1)-Cl(1)#1	2.8531(11)
Ce(1)-Zr(1)	3.5475(5)
Ce(1)-Zr(2)	3.5484(5)
Zr(1)-O(8)	1.917(4)
Zr(1)-O(9)	1.921(4)
Zr(1)-O(3)	2.075(3)
Zr(1)-O(5)	2.176(3)
Zr(1)-O(2)	2.299(3)
Zr(1)-O(1)	2.300(3)
Zr(1)-Zr(2)	3.3347(6)
Zr(2)-O(6)	1.920(3)
Zr(2)-O(7)	1.922(3)
Zr(2)-O(4)	2.106(3)
Zr(2)-O(5)	2.158(3)
Zr(2)-O(1)	2.256(3)
Zr(2)-O(2)	2.296(3)
Cl(1)-Ce(1)#1	2.8531(11)
O(1)-C(1)	1.465(5)
O(2)-C(4)	1.460(5)
O(3)-C(7)	1.445(7)
O(3)-C(7')	1.49(3)
O(4)-C(10)	1.445(5)
O(5)-C(13)	1.444(6)
O(6)-C(16)	1.433(7)
O(7)-C(19)	1.427(9)
O(7)-C(19')	1.49(2)
O(8)-C(22)	1.425(7)
O(9)-C(25')	1.43(2)

O(9)-C(25)	1.434(10)
C(1)-C(3)	1.514(7)
C(1)-C(2)	1.518(7)
C(4)-C(5)	1.517(7)
C(4)-C(6)	1.523(7)
C(7)-C(9)	1.499(9)
C(7)-C(8)	1.559(9)
C(7')-C(8)	1.38(3)
C(7')-C(9)	1.52(3)
C(10)-C(12)	1.484(9)
C(10)-C(11)	1.514(8)
C(13)-C(15)	1.481(10)
C(13)-C(14)	1.506(9)
C(16)-C(17)	1.483(9)
C(16)-C(18)	1.501(10)
C(19)-C(21)	1.412(13)
C(19)-C(20)	1.474(11)
C(19')-C(21')	1.21(2)
C(19')-C(20)	1.51(2)
C(22)-C(24)	1.438(13)
C(22)-C(23)	1.506(12)
C(25)-C(26)	1.489(13)
C(25)-C(27)	1.527(15)
C(25')-C(27')	1.45(2)
C(25')-C(26)	1.58(2)
Ce(2)-O(12)	2.455(3)
Ce(2)-O(13)	2.483(3)
Ce(2)-O(11)	2.532(3)
Ce(2)-O(10)	2.547(3)
Ce(2)-Cl(4)	2.6868(12)
Ce(2)-Cl(3)#2	2.8364(11)
Ce(2)-Cl(3)	2.8726(11)
Ce(2)-Zr(3)	3.5527(5)
Ce(2)-Zr(4)	3.5576(5)
Zr(3)-O(18)	1.913(3)
Zr(3)-O(17)	1.937(3)

Zr(3)-O(13)	2.105(3)
Zr(3)-O(14)	2.168(3)
Zr(3)-O(10)	2.265(3)
Zr(3)-O(11)	2.285(3)
Zr(3)-Zr(4)	3.3388(6)
Zr(4)-O(16)	1.917(3)
Zr(4)-O(15)	1.931(3)
Zr(4)-O(12)	2.075(3)
Zr(4)-O(14)	2.181(3)
Zr(4)-O(11)	2.278(3)
Zr(4)-O(10)	2.323(3)
Cl(3)-Ce(2)#2	2.8364(11)
O(10)-C(28)	1.457(5)
O(11)-C(31)	1.463(5)
O(12)-C(34)	1.453(5)
O(13)-C(37)	1.438(6)
O(13)-C(37')	1.548(6)
O(14)-C(40)	1.437(6)
O(15)-C(43)	1.424(7)
O(15)-C(43')	1.520(8)
O(16)-C(46)	1.424(6)
O(17)-C(49)	1.412(6)
O(18)-C(52)	1.424(6)
C(28)-C(30)	1.525(6)
C(28)-C(29)	1.526(7)
C(31)-C(32)	1.516(6)
C(31)-C(33)	1.519(6)
C(34)-C(36)	1.516(7)
C(34)-C(35)	1.522(7)
C(37)-C(39)	1.490(10)
C(37)-C(38)	1.506(8)
C(37')-C(38)	1.589(8)
C(37')-C(39')	1.628(10)
C(40)-C(42)	1.478(8)
C(40)-C(41)	1.501(8)
C(43)-C(44)	1.479(9)

C(43)-C(45)	1.573(10)
C(43')-C(44')	1.432(9)
C(43')-C(45')	1.445(10)
C(46)-C(47)	1.514(8)
C(46)-C(48)	1.523(8)
C(49)-C(50)	1.506(9)
C(49)-C(51)	1.508(10)
C(52)-C(54)	1.504(8)
C(52)-C(53)	1.511(8)
O(19)-C(58')	1.45(3)
O(19)-C(55)	1.60(2)
O(19)-C(58)	1.63(2)
C(55)-C(56)	1.38(2)
C(56)-C(57')	1.36(3)
C(56)-C(57)	1.48(2)
C(57')-C(58)	1.45(3)
C(57)-C(58')	1.26(3)
O(20)-C(64)	1.39(2)
O(20)-C(61)	1.64(2)
C(61)-C(62)	1.67(2)
C(62)-C(63)	1.382(19)
C(63)-C(64)	1.34(2)

O(3)-Ce(1)-O(4)	126.13(10)
O(3)-Ce(1)-O(2)	69.06(10)
O(4)-Ce(1)-O(2)	67.83(10)
O(3)-Ce(1)-O(1)	64.78(10)
O(4)-Ce(1)-O(1)	66.23(10)
O(2)-Ce(1)-O(1)	59.54(9)
O(3)-Ce(1)-Cl(2)	83.71(8)
O(4)-Ce(1)-Cl(2)	126.89(8)
O(2)-Ce(1)-Cl(2)	90.63(7)
O(1)-Ce(1)-Cl(2)	142.06(7)
O(3)-Ce(1)-Cl(1)	80.06(8)
O(4)-Ce(1)-Cl(1)	125.34(8)
O(2)-Ce(1)-Cl(1)	146.01(7)

O(1)-Ce(1)-Cl(1)	94.99(7)
Cl(2)-Ce(1)-Cl(1)	100.00(4)
O(3)-Ce(1)-Cl(1)#1	149.47(8)
O(4)-Ce(1)-Cl(1)#1	83.14(7)
O(2)-Ce(1)-Cl(1)#1	138.92(7)
O(1)-Ce(1)-Cl(1)#1	133.69(7)
Cl(2)-Ce(1)-Cl(1)#1	84.06(4)
Cl(1)-Ce(1)-Cl(1)#1	74.68(3)
O(3)-Ce(1)-Zr(1)	34.85(7)
O(4)-Ce(1)-Zr(1)	91.73(7)
O(2)-Ce(1)-Zr(1)	40.20(7)
O(1)-Ce(1)-Zr(1)	40.31(7)
Cl(2)-Ce(1)-Zr(1)	101.83(3)
Cl(1)-Ce(1)-Zr(1)	105.81(2)
Cl(1)#1-Ce(1)-Zr(1)	173.82(3)
O(3)-Ce(1)-Zr(2)	90.66(7)
O(4)-Ce(1)-Zr(2)	35.68(7)
O(2)-Ce(1)-Zr(2)	40.12(7)
O(1)-Ce(1)-Zr(2)	39.31(6)
Cl(2)-Ce(1)-Zr(2)	127.50(3)
Cl(1)-Ce(1)-Zr(2)	130.38(3)
Cl(1)#1-Ce(1)-Zr(2)	118.79(3)
Zr(1)-Ce(1)-Zr(2)	56.061(11)
O(8)-Zr(1)-O(9)	100.09(17)
O(8)-Zr(1)-O(3)	101.96(15)
O(9)-Zr(1)-O(3)	102.26(15)
O(8)-Zr(1)-O(5)	103.00(15)
O(9)-Zr(1)-O(5)	98.67(14)
O(3)-Zr(1)-O(5)	143.83(12)
O(8)-Zr(1)-O(2)	95.19(14)
O(9)-Zr(1)-O(2)	163.65(14)
O(3)-Zr(1)-O(2)	80.04(12)
O(5)-Zr(1)-O(2)	72.02(11)
O(8)-Zr(1)-O(1)	161.44(14)
O(9)-Zr(1)-O(1)	98.38(14)
O(3)-Zr(1)-O(1)	75.72(11)

