Inorganic Chemistry
including bioinorganic chemistry
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TABLE S1 - Data collection and refinement parameters for complex 4.

	Complex 4
Diffractometer Used	
Radiation	
Temperature (K)	
Monochromator	
2θ Range	2.0 to 48.0°
Scan Type	ω
Scan Speed	Variable; 4.00 to 19.00°/min.
Scan Range (ω)	2.20°
Reflections Collected	7383
Independent Reflections	7165 (R_{int} = 4.19%)
Observed Reflections	5142 ($F > 4.0\sigma(F)$)
Refinement Method	
Quantity Minimized	
Hydrogen Atoms	
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0050F^2$
Number of Parameters Refined	1018
Final R Indices (obs. data)	R = 7.60 %, wR = 10.61 %
R Indices (all data)	R = 11.10 %, wR = 24.17 %
Goodness-of-Fit	1.23
Largest and Mean Δ/σ	0.297, 0.019
Data-to-Parameter Ratio	5.1:1
Largest Difference Peak	0.93 eÅ^{-3}
Largest Difference Hole	-0.58 eÅ^{-3}

Table S1 (cont.)

	Complex 4
Empirical Formula	$C_{74}H_{114}Na_3O_{36.5}V$
Color; Habit	green, prism
Crystal Size (mm)	0.28x0.40x0.64
Crystal System	Monoclinic
Space Group	$P2_1$
Unit Cell Dimensions	$\underline{a}$ = 14.735(10) Å
	$\underline{b}$ = 15.033(9) Å
	$\underline{c}$ = 21.021(10) Å
	β = 107.34(2)°
Volume	4445(5) $Å^3$
Z	2
Formula Weight	1707.6
Density(calc.)	1.276 Mg/m^3
Absorption Coefficient	0.210 mm^{-1}
F(000)	1812

TABLE S2 – Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$) for complex 4

	x	y	z	U(eq)
V	8223(1)	0	2335(1)	14(1)
O(1A)	6889(6)	516(7)	2231(4)	18(3)
C(1A)	6022(8)	96(10)	1988(6)	21(4)
C(2A)	5168(10)	660(11)	2023(7)	31(5)
O(2A)	4925(7)	1208(7)	1424(4)	30(3)
C(3A)	5064(10)	688(11)	899(7)	35(5)
C(4A)	5729(8)	-62(11)	1228(6)	21(4)
O(3A)	5131(6)	-840(7)	1055(4)	21(3)
C(5A)	4384(9)	-634(10)	473(7)	25(5)
C(6A)	3499(9)	-1141(12)	445(7)	37(6)
C(7A)	4670(10)	-797(13)	-145(7)	42(6)
O(4A)	4202(7)	303(7)	528(5)	33(4)
C(8A)	5342(9)	1326(10)	2590(6)	24(5)
C(9A)	4440(9)	1703(12)	2728(7)	33(5)
O(5A)	4210(6)	1041(9)	3115(5)	37(4)
C(10A)	5095(11)	728(13)	3541(8)	45(6)
C(11A)	4989(13)	-253(15)	3561(10)	67(9)
C(12A)	5328(14)	1177(18)	4175(8)	71(9)
O(6A)	5802(6)	933(8)	3215(4)	25(3)
O(1B)	8690(6)	585(7)	3252(4)	18(3)
C(1B)	9582(8)	975(9)	3571(6)	14(4)
C(2B)	9679(9)	1309(10)	4303(6)	20(4)
O(2B)	10067(6)	560(7)	4715(4)	22(3)
C(3B)	10685(8)	85(10)	4460(5)	16(4)
C(4B)	10421(8)	335(10)	3710(6)	19(4)
O(3B)	11251(6)	775(7)	3637(4)	28(3)
C(5B)	12036(9)	602(10)	4205(7)	24(5)
C(6B)	12577(10)	-188(11)	4090(7)	34(5)
C(7B)	12607(11)	1435(12)	4381(10)	52(7)
O(4B)	11624(6)	420(8)	4724(4)	32(3)
C(8B)	8767(9)	1535(10)	4418(6)	22(3)
C(9B)	8899(10)	1973(9)	5107(6)	26(5)
O(5B)	9032(7)	2886(7)	4989(4)	26(3)
C(10B)	8426(10)	3076(10)	4311(7)	27(5)
C(11B)	8997(10)	3678(11)	3988(6)	28(5)
C(12B)	7506(11)	3448(11)	4304(8)	41(6)
O(6B)	8272(6)	2231(7)	3975(4)	24(3)
O(1C)	9532(6)	-538(6)	2437(4)	16(3)
C(1C)	9717(9)	-1391(9)	2270(6)	17(4)
C(2C)	10775(8)	-1578(10)	2312(6)	18(4)
O(2C)	11219(7)	-1890(8)	2987(5)	32(2)
C(3C)	10536(9)	-2277(10)	3233(6)	24(3)
C(4C)	9559(10)	-2092(9)	2761(6)	21(4)
O(3C)	9309(7)	-2938(7)	2417(4)	29(3)
C(5C)	9767(11)	-3639(10)	2853(7)	32(5)
C(6C)	9202(12)	-3953(12)	3290(8)	45(6)
C(7C)	10072(16)	-4338(13)	2454(11)	74(9)
O(4C)	10640(7)	-3220(7)	3280(5)	30(3)
C(8C)	11394(9)	-781(9)	2284(7)	22(5)
C(9C)	12344(10)	-1045(12)	2212(6)	30(5)
O(5C)	12166(6)	-1069(7)	1493(5)	29(3)
C(10C)	11507(9)	-363(10)	1221(6)	23(5)
C(11C)	10855(11)	-615(12)	541(6)	40(6)
C(12C)	12036(11)	502(12)	1221(8)	44(6)

Tab 1

O(6C)	10954(6)	-269(7)	1681(4)	26(3)
O(1D)	8661(6)	1125(6)	1964(4)	18(3)
C(1D)	8475(9)	1999(9)	2075(6)	20(4)
C(2D)	8895(9)	2701(10)	1709(6)	20(4)
O(2D)	8131(6)	2867(7)	1081(4)	26(3)
C(3D)	7269(9)	2827(10)	1227(6)	25(5)
C(4D)	7393(9)	2253(9)	1825(7)	21(5)
O(3D)	7167(7)	2817(7)	2319(4)	28(3)
C(5D)	6685(10)	3592(11)	1965(6)	30(5)
C(6D)	5645(10)	3475(12)	1767(8)	40(6)
C(7D)	7026(16)	4404(13)	2419(9)	68(8)
O(4D)	7053(7)	3698(7)	1425(5)	31(4)
C(8D)	9736(9)	2443(10)	1501(6)	25(5)
C(9D)	10170(12)	3222(11)	1221(7)	38(6)
O(5D)	10774(7)	3618(7)	1831(5)	34(4)
C(10D)	11173(9)	2907(10)	2283(7)	31(5)
C(11D)	12150(11)	2627(11)	2265(8)	40(6)
C(12D)	11177(11)	3198(12)	2965(7)	40(6)
O(6D)	10519(6)	2176(7)	2072(4)	24(3)
O(1E)	7736(6)	-553(7)	1404(4)	19(3)
C(1E)	8141(9)	-465(9)	890(6)	15(4)
C(2E)	7656(9)	-1036(9)	266(6)	18(4)
O(2E)	6905(7)	-499(8)	-174(5)	32(4)
C(3E)	7080(10)	421(10)	16(7)	27(5)
C(4E)	7980(8)	471(10)	568(6)	18(4)
O(3E)	8658(6)	611(7)	196(4)	27(3)
C(5E)	8200(10)	1007(11)	-440(6)	28(5)
C(6E)	8470(11)	460(12)	-952(7)	43(6)
C(7E)	8441(11)	1980(11)	-434(7)	33(5)
O(4E)	7193(7)	920(7)	-512(4)	30(3)
C(8E)	7150(10)	-1853(11)	395(6)	30(5)
C(9E)	6814(11)	-2464(10)	-218(7)	35(5)
O(5E)	7647(7)	-2989(8)	-149(4)	34(4)
C(10E)	8081(11)	-3167(11)	534(7)	31(5)
C(11E)	7765(11)	-4042(11)	753(8)	39(6)
C(12E)	9136(10)	-3091(11)	674(8)	38(6)
O(6E)	7751(6)	-2436(7)	882(4)	22(3)
O(1F)	7846(6)	-1104(7)	2765(4)	19(3)
C(1F)	7386(9)	-1068(10)	3255(6)	20(4)
C(2F)	7004(9)	-2009(10)	3380(6)	22(5)
O(2F)	7710(8)	-2420(7)	3923(5)	44(4)
C(3F)	8374(9)	-1794(10)	4278(6)	20(5)
C(4F)	8067(8)	-912(10)	3938(6)	20(4)
O(3F)	7532(7)	-519(7)	4350(4)	27(3)
C(5F)	7812(9)	-914(10)	4999(6)	20(5)
C(6F)	6926(11)	-1164(12)	5198(7)	40(6)
C(7F)	8512(11)	-320(10)	5502(7)	33(5)
O(4F)	8327(7)	-1706(7)	4949(4)	28(3)
C(8F)	6806(10)	-2713(10)	2849(6)	24(5)
C(9F)	6299(11)	-3510(10)	3002(7)	32(5)
O(5F)	5697(7)	-3776(7)	2350(5)	34(4)
C(10F)	5391(9)	-2985(10)	1965(8)	28(5)
C(11F)	4512(11)	-2591(13)	2129(9)	54(7)
C(12F)	5278(12)	-3190(12)	1245(7)	41(6)
O(6F)	6191(6)	-2372(7)	2221(4)	25(3)
Na(1)	7337(4)	1370(5)	3146(3)	30(2)
Na(2)	10198(4)	718(5)	2212(3)	33(2)
Na(3)	7418(5)	-1883(5)	1803(3)	36(2)
C(1)	5831(37)	2501(41)	5809(25)	95(16)

Table S2 (cont.)

C(2)	6649(24)	2165(27)	6037(17)	48(9)
O(3)	6937(21)	1467(24)	6556(14)	84(9)
C(4)	6141(35)	717(39)	6456(24)	89(14)
C(5)	6503(38)	192(42)	7025(26)	33(13)
C(5')	5360(31)	911(33)	6044(21)	9(10)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table S3. . Bond lengths (Å) for complex 4

V-O(1A)	2.064 (9)	V-O(1B)	2.041 (8)
V-O(1C)	2.042 (9)	V-O(1D)	2.046 (10)
V-O(1E)	2.049 (8)	V-O(1F)	2.043 (10)
V-Na(1)	3.190 (7)	V-Na(2)	3.185 (7)
V-Na(3)	3.143 (7)	O(1A)-C(1A)	1.382 (15)
O(1A)-Na(1)	2.240 (11)	C(1A)-C(2A)	1.532 (21)
C(1A)-C(4A)	1.543 (17)	C(2A)-O(2A)	1.455 (17)
C(2A)-C(8A)	1.521 (20)	O(2A)-C(3A)	1.413 (19)
C(3A)-C(4A)	1.523 (21)	C(3A)-O(4A)	1.402 (16)
C(4A)-O(3A)	1.442 (17)	O(3A)-C(5A)	1.414 (14)
C(5A)-C(6A)	1.495 (21)	C(5A)-C(7A)	1.501 (22)
C(5A)-O(4A)	1.447 (19)	C(8A)-C(9A)	1.546 (21)
C(8A)-O(6A)	1.415 (15)	C(8A)-Na(1)	2.822 (14)
C(9A)-O(5A)	1.391 (21)	O(5A)-C(10A)	1.426 (17)
C(10A)-C(11A)	1.486 (30)	C(10A)-C(12A)	1.442 (25)
C(10A)-O(6A)	1.439 (21)	O(6A)-Na(1)	2.402 (11)
O(1B)-C(1B)	1.415 (14)	O(1B)-Na(1)	2.270 (11)
C(1B)-C(2B)	1.586 (17)	C(1B)-C(4B)	1.523 (18)
C(2B)-O(2B)	1.432 (16)	C(2B)-C(8B)	1.473 (20)
O(2B)-C(3B)	1.385 (17)	C(3B)-C(4B)	1.550 (16)
C(3B)-O(4B)	1.422 (15)	C(4B)-O(3B)	1.439 (17)
O(3B)-C(5B)	1.416 (14)	O(3B)-Na(2)	2.937 (10)
C(5B)-C(6B)	1.489 (22)	C(5B)-C(7B)	1.495 (23)
C(5B)-O(4B)	1.424 (18)	C(8B)-C(9B)	1.547 (19)
C(8B)-O(6B)	1.445 (16)	C(8B)-Na(1)	2.880 (12)
C(9B)-O(5B)	1.419 (17)	O(5B)-C(10B)	1.465 (15)
C(10B)-C(11B)	1.530 (22)	C(10B)-C(12B)	1.462 (23)
C(10B)-O(6B)	1.436 (17)	O(6B)-Na(1)	2.277 (10)
O(1C)-C(1C)	1.379 (17)	O(1C)-Na(2)	2.243 (12)
C(1C)-C(2C)	1.561 (18)	C(1C)-C(4C)	1.538 (19)
C(2C)-O(2C)	1.453 (14)	C(2C)-C(8C)	1.517 (20)
O(2C)-C(3C)	1.390 (19)	C(3C)-C(4C)	1.509 (17)
C(3C)-O(4C)	1.426 (18)	C(4C)-O(3C)	1.455 (16)
O(3C)-C(5C)	1.428 (17)	C(5C)-C(6C)	1.490 (25)
C(5C)-C(7C)	1.494 (28)	C(5C)-O(4C)	1.472 (16)
C(8C)-C(9C)	1.506 (21)	C(8C)-O(6C)	1.458 (15)
C(8C)-Na(2)	2.837 (15)	C(9C)-O(5C)	1.454 (16)
O(5C)-C(10C)	1.437 (17)	C(10C)-C(11C)	1.515 (17)
C(10C)-C(12C)	1.514 (23)	C(10C)-O(6C)	1.444 (18)
O(6C)-Na(2)	2.330 (12)	O(1D)-C(1D)	1.375 (17)
O(1D)-Na(2)	2.253 (10)	C(1D)-C(2D)	1.543 (20)
C(1D)-C(4D)	1.569 (18)	C(2D)-O(2D)	1.481 (13)
C(2D)-C(8D)	1.483 (20)	O(2D)-C(3D)	1.394 (18)
C(3D)-C(4D)	1.490 (19)	C(3D)-O(4D)	1.438 (19)
C(4D)-O(3D)	1.454 (18)	O(3D)-C(5D)	1.449 (18)
O(3D)-Na(1)	2.749 (12)	C(5D)-C(6D)	1.474 (21)
C(5D)-C(7D)	1.539 (24)	C(5D)-O(4D)	1.404 (19)
C(8D)-C(9D)	1.531 (23)	C(8D)-O(6D)	1.452 (14)
C(8D)-Na(2)	2.971 (16)	C(9D)-O(5D)	1.453 (17)
O(5D)-C(10D)	1.432 (18)	C(10D)-C(11D)	1.513 (22)
C(10D)-C(12D)	1.495 (23)	C(10D)-O(6D)	1.443 (17)
O(6D)-Na(2)	2.279 (13)	O(1E)-C(1E)	1.390 (16)
O(1E)-Na(3)	2.271 (12)	C(1E)-C(2E)	1.548 (16)
C(1E)-C(4E)	1.545 (19)	C(2E)-O(2E)	1.457 (15)
C(2E)-C(8E)	1.505 (21)	O(2E)-C(3E)	1.438 (19)
C(3E)-C(4E)	1.482 (16)	C(3E)-O(4E)	1.391 (18)

C(4E)-O(3E)	1.454 (17)	O(3E)-C(5E)	1.435 (15)
C(5E)-C(6E)	1.498 (24)	C(5E)-C(7E)	1.506 (23)
C(5E)-O(4E)	1.453 (18)	C(8E)-C(9E)	1.539 (20)
C(8E)-O(6E)	1.434 (16)	C(8E)-Na(3)	2.866 (15)
C(9E)-O(5E)	1.429 (19)	O(5E)-C(10E)	1.412 (16)
C(10E)-C(11E)	1.514 (23)	C(10E)-C(12E)	1.495 (21)
C(10E)-O(6E)	1.482 (19)	O(6E)-Na(3)	2.290 (12)
O(1F)-C(1F)	1.394 (17)	O(1F)-Na(3)	2.256 (10)
C(1F)-C(2F)	1.574 (21)	C(1F)-C(4F)	1.506 (15)
C(2F)-O(2F)	1.436 (15)	C(2F)-C(8F)	1.500 (19)
O(2F)-C(3F)	1.400 (16)	C(3F)-C(4F)	1.508 (19)
C(3F)-O(4F)	1.439 (16)	C(4F)-O(3F)	1.459 (18)
O(3F)-C(5F)	1.431 (15)	C(5F)-C(6F)	1.533 (23)
C(5F)-C(7F)	1.530 (18)	C(5F)-O(4F)	1.428 (18)
C(8F)-C(9F)	1.498 (22)	C(8F)-O(6F)	1.453 (14)
C(8F)-Na(3)	2.894 (16)	C(9F)-O(5F)	1.450 (15)
O(5F)-C(10F)	1.431 (18)	C(10F)-C(11F)	1.550 (24)
C(10F)-C(12F)	1.511 (23)	C(10F)-O(6F)	1.467 (16)
O(6F)-Na(3)	2.348 (12)	C(1)-C(2)	1.254 (63)
C(2)-O(3)	1.492 (49)	O(3)-C(4)	1.590 (66)
C(4)-C(5)	1.396 (85)	C(4)-C(5')	1.258 (79)

Table S4 . Bond angles (°) for complex 4

O(1A)-V-O(1B)	88.9(3)	O(1A)-V-O(1C)	178.8(4)
O(1B)-V-O(1C)	91.7(3)	O(1A)-V-O(1D)	92.6(4)
O(1B)-V-O(1D)	87.0(4)	O(1C)-V-O(1D)	88.5(4)
O(1A)-V-O(1E)	90.0(4)	O(1B)-V-O(1E)	178.3(4)
O(1C)-V-O(1E)	89.5(4)	O(1D)-V-O(1E)	91.8(4)
O(1A)-V-O(1F)	88.7(4)	O(1B)-V-O(1F)	89.6(4)
O(1C)-V-O(1F)	90.3(4)	O(1D)-V-O(1F)	176.3(3)
O(1E)-V-O(1F)	91.6(4)	O(1A)-V-Na(1)	44.3(3)
O(1B)-V-Na(1)	45.1(3)	O(1C)-V-Na(1)	136.4(3)
O(1D)-V-Na(1)	84.0(3)	O(1E)-V-Na(1)	133.6(3)
O(1F)-V-Na(1)	94.6(3)	O(1A)-V-Na(2)	136.7(3)
O(1B)-V-Na(2)	82.6(3)	O(1C)-V-Na(2)	44.4(3)
O(1D)-V-Na(2)	44.8(3)	O(1E)-V-Na(2)	97.4(3)
O(1F)-V-Na(2)	133.3(3)	Na(1)-V-Na(2)	110.7(2)
O(1A)-V-Na(3)	93.1(3)	O(1B)-V-Na(3)	135.1(3)
O(1C)-V-Na(3)	85.7(3)	O(1D)-V-Na(3)	137.5(3)
O(1E)-V-Na(3)	46.2(3)	O(1F)-V-Na(3)	45.7(3)
Na(1)-V-Na(3)	126.9(2)	Na(2)-V-Na(3)	122.2(2)
V-O(1A)-C(1A)	128.0(9)	V-O(1A)-Na(1)	95.6(3)
C(1A)-O(1A)-Na(1)	125.7(8)	O(1A)-C(1A)-C(2A)	114.2(12)
O(1A)-C(1A)-C(4A)	113.3(11)	C(2A)-C(1A)-C(4A)	99.0(9)
C(1A)-C(2A)-O(2A)	105.6(12)	C(1A)-C(2A)-C(8A)	117.1(11)
O(2A)-C(2A)-C(8A)	104.5(12)	C(2A)-O(2A)-C(3A)	107.9(11)
O(2A)-C(3A)-C(4A)	106.1(10)	O(2A)-C(3A)-O(4A)	110.2(13)
C(4A)-C(3A)-O(4A)	107.4(13)	C(1A)-C(4A)-C(3A)	107.3(12)
C(1A)-C(4A)-O(3A)	110.5(11)	C(3A)-C(4A)-O(3A)	102.9(9)
C(4A)-O(3A)-C(5A)	107.6(10)	O(3A)-C(5A)-C(6A)	111.5(12)
O(3A)-C(5A)-C(7A)	111.4(11)	C(6A)-C(5A)-C(7A)	110.4(12)
O(3A)-C(5A)-O(4A)	105.0(10)	C(6A)-C(5A)-O(4A)	108.6(12)
C(7A)-C(5A)-O(4A)	109.6(13)	C(3A)-O(4A)-C(5A)	106.8(10)
C(2A)-C(8A)-C(9A)	115.8(11)	C(2A)-C(8A)-O(6A)	112.1(12)
C(9A)-C(8A)-O(6A)	100.6(11)	C(2A)-C(8A)-Na(1)	104.4(9)
C(9A)-C(8A)-Na(1)	139.6(9)	O(6A)-C(8A)-Na(1)	58.3(6)
C(8A)-C(9A)-O(5A)	102.7(12)	C(9A)-O(5A)-C(10A)	105.4(11)
O(5A)-C(10A)-C(11A)	105.1(13)	O(5A)-C(10A)-C(12A)	110.4(16)
C(11A)-C(10A)-C(12A)	115.8(17)	O(5A)-C(10A)-O(6A)	106.7(12)
C(11A)-C(10A)-O(6A)	108.8(16)	C(12A)-C(10A)-O(6A)	109.5(15)
C(8A)-O(6A)-C(10A)	108.4(10)	C(8A)-O(6A)-Na(1)	91.6(8)
C(10A)-O(6A)-Na(1)	156.3(7)	V-O(1B)-C(1B)	129.1(8)
V-O(1B)-Na(1)	95.3(3)	C(1B)-O(1B)-Na(1)	119.8(8)
O(1B)-C(1B)-C(2B)	113.0(10)	O(1B)-C(1B)-C(4B)	114.4(11)
C(2B)-C(1B)-C(4B)	100.5(9)	C(1B)-C(2B)-O(2B)	104.0(11)
C(1B)-C(2B)-C(8B)	114.3(9)	O(2B)-C(2B)-C(8B)	107.7(11)
C(2B)-O(2B)-C(3B)	111.1(10)	O(2B)-C(3B)-C(4B)	106.1(10)
O(2B)-C(3B)-O(4B)	109.9(10)	C(4B)-C(3B)-O(4B)	103.5(10)
C(1B)-C(4B)-C(3B)	106.9(11)	C(1B)-C(4B)-O(3B)	110.7(11)
C(3B)-C(4B)-O(3B)	104.8(8)	C(4B)-O(3B)-C(5B)	109.3(10)
C(4B)-O(3B)-Na(2)	83.5(6)	C(5B)-O(3B)-Na(2)	154.9(9)
O(3B)-C(5B)-C(6B)	110.5(11)	O(3B)-C(5B)-C(7B)	108.2(12)
C(6B)-C(5B)-C(7B)	114.8(12)	O(3B)-C(5B)-O(4B)	104.8(10)
C(6B)-C(5B)-O(4B)	109.9(12)	C(7B)-C(5B)-O(4B)	108.1(13)
C(3B)-O(4B)-C(5B)	110.7(9)	C(2B)-C(8B)-C(9B)	112.5(10)
C(2B)-C(8B)-O(6B)	111.9(12)	C(9B)-C(8B)-O(6B)	101.2(11)
C(2B)-C(8B)-Na(1)	106.2(8)	C(9B)-C(8B)-Na(1)	139.4(9)
O(6B)-C(8B)-Na(1)	51.4(5)	C(8B)-C(9B)-O(5B)	103.5(11)
C(9B)-O(5B)-C(10B)	106.4(9)	O(5B)-C(10B)-C(11B)	107.0(10)

Table S4 (cont.)