O(5)-Zr(1)-O(1)	72.28(11)
O(2)-Zr(1)-O(1)	66.25(10)
O(8)-Zr(1)-Zr(2)	123.44(12)
O(9)-Zr(1)-Zr(2)	121.32(12)
O(3)-Zr(1)-Zr(2)	104.42(8)
O(5)-Zr(1)-Zr(2)	39.49(8)
O(2)-Zr(1)-Zr(2)	43.44(7)
O(1)-Zr(1)-Zr(2)	42.43(7)
O(8)-Zr(1)-Ce(1)	120.57(12)
O(9)-Zr(1)-Ce(1)	128.26(12)
O(3)-Zr(1)-Ce(1)	42.76(8)
O(5)-Zr(1)-Ce(1)	101.44(8)
O(2)-Zr(1)-Ce(1)	44.71(8)
O(1)-Zr(1)-Ce(1)	45.96(7)
Zr(2)-Zr(1)-Ce(1)	61.982(10)
O(6)-Zr(2)-O(7)	100.22(16)
O(6)-Zr(2)-O(4)	100.70(14)
O(7)-Zr(2)-O(4)	102.63(15)
O(6)-Zr(2)-O(5)	100.51(14)
O(7)-Zr(2)-O(5)	100.04(15)
O(4)-Zr(2)-O(5)	145.46(12)
O(6)-Zr(2)-O(1)	163.11(13)
O(7)-Zr(2)-O(1)	96.40(13)
O(4)-Zr(2)-O(1)	78.37(11)
O(5)-Zr(2)-O(1)	73.48(12)
O(6)-Zr(2)-O(2)	96.19(13)
O(7)-Zr(2)-O(2)	162.99(13)
O(4)-Zr(2)-O(2)	78.49(11)
O(5)-Zr(2)-O(2)	72.39(11)
O(1)-Zr(2)-O(2)	67.02(11)
O(6)-Zr(2)-Zr(1)	122.70(11)
O(7)-Zr(2)-Zr(1)	121.56(11)
O(4)-Zr(2)-Zr(1)	105.60(8)
O(5)-Zr(2)-Zr(1)	39.88(8)
O(1)-Zr(2)-Zr(1)	43.47(7)
O(2)-Zr(2)-Zr(1)	43.51(7)

O(6)-Zr(2)-Ce(1)	123.07(11)
O(7)-Zr(2)-Ce(1)	125.94(12)
O(4)-Zr(2)-Ce(1)	43.65(8)
O(5)-Zr(2)-Ce(1)	101.81(8)
O(1)-Zr(2)-Ce(1)	45.86(7)
O(2)-Zr(2)-Ce(1)	44.69(8)
Zr(1)-Zr(2)-Ce(1)	61.956(11)
Ce(1)-Cl(1)-Ce(1)#1	105.32(3)
C(1)-O(1)-Zr(2)	130.7(3)
C(1)-O(1)-Zr(1)	122.6(3)
Zr(2)-O(1)-Zr(1)	94.10(11)
C(1)-O(1)-Ce(1)	112.3(2)
Zr(2)-O(1)-Ce(1)	94.83(10)
Zr(1)-O(1)-Ce(1)	93.73(10)
C(4)-O(2)-Zr(2)	126.2(3)
C(4)-O(2)-Zr(1)	123.1(3)
Zr(2)-O(2)-Zr(1)	93.06(11)
C(4)-O(2)-Ce(1)	116.8(2)
Zr(2)-O(2)-Ce(1)	95.19(11)
Zr(1)-O(2)-Ce(1)	95.09(11)
C(7)-O(3)-C(7')	31.9(11)
C(7)-O(3)-Zr(1)	140.4(3)
C(7')-O(3)-Zr(1)	109.4(12)
C(7)-O(3)-Ce(1)	116.7(3)
C(7')-O(3)-Ce(1)	148.2(12)
Zr(1)-O(3)-Ce(1)	102.39(12)
C(10)-O(4)-Zr(2)	118.0(3)
C(10)-O(4)-Ce(1)	141.3(3)
Zr(2)-O(4)-Ce(1)	100.67(11)
C(13)-O(5)-Zr(2)	124.4(3)
C(13)-O(5)-Zr(1)	135.0(3)
Zr(2)-O(5)-Zr(1)	100.63(12)
C(16)-O(6)-Zr(2)	178.1(4)
C(19)-O(7)-C(19')	24.6(9)
C(19)-O(7)-Zr(2)	160.1(4)
C(19')-O(7)-Zr(2)	158.3(10)

C(22)-O(8)-Zr(1)	172.8(5)
C(25')-O(9)-C(25)	30.1(8)
C(25')-O(9)-Zr(1)	151.9(10)
C(25)-O(9)-Zr(1)	171.5(5)
O(1)-C(1)-C(3)	111.0(4)
O(1)-C(1)-C(2)	110.4(4)
C(3)-C(1)-C(2)	110.0(4)
O(2)-C(4)-C(5)	110.3(4)
O(2)-C(4)-C(6)	111.5(4)
C(5)-C(4)-C(6)	110.8(4)
O(3)-C(7)-C(9)	110.9(5)
O(3)-C(7)-C(8)	107.7(5)
C(9)-C(7)-C(8)	113.3(6)
C(8)-C(7')-O(3)	115(2)
C(8)-C(7')-C(9)	123(2)
O(3)-C(7')-C(9)	107.3(19)
C(7')-C(8)-C(7)	31.1(12)
C(7)-C(9)-C(7')	31.0(11)
O(4)-C(10)-C(12)	111.4(5)
O(4)-C(10)-C(11)	110.8(5)
C(12)-C(10)-C(11)	114.5(5)
O(5)-C(13)-C(15)	111.3(5)
O(5)-C(13)-C(14)	110.5(5)
C(15)-C(13)-C(14)	113.5(6)
O(6)-C(16)-C(17)	110.4(5)
O(6)-C(16)-C(18)	108.7(5)
C(17)-C(16)-C(18)	113.1(6)
C(21)-C(19)-O(7)	114.4(7)
C(21)-C(19)-C(20)	120.6(8)
O(7)-C(19)-C(20)	110.0(6)
C(21')-C(19')-O(7)	125.4(19)
C(21')-C(19')-C(20)	129.4(19)
O(7)-C(19')-C(20)	104.8(15)
C(19)-C(20)-C(19')	24.0(9)
O(8)-C(22)-C(24)	112.5(8)
O(8)-C(22)-C(23)	109.9(6)

C(24)-C(22)-C(23)	115.5(8)
O(9)-C(25)-C(26)	110.0(7)
O(9)-C(25)-C(27)	106.8(8)
C(26)-C(25)-C(27)	112.1(9)
O(9)-C(25')-C(27')	110.9(15)
O(9)-C(25')-C(26)	105.4(14)
C(27')-C(25')-C(26)	111.5(16)
O(12)-Ce(2)-O(13)	126.10(10)
O(12)-Ce(2)-O(11)	67.16(10)
O(13)-Ce(2)-O(11)	67.13(10)
O(12)-Ce(2)-O(10)	66.32(10)
O(13)-Ce(2)-O(10)	66.64(10)
O(11)-Ce(2)-O(10)	59.31(9)
O(12)-Ce(2)-Cl(4)	84.21(8)
O(13)-Ce(2)-Cl(4)	123.44(8)
O(11)-Ce(2)-Cl(4)	146.24(7)
O(10)-Ce(2)-Cl(4)	93.63(7)
O(12)-Ce(2)-Cl(3)#2	79.77(8)
O(13)-Ce(2)-Cl(3)#2	129.31(8)
O(11)-Ce(2)-Cl(3)#2	93.01(7)
O(10)-Ce(2)-Cl(3)#2	142.17(7)
Cl(4)-Ce(2)-Cl(3)#2	99.34(4)
O(12)-Ce(2)-Cl(3)	149.65(8)
O(13)-Ce(2)-Cl(3)	83.26(8)
O(11)-Ce(2)-Cl(3)	129.06(7)
O(10)-Ce(2)-Cl(3)	142.62(7)
Cl(4)-Ce(2)-Cl(3)	84.63(4)
Cl(3)#2-Ce(2)-Cl(3)	74.34(3)
O(12)-Ce(2)-Zr(3)	90.57(7)
O(13)-Ce(2)-Zr(3)	35.54(7)
O(11)-Ce(2)-Zr(3)	39.85(6)
O(10)-Ce(2)-Zr(3)	39.42(7)
Cl(4)-Ce(2)-Zr(3)	128.39(3)
Cl(3)#2-Ce(2)-Zr(3)	130.19(3)
Cl(3)-Ce(2)-Zr(3)	118.25(2)
O(12)-Ce(2)-Zr(4)	34.60(7)

O(13)-Ce(2)-Zr(4)	91.55(7)
O(11)-Ce(2)-Zr(4)	39.62(6)
O(10)-Ce(2)-Zr(4)	40.67(7)
Cl(4)-Ce(2)-Zr(4)	106.79(3)
Cl(3)#2-Ce(2)-Zr(4)	101.51(2)
Cl(3)-Ce(2)-Zr(4)	168.45(3)
Zr(3)-Ce(2)-Zr(4)	56.012(10)
O(18)-Zr(3)-O(17)	100.44(15)
O(18)-Zr(3)-O(13)	102.32(14)
O(17)-Zr(3)-O(13)	102.41(14)
O(18)-Zr(3)-O(14)	99.30(14)
O(17)-Zr(3)-O(14)	99.90(14)
O(13)-Zr(3)-O(14)	145.34(12)
O(18)-Zr(3)-O(10)	163.05(13)
O(17)-Zr(3)-O(10)	95.90(13)
O(13)-Zr(3)-O(10)	78.35(11)
O(14)-Zr(3)-O(10)	73.24(12)
O(18)-Zr(3)-O(11)	96.35(12)
O(17)-Zr(3)-O(11)	162.61(13)
O(13)-Zr(3)-O(11)	78.21(11)
O(14)-Zr(3)-O(11)	72.72(11)
O(10)-Zr(3)-O(11)	67.04(10)
O(18)-Zr(3)-Zr(4)	121.21(10)
O(17)-Zr(3)-Zr(4)	122.10(11)
O(13)-Zr(3)-Zr(4)	105.34(8)
O(14)-Zr(3)-Zr(4)	40.00(8)
O(10)-Zr(3)-Zr(4)	44.00(7)
O(11)-Zr(3)-Zr(4)	42.90(7)
O(18)-Zr(3)-Ce(2)	124.68(10)
O(17)-Zr(3)-Ce(2)	124.72(11)
O(13)-Zr(3)-Ce(2)	43.27(8)
O(14)-Zr(3)-Ce(2)	102.06(8)
O(10)-Zr(3)-Ce(2)	45.57(7)
O(11)-Zr(3)-Ce(2)	45.23(7)
Zr(4)-Zr(3)-Ce(2)	62.067(11)
O(16)-Zr(4)-O(15)	99.42(15)

O(16)-Zr(4)-O(12)	101.19(15)
O(15)-Zr(4)-O(12)	103.09(15)
O(16)-Zr(4)-O(14)	103.61(14)
O(15)-Zr(4)-O(14)	98.50(14)
O(12)-Zr(4)-O(14)	143.73(12)
O(16)-Zr(4)-O(11)	96.94(12)
O(15)-Zr(4)-O(11)	162.88(13)
O(12)-Zr(4)-O(11)	78.51(11)
O(14)-Zr(4)-O(11)	72.60(11)
O(16)-Zr(4)-O(10)	163.11(12)
O(15)-Zr(4)-O(10)	97.36(13)
O(12)-Zr(4)-O(10)	76.73(11)
O(14)-Zr(4)-O(10)	71.84(11)
O(11)-Zr(4)-O(10)	66.18(10)
O(16)-Zr(4)-Zr(3)	124.22(10)
O(15)-Zr(4)-Zr(3)	121.43(12)
O(12)-Zr(4)-Zr(3)	104.08(8)
O(14)-Zr(4)-Zr(3)	39.70(8)
O(11)-Zr(4)-Zr(3)	43.06(7)
O(10)-Zr(4)-Zr(3)	42.62(7)
O(16)-Zr(4)-Ce(2)	122.69(11)
O(15)-Zr(4)-Ce(2)	126.35(12)
O(12)-Zr(4)-Ce(2)	42.22(8)
O(14)-Zr(4)-Ce(2)	101.62(8)
O(11)-Zr(4)-Ce(2)	45.12(7)
O(10)-Zr(4)-Ce(2)	45.58(7)
Zr(3)-Zr(4)-Ce(2)	61.921(10)
Ce(2)#2-Cl(3)-Ce(2)	105.66(3)
C(28)-O(10)-Zr(3)	129.3(3)
C(28)-O(10)-Zr(4)	122.4(3)
Zr(3)-O(10)-Zr(4)	93.38(11)
C(28)-O(10)-Ce(2)	114.8(3)
Zr(3)-O(10)-Ce(2)	95.01(10)
Zr(4)-O(10)-Ce(2)	93.75(10)
C(31)-O(11)-Zr(4)	122.3(2)
C(31)-O(11)-Zr(3)	128.7(2)

Zr(4)-O(11)-Zr(3)	94.04(10)
C(31)-O(11)-Ce(2)	114.1(2)
Zr(4)-O(11)-Ce(2)	95.25(10)
Zr(3)-O(11)-Ce(2)	94.92(10)
C(34)-O(12)-Zr(4)	137.6(3)
C(34)-O(12)-Ce(2)	119.2(3)
Zr(4)-O(12)-Ce(2)	103.18(12)
C(37)-O(13)-C(37')	25.83(11)
C(37)-O(13)-Zr(3)	117.2(3)
C(37')-O(13)-Zr(3)	141.8(3)
C(37)-O(13)-Ce(2)	141.6(3)
C(37')-O(13)-Ce(2)	116.3(3)
Zr(3)-O(13)-Ce(2)	101.19(11)
C(40)-O(14)-Zr(3)	122.6(3)
C(40)-O(14)-Zr(4)	137.1(3)
Zr(3)-O(14)-Zr(4)	100.30(12)
C(43)-O(15)-C(43')	30.60(15)
C(43)-O(15)-Zr(4)	166.2(4)
C(43')-O(15)-Zr(4)	149.5(4)
C(46)-O(16)-Zr(4)	165.2(3)
C(49)-O(17)-Zr(3)	166.3(4)
C(52)-O(18)-Zr(3)	174.9(3)
C(25)-C(26)-C(25')	27.8(8)
O(10)-C(28)-C(30)	111.6(4)
O(10)-C(28)-C(29)	110.3(4)
C(30)-C(28)-C(29)	109.9(4)
O(11)-C(31)-C(32)	111.2(4)
O(11)-C(31)-C(33)	109.8(3)
C(32)-C(31)-C(33)	110.5(4)
O(12)-C(34)-C(36)	110.1(4)
O(12)-C(34)-C(35)	108.8(4)
C(36)-C(34)-C(35)	113.4(4)
O(13)-C(37)-C(39)	109.8(5)
O(13)-C(37)-C(38)	111.4(4)
C(39)-C(37)-C(38)	112.6(6)
O(13)-C(37')-C(38)	101.7(4)