O(5B)-C(10B)-C(12B)	112.3(13)	C(11B)-C(10B)-C(12B)	113.6(12)
O(5B)-C(10B)-O(6B)	105.6(10)	C(11B)-C(10B)-O(6B)	109.2(12)
C(12B)-C(10B)-O(6B)	108.8(11)	C(8B)-O(6B)-C(10B)	110.2(9)
C(8B)-O(6B)-Na(1)	98.9(7)	C(10B)-O(6B)-Na(1)	148.2(8)
V-O(1C)-C(1C)	126.5(7)	V-O(1C)-Na(2)	95.9(4)
C(1C)-O(1C)-Na(2)	126.6(8)	O(1C)-C(1C)-C(2C)	115.1(11)
O(1C)-C(1C)-C(4C)	112.7(11)	C(2C)-C(1C)-C(4C)	100.8(10)
C(1C)-C(2C)-O(2C)	105.2(10)	C(1C)-C(2C)-C(8C)	117.2(11)
O(2C)-C(2C)-C(8C)	101.0(9)	C(2C)-O(2C)-C(3C)	109.5(9)
O(2C)-C(3C)-C(4C)	109.4(11)	O(2C)-C(3C)-O(4C)	111.5(12)
C(4C)-C(3C)-O(4C)	106.9(10)	C(1C)-C(4C)-C(3C)	105.3(11)
C(1C)-C(4C)-O(3C)	109.5(10)	C(3C)-C(4C)-O(3C)	102.6(11)
C(4C)-O(3C)-C(5C)	109.0(9)	O(3C)-C(5C)-C(6C)	112.5(13)
O(3C)-C(5C)-C(7C)	108.8(13)	C(6C)-C(5C)-C(7C)	116.2(15)
O(3C)-C(5C)-O(4C)	103.7(11)	C(6C)-C(5C)-O(4C)	107.8(11)
C(7C)-C(5C)-O(4C)	107.0(14)	C(3C)-O(4C)-C(5C)	109.0(9)
C(2C)-C(8C)-C(9C)	112.5(12)	C(2C)-C(8C)-O(6C)	109.5(9)
C(9C)-C(8C)-O(6C)	103.7(12)	C(2C)-C(8C)-Na(2)	105.0(8)
C(9C)-C(8C)-Na(2)	141.8(10)	O(6C)-C(8C)-Na(2)	55.0(6)
C(8C)-C(9C)-O(5C)	103.1(10)	C(9C)-O(5C)-C(10C)	106.6(11)
O(5C)-C(10C)-C(11C)	110.6(12)	O(5C)-C(10C)-C(12C)	110.3(11)
C(11C)-C(10C)-C(12C)	113.4(13)	O(5C)-C(10C)-O(6C)	104.8(10)
C(11C)-C(10C)-O(6C)	109.5(11)	C(12C)-C(10C)-O(6C)	107.9(12)
C(8C)-O(6C)-C(10C)	109.7(10)	C(8C)-O(6C)-Na(2)	94.2(8)
C(10C)-O(6C)-Na(2)	145.9(9)	V-O(1D)-C(1D)	128.5(9)
V-O(1D)-Na(2)	95.5(4)	C(1D)-O(1D)-Na(2)	117.2(7)
O(1D)-C(1D)-C(2D)	116.1(12)	O(1D)-C(1D)-C(4D)	114.1(10)
C(2D)-C(1D)-C(4D)	100.7(10)	C(1D)-C(2D)-O(2D)	104.3(9)
C(1D)-C(2D)-C(8D)	117.7(12)	O(2D)-C(2D)-C(8D)	105.1(10)
C(2D)-O(2D)-C(3D)	107.3(9)	O(2D)-C(3D)-C(4D)	108.7(10)
O(2D)-C(3D)-O(4D)	108.5(11)	C(4D)-C(3D)-O(4D)	105.4(11)
C(1D)-C(4D)-C(3D)	106.3(12)	C(1D)-C(4D)-O(3D)	109.2(9)
C(3D)-C(4D)-O(3D)	105.5(11)	C(4D)-O(3D)-C(5D)	106.6(10)
C(4D)-O(3D)-Na(1)	89.5(7)	C(5D)-O(3D)-Na(1)	154.0(9)
O(3D)-C(5D)-C(6D)	111.0(13)	O(3D)-C(5D)-C(7D)	107.5(11)
C(6D)-C(5D)-C(7D)	113.0(15)	O(3D)-C(5D)-O(4D)	104.9(12)
C(6D)-C(5D)-O(4D)	113.9(11)	C(7D)-C(5D)-O(4D)	106.1(14)
C(3D)-O(4D)-C(5D)	107.6(11)	C(2D)-C(8D)-C(9D)	113.3(13)
C(2D)-C(8D)-O(6D)	110.7(11)	C(9D)-C(8D)-O(6D)	102.2(10)
C(2D)-C(8D)-Na(2)	99.5(9)	C(9D)-C(8D)-Na(2)	143.2(9)
O(6D)-C(8D)-Na(2)	48.3(6)	C(8D)-C(9D)-O(5D)	100.9(11)
C(9D)-O(5D)-C(10D)	107.6(11)	O(5D)-C(10D)-C(11D)	113.3(13)
O(5D)-C(10D)-C(12D)	107.8(13)	C(11D)-C(10D)-C(12D)	111.9(11)
O(5D)-C(10D)-O(6D)	105.1(9)	C(11D)-C(10D)-O(6D)	109.4(12)
C(12D)-C(10D)-O(6D)	109.1(13)	C(8D)-O(6D)-C(10D)	109.5(10)
C(8D)-O(6D)-Na(2)	103.3(8)	C(10D)-O(6D)-Na(2)	147.1(8)
V-O(1E)-C(1E)	126.5(7)	V-O(1E)-Na(3)	93.2(4)
C(1E)-O(1E)-Na(3)	123.9(8)	O(1E)-C(1E)-C(2E)	114.0(11)
O(1E)-C(1E)-C(4E)	112.6(11)	C(2E)-C(1E)-C(4E)	99.4(9)
C(1E)-C(2E)-O(2E)	107.5(11)	C(1E)-C(2E)-C(8E)	115.5(11)
O(2E)-C(2E)-C(8E)	104.1(10)	C(2E)-O(2E)-C(3E)	108.5(9)
O(2E)-C(3E)-C(4E)	108.0(11)	O(2E)-C(3E)-O(4E)	110.8(11)
C(4E)-C(3E)-O(4E)	107.7(12)	C(1E)-C(4E)-C(3E)	106.3(11)
C(1E)-C(4E)-O(3E)	109.2(11)	C(3E)-C(4E)-O(3E)	100.7(10)
C(4E)-O(3E)-C(5E)	110.8(9)	O(3E)-C(5E)-C(6E)	106.9(12)
O(3E)-C(5E)-C(7E)	110.5(10)	C(6E)-C(5E)-C(7E)	115.5(14)
O(3E)-C(5E)-O(4E)	104.0(11)	C(6E)-C(5E)-O(4E)	111.0(11)
C(7E)-C(5E)-O(4E)	108.4(12)	C(3E)-O(4E)-C(5E)	109.1(10)
C(2E)-C(8E)-C(9E)	112.9(12)	C(2E)-C(8E)-O(6E)	113.2(10)

Table S1 (cont.)

C(9E)-C(8E)-O(6E)	102.1(12)	C(2E)-C(8E)-Na(3)	106.0(8)
C(9E)-C(8E)-Na(3)	140.0(11)	O(6E)-C(8E)-Na(3)	52.3(6)
C(8E)-C(9E)-O(5E)	101.1(10)	C(9E)-O(5E)-C(10E)	108.8(11)
O(5E)-C(10E)-C(11E)	112.8(12)	O(5E)-C(10E)-C(12E)	108.3(13)
C(11E)-C(10E)-C(12E)	113.7(13)	O(5E)-C(10E)-O(6E)	104.2(11)
C(11E)-C(10E)-O(6E)	108.5(13)	C(12E)-C(10E)-O(6E)	108.9(12)
C(8E)-O(6E)-C(10E)	108.9(10)	C(8E)-O(6E)-Na(3)	98.0(8)
C(10E)-O(6E)-Na(3)	150.7(8)	V-O(1F)-C(1F)	123.5(9)
V-O(1F)-Na(3)	93.8(4)	C(1F)-O(1F)-Na(3)	127.8(8)
O(1F)-C(1F)-C(2F)	111.4(11)	O(1F)-C(1F)-C(4F)	112.2(11)
C(2F)-C(1F)-C(4F)	98.5(10)	C(1F)-C(2F)-O(2F)	108.0(10)
C(1F)-C(2F)-C(8F)	120.6(12)	O(2F)-C(2F)-C(8F)	102.8(11)
C(2F)-O(2F)-C(3F)	111.2(11)	O(2F)-C(3F)-C(4F)	105.8(9)
O(2F)-C(3F)-O(4F)	110.8(12)	C(4F)-C(3F)-O(4F)	106.6(11)
C(1F)-C(4F)-C(3F)	109.8(11)	C(1F)-C(4F)-O(3F)	107.7(10)
C(3F)-C(4F)-O(3F)	102.5(11)	C(4F)-O(3F)-C(5F)	110.0(10)
O(3F)-C(5F)-C(6F)	109.6(10)	O(3F)-C(5F)-C(7F)	111.0(12)
C(6F)-C(5F)-C(7F)	114.2(12)	O(3F)-C(5F)-O(4F)	106.5(10)
C(6F)-C(5F)-O(4F)	109.4(12)	C(7F)-C(5F)-O(4F)	105.9(10)
C(3F)-O(4F)-C(5F)	109.4(9)	C(2F)-C(8F)-C(9F)	113.8(12)
C(2F)-C(8F)-O(6F)	111.0(11)	C(9F)-C(8F)-O(6F)	105.1(10)
C(2F)-C(8F)-Na(3)	103.0(9)	C(9F)-C(8F)-Na(3)	142.7(9)
O(6F)-C(8F)-Na(3)	53.8(6)	C(8F)-C(9F)-O(5F)	102.9(11)
C(9F)-O(5F)-C(10F)	107.6(11)	O(5F)-C(10F)-C(11F)	109.8(14)
O(5F)-C(10F)-C(12F)	108.5(13)	C(11F)-C(10F)-C(12F)	116.6(12)
O(5F)-C(10F)-O(6F)	103.5(9)	C(11F)-C(10F)-O(6F)	108.4(12)
C(12F)-C(10F)-O(6F)	109.2(13)	C(8F)-O(6F)-C(10F)	109.0(10)
C(8F)-O(6F)-Na(3)	96.3(7)	C(10F)-O(6F)-Na(3)	133.3(9)
V-Na(1)-O(1A)	40.1(2)	V-Na(1)-C(8A)	107.8(4)
O(1A)-Na(1)-C(8A)	68.2(4)	V-Na(1)-O(6A)	113.5(3)
O(1A)-Na(1)-O(6A)	81.6(4)	C(8A)-Na(1)-O(6A)	30.1(4)
V-Na(1)-O(1B)	39.6(2)	O(1A)-Na(1)-O(1B)	79.2(4)
C(8A)-Na(1)-O(1B)	143.6(5)	O(6A)-Na(1)-O(1B)	131.9(5)
V-Na(1)-C(8B)	104.4(3)	O(1A)-Na(1)-C(8B)	142.5(5)
C(8A)-Na(1)-C(8B)	140.3(5)	O(6A)-Na(1)-C(8B)	114.1(4)
O(1B)-Na(1)-C(8B)	64.9(4)	V-Na(1)-O(6B)	121.7(3)
O(1A)-Na(1)-O(6B)	159.9(5)	C(8A)-Na(1)-O(6B)	130.3(5)
O(6A)-Na(1)-O(6B)	118.4(4)	O(1B)-Na(1)-O(6B)	84.7(4)
C(8B)-Na(1)-O(6B)	29.7(4)	V-Na(1)-O(3D)	98.5(3)
O(1A)-Na(1)-O(3D)	87.9(4)	C(8A)-Na(1)-O(3D)	82.5(4)
O(6A)-Na(1)-O(3D)	110.2(4)	O(1B)-Na(1)-O(3D)	112.7(4)
C(8B)-Na(1)-O(3D)	115.0(4)	O(6B)-Na(1)-O(3D)	87.4(4)
V-Na(2)-O(3B)	98.3(3)	V-Na(2)-O(1C)	39.6(2)
O(3B)-Na(2)-O(1C)	86.6(3)	V-Na(2)-C(8C)	107.1(4)
O(3B)-Na(2)-C(8C)	80.6(4)	O(1C)-Na(2)-C(8C)	67.9(4)
V-Na(2)-O(6C)	113.7(3)	O(3B)-Na(2)-O(6C)	108.9(3)
O(1C)-Na(2)-O(6C)	82.4(4)	C(8C)-Na(2)-O(6C)	30.8(4)
V-Na(2)-O(1D)	39.7(3)	O(3B)-Na(2)-O(1D)	114.7(4)
O(1C)-Na(2)-O(1D)	78.7(4)	C(8C)-Na(2)-O(1D)	142.6(4)
O(6C)-Na(2)-O(1D)	130.9(4)	V-Na(2)-C(8D)	105.0(3)
O(3B)-Na(2)-C(8D)	117.4(4)	O(1C)-Na(2)-C(8D)	142.4(4)
C(8C)-Na(2)-C(8D)	140.0(5)	O(6C)-Na(2)-C(8D)	112.7(4)
O(1D)-Na(2)-C(8D)	65.3(4)	V-Na(2)-O(6D)	124.5(3)
O(3B)-Na(2)-O(6D)	92.1(3)	O(1C)-Na(2)-O(6D)	163.2(5)
C(8C)-Na(2)-O(6D)	128.4(5)	O(6C)-Na(2)-O(6D)	113.8(5)
O(1D)-Na(2)-O(6D)	86.7(4)	C(8D)-Na(2)-O(6D)	28.4(3)
V-Na(3)-O(1E)	40.6(2)	V-Na(3)-C(8E)	105.9(4)
O(1E)-Na(3)-C(8E)	65.5(4)	V-Na(3)-O(6E)	118.3(4)
O(1E)-Na(3)-O(6E)	83.5(4)	C(8E)-Na(3)-O(6E)	29.7(4)

Table S4 (cont.)

V-Na(3)-O(1F)	40.4(3)	O(1E)-Na(3)-O(1F)	80.8(4)
C(8E)-Na(3)-O(1F)	146.3(5)	O(6E)-Na(3)-O(1F)	150.7(5)
V-Na(3)-C(8F)	106.7(3)	O(1E)-Na(3)-C(8F)	143.7(5)
C(8E)-Na(3)-C(8F)	144.3(5)	O(6E)-Na(3)-C(8F)	132.8(5)
O(1F)-Na(3)-C(8F)	67.1(4)	V-Na(3)-O(6F)	113.6(3)
O(1E)-Na(3)-O(6F)	132.9(5)	C(8E)-Na(3)-O(6F)	120.4(4)
O(6E)-Na(3)-O(6F)	125.7(4)	O(1F)-Na(3)-O(6F)	82.5(4)
C(8F)-Na(3)-O(6F)	29.9(3)	C(1)-C(2)-O(3)	125.6(43)
C(2)-O(3)-C(4)	111.5(27)	O(3)-C(4)-C(5)	101.4(41)
O(3)-C(4)-C(5')	115.5(55)	C(5)-C(4)-C(5')	139.4(67)

TABLE S5 – Anisotropic displacement coefficients ($Å^2 x 10^3$) for complex 4.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
V	19(1)	6(1)	15(1)	1(1)	2(1)	-1(1)
O(1A)	17(4)	11(5)	24(5)	8(4)	4(4)	-3(4)
C(1A)	21(6)	19(8)	24(6)	4(7)	10(5)	2(6)
C(2A)	40(8)	24(8)	28(7)	0(7)	9(6)	-4(7)
O(2A)	38(6)	19(6)	23(5)	18(5)	-4(4)	-1(4)
C(3A)	32(8)	28(9)	31(8)	8(7)	-11(7)	-9(7)
C(4A)	19(6)	26(8)	14(6)	-3(7)	-3(5)	-10(6)
O(3A)	18(4)	19(5)	22(5)	1(4)	-1(4)	-8(4)
C(5A)	18(7)	18(8)	34(8)	4(6)	1(6)	8(7)
C(6A)	18(7)	42(10)	48(9)	2(7)	6(7)	-8(8)
C(7A)	32(8)	60(12)	34(8)	-11(9)	11(7)	-17(8)
O(4A)	31(5)	22(6)	37(5)	6(5)	-3(4)	-8(5)
C(8A)	23(7)	23(8)	25(7)	14(6)	3(6)	-7(6)
C(9A)	20(7)	40(10)	37(8)	11(7)	5(6)	-8(8)
O(5A)	27(5)	53(8)	35(6)	8(5)	16(5)	-4(6)
C(10A)	38(9)	55(13)	35(9)	14(9)	0(7)	-16(9)
C(11A)	43(11)	75(17)	82(14)	-17(11)	16(10)	27(12)
C(12A)	67(12)	109(20)	43(10)	32(14)	23(9)	-6(12)
O(6A)	22(5)	35(6)	16(4)	3(4)	4(4)	-1(4)
O(1B)	26(5)	8(5)	15(4)	-3(4)	1(4)	-1(4)
C(1B)	20(6)	1(6)	15(6)	4(5)	-3(5)	-2(5)
C(2B)	24(7)	17(7)	15(6)	-3(6)	1(5)	0(6)
O(2B)	32(5)	16(5)	14(4)	2(4)	3(4)	7(4)
C(3B)	23(6)	15(7)	13(6)	-1(6)	9(5)	-2(6)
C(4B)	22(7)	23(8)	14(6)	-6(6)	7(5)	-3(5)
O(3B)	24(5)	23(6)	35(5)	4(4)	6(4)	8(5)
C(5B)	19(7)	18(8)	36(8)	0(6)	9(6)	-6(7)
C(6B)	25(7)	31(10)	41(9)	20(7)	0(7)	-4(7)
C(7B)	33(9)	24(9)	94(14)	0(8)	10(9)	-8(10)
O(4B)	29(5)	43(7)	18(5)	2(5)	-1(4)	1(5)
C(9B)	44(9)	7(7)	21(7)	-2(6)	1(6)	2(6)
O(5B)	42(6)	11(5)	23(5)	3(4)	6(4)	1(4)
C(10B)	30(8)	12(8)	33(8)	6(6)	0(6)	-9(6)
C(11B)	34(8)	24(9)	28(7)	-3(7)	10(6)	4(6)
C(12B)	52(10)	15(8)	47(9)	-5(8)	0(8)	1(7)
O(6B)	35(5)	8(5)	21(5)	3(4)	-2(4)	-6(4)
O(1C)	17(4)	7(5)	26(5)	1(4)	6(4)	-3(4)
C(1C)	24(7)	14(7)	15(6)	10(6)	7(5)	3(5)
C(2C)	19(7)	17(7)	15(6)	2(6)	-2(5)	-4(6)
C(4C)	35(8)	2(6)	23(7)	0(6)	5(6)	-4(5)
O(3C)	41(6)	13(5)	27(5)	5(5)	0(4)	0(4)
C(5C)	42(9)	13(8)	31(8)	6(7)	-5(7)	4(7)
C(6C)	54(10)	26(9)	43(9)	-5(8)	-2(8)	14(8)
C(7C)	90(15)	33(11)	90(15)	26(11)	13(12)	-29(11)
O(4C)	32(5)	2(5)	50(6)	6(4)	1(5)	8(4)
C(8C)	22(7)	5(7)	38(8)	4(6)	9(6)	11(6)
C(9C)	32(8)	32(9)	32(8)	-6(7)	19(6)	3(7)
O(5C)	33(5)	19(5)	40(6)	0(5)	20(4)	5(5)
C(10C)	24(7)	26(8)	19(7)	-3(7)	7(6)	1(6)
C(11C)	56(10)	38(10)	23(7)	2(9)	7(7)	-14(7)
C(12C)	35(9)	35(10)	61(11)	-7(8)	14(8)	7(9)
O(6C)	37(5)	19(5)	21(5)	2(4)	10(4)	13(4)
O(1D)	27(5)	6(5)	19(4)	0(4)	1(4)	-1(4)
C(1D)	33(7)	8(7)	13(6)	-5(6)	-1(5)	2(5)

C(2D)	26(7)	19(8)	18(6)	3(6)	11(6)	1(6)
O(2D)	29(5)	23(5)	23(5)	7(4)	5(4)	12(4)
C(3D)	24(7)	23(8)	25(7)	-2(6)	3(6)	5(6)
C(4D)	25(7)	3(6)	36(8)	5(6)	9(6)	4(6)
O(3D)	38(5)	17(5)	30(5)	18(5)	12(4)	6(4)
C(5D)	38(8)	29(9)	24(7)	19(7)	14(7)	7(7)
C(6D)	32(8)	40(10)	48(9)	15(8)	13(7)	13(8)
C(7D)	99(16)	34(11)	44(10)	32(11)	-21(10)	-9(9)
O(4D)	33(5)	24(6)	34(5)	11(5)	6(4)	7(5)
C(8D)	29(7)	22(8)	28(7)	-6(7)	15(6)	-9(6)
C(9D)	56(10)	16(8)	43(9)	-14(8)	18(8)	3(7)
O(5D)	33(6)	13(5)	56(6)	-6(5)	12(5)	2(5)
C(10D)	25(8)	9(7)	48(9)	0(6)	-4(7)	-9(7)
C(11D)	47(9)	18(8)	58(10)	3(8)	21(8)	-8(8)
C(12D)	45(9)	24(9)	46(9)	-3(8)	9(7)	-12(8)
O(6D)	29(5)	12(5)	29(5)	3(4)	5(4)	2(4)
O(1E)	34(5)	17(5)	10(4)	-4(4)	12(4)	-10(4)
C(1E)	24(7)	4(6)	14(6)	6(6)	1(5)	-6(5)
C(2E)	26(7)	11(7)	12(6)	5(6)	-1(5)	0(5)
O(2E)	30(5)	29(6)	26(5)	-6(5)	-8(4)	5(5)
C(3E)	40(8)	18(8)	29(8)	-6(7)	18(7)	-8(6)
C(4E)	19(6)	19(8)	15(6)	-2(6)	4(5)	2(6)
O(3E)	30(5)	21(5)	32(5)	2(5)	11(4)	12(5)
C(5E)	30(8)	29(9)	20(7)	-2(7)	-1(6)	3(6)
C(6E)	45(9)	42(11)	40(9)	6(9)	7(7)	0(8)
C(7E)	46(9)	26(9)	26(8)	-4(7)	9(7)	7(7)
O(4E)	48(6)	23(6)	17(5)	-6(5)	8(4)	8(4)
C(8E)	35(8)	27(9)	25(7)	-5(7)	7(6)	-14(7)
C(9E)	48(9)	11(7)	35(8)	1(7)	-3(7)	-15(7)
O(5E)	37(5)	34(6)	26(5)	9(5)	4(4)	-18(5)
C(10E)	42(9)	20(8)	31(8)	-5(7)	10(7)	-23(7)
C(11E)	44(9)	14(8)	57(10)	-4(7)	12(8)	0(7)
C(12E)	35(9)	25(9)	54(10)	5(7)	14(7)	-11(8)
O(6E)	29(5)	17(5)	22(5)	6(4)	10(4)	-1(4)
O(1F)	29(5)	8(5)	17(4)	-3(4)	4(4)	-1(4)
C(1F)	28(7)	15(7)	12(6)	1(6)	-1(5)	8(6)
C(2F)	31(7)	15(7)	25(7)	0(6)	14(6)	-1(6)
O(2F)	81(8)	16(6)	24(5)	-17(6)	-4(5)	7(5)
C(3F)	33(8)	16(7)	21(7)	3(6)	20(6)	6(6)
C(4F)	15(6)	15(8)	28(7)	2(6)	3(6)	2(6)
O(3F)	38(5)	13(5)	21(5)	2(4)	-4(4)	1(4)
C(5F)	28(7)	22(8)	13(6)	2(6)	9(5)	-2(6)
C(6F)	53(10)	36(10)	31(8)	6(9)	10(7)	12(8)
C(7F)	54(10)	18(8)	32(8)	-5(7)	19(7)	-5(6)
O(4F)	42(6)	22(6)	18(5)	8(5)	7(4)	5(4)
C(8F)	32(7)	20(8)	22(7)	3(7)	12(6)	-1(6)
C(9F)	55(9)	17(8)	28(7)	-25(8)	18(7)	-8(7)
O(5F)	38(6)	19(6)	40(6)	-3(5)	3(5)	-3(5)
C(10F)	16(7)	12(8)	54(9)	-1(6)	7(6)	-3(7)
C(11F)	36(9)	45(12)	85(13)	-8(9)	22(9)	-7(10)
C(12F)	47(10)	32(10)	39(9)	-4(8)	6(8)	-13(8)
O(6F)	27(5)	14(5)	29(5)	-8(4)	2(4)	-10(4)
Na(1)	25(3)	30(3)	33(3)	4(3)	6(2)	-18(3)
Na(2)	37(3)	9(3)	60(4)	4(3)	26(3)	7(3)
Na(3)	74(4)	14(3)	28(3)	-20(3)	24(3)	-11(2)