O(13)-C(37')-C(39')	101.4(5)
C(38)-C(37')-C(39')	102.8(5)
C(37)-C(38)-C(37')	25.05(13)
O(14)-C(40)-C(42)	110.7(4)
O(14)-C(40)-C(41)	111.5(4)
C(42)-C(40)-C(41)	115.2(5)
O(15)-C(43)-C(44)	110.7(6)
O(15)-C(43)-C(45)	104.9(5)
C(44)-C(43)-C(45)	117.6(6)
C(44')-C(43')-C(45')	125.3(7)
C(44')-C(43')-O(15)	113.1(5)
C(45')-C(43')-O(15)	107.2(6)
O(16)-C(46)-C(47)	110.5(4)
O(16)-C(46)-C(48)	109.5(4)
C(47)-C(46)-C(48)	112.7(5)
O(17)-C(49)-C(50)	110.6(5)
O(17)-C(49)-C(51)	109.5(6)
C(50)-C(49)-C(51)	114.2(6)
O(18)-C(52)-C(54)	109.4(4)
O(18)-C(52)-C(53)	109.5(4)
C(54)-C(52)-C(53)	114.0(5)
C(58')-O(19)-C(55)	95.2(16)
C(58')-O(19)-C(58)	25.7(11)
C(55)-O(19)-C(58)	97.6(14)
C(56)-C(55)-O(19)	109.6(16)
C(57')-C(56)-C(55)	97.9(18)
C(57')-C(56)-C(57)	52.1(13)
C(55)-C(56)-C(57)	105.6(17)
C(56)-C(57')-C(58)	116(2)
C(58')-C(57)-C(56)	106.7(19)
C(57')-C(58)-O(19)	98.8(15)
C(57)-C(58')-O(19)	119(2)
C(64)-O(20)-C(61)	111.1(15)
O(20)-C(61)-C(62)	92.3(12)
C(63)-C(62)-C(61)	105.6(13)
C(64)-C(63)-C(62)	116.0(18)

C(63)-C(64)-O(20)	108(2)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for (1). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ce(1)	21(1)	23(1)	21(1)	9(1)	2(1)	0(1)
Zr(1)	25(1)	26(1)	23(1)	10(1)	-1(1)	4(1)
Zr(2)	21(1)	25(1)	22(1)	7(1)	4(1)	-2(1)
Cl(1)	32(1)	27(1)	33(1)	13(1)	-9(1)	-4(1)
Cl(2)	39(1)	57(1)	31(1)	18(1)	14(1)	13(1)
O(1)	21(1)	22(1)	18(1)	2(1)	1(1)	-2(1)
O(2)	25(1)	23(2)	19(1)	4(1)	2(1)	2(1)
O(3)	20(1)	32(2)	35(2)	14(1)	3(1)	3(1)
O(4)	19(1)	28(2)	29(2)	10(1)	1(1)	4(1)
O(5)	33(2)	29(2)	29(2)	16(1)	2(1)	-2(1)
O(6)	31(2)	34(2)	37(2)	7(2)	-2(1)	-10(1)
O(7)	27(2)	49(2)	32(2)	4(2)	14(1)	-2(2)
O(8)	42(2)	32(2)	47(2)	11(2)	7(2)	13(2)
O(9)	35(2)	53(2)	33(2)	19(2)	-8(2)	2(2)
C(1)	31(2)	34(2)	23(2)	1(2)	1(2)	-5(2)
C(2)	42(3)	31(3)	33(3)	-3(2)	6(2)	0(2)
C(3)	46(3)	54(3)	20(2)	5(2)	5(2)	5(3)
C(4)	35(2)	26(2)	23(2)	-2(2)	3(2)	2(2)
C(5)	44(3)	46(3)	21(2)	3(2)	-1(2)	5(2)
C(6)	49(3)	28(2)	35(3)	-4(2)	4(2)	3(2)
C(8)	29(3)	60(4)	78(5)	22(4)	-17(3)	-9(3)
C(9)	38(3)	65(4)	83(5)	19(4)	23(3)	10(3)
C(10)	27(2)	57(4)	45(3)	12(3)	-4(2)	16(2)
C(11)	35(3)	61(4)	46(3)	18(3)	-10(2)	5(3)
C(12)	60(4)	65(4)	58(4)	10(3)	-3(3)	30(4)
C(13)	58(3)	39(3)	44(3)	25(3)	7(3)	-8(3)
C(14)	102(6)	58(4)	40(3)	28(3)	21(4)	2(4)
C(15)	135(8)	34(3)	74(5)	32(4)	28(5)	7(4)
C(16)	40(3)	49(3)	49(3)	2(3)	1(3)	-14(3)
C(17)	78(5)	51(4)	69(5)	12(4)	3(4)	-28(4)
C(18)	44(4)	62(5)	92(6)	5(4)	-24(4)	-10(3)

C(22)	70(5)	54(4)	85(6)	11(4)	8(4)	34(4)
C(23)	66(5)	70(5)	80(6)	-11(4)	22(4)	17(4)
C(24)	140(10)	105(8)	122(9)	39(7)	12(8)	88(8)
Ce(2)	20(1)	17(1)	21(1)	3(1)	1(1)	2(1)
Zr(3)	19(1)	21(1)	23(1)	7(1)	1(1)	0(1)
Zr(4)	20(1)	21(1)	23(1)	4(1)	2(1)	6(1)
Cl(3)	29(1)	21(1)	31(1)	5(1)	10(1)	4(1)
Cl(4)	44(1)	41(1)	31(1)	4(1)	-11(1)	6(1)
O(10)	23(1)	23(1)	20(1)	9(1)	2(1)	2(1)
O(11)	19(1)	20(1)	18(1)	6(1)	1(1)	3(1)
O(12)	16(1)	27(2)	34(2)	4(1)	2(1)	2(1)
O(13)	20(1)	29(2)	28(2)	7(1)	6(1)	5(1)
O(14)	28(2)	15(1)	34(2)	1(1)	1(1)	1(1)
O(15)	36(2)	37(2)	42(2)	14(2)	1(2)	17(2)
O(16)	28(2)	43(2)	25(2)	4(2)	7(1)	9(1)
O(17)	32(2)	38(2)	37(2)	18(2)	7(1)	-4(1)
O(18)	23(2)	36(2)	31(2)	7(1)	-4(1)	-2(1)
C(26)	80(6)	130(9)	49(4)	2(5)	-22(4)	-30(6)
C(28)	32(2)	40(3)	26(2)	15(2)	-5(2)	0(2)
C(29)	51(3)	54(3)	21(2)	13(2)	2(2)	-4(3)
C(30)	48(3)	36(3)	54(4)	27(3)	1(3)	6(2)
C(31)	23(2)	29(2)	20(2)	12(2)	2(2)	0(2)
C(32)	31(2)	41(3)	19(2)	9(2)	-1(2)	1(2)
C(33)	33(2)	34(3)	37(3)	18(2)	-6(2)	7(2)
C(34)	19(2)	35(3)	50(3)	1(2)	-1(2)	-3(2)
C(35)	30(3)	59(4)	69(4)	15(3)	21(3)	1(3)
C(36)	29(3)	63(4)	79(5)	25(4)	-14(3)	2(3)
C(38)	25(2)	46(3)	54(3)	9(3)	5(2)	14(2)
C(40)	48(3)	24(2)	44(3)	-1(2)	-9(2)	-3(2)
C(41)	79(5)	25(3)	78(5)	10(3)	-1(4)	0(3)
C(42)	96(6)	45(4)	57(4)	-13(3)	16(4)	-15(4)
C(46)	36(3)	53(3)	37(3)	9(3)	14(2)	8(2)
C(47)	54(4)	85(5)	51(4)	28(4)	22(3)	12(4)
C(48)	58(4)	76(5)	46(4)	-7(3)	24(3)	-2(3)
C(49)	49(3)	71(5)	60(4)	40(4)	1(3)	-18(3)
C(50)	50(4)	66(5)	88(6)	38(4)	-6(4)	-27(3)