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

TABLE S6 – H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$) for complex 4.

	x	y	z	U
H(1AA)	6030	-459	2215	80
H(2AA)	4644	279	2020	80
H(3AA)	5328	1045	619	80
H(4AA)	6274	-104	1068	80
H(6AA)	3337	-1030	848	80
H(6AB)	2992	-941	69	80
H(6AC)	3597	-1767	403	80
H(7AA)	5244	-470	-108	80
H(7AB)	4781	-1419	-194	80
H(7AC)	4177	-592	-528	80
H(8AA)	5722	1808	2511	80
H(9AA)	3935	1776	2320	80
H(9AB)	4560	2262	2958	80
H(11A)	4518	-385	3779	80
H(11B)	4794	-497	3119	80
H(11C)	5586	-511	3809	80
H(12A)	5391	1807	4126	80
H(12B)	4827	1062	4369	80
H(12C)	5915	941	4459	80
H(1BA)	9686	1460	3304	80
H(2BA)	10113	1801	4409	80
H(3BA)	10648	-544	4526	80
H(4BA)	10270	-186	3434	80
H(6BA)	12176	-703	3974	80
H(6BB)	12835	-50	3733	80
H(6BC)	13086	-307	4489	80
H(7BA)	12220	1916	4452	80
H(7BB)	13117	1329	4781	80
H(7BC)	12865	1586	4026	80
H(8BA)	8373	1015	4370	80
H(9BA)	9457	1743	5429	80
H(9BB)	8356	1872	5260	80
H(11D)	9589	3400	4001	80
H(11E)	8628	3774	3533	80
H(11F)	9119	4237	4217	80
H(12D)	7186	3048	4521	80
H(12E)	7612	4006	4538	80
H(12F)	7122	3543	3853	80
H(1CA)	9315	-1524	1830	80
H(2CA)	10813	-2016	1988	80
H(3CA)	10592	-2033	3666	80
H(4CA)	9111	-1907	2985	80
H(6CA)	9054	-3455	3529	80
H(6CB)	8622	-4221	3022	80
H(6CC)	9563	-4382	3602	80
H(7CA)	10430	-4065	2193	80
H(7CB)	10456	-4777	2743	80
H(7CC)	9516	-4616	2163	80
H(8CA)	11467	-412	2669	80
H(9CA)	12553	-1612	2413	80
H(9CB)	12811	-602	2410	80
H(11G)	10559	-1171	584	80
H(11H)	10376	-165	392	80
H(11I)	11202	-676	222	80

Table S6 (cont.)

H(12G)	12444	610	1665	80
H(12H)	12412	468	919	80
H(12I)	11586	979	1089	80
H(1DA)	8703	2112	2545	80
H(2DA)	9035	3239	1966	80
H(3DA)	6771	2614	851	80
H(4DA)	6997	1733	1726	80
H(6DA)	5480	2970	1476	80
H(6DB)	5452	3372	2158	80
H(6DC)	5329	3994	1540	80
H(7DA)	7704	4453	2523	80
H(7DB)	6734	4939	2203	80
H(7DC)	6858	4317	2822	80
H(8DA)	9569	1974	1177	80
H(9DA)	9691	3632	982	80
H(9DB)	10534	3027	937	80
H(11J)	12113	2440	1821	80
H(11K)	12589	3113	2393	80
H(11L)	12365	2139	2568	80
H(12J)	10548	3379	2954	80
H(12K)	11381	2718	3276	80
H(12L)	11605	3691	3101	80
H(1EA)	8809	-593	1049	80
H(2EA)	8109	-1208	43	80
H(3EA)	6563	656	154	80
H(4EA)	7996	937	883	80
H(6EA)	8303	-153	-924	80
H(6EB)	8141	687	-1386	80
H(6EC)	9144	508	-877	80
H(7EA)	8245	2275	-92	80
H(7EB)	9113	2055	-350	80
H(7EC)	8111	2233	-859	80
H(8EA)	6621	-1681	547	80
H(9EA)	6635	-2125	-623	80
H(9EB)	6294	-2839	-201	80
H(11M)	7085	-4036	652	80
H(11N)	7951	-4522	518	80
H(11O)	8048	-4123	1224	80
H(12M)	9295	-2523	528	80
H(12N)	9442	-3156	1143	80
H(12O)	9346	-3555	437	80
H(1FA)	6888	-632	3147	80
H(2FA)	6434	-1934	3507	80
H(3FA)	9008	-1947	4281	80
H(4FA)	8590	-542	3922	80
H(6FA)	6533	-1541	4858	80
H(6FB)	7105	-1477	5616	80
H(6FC)	6578	-637	5238	80
H(7FA)	9053	-186	5353	80
H(7FB)	8193	223	5547	80
H(7FC)	8720	-617	5925	80
H(8FA)	7401	-2887	2788	80
H(9FA)	5935	-3362	3298	80
H(9FB)	6736	-3980	3194	80
H(11P)	4646	-2486	2598	80
H(11Q)	4348	-2039	1892	80
H(11R)	3991	-3000	1983	80
H(12P)	5863	-3434	1209	80
H(12Q)	4775	-3613	1079	80
H(12R)	5132	-2653	988	80

Table S7. Data collection and refinement parameters for complex 5.

Empirical Formula	$C_{79}\ H_{114}\ Cr\ Li_3\ O_{36}$
Color; Habit	Green ; Prismatic
Crystal Size (mm)	0.32 x 0.40 x 0.52
Crystal System	Monoclinic
Space Group	C2
Unit Cell Dimensions	$\underline{a}$ = 22.671(9) Å
	$\underline{b}$ = 18.785(5) Å
	$\underline{c}$ = 13.886(4) Å
	β = 126.39(2)°
Volume	4761(3) $Å^3$
Z	2
Formula Weight	1712.5
Density(calc.)	1.195 g/cm^3
Absorption Coefficient	0.199 mm^{-1}
F(000)	1818
Diffractometer Used	Siemens P4
Radiation	MoKα (λ = 0.71069 Å)
Temperature (K)	293
Monochromator	Highly oriented graphite crystal
2θ Range	2.0 to 50.0°
Scan Type	ω
Scan Speed	Variable; 4.00 to 20.00°/min.
Scan Range	1.40°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 30.0% of total scan time
Standard Reflections	2 measured every 50 reflections
Index Ranges	$0 \le h \le 26$, $0 \le k \le 22$
	$-16 \le \ell \le 13$
Reflections Collected	4453
Independent Reflections	4335 (R_{int} = 2.84%)
Observed Reflections	3055 ($F > 4.0\sigma(F)$)
Absorption Correction	Semi-empirical
Min./Max. Transmission	0.8923 / 0.9265
System Used	Siemens SHELXTL IRIS
Solution	Direct Methods

Table 3. (cont.)

Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0130F^2$
Number of Parameters Refined	510
Final R Indices (obs. data)	R = 7.32 %, wR = 10.20 %
R Indices (all data)	R = 10.56 %, wR = 100.24 %
Goodness-of-Fit	0.82
Largest and Mean Δ/σ	0.322, 0.022
Data-to-Parameter Ratio	6.0:1
Largest Difference Peak	0.64 $eÅ^{-3}$
Largest Difference Hole	-0.41 $eÅ^{-3}$

Table S8. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$) for complex 5.

	x	y	z	U(eq)
Cr	-10000	-190	-10000	25(1)
Li(1)	-9129(9)	549(10)	-7763(15)	52(4)
Li(2)	-10000	-1712(15)	-10000	61(6)
C(1A)	-9172(5)	1166(5)	-9742(8)	41(4)
C(2A)	-8521(5)	1653(6)	-8821(8)	49(5)
C(3A)	-8140(6)	1123(6)	-9884(10)	57(6)
C(4A)	-8974(6)	1030(6)	-10598(9)	54(5)
C(5A)	-8722(6)	1813(6)	-11612(9)	58(6)
C(6A)	-8750(9)	2615(9)	-11647(17)	112(12)
C(7A)	-8845(10)	1460(12)	-12708(14)	114(12)
C(8A)	-8263(5)	1592(6)	-7530(9)	53(5)
C(9A)	-7762(7)	2193(8)	-6728(10)	76(7)
C(10A)	-8774(8)	2241(8)	-6753(15)	83(9)
C(11A)	-8994(9)	2073(8)	-5961(14)	91(11)
C(12A)	-9235(12)	2814(9)	-7651(19)	118(16)
O(1A)	-9209(3)	554(3)	-9198(5)	35(3)
O(2A)	-7915(4)	1442(6)	-8807(6)	72(5)
O(3A)	-9261(4)	1590(4)	-11454(6)	55(4)
O(4A)	-8037(4)	1578(6)	-10568(7)	75(5)
O(5A)	-8008(5)	2401(6)	-6047(8)	89(6)
O(6A)	-8840(4)	1611(4)	-7416(6)	54(4)
C(1B)	-9931(4)	-719(5)	-7868(7)	35(4)
C(2B)	-9734(5)	-510(6)	-6624(8)	47(5)
C(3B)	-10985(7)	-665(8)	-7814(11)	69(7)
C(4B)	-10692(5)	-1036(6)	-8431(7)	48(4)
C(5B)	-11104(6)	-1884(8)	-7740(10)	64(6)
C(6B)	-11780(9)	-2224(12)	-8685(14)	128(12)
C(7B)	-10701(11)	-2301(14)	-6603(16)	154(16)
C(8B)	-9257(6)	139(7)	-6055(8)	56(5)
C(9B)	-8935(8)	218(10)	-4718(10)	93(9)
C(10B)	-7978(6)	81(7)	-4815(9)	66(6)
C(11B)	-7400(7)	564(9)	-4682(10)	86(7)
C(12B)	-7750(10)	-687(8)	-4510(14)	100(11)
O(1B)	-9905(3)	-139(4)	-8468(4)	35(3)
O(2B)	-10413(4)	-312(5)	-6830(7)	75(5)
O(3B)	-10622(5)	-1757(4)	-8061(7)	65(5)
O(4B)	-11249(6)	-1222(7)	-7486(11)	110(9)
O(5B)	-8203(5)	401(6)	-4170(7)	86(5)
O(6B)	-8628(3)	118(4)	-6047(5)	51(3)
C(1C)	-11413(4)	-981(5)	-11761(7)	40(4)
C(2C)	-11789(6)	-1727(6)	-12067(10)	55(5)
C(3C)	-12437(6)	-977(7)	-11597(9)	60(6)
C(4C)	-11990(5)	-522(6)	-11849(7)	42(4)
C(5C)	-13254(6)	-418(7)	-13418(10)	66(6)
C(6C)	-13584(8)	273(8)	-13532(14)	90(9)
C(7C)	-13678(8)	-916(12)	-14510(13)	113(10)
C(8C)	-11299(7)	-2367(6)	-11389(11)	68(7)
C(9C)	-11676(7)	-3088(7)	-11946(15)	92(9)
C(10C)	-10721(8)	-2997(7)	-12061(11)	77(7)
C(11C)	-9983(8)	-3322(8)	-11471(14)	106(10)
C(12C)	-11060(8)	-2750(9)	-13337(10)	96(8)
O(1C)	-10730(3)	-987(4)	-10625(5)	34(3)
O(2C)	-12285(5)	-1698(5)	-11736(9)	85(6)
O(3C)	-12529(3)	-340(5)	-13104(6)	60(4)

O(4C)	-13160(4)	-805(5)	-12444(7)	77(5)
O(5C)	-11157(7)	-3482(5)	-11955(10)	104(7)
O(6C)	-10678(4)	-2376(4)	-11418(6)	59(4)
C(1)	2934(10)	-222(15)	-1248(13)	102(8)
C(2)	3070	330	-468	114(11)
C(3)	3655	281	742	97(9)
C(4)	4103	-321	1172	65(6)
C(5)	3967	-873	392	135(14)
C(6)	3382	-823	-818	169(19)
C(7)	4816	-504	2262	153(16)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table S9. Bond lengths (Å) for complex 5.