C(51)	126(9)	186(13)	76(7)	2(7)	58(7)	-80(9)
C(52)	28(2)	42(3)	31(2)	14(2)	-6(2)	-2(2)
C(53)	78(5)	66(5)	68(5)	-6(4)	-38(4)	16(4)
C(54)	32(3)	128(8)	69(5)	-2(5)	-11(3)	14(4)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (1).

	x	y	z	U(eq)
H(1A)	10411	4316	1825	37
H(2A)	9033	4860	1279	55
H(2B)	9082	5148	2123	55
H(2C)	8154	4550	1715	55
H(3A)	9938	3525	2541	61
H(3B)	8710	3739	2489	61
H(3C)	9642	4335	2893	61
H(4A)	9995	1992	-799	35
H(5A)	8648	2663	-1206	57
H(5B)	7728	2157	-989	57
H(5C)	8468	1822	-1610	57
H(6A)	9519	1114	-173	59
H(6B)	9005	870	-977	59
H(6C)	8264	1202	-355	59
H(7A)	12294	3914	135	40
H(7'A)	12562	2968	1027	28
H(8A)	12562	4362	1392	85
H(8B)	13695	4148	1085	85
H(8C)	13054	3619	1467	85
H(8D)	12566	4122	1577	85
H(8E)	12996	4331	891	85
H(8F)	13717	3877	1320	85
H(9A)	12534	2704	-408	91
H(9B)	13032	2576	328	91
H(9C)	13668	3110	-51	91
H(9D)	12491	2492	-180	91
H(9E)	13687	2801	147	91
H(9F)	12967	3255	-282	91
H(10A)	6217	3481	159	51
H(11A)	6651	3182	-1016	71

H(11B)	7044	4011	-958	71
H(11C)	5796	3794	-902	71
H(12A)	6732	4591	924	92
H(12B)	5843	4673	318	92
H(12C)	7089	4906	276	92
H(13A)	7839	1453	1426	53
H(14A)	8225	2350	2474	95
H(14B)	9403	2064	2574	95
H(14C)	8349	1562	2617	95
H(15A)	9155	749	892	115
H(15B)	8921	566	1630	115
H(15C)	9984	1055	1577	115
H(16A)	6516	1257	-661	58
H(17A)	6542	729	299	101
H(17B)	5401	539	-163	101
H(17C)	5505	1147	570	101
H(18A)	5406	2200	-722	106
H(18B)	4807	2072	-57	106
H(18C)	4681	1463	-789	106
H(19)	6724	2910	2415	29
H(19')	6455	3295	2392	99
H(20A)	5566	2267	1481	89
H(20B)	4887	2970	1542	89
H(20C)	4997	2589	2191	89
H(20D)	5705	2312	1496	89
H(20E)	4671	2787	1573	89
H(20F)	5255	2594	2256	89
H(21A)	7011	4114	2687	118
H(21B)	5941	3826	2975	118
H(21C)	5849	4171	2302	118
H(21D)	6581	4322	2217	78
H(21E)	5322	4192	2061	78
H(21F)	5894	4003	2731	78
H(22A)	11091	617	237	83
H(23A)	11422	1065	-743	114
H(23B)	12275	489	-633	114

H(23C)	12627	1339	-408	114
H(24A)	12178	905	1255	177
H(24B)	13094	1248	870	177
H(24C)	12751	397	627	177
H(25A)	11138	2772	2957	56
H(25B)	12812	2514	2129	62
H(26A)	12006	3875	2919	138
H(26B)	13008	3467	2574	138
H(26C)	12775	3472	3373	138
H(26D)	12616	3790	2604	138
H(26E)	13058	3457	3241	138
H(26F)	11806	3610	3152	138
H(27A)	11868	1662	2436	114
H(27B)	12691	2107	3080	114
H(27C)	12932	2089	2280	114
H(27D)	11771	1675	2493	125
H(27E)	12514	2129	3148	125
H(27F)	11287	2279	3061	125
H(28A)	4126	2572	4229	38
H(29A)	5519	1848	3744	63
H(29B)	6355	2549	3934	63
H(29C)	5357	2491	3353	63
H(30A)	4568	3797	4834	66
H(30B)	5752	3737	4603	66
H(30C)	4778	3679	4032	66
H(31A)	4958	1518	6796	28
H(32A)	5445	2696	7508	46
H(32B)	6694	2580	7393	46
H(32C)	6048	2105	7827	46
H(33A)	6280	836	6175	50
H(33B)	6556	965	7012	50
H(33C)	7207	1437	6577	50
H(34A)	2450	998	4993	44
H(35A)	2408	1150	6224	78
H(35B)	1211	1176	5872	78
H(35C)	1881	1912	6289	78

H(36A)	2035	1937	4450	84
H(36B)	998	1677	4760	84
H(36C)	1662	2397	5163	84
H(37A)	8480	1940	5019	32
H(37B)	7389	841	4226	53
H(38A)	8434	1104	5724	63
H(38B)	9141	827	5069	63
H(38C)	7936	479	5057	63
H(38D)	7973	551	5353	63
H(38E)	8621	1329	5622	63
H(38F)	9059	720	5007	63
H(39A)	7634	1650	3872	70
H(39B)	7460	818	3903	70
H(39C)	8658	1180	3924	70
H(39D)	8181	2030	4084	72
H(39E)	9189	1593	4266	72
H(39F)	8740	2202	4876	72
H(40A)	6905	4248	6695	49
H(41A)	6121	4620	5736	92
H(41B)	6168	5255	6447	92
H(41C)	5050	4796	6139	92
H(42A)	5929	4046	7598	106
H(42B)	6041	4876	7615	106
H(42C)	4951	4419	7316	106
H(43A)	3261	4555	5662	42
H(43B)	1774	3557	5849	56
H(44A)	2617	3889	4553	83
H(44B)	1710	4405	4887	83
H(44C)	1607	3557	4869	83
H(44D)	1098	4003	4959	80
H(44E)	2253	3991	4681	80
H(44F)	1645	3266	4734	80
H(45A)	2551	4402	6725	91
H(45B)	1667	4727	6300	91
H(45C)	1576	3899	6287	91
H(45D)	1653	4766	6192	66

Table 1. Crystal data and structure refinement for 2.

Identification code	maj15	
Empirical formula	$C_{54}H_{126}Cl_4Ho_2O_{18}Zr_4$	
Formula weight	1900.09	
Temperature	158 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*C*2/*c*	
Unit cell dimensions	a = 25.1290(12) Å	α= 90°.
	b = 21.4085(10) Å	β= 119.3880(10)°.
	c = 17.9501(9) Å	γ = 90°.
Volume	8414.0(7) Å^3	
Z	4	
Density (calculated)	1.500 Mg/m^3	
Absorption coefficient	2.514 mm^{-1}	
F(000)	3824	
Crystal size	0.33 x 0.23 x 0.23 mm^3	
Theta range for data collection	1.33 to 28.35°.	
Index ranges	$-32 \le h \le 33$, $-28 \le k \le 12$, $-23 \le l \le 23$	
Reflections collected	26586	
Independent reflections	9910 [R(int) = 0.0227]	
Completeness to theta = 28.35°	94.4 %	
Absorption correction	Semi-empirical via SADABS	
Max. and min. transmission	0.5956 and 0.4909	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9910 / 0 / 370	
Goodness-of-fit on F^2	1.087	
Final R indices [I>2sigma(I)]	R1 = 0.0443, wR2 = 0.1399	
R indices (all data)	R1 = 0.0492, wR2 = 0.1442	
Largest diff. peak and hole	4.883 and -0.942 e.Å^{-3}	

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

	x	y	z	U(eq)
Ho(1)	7367(1)	7195(1)	6067(1)	21(1)
Zr(1)	8267(1)	6410(1)	7954(1)	24(1)
Zr(2)	6924(1)	5807(1)	6521(1)	28(1)
Cl(1)	7878(1)	8102(1)	5549(1)	26(1)
Cl(2)	6596(1)	8047(1)	5876(1)	37(1)
O(1)	8287(2)	7248(2)	7348(2)	26(1)
O(2)	7721(2)	5584(2)	7764(3)	36(1)
O(3)	6552(2)	6494(2)	5590(2)	27(1)
O(4)	7775(2)	6174(2)	6518(2)	25(1)
O(5)	7283(2)	6729(2)	7252(2)	24(1)
O(6)	9067(2)	6098(2)	8247(3)	39(1)
O(7)	8434(2)	6683(2)	9067(3)	35(1)
O(8)	6847(3)	5085(2)	5852(4)	54(2)
O(9)	6260(3)	5649(3)	6738(3)	55(2)
C(1)	8815(3)	7646(4)	7818(4)	39(2)
C(2)	8623(4)	8300(4)	7843(5)	49(2)
C(3)	9255(3)	7602(4)	7469(5)	45(2)
C(4)	7825(6)	5060(6)	8316(8)	109(6)
C(5)	7466(7)	4560(6)	7992(9)	134(8)
C(6)	8417(6)	5011(6)	9045(9)	119(6)
C(7)	5974(3)	6616(3)	4835(4)	37(2)
C(8)	5486(4)	6748(5)	5075(7)	66(3)
C(9)	5809(4)	6087(4)	4211(5)	54(2)
C(10)	8059(3)	5851(3)	6076(4)	39(2)
C(11)	8547(3)	6247(4)	6068(4)	45(2)
C(12)	8308(4)	5216(4)	6479(5)	53(2)
C(13)	6950(3)	7052(3)	7617(4)	31(1)
C(14)	6896(3)	6646(4)	8274(4)	43(2)
C(15)	7246(3)	7669(3)	8008(4)	38(1)
C(16)	9714(4)	6005(5)	8639(6)	64(3)
C(17)	9882(5)	5377(7)	8668(11)	130(7)

C(18)	10020(4)	6288(7)	9502(8)	110(6)
C(19)	8679(6)	6852(5)	9939(5)	79(3)
C(20)	8526(11)	6526(11)	10414(8)	214(15)
C(21)	8986(6)	7474(5)	10134(6)	84(4)
C(22)	6696(7)	4533(8)	5368(15)	180(12)
C(23)	6020(7)	4310(6)	5229(11)	131(7)
C(24)	6896(11)	4390(19)	5000(30)	440(40)
C(25)	5740(9)	5377(11)	6692(10)	176(12)
C(26)	5399(8)	5904(16)	6898(12)	234(19)
C(27)	5704(9)	4985(8)	7183(13)	128(7)

Table 3. Bond lengths [Å] and angles [°] for 2.

Ho(1)-O(1)	2.329(4)	C(4)-C(5)	1.336(15)
Ho(1)-O(3)	2.338(4)	C(4)-C(6)	1.422(14)
Ho(1)-O(4)	2.382(4)	C(7)-C(9)	1.500(11)
Ho(1)-O(5)	2.452(4)	C(7)-C(8)	1.512(11)
Ho(1)-Cl(2)	2.5581(15)	C(10)-C(11)	1.499(11)
Ho(1)-Cl(1)#1	2.7288(13)	C(10)-C(12)	1.522(10)
Ho(1)-Cl(1)	2.7290(13)	C(13)-C(15)	1.510(9)
Ho(1)-Zr(2)	3.4106(6)	C(13)-C(14)	1.521(9)
Ho(1)-Zr(1)	3.4489(6)	C(16)-C(17)	1.402(15)
Zr(1)-O(7)	1.919(4)	C(16)-C(18)	1.479(14)
Zr(1)-O(6)	1.932(5)	C(19)-C(20)	1.298(16)
Zr(1)-O(1)	2.111(4)	C(19)-C(21)	1.492(15)
Zr(1)-O(2)	2.162(4)	C(22)-C(24)	1.05(3)
Zr(1)-O(5)	2.261(4)	C(22)-C(23)	1.66(3)
Zr(1)-O(4)	2.303(4)	C(25)-C(27)	1.25(2)
Zr(1)-Zr(2)	3.3392(8)	C(25)-C(26)	1.57(4)
Zr(2)-O(8)	1.908(5)	O(1)-Ho(1)-O(3)	131.23(13)
Zr(2)-O(9)	1.922(6)	O(1)-Ho(1)-O(4)	69.88(13)
Zr(2)-O(3)	2.073(4)	O(3)-Ho(1)-O(4)	71.84(14)
Zr(2)-O(2)	2.197(4)	O(1)-Ho(1)-O(5)	68.25(13)
Zr(2)-O(4)	2.281(4)	O(3)-Ho(1)-O(5)	67.81(13)
Zr(2)-O(5)	2.295(4)	O(4)-Ho(1)-O(5)	62.45(13)
Cl(1)-Ho(1)#1	2.7288(13)	O(1)-Ho(1)-Cl(2)	114.64(11)
O(1)-C(1)	1.450(7)	O(3)-Ho(1)-Cl(2)	86.50(11)
O(2)-C(4)	1.433(9)	O(4)-Ho(1)-Cl(2)	150.62(10)
O(3)-C(7)	1.443(7)	O(5)-Ho(1)-Cl(2)	91.39(10)
O(4)-C(10)	1.472(7)	O(1)-Ho(1)-Cl(1)#1	131.14(11)
O(5)-C(13)	1.465(7)	O(3)-Ho(1)-Cl(1)#1	76.18(10)
O(6)-C(16)	1.433(9)	O(4)-Ho(1)-Cl(1)#1	88.96(9)
O(7)-C(19)	1.419(8)	O(5)-Ho(1)-Cl(1)#1	139.20(10)
O(8)-C(22)	1.404(11)	Cl(2)-Ho(1)-Cl(1)#1	105.24(5)
O(9)-C(25)	1.393(13)	O(1)-Ho(1)-Cl(1)	84.09(10)
C(1)-C(2)	1.490(11)	O(3)-Ho(1)-Cl(1)	143.76(10)
C(1)-C(3)	1.516(10)	O(4)-Ho(1)-Cl(1)	124.92(10)