Cr-Li(1)	2.864	(17)	Cr-Li(2)	2.859	(28)
Cr-O(1A)	2.010	(6)	Cr-O(1B)	2.009	(7)
Cr-O(1C)	2.008	(6)	Cr-Li(1A)	2.864	(17)
Cr-O(1AA)	2.010	(6)	Cr-O(1BA)	2.009	(7)
Cr-O(1CA)	2.008	(6)	Li(1)-C(8A)	2.656	(24)
Li(1)-O(1A)	1.890	(25)	Li(1)-O(6A)	2.065	(19)
Li(1)-C(8B)	2.668	(29)	Li(1)-O(1B)	1.919	(19)
Li(1)-O(6B)	2.101	(20)	Li(2)-C(8C)	2.677	(17)
Li(2)-O(1C)	1.909	(21)	Li(2)-O(6C)	2.050	(18)
Li(2)-C(8CA)	2.677	(17)	Li(2)-O(1CA)	1.909	(21)
Li(2)-O(6CA)	2.050	(18)	C(1A)-C(2A)	1.553	(12)
C(1A)-C(4A)	1.520	(20)	C(1A)-O(1A)	1.405	(13)
C(2A)-C(8A)	1.524	(17)	C(2A)-O(2A)	1.421	(17)
C(3A)-C(4A)	1.539	(15)	C(3A)-O(2A)	1.397	(16)
C(3A)-O(4A)	1.395	(18)	C(4A)-O(3A)	1.422	(13)
C(5A)-C(6A)	1.507	(21)	C(5A)-C(7A)	1.526	(25)
C(5A)-O(3A)	1.427	(18)	C(5A)-O(4A)	1.427	(11)
C(8A)-C(9A)	1.516	(16)	C(8A)-O(6A)	1.410	(18)
C(9A)-O(5A)	1.410	(23)	C(10A)-C(11A)	1.487	(34)
C(10A)-C(12A)	1.503	(22)	C(10A)-O(5A)	1.430	(18)
C(10A)-O(6A)	1.452	(19)	C(1B)-C(2B)	1.556	(15)
C(1B)-C(4B)	1.531	(13)	C(1B)-O(1B)	1.394	(12)
C(2B)-C(8B)	1.506	(16)	C(2B)-O(2B)	1.438	(16)
C(3B)-C(4B)	1.528	(22)	C(3B)-O(2B)	1.374	(13)
C(3B)-O(4B)	1.407	(23)	C(4B)-O(3B)	1.423	(14)
C(5B)-C(6B)	1.446	(19)	C(5B)-C(7B)	1.493	(24)
C(5B)-O(3B)	1.422	(21)	C(5B)-O(4B)	1.386	(21)
C(8B)-C(9B)	1.547	(18)	C(8B)-O(6B)	1.420	(17)
C(9B)-O(5B)	1.398	(19)	C(10B)-C(11B)	1.511	(22)
C(10B)-C(12B)	1.506	(20)	C(10B)-O(5B)	1.403	(20)
C(10B)-O(6B)	1.453	(10)	C(1C)-C(2C)	1.564	(14)
C(1C)-C(4C)	1.510	(15)	C(1C)-O(1C)	1.409	(8)
C(2C)-C(8C)	1.525	(15)	C(2C)-O(2C)	1.447	(21)
C(3C)-C(4C)	1.516	(19)	C(3C)-O(2C)	1.438	(17)
C(3C)-O(4C)	1.374	(11)	C(4C)-O(3C)	1.457	(10)
C(5C)-C(6C)	1.457	(21)	C(5C)-C(7C)	1.539	(21)
C(5C)-O(3C)	1.439	(16)	C(5C)-O(4C)	1.435	(18)
C(8C)-C(9C)	1.542	(17)	C(8C)-O(6C)	1.433	(20)
C(9C)-O(5C)	1.395	(24)	C(10C)-C(11C)	1.489	(22)
C(10C)-C(12C)	1.527	(20)	C(10C)-O(5C)	1.414	(23)
C(10C)-O(6C)	1.437	(17)			

Table S10 Bond angles (°) for complex 5.

Li(1)-Cr-Li(2)	119.0(4)	Li(1)-Cr-O(1A)	41.2(5)
Li(2)-Cr-O(1A)	134.1(2)	Li(1)-Cr-O(1B)	42.0(5)
Li(2)-Cr-O(1B)	92.7(2)	O(1A)-Cr-O(1B)	83.1(3)
Li(1)-Cr-O(1C)	133.8(5)	Li(2)-Cr-O(1C)	41.8(2)
O(1A)-Cr-O(1C)	173.7(2)	O(1B)-Cr-O(1C)	92.1(3)
Li(1)-Cr-Li(1A)	122.0(7)	Li(2)-Cr-Li(1A)	119.0(4)
O(1A)-Cr-Li(1A)	94.5(4)	O(1B)-Cr-Li(1A)	134.3(5)
O(1C)-Cr-Li(1A)	91.8(4)	Li(1)-Cr-O(1AA)	94.5(4)
Li(2)-Cr-O(1AA)	134.1(2)	O(1A)-Cr-O(1AA)	91.9(3)
O(1B)-Cr-O(1AA)	93.1(3)	O(1C)-Cr-O(1AA)	92.5(2)
Li(1A)-Cr-O(1AA)	41.2(5)	Li(1)-Cr-O(1BA)	134.3(5)
Li(2)-Cr-O(1BA)	92.7(2)	O(1A)-Cr-O(1BA)	93.1(3)
O(1B)-Cr-O(1BA)	174.6(4)	O(1C)-Cr-O(1BA)	92.0(3)
Li(1A)-Cr-O(1BA)	42.0(5)	O(1AA)-Cr-O(1BA)	83.1(3)
Li(1)-Cr-O(1CA)	91.8(4)	Li(2)-Cr-O(1CA)	41.8(2)
O(1A)-Cr-O(1CA)	92.5(2)	O(1B)-Cr-O(1CA)	92.0(3)
O(1C)-Cr-O(1CA)	83.6(4)	Li(1A)-Cr-O(1CA)	133.8(5)
O(1AA)-Cr-O(1CA)	173.7(2)	O(1BA)-Cr-O(1CA)	92.1(3)
Cr-Li(1)-C(8A)	118.3(9)	Cr-Li(1)-O(1A)	44.4(4)
C(8A)-Li(1)-O(1A)	74.1(8)	Cr-Li(1)-O(6A)	129.8(8)
C(8A)-Li(1)-O(6A)	31.7(5)	O(1A)-Li(1)-O(6A)	93.4(10)
Cr-Li(1)-C(8B)	117.1(7)	C(8A)-Li(1)-C(8B)	124.6(7)
O(1A)-Li(1)-C(8B)	160.9(9)	O(6A)-Li(1)-C(8B)	105.0(9)
Cr-Li(1)-O(1B)	44.4(4)	C(8A)-Li(1)-O(1B)	161.4(10)
O(1A)-Li(1)-O(1B)	88.8(7)	O(6A)-Li(1)-O(1B)	146.9(11)
C(8B)-Li(1)-O(1B)	73.1(8)	Cr-Li(1)-O(6B)	127.2(8)
C(8A)-Li(1)-O(6B)	106.5(6)	O(1A)-Li(1)-O(6B)	147.8(12)
O(6A)-Li(1)-O(6B)	103.0(8)	C(8B)-Li(1)-O(6B)	31.9(5)
O(1B)-Li(1)-O(6B)	91.9(9)	Cr-Li(2)-C(8C)	117.4(6)
Cr-Li(2)-O(1C)	44.5(6)	C(8C)-Li(2)-O(1C)	73.4(3)
Cr-Li(2)-O(6C)	127.5(7)	C(8C)-Li(2)-O(6C)	31.9(5)
O(1C)-Li(2)-O(6C)	92.5(3)	Cr-Li(2)-C(8CA)	117.4(6)
C(8C)-Li(2)-C(8CA)	125.2(12)	O(1C)-Li(2)-C(8CA)	160.4(11)
O(6C)-Li(2)-C(8CA)	106.8(10)	Cr-Li(2)-O(1CA)	44.5(6)
C(8C)-Li(2)-O(1CA)	160.4(11)	O(1C)-Li(2)-O(1CA)	89.0(12)
O(6C)-Li(2)-O(1CA)	145.5(5)	C(8CA)-Li(2)-O(1CA)	73.4(3)
Cr-Li(2)-O(6CA)	127.5(7)	C(8C)-Li(2)-O(6CA)	106.8(10)
O(1C)-Li(2)-O(6CA)	145.5(5)	O(6C)-Li(2)-O(6CA)	105.1(13)
C(8CA)-Li(2)-O(6CA)	31.9(5)	O(1CA)-Li(2)-O(6CA)	92.5(3)
C(2A)-C(1A)-C(4A)	99.6(10)	C(2A)-C(1A)-O(1A)	111.7(7)
C(4A)-C(1A)-O(1A)	115.1(9)	C(1A)-C(2A)-C(8A)	116.1(11)
C(1A)-C(2A)-O(2A)	106.5(9)	C(8A)-C(2A)-O(2A)	105.6(7)
C(4A)-C(3A)-O(2A)	105.4(12)	C(4A)-C(3A)-O(4A)	105.6(8)
O(2A)-C(3A)-O(4A)	111.3(10)	C(1A)-C(4A)-C(3A)	107.3(8)
C(1A)-C(4A)-O(3A)	109.2(10)	C(3A)-C(4A)-O(3A)	103.4(10)
C(6A)-C(5A)-C(7A)	115.0(15)	C(6A)-C(5A)-O(3A)	105.9(14)
C(7A)-C(5A)-O(3A)	111.0(11)	C(6A)-C(5A)-O(4A)	110.0(9)
C(7A)-C(5A)-O(4A)	108.9(12)	O(3A)-C(5A)-O(4A)	105.5(10)
Li(1)-C(8A)-C(2A)	99.9(7)	Li(1)-C(8A)-C(9A)	144.6(12)
C(2A)-C(8A)-C(9A)	114.0(11)	Li(1)-C(8A)-O(6A)	50.4(7)
C(2A)-C(8A)-O(6A)	113.3(7)	C(9A)-C(8A)-O(6A)	103.9(11)
C(8A)-C(9A)-O(5A)	106.1(13)	C(11A)-C(10A)-C(12A)	113.1(19)
C(11A)-C(10A)-O(5A)	110.0(13)	C(12A)-C(10A)-O(5A)	112.5(15)
C(11A)-C(10A)-O(6A)	110.0(13)	C(12A)-C(10A)-O(6A)	107.3(14)
O(5A)-C(10A)-O(6A)	103.5(14)	Cr-O(1A)-Li(1)	94.4(6)
Cr-O(1A)-C(1A)	126.1(4)	Li(1)-O(1A)-C(1A)	124.9(8)

Table S15 (cont.)