O(5)-Ho(1)-Cl(1)	147.19(9)	O(2)-Zr(1)-Zr(2)	40.39(11)
Cl(2)-Ho(1)-Cl(1)	84.22(5)	O(5)-Zr(1)-Zr(2)	43.27(10)
Cl(1)#1-Ho(1)-Cl(1)	72.69(4)	O(4)-Zr(1)-Zr(2)	43.00(10)
O(1)-Ho(1)-Zr(2)	95.06(10)	O(7)-Zr(1)-Ho(1)	125.28(14)
O(3)-Ho(1)-Zr(2)	36.61(9)	O(6)-Zr(1)-Ho(1)	121.96(15)
O(4)-Ho(1)-Zr(2)	41.86(10)	O(1)-Zr(1)-Ho(1)	41.37(11)
O(5)-Ho(1)-Zr(2)	42.27(9)	O(2)-Zr(1)-Ho(1)	100.63(11)
Cl(2)-Ho(1)-Zr(2)	109.80(4)	O(5)-Zr(1)-Ho(1)	45.17(9)
Cl(1)#1-Ho(1)-Zr(2)	96.96(3)	O(4)-Zr(1)-Ho(1)	43.49(10)
Cl(1)-Ho(1)-Zr(2)	164.68(3)	Zr(2)-Zr(1)-Ho(1)	60.297(13)
O(1)-Ho(1)-Zr(1)	36.80(10)	O(8)-Zr(2)-O(9)	99.0(3)
O(3)-Ho(1)-Zr(1)	94.63(9)	O(8)-Zr(2)-O(3)	101.5(2)
O(4)-Ho(1)-Zr(1)	41.72(9)	O(9)-Zr(2)-O(3)	101.2(2)
O(5)-Ho(1)-Zr(1)	40.83(9)	O(8)-Zr(2)-O(2)	102.9(2)
Cl(2)-Ho(1)-Zr(1)	124.56(4)	O(9)-Zr(2)-O(2)	101.8(2)
Cl(1)#1-Ho(1)-Zr(1)	128.88(3)	O(3)-Zr(2)-O(2)	143.01(16)
Cl(1)-Ho(1)-Zr(1)	119.32(3)	O(8)-Zr(2)-O(4)	94.7(2)
Zr(2)-Ho(1)-Zr(1)	58.258(13)	O(9)-Zr(2)-O(4)	166.0(2)
O(7)-Zr(1)-O(6)	98.9(2)	O(3)-Zr(2)-O(4)	78.83(15)
O(7)-Zr(1)-O(1)	103.29(18)	O(2)-Zr(2)-O(4)	71.92(16)
O(6)-Zr(1)-O(1)	98.64(19)	O(8)-Zr(2)-O(5)	161.1(2)
O(7)-Zr(1)-O(2)	102.18(19)	O(9)-Zr(2)-O(5)	99.9(2)
O(6)-Zr(1)-O(2)	104.7(2)	O(3)-Zr(2)-O(5)	75.28(15)
O(1)-Zr(1)-O(2)	141.99(15)	O(2)-Zr(2)-O(5)	72.57(15)
O(7)-Zr(1)-O(5)	96.28(17)	O(4)-Zr(2)-O(5)	66.41(13)
O(6)-Zr(1)-O(5)	164.65(17)	O(8)-Zr(2)-Zr(1)	123.38(18)
O(1)-Zr(1)-O(5)	75.66(15)	O(9)-Zr(2)-Zr(1)	124.20(16)
O(2)-Zr(1)-O(5)	73.91(16)	O(3)-Zr(2)-Zr(1)	103.43(11)
O(7)-Zr(1)-O(4)	162.80(17)	O(2)-Zr(2)-Zr(1)	39.61(12)
O(6)-Zr(1)-O(4)	98.24(17)	O(4)-Zr(2)-Zr(1)	43.51(9)
O(1)-Zr(1)-O(4)	75.23(15)	O(5)-Zr(2)-Zr(1)	42.46(10)
O(2)-Zr(1)-O(4)	72.12(15)	O(8)-Zr(2)-Ho(1)	119.9(2)
O(5)-Zr(1)-O(4)	66.62(13)	O(9)-Zr(2)-Ho(1)	128.3(2)
O(7)-Zr(1)-Zr(2)	122.80(14)	O(3)-Zr(2)-Ho(1)	42.26(11)
O(6)-Zr(1)-Zr(2)	126.79(14)	O(2)-Zr(2)-Ho(1)	101.00(12)
O(1)-Zr(1)-Zr(2)	101.66(11)	O(4)-Zr(2)-Ho(1)	44.17(10)

O(5)-Zr(2)-Ho(1)	45.93(9)	O(1)-C(1)-C(2)	110.6(6)
Zr(1)-Zr(2)-Ho(1)	61.445(14)	O(1)-C(1)-C(3)	111.7(6)
Ho(1)#1-Cl(1)-Ho(1)	107.31(4)	C(2)-C(1)-C(3)	112.5(6)
C(1)-O(1)-Zr(1)	116.5(4)	C(5)-C(4)-C(6)	121.3(10)
C(1)-O(1)-Ho(1)	141.7(4)	C(5)-C(4)-O(2)	118.1(9)
Zr(1)-O(1)-Ho(1)	101.82(16)	C(6)-C(4)-O(2)	116.6(9)
C(4)-O(2)-Zr(1)	130.2(5)	O(3)-C(7)-C(9)	110.4(6)
C(4)-O(2)-Zr(2)	129.7(5)	O(3)-C(7)-C(8)	110.4(6)
Zr(1)-O(2)-Zr(2)	100.00(17)	C(9)-C(7)-C(8)	112.7(7)
C(7)-O(3)-Zr(2)	137.2(4)	O(4)-C(10)-C(11)	110.7(5)
C(7)-O(3)-Ho(1)	121.6(3)	O(4)-C(10)-C(12)	111.1(6)
Zr(2)-O(3)-Ho(1)	101.13(15)	C(11)-C(10)-C(12)	111.3(6)
C(10)-O(4)-Zr(2)	122.8(4)	O(5)-C(13)-C(15)	111.1(5)
C(10)-O(4)-Zr(1)	124.8(3)	O(5)-C(13)-C(14)	111.4(5)
Zr(2)-O(4)-Zr(1)	93.50(14)	C(15)-C(13)-C(14)	110.5(5)
C(10)-O(4)-Ho(1)	119.4(4)	C(17)-C(16)-O(6)	113.5(9)
Zr(2)-O(4)-Ho(1)	93.97(14)	C(17)-C(16)-C(18)	111.3(11)
Zr(1)-O(4)-Ho(1)	94.79(14)	O(6)-C(16)-C(18)	109.8(8)
C(13)-O(5)-Zr(1)	127.0(3)	C(20)-C(19)-O(7)	118.7(10)
C(13)-O(5)-Zr(2)	120.7(3)	C(20)-C(19)-C(21)	127.7(11)
Zr(1)-O(5)-Zr(2)	94.26(15)	O(7)-C(19)-C(21)	112.4(7)
C(13)-O(5)-Ho(1)	120.5(3)	C(24)-C(22)-O(8)	125(3)
Zr(1)-O(5)-Ho(1)	94.00(13)	C(24)-C(22)-C(23)	126.1(17)
Zr(2)-O(5)-Ho(1)	91.79(13)	O(8)-C(22)-C(23)	106.3(13)
C(16)-O(6)-Zr(1)	163.7(5)	C(27)-C(25)-O(9)	129(2)
C(19)-O(7)-Zr(1)	168.6(7)	C(27)-C(25)-C(26)	94.5(15)
C(22)-O(8)-Zr(2)	169.8(11)	O(9)-C(25)-C(26)	106.9(15)
C(25)-O(9)-Zr(2)	160.5(9)		

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for maj15. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ho(1)	23(1)	21(1)	17(1)	3(1)	10(1)	-1(1)
Zr(1)	28(1)	25(1)	16(1)	2(1)	7(1)	1(1)
Zr(2)	34(1)	22(1)	20(1)	2(1)	8(1)	-5(1)
Cl(1)	32(1)	25(1)	19(1)	-1(1)	12(1)	-8(1)
Cl(2)	41(1)	34(1)	41(1)	11(1)	26(1)	13(1)
O(1)	26(2)	29(2)	20(2)	0(2)	9(2)	-6(2)
O(2)	45(3)	25(2)	23(2)	6(2)	5(2)	-1(2)
O(3)	24(2)	31(2)	22(2)	6(2)	7(2)	-2(2)
O(4)	27(2)	26(2)	19(2)	-2(1)	9(2)	4(2)
O(5)	29(2)	27(2)	18(2)	1(1)	13(2)	-1(2)
O(6)	34(2)	42(3)	28(2)	-1(2)	6(2)	10(2)
O(7)	43(2)	40(2)	18(2)	-2(2)	13(2)	-5(2)
O(8)	54(3)	31(3)	47(3)	-16(2)	1(2)	0(2)
O(9)	64(3)	63(4)	41(3)	-1(3)	27(3)	-35(3)
C(1)	38(3)	49(4)	25(3)	-8(3)	13(3)	-18(3)
C(2)	57(5)	47(4)	40(4)	-9(3)	22(3)	-12(4)
C(3)	34(3)	60(5)	40(4)	3(3)	16(3)	-9(3)
C(4)	91(8)	75(7)	83(8)	63(6)	-17(6)	-29(6)
C(5)	115(11)	69(8)	109(10)	57(7)	-30(8)	-32(7)
C(6)	83(8)	96(9)	96(9)	69(8)	-19(7)	-24(7)
C(7)	24(3)	35(3)	39(3)	13(3)	5(2)	-5(2)
C(8)	31(4)	63(5)	105(8)	31(5)	34(4)	10(4)
C(9)	44(4)	43(4)	42(4)	8(3)	-5(3)	-16(3)
C(10)	41(3)	46(4)	22(3)	-7(3)	10(3)	17(3)
C(11)	36(3)	74(5)	29(3)	3(3)	20(3)	15(3)
C(12)	61(5)	49(4)	35(4)	-6(3)	12(3)	30(4)
C(13)	31(3)	39(3)	26(3)	1(2)	17(2)	4(2)
C(14)	46(4)	60(5)	33(3)	1(3)	26(3)	-6(3)
C(15)	46(4)	38(3)	34(3)	-8(3)	23(3)	4(3)
C(16)	38(4)	92(7)	51(5)	-6(5)	12(4)	17(4)
C(17)	51(6)	97(10)	167(15)	-53(10)	-5(8)	25(6)

C(18)	34(4)	155(13)	90(8)	-61(9)	-9(5)	13(6)
C(19)	132(10)	81(7)	28(4)	-17(4)	42(5)	-35(7)
C(20)	290(30)	310(30)	36(6)	-45(11)	71(11)	-210(20)
C(21)	116(9)	69(7)	33(4)	-8(4)	11(5)	-12(6)
C(22)	72(8)	119(12)	230(20)	-142(15)	-14(11)	11(8)
C(23)	121(12)	68(8)	114(12)	-9(8)	-12(9)	-14(8)
C(24)	133(18)	560(60)	590(70)	-530(60)	160(30)	-80(30)
C(25)	196(18)	280(30)	89(9)	-73(13)	99(12)	-200(20)
C(26)	112(14)	520(60)	105(13)	-80(20)	80(12)	-150(20)
C(27)	163(17)	100(11)	169(18)	-11(11)	118(15)	-42(11)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2.

	x	y	z	U(eq)
H(1A)	9036	7490	8420	46
H(2A)	8343	8305	8076	73
H(2B)	8417	8473	7262	73
H(2C)	8984	8554	8206	73
H(3A)	9370	7165	7469	67
H(3B)	9622	7849	7830	67
H(3C)	9058	7766	6884	67
H(4A)	7617	5236	8621	130
H(5A)	7077	4686	7499	201
H(5B)	7389	4374	8429	201
H(5C)	7668	4252	7810	201
H(6A)	8432	4644	9381	178
H(6B)	8504	5388	9396	178
H(6C)	8722	4967	8859	178
H(7A)	6024	7000	4557	45
H(8A)	5617	7096	5481	99
H(8B)	5422	6375	5338	99
H(8C)	5104	6858	4560	99
H(9A)	6137	6024	4073	81
H(9B)	5429	6188	3687	81
H(9C)	5752	5705	4464	81
H(10A)	7735	5780	5470	47
H(11A)	8373	6652	5805	67
H(11B)	8710	6037	5737	67
H(11C)	8876	6312	6655	67
H(12A)	7980	4967	6475	80
H(12B)	8636	5273	7070	80
H(12C)	8469	4999	6151	80
H(13A)	6527	7139	7143	37
H(14A)	6700	6249	8009	65

H(14B)	6650	6863	8479	65
H(14C)	7305	6565	8756	65
H(15A)	7274	7925	7576	57
H(15B)	7657	7594	8488	57
H(15C)	7000	7887	8213	57
H(16A)	9859	6234	8287	77
H(17A)	9680	5204	8087	195
H(17B)	9758	5140	9024	195
H(17C)	10326	5348	8911	195
H(18A)	10463	6230	9763	166
H(18B)	9874	6087	9858	166
H(18C)	9926	6736	9456	166
H(19A)	9068	6616	10125	94
H(20A)	8341	6131	10126	321
H(20B)	8231	6762	10510	321
H(20C)	8890	6438	10964	321
H(21A)	9155	7566	10743	125
H(21B)	8688	7796	9793	125
H(21C)	9317	7468	9993	125
H(22A)	6943	4250	5862	216
H(23A)	5901	3915	4913	197
H(23B)	5714	4631	4905	197
H(23C)	6045	4254	5788	197
H(24A)	7318	4539	5268	658
H(24B)	6663	4563	4423	658
H(24C)	6891	3932	4969	658
H(25A)	5470	5235	6090	212
H(26A)	5028	5732	6869	351
H(26B)	5289	6243	6481	351
H(26C)	5667	6067	7474	351
H(27A)	5886	4589	7146	192
H(27B)	5274	4917	7016	192
H(27C)	5924	5141	7772	192

H(45E)	2470	4437	6660	66
H(45F)	2899	4858	6123	66
H(46A)	2262	3015	7342	50
H(47A)	2870	1901	7473	90
H(47B)	2621	2393	8226	90
H(47C)	3845	2316	8024	90
H(48A)	3310	4106	7838	94
H(48B)	2907	3772	8444	94
H(48C)	4105	3698	8244	94
H(49A)	7676	4187	4759	68
H(50A)	8543	4516	5901	100
H(50B)	9361	4639	5334	100
H(50C)	9437	3948	5667	100
H(51A)	8146	3180	3915	203
H(51B)	9095	3787	4086	203
H(51C)	9165	3110	4410	203
H(52A)	8565	2597	7332	40
H(53A)	8052	3792	7638	114
H(53B)	8931	4036	7163	114
H(53C)	9315	3775	7857	114
H(54A)	9743	2227	6457	121
H(54B)	9983	3033	6418	121
H(54C)	10364	2787	7103	121

Table 1. Crystal data and structure refinement for 3.

Identification code	jb1
Empirical formula	$C_{61}H_{134}Cl_4O_{18}Y_2Zr_4$
Formula weight	1840.18
Temperature	158 K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 25.1194(13) Å alpha = 90° b = 21.4503(11) Å beta = 119.2770(10)° c = 17.9466(9) Å gamma = 90°
Volume, Z	8434.8(7) $Å^3$, 4
Density (calculated)	1.449 Mg/m^3
Absorption coefficient	2.018 mm^{-1}
F(000)	3800
Crystal size	0.53 x 0.20 x 0.20 mm
θ range for data collection	1.33 to 28.33°
Limiting indices	$-32 \le h \le 33$, $-19 \le k \le 28$, $-20 \le l \le 23$
Reflections collected	25787
Independent reflections	9850 (R_{int} = 0.0362)
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9850 / 0 / 412
Goodness-of-fit on F^2	1.071
Final R indices [$I>2\sigma(I)$]	R1 = 0.0528, wR2 = 0.1025
R indices (all data)	R1 = 0.0780, wR2 = 0.1123
Largest diff. peak and hole	0.937 and -0.697 $eÅ^{-3}$