C(2A)-O(2A)-C(3A)	111.7(8)	C(4A)-O(3A)-C(5A)	109.7(8)
C(3A)-O(4A)-C(5A)	111.2(10)	C(9A)-O(5A)-C(10A)	106.5(12)
Li(1)-O(6A)-C(8A)	97.9(9)	Li(1)-O(6A)-C(10A)	146.6(13)
C(8A)-O(6A)-C(10A)	109.7(10)	C(2B)-C(1B)-C(4B)	99.2(9)
C(2B)-C(1B)-O(1B)	112.3(8)	C(4B)-C(1B)-O(1B)	115.7(6)
C(1B)-C(2B)-C(8B)	115.5(11)	C(1B)-C(2B)-O(2B)	106.0(6)
C(8B)-C(2B)-O(2B)	104.2(10)	C(4B)-C(3B)-O(2B)	108.1(11)
C(4B)-C(3B)-O(4B)	104.6(12)	O(2B)-C(3B)-O(4B)	111.6(12)
C(1B)-C(4B)-C(3B)	105.7(8)	C(1B)-C(4B)-O(3B)	109.5(7)
C(3B)-C(4B)-O(3B)	102.9(11)	C(6B)-C(5B)-C(7B)	112.5(16)
C(6B)-C(5B)-O(3B)	112.9(14)	C(7B)-C(5B)-O(3B)	108.5(14)
C(6B)-C(5B)-O(4B)	110.0(13)	C(7B)-C(5B)-O(4B)	106.8(15)
O(3B)-C(5B)-O(4B)	105.7(13)	Li(1)-C(8B)-C(2B)	101.0(8)
Li(1)-C(8B)-C(9B)	144.8(10)	C(2B)-C(8B)-C(9B)	112.8(12)
Li(1)-C(8B)-O(6B)	51.5(6)	C(2B)-C(8B)-O(6B)	112.7(11)
C(9B)-C(8B)-O(6B)	103.7(9)	C(8B)-C(9B)-O(5B)	103.8(14)
C(11B)-C(10B)-C(12B)	114.4(14)	C(11B)-C(10B)-O(5B)	106.4(11)
C(12B)-C(10B)-O(5B)	115.1(14)	C(11B)-C(10B)-O(6B)	108.4(11)
C(12B)-C(10B)-O(6B)	108.4(10)	O(5B)-C(10B)-O(6B)	103.4(10)
Cr-O(1B)-Li(1)	93.6(8)	Cr-O(1B)-C(1B)	125.5(6)
Li(1)-O(1B)-C(1B)	125.0(6)	C(2B)-O(2B)-C(3B)	109.9(11)
C(4B)-O(3B)-C(5B)	109.4(10)	C(3B)-O(4B)-C(5B)	111.9(16)
C(9B)-O(5B)-C(10B)	108.2(10)	Li(1)-O(6B)-C(8B)	96.6(8)
Li(1)-O(6B)-C(10B)	147.3(10)	C(8B)-O(6B)-C(10B)	108.9(10)
C(2C)-C(1C)-C(4C)	100.5(9)	C(2C)-C(1C)-O(1C)	110.9(7)
C(4C)-C(1C)-O(1C)	114.7(8)	C(1C)-C(2C)-C(8C)	117.3(8)
C(1C)-C(2C)-O(2C)	106.3(10)	C(8C)-C(2C)-O(2C)	104.7(12)
C(4C)-C(3C)-O(2C)	104.7(12)	C(4C)-C(3C)-O(4C)	107.0(10)
O(2C)-C(3C)-O(4C)	111.4(9)	C(1C)-C(4C)-C(3C)	109.1(9)
C(1C)-C(4C)-O(3C)	107.6(9)	C(3C)-C(4C)-O(3C)	102.0(7)
C(6C)-C(5C)-C(7C)	117.0(10)	C(6C)-C(5C)-O(3C)	111.2(11)
C(7C)-C(5C)-O(3C)	107.0(13)	C(6C)-C(5C)-O(4C)	109.5(14)
C(7C)-C(5C)-O(4C)	106.1(12)	O(3C)-C(5C)-O(4C)	105.2(7)
Li(2)-C(8C)-C(2C)	99.8(9)	Li(2)-C(8C)-C(9C)	144.1(11)
C(2C)-C(8C)-C(9C)	113.5(8)	Li(2)-C(8C)-O(6C)	49.2(5)
C(2C)-C(8C)-O(6C)	111.1(12)	C(9C)-C(8C)-O(6C)	103.7(13)
C(8C)-C(9C)-O(5C)	104.5(12)	C(11C)-C(10C)-C(12C)	113.0(17)
C(11C)-C(10C)-O(5C)	107.8(12)	C(12C)-C(10C)-O(5C)	114.5(10)
C(11C)-C(10C)-O(6C)	110.5(10)	C(12C)-C(10C)-O(6C)	106.0(11)
O(5C)-C(10C)-O(6C)	104.7(15)	Cr-O(1C)-Li(2)	93.7(6)
Cr-O(1C)-C(1C)	123.6(6)	Li(2)-O(1C)-C(1C)	126.5(7)
C(2C)-O(2C)-C(3C)	111.8(11)	C(4C)-O(3C)-C(5C)	109.5(9)
C(3C)-O(4C)-C(5C)	111.2(11)	C(9C)-O(5C)-C(10C)	107.7(11)
Li(2)-O(6C)-C(8C)	98.9(7)	Li(2)-O(6C)-C(10C)	145.8(8)
C(8C)-O(6C)-C(10C)	108.7(10)		

Table S11. Anisotropic displacement coefficients ($Å^2 x 10^3$) for complex 5.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cr	26(1)	24(1)	24(1)	0	15(1)	0
C(1A)	39(5)	43(5)	37(4)	-12(4)	21(4)	-4(4)
C(2A)	52(6)	46(6)	45(5)	-24(5)	27(5)	-8(5)
C(3A)	50(6)	60(7)	67(7)	-8(5)	39(6)	0(5)
C(4A)	56(6)	57(6)	45(5)	-21(5)	29(5)	-9(5)
C(5A)	50(6)	65(7)	53(6)	-28(5)	27(5)	0(5)
C(6A)	89(11)	103(12)	131(14)	-12(9)	58(10)	43(11)
C(7A)	118(13)	184(20)	86(10)	-52(13)	86(10)	-26(11)
C(8A)	45(6)	61(7)	44(5)	-10(5)	21(5)	-4(5)
C(9A)	84(9)	89(9)	44(6)	-45(7)	32(6)	-34(6)
C(10A)	76(8)	63(8)	101(10)	-12(7)	47(8)	-28(7)
C(11A)	120(12)	64(8)	109(11)	-4(8)	79(10)	-39(8)
C(12A)	150(16)	65(10)	159(17)	14(10)	103(15)	-6(11)
O(1A)	40(3)	30(3)	35(3)	-10(3)	23(3)	-3(3)
O(2A)	41(4)	124(8)	49(4)	-29(4)	26(4)	-15(4)
O(3A)	48(4)	70(5)	44(4)	-15(3)	25(3)	14(3)
O(4A)	44(4)	127(8)	61(4)	-19(4)	35(4)	9(5)
O(5A)	86(6)	92(7)	78(6)	-32(5)	43(5)	-40(5)
O(6A)	62(4)	46(4)	56(4)	-18(3)	37(4)	-25(3)
C(1B)	26(4)	49(5)	24(4)	-2(3)	12(3)	6(4)
C(2B)	48(5)	67(6)	30(4)	-12(5)	25(4)	-7(4)
C(3B)	60(7)	84(9)	66(7)	-3(6)	40(6)	4(6)
C(4B)	41(5)	63(6)	26(4)	-13(5)	13(4)	8(4)
C(5B)	50(6)	88(9)	46(6)	-17(6)	24(5)	10(6)
C(6B)	105(12)	184(20)	86(10)	-83(14)	52(9)	-8(12)
C(7B)	152(17)	215(24)	104(13)	-23(17)	81(13)	77(15)
C(8B)	54(6)	82(7)	34(5)	-26(5)	27(4)	-16(5)
C(9B)	107(10)	136(12)	53(7)	-49(10)	56(8)	-48(8)
C(10B)	63(7)	93(9)	34(5)	-14(6)	24(5)	-9(5)
C(11B)	53(7)	112(11)	52(7)	-35(7)	8(6)	-44(7)
C(12B)	117(13)	63(9)	84(10)	5(9)	40(10)	8(7)
O(1B)	38(3)	39(3)	32(2)	-6(3)	23(2)	-7(3)
O(2B)	68(5)	101(7)	81(5)	-29(5)	57(4)	-34(5)
O(3B)	72(5)	61(5)	60(4)	-28(4)	39(4)	-6(4)
O(4B)	109(8)	138(11)	135(9)	-31(7)	102(8)	5(8)
O(5B)	83(6)	126(8)	39(4)	-25(6)	31(4)	-22(5)
O(6B)	47(4)	71(4)	38(3)	-23(3)	27(3)	-19(3)
C(1C)	31(4)	55(6)	27(4)	-13(4)	13(3)	-2(4)
C(2C)	43(5)	47(6)	49(6)	-12(5)	14(5)	-2(5)
C(3C)	45(6)	86(8)	47(5)	0(5)	26(5)	9(6)
C(4C)	30(4)	52(5)	32(4)	7(4)	13(4)	8(4)
C(5C)	41(5)	79(8)	60(6)	-6(5)	20(5)	2(6)
C(6C)	68(8)	85(10)	106(11)	28(7)	46(8)	16(9)
C(7C)	61(8)	155(17)	83(10)	-28(10)	20(7)	-37(11)
C(8C)	72(8)	38(6)	59(7)	-10(5)	20(6)	-3(5)
C(9C)	72(9)	47(7)	117(12)	-18(6)	34(8)	-10(7)
C(10C)	83(9)	46(7)	68(7)	-6(6)	26(7)	-25(6)
C(11C)	103(11)	70(9)	92(10)	37(8)	28(9)	-22(8)
C(12C)	83(10)	95(11)	42(6)	-4(8)	0(7)	-10(7)
O(1C)	25(3)	40(3)	25(3)	-3(3)	9(2)	3(3)
O(2C)	55(5)	72(6)	123(8)	-11(4)	49(5)	21(6)
O(3C)	33(3)	89(7)	42(3)	10(3)	14(3)	21(4)
O(4C)	38(4)	104(7)	78(5)	-7(4)	29(4)	18(5)
O(5C)	121(9)	44(5)	111(8)	-14(6)	49(7)	-23(5)
O(6C)	50(4)	35(3)	58(4)	-5(3)	14(3)	-13(3)

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table S12. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$) for complex 5.

	x	y	z	U
H(1AA)	-9630	1416	-10160	80
H(2AA)	-8639	2141	-9071	80
H(3AA)	-7889	677	-9719	80
H(4AA)	-9135	572	-10977	80
H(6AA)	-8408	2811	-11769	80
H(6AB)	-9233	2788	-12256	80
H(6AC)	-8614	2755	-10875	80
H(7AA)	-8831	949	-12688	80
H(7AB)	-9326	1616	-13360	80
H(7AC)	-8491	1637	-12818	80
H(8AA)	-8012	1146	-7218	80
H(9AA)	-7258	2046	-6209	80
H(9AB)	-7805	2587	-7205	80
H(11A)	-8979	2484	-5537	80
H(11B)	-9471	1859	-6388	80
H(11C)	-8632	1736	-5403	80
H(12A)	-9074	2895	-8145	80
H(12B)	-9741	2676	-8144	80
H(12C)	-9177	3243	-7228	80
H(1BA)	-9605	-1084	-7781	80
H(2BA)	-9529	-916	-6102	80
H(3BA)	-11372	-338	-8340	80
H(4BA)	-11005	-992	-9287	80
H(6BA)	-12089	-1901	-9335	80
H(6BB)	-11634	-2607	-8956	80
H(6BC)	-12045	-2411	-8400	80
H(7BA)	-11010	-2429	-6371	80
H(7BB)	-10695	-2681	-7060	80
H(7BC)	-10212	-2217	-5901	80
H(8BA)	-9539	552	-6494	80
H(9BA)	-9181	605	-4640	80
H(9BB)	-8986	-206	-4387	80
H(11D)	-6948	536	-3893	80
H(11E)	-7313	446	-5261	80
H(11F)	-7592	1039	-4826	80
H(12D)	-7307	-703	-3709	80
H(12E)	-8128	-947	-4546	80
H(12F)	-7665	-898	-5048	80
H(1CA)	-11354	-835	-12363	80
H(2CA)	-12069	-1809	-12913	80
H(3CA)	-12303	-901	-10807	80
H(4CA)	-11787	-107	-11351	80
H(6CA)	-13297	559	-12822	80
H(6CB)	-13629	513	-14183	80
H(6CC)	-14062	197	-13726	80
H(7CA)	-13445	-1368	-14385	80
H(7CB)	-14156	-988	-14702	80
H(7CC)	-13723	-672	-15158	80
H(8CA)	-11125	-2339	-10569	80
H(9CA)	-11749	-3333	-11418	80
H(9CB)	-12137	-3043	-12719	80
H(11G)	-9797	-3423	-10658	80
H(11H)	-10023	-3757	-11868	80
H(11I)	-9655	-3004	-11479	80
H(12G)	-11075	-3160	-13764	80
H(12H)	-11551	-2592	-13684	80
H(12I)	-10791	-2376	-13387	80

Table S13. Data collection and refinement parameters for complex 6.

Empirical Formula	$C_{72}\ H_{114}\ Li_3\ O_{36}\ Ti$
Color; Habit	Colorless ; Prismatic
Crystal Size (mm)	0.3 x 0.3 x 0.7
Crystal System	Monoclinic
Space Group	$P2_1$
Unit Cell Dimensions	$\underline{a}$ = 13.888(5) Å
	$\underline{b}$ = 18.750(5) Å
	$\underline{c}$ = 17.933(5) Å
	β = 91.84(2)°
Volume	4667(2) $Å^3$
Z	2
Formula Weight	1624.4
Density(calc.)	1.156 g/cm^3
Absorption Coefficient	0.169 mm^{-1}
F(000)	1730
Diffractometer Used	Siemens P4
Radiation	MoKα (λ = 0.71069 Å)
Temperature (K)	150
Monochromator	Highly oriented graphite crystal
2θ Range	2.0 to 50.0°
Scan Type	ω
Scan Speed	Variable; 4.00 to 20.00°/min.
Scan Range	1.50°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 35.0% of total scan time
Standard Reflections	2 measured every 50 reflections
Index Ranges	$-13 \le h \le 16$, $-22 \le k \le 0$
	$-13 \le \ell \le 21$
Reflections Collected	8748
Independent Reflections	8520 (R_{int} = 1.52%)
Observed Reflections	5011 ($F > 4.0\sigma(F)$)
System Used	Siemens SHELXTL IRIS
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Hydrogen Atoms	Riding model, fixed isotropic U

Table S15 (cont.)

Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0146F^2$
Number of Parameters Refined	511
Final R Indices (obs. data)	R = 8.75 %, wR = 12.59 %
R Indices (all data)	R = 14.30 %, wR = 20.63 %
Goodness-of-Fit	0.89
Largest and Mean Δ/σ	0.070, 0.013
Data-to-Parameter Ratio	9.8:1
Largest Difference Peak	1.27 $e\text{Å}^{-3}$
Largest Difference Hole	-0.50 $e\text{Å}^{-3}$

Table S14. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$) for complex 6.

	x	y	z	U(eq)
Ti	2402(1)	3418	7535(1)	11(1)
Li(1)	3788(15)	4233(12)	6694(12)	25(5)
Li(2)	2400(16)	1888(13)	7470(13)	30(5)
Li(3)	1039(15)	4122(12)	8476(12)	26(5)
C(1A)	285(8)	2883(7)	7619(6)	15(2)
C(2A)	-738(8)	3063(7)	7867(6)	16(2)
C(3A)	-922(8)	2922(7)	6578(7)	21(3)
C(4A)	73(8)	2602(7)	6811(7)	18(3)
C(5A)	-919(9)	1698(7)	6359(7)	20(3)
C(6A)	-1460(11)	1075(9)	6642(9)	41(4)
C(7A)	-618(12)	1614(10)	5571(9)	51(4)
C(8A)	-814(9)	3705(7)	8382(7)	21(3)
C(9A)	-1758(10)	3766(8)	8751(8)	34(3)
C(10A)	-640(9)	3640(7)	9683(7)	21(3)
C(11A)	-736(12)	2872(9)	9904(9)	45(4)
C(12A)	-144(9)	4108(7)	10260(7)	25(3)
O(1A)	933(5)	3462(5)	7646(4)	13(2)
O(2A)	-1223(6)	3299(5)	7190(5)	28(2)
O(3A)	-88(6)	1839(5)	6843(5)	26(2)
O(4A)	-1497(7)	2317(6)	6433(5)	34(2)
O(5A)	-1530(6)	3970(5)	9505(5)	30(2)
O(6A)	-115(6)	3662(5)	8988(4)	18(2)
C(1B)	1843(8)	4836(7)	6702(7)	19(3)
C(2B)	2093(9)	5293(7)	6020(7)	21(3)
C(3B)	640(9)	4766(7)	5678(7)	25(3)
C(4B)	789(8)	4702(7)	6521(7)	19(3)
C(5B)	-479(9)	5485(7)	6258(7)	24(3)
C(6B)	-1408(10)	5090(8)	6393(8)	36(4)
C(7B)	-555(11)	6279(9)	6270(9)	41(4)
C(8B)	3121(8)	5237(7)	5769(7)	21(3)
C(9B)	3447(9)	5859(7)	5284(7)	27(3)
C(10B)	4099(14)	6053(11)	6495(11)	56(5)
C(11B)	3634(16)	6407(14)	7106(12)	84(7)
C(12B)	5197(17)	5997(15)	6549(14)	97(8)
O(1B)	2426(6)	4220(5)	6743(4)	17(2)
O(2B)	1521(6)	5027(5)	5408(5)	28(2)
O(3B)	242(6)	5284(5)	6805(5)	21(2)
O(4B)	-118(6)	5256(5)	5554(5)	28(2)
O(5B)	3735(11)	6371(9)	5832(9)	88(5)
O(6B)	3791(6)	5296(5)	6414(5)	28(2)
C(1C)	2790(9)	2650(7)	6061(7)	21(3)
C(2C)	2750(9)	1929(7)	5655(7)	22(3)
C(3C)	1632(9)	2689(8)	5019(7)	26(3)
C(4C)	2301(8)	3154(7)	5470(6)	16(3)
C(5C)	2655(9)	3265(8)	4204(7)	30(3)
C(6C)	3354(12)	2844(10)	3773(9)	52(5)
C(7C)	2437(12)	4007(9)	3896(9)	46(4)
C(8C)	2558(10)	1285(8)	6112(8)	28(3)
C(9C)	2759(11)	569(9)	5761(8)	39(4)
C(10C)	3803(9)	668(7)	6731(7)	26(3)
C(11C)	3971(11)	374(9)	7510(9)	42(4)
C(12C)	4742(11)	865(9)	6366(9)	43(4)
O(1C)	2280(5)	2646(4)	6736(4)	14(2)
O(2C)	1923(8)	1987(6)	5131(6)	45(3)

Table 3.1 (cont.)

O(3C)	3033(6)	3342(5)	4957(5)	28(2)
O(4C)	1755(7)	2916(6)	4260(5)	39(2)
O(5C)	3256(7)	180(6)	6300(6)	40(3)
O(6C)	3197(6)	1284(5)	6776(5)	21(2)
C(1D)	4574(8)	2934(6)	7407(6)	14(2)
C(2D)	5605(8)	3235(6)	7299(6)	15(3)
C(3D)	5537(9)	2982(8)	8569(8)	30(3)
C(4D)	4753(8)	2545(6)	8160(6)	15(2)
C(5D)	5985(10)	1798(8)	8545(8)	32(3)
C(6D)	5725(13)	1295(10)	9153(10)	53(5)
C(7D)	6871(14)	1548(12)	8157(12)	72(6)
C(8D)	5618(9)	3924(8)	6877(7)	28(3)
C(9D)	6607(14)	4119(12)	6574(11)	64(5)
C(10D)	5620(10)	3777(8)	5569(8)	32(3)
C(11D)	5300(13)	4295(11)	4960(11)	60(5)
C(12D)	5509(12)	3026(10)	5297(10)	51(4)
O(1D)	3867(5)	3477(5)	7435(4)	15(2)
O(2D)	5980(7)	3397(6)	8031(5)	41(2)
O(3D)	5228(6)	1892(5)	8011(5)	31(2)
O(4D)	6192(7)	2465(6)	8866(6)	43(3)
O(5D)	6562(10)	3927(8)	5874(8)	73(4)
O(6D)	4999(6)	3883(5)	6204(5)	27(2)
C(1E)	2058(8)	2552(7)	8955(6)	16(3)
C(2E)	2139(9)	1806(7)	9328(7)	25(3)
C(3E)	3300(9)	2494(7)	9966(7)	22(3)
C(4E)	2594(8)	2991(7)	9560(6)	18(3)
C(5E)	2407(9)	3075(7)	10850(7)	24(3)
C(6E)	1774(12)	2625(10)	11306(9)	50(4)
C(7E)	2675(12)	3784(9)	11197(9)	44(4)
C(8E)	2328(9)	1184(7)	8807(7)	21(3)
C(9E)	2165(10)	451(8)	9149(8)	30(3)
C(10E)	1143(9)	562(7)	8138(7)	23(3)
C(11E)	167(10)	714(9)	8482(8)	38(4)
C(12E)	1055(10)	282(9)	7353(8)	36(3)
O(1E)	2513(5)	2576(5)	8269(4)	16(2)
O(2E)	2955(7)	1810(6)	9852(6)	41(3)
O(3E)	1947(6)	3180(5)	10131(5)	25(2)
O(4E)	3285(6)	2709(5)	10718(5)	30(2)
O(5E)	1682(7)	51(5)	8565(5)	33(2)
O(6E)	1715(6)	1186(5)	8148(5)	23(2)
C(1F)	2977(8)	4759(7)	8448(7)	18(3)
C(2F)	2708(9)	5249(7)	9107(7)	24(3)
C(3F)	4167(9)	4709(7)	9481(7)	24(3)
C(4F)	4049(9)	4609(7)	8652(7)	22(3)
C(5F)	5291(10)	5420(8)	8884(8)	29(3)
C(6F)	6283(12)	5104(10)	8760(10)	53(5)
C(7F)	5277(13)	6225(11)	8896(11)	60(5)
C(8F)	1693(9)	5181(8)	9368(7)	27(3)
C(9F)	1396(9)	5803(7)	9863(7)	23(3)
C(10F)	388(9)	5816(7)	8855(7)	24(3)
C(11F)	-643(10)	5616(8)	8616(8)	31(3)
C(12F)	779(11)	6405(9)	8394(9)	45(4)
O(1F)	2414(6)	4144(5)	8400(4)	17(2)
O(2F)	3327(6)	5033(5)	9718(5)	27(2)
O(3F)	4617(7)	5178(5)	8334(5)	30(2)
O(4F)	4976(7)	5160(5)	9576(5)	33(2)
O(5F)	435(7)	5953(6)	9627(5)	35(2)
O(6F)	1007(6)	5195(5)	8765(5)	23(2)
C(1)	632(12)	8242(10)	6576(9)	50(4)

C(2)	1348(13)	7742(12)	6510(11)	62(5)
C(3)	1941(15)	7721(13)	5903(11)	71(6)
C(4)	1893(13)	8273(11)	5403(10)	58(5)
C(5)	1169(13)	8823(11)	5463(10)	57(5)
C(6)	541(13)	8795(10)	6059(10)	52(4)
C(7)	-22(15)	8203(13)	7241(11)	78(6)
C(1')	3645(13)	8354(12)	8591(7)	78(12)
C(2')	2977	8590	8047	72(6)
C(3')	3234	8628	7303	123(21)
C(4')	4159	8430	7101	92(7)
C(5')	4826	8195	7645	68(11)
C(6')	4570	8157	8389	77(6)
C(7')	3369(16)	8252(13)	9333(10)	105(9)
C(2")	2712	8521	8800	47(8)
C(2')	2963	8565	8054	50(162)
C(4")	3871	8340	7842	58(9)
C(6')	4529	8070	8375	50(162)
C(6")	4278	8026	9121	62(10)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table S15. Bond lengths (Å) for complex 6

Ti-Li(1)	2.917 (22)	Ti-Li(2)	2.871 (24)
Ti-Li(3)	2.894 (22)	Ti-O(1A)	2.057 (7)
Ti-O(1B)	2.069 (8)	Ti-O(1C)	2.040 (8)
Ti-O(1D)	2.051 (7)	Ti-O(1E)	2.058 (8)
Ti-O(1F)	2.063 (8)	Li(1)-C(8B)	2.657 (25)
Li(1)-O(1B)	1.898 (22)	Li(1)-O(6B)	2.056 (24)
Li(1)-C(8D)	2.617 (25)	Li(1)-O(1D)	1.943 (23)
Li(1)-O(6D)	2.032 (23)	Li(2)-C(8C)	2.701 (27)
Li(2)-O(1C)	1.942 (25)	Li(2)-O(6C)	2.036 (25)
Li(2)-C(8E)	2.741 (26)	Li(2)-O(1E)	1.930 (25)
Li(2)-O(6E)	2.045 (25)	Li(3)-C(8A)	2.690 (24)
Li(3)-O(1A)	1.937 (24)	Li(3)-O(6A)	2.062 (23)
Li(3)-C(8F)	2.690 (26)	Li(3)-O(1F)	1.918 (23)
Li(3)-O(6F)	2.077 (25)	C(1A)-C(2A)	1.540 (16)
C(1A)-C(4A)	1.560 (16)	C(1A)-O(1A)	1.410 (14)
C(2A)-C(8A)	1.524 (18)	C(2A)-O(2A)	1.438 (14)
C(3A)-C(4A)	1.552 (17)	C(3A)-O(2A)	1.381 (15)
C(3A)-O(4A)	1.406 (16)	C(4A)-O(3A)	1.450 (16)
C(5A)-C(6A)	1.487 (20)	C(5A)-C(7A)	1.494 (21)
C(5A)-O(3A)	1.445 (15)	C(5A)-O(4A)	1.419 (16)
C(8A)-C(9A)	1.491 (19)	C(8A)-O(6A)	1.436 (14)
C(9A)-O(5A)	1.431 (17)	C(10A)-C(11A)	1.501 (21)
C(10A)-C(12A)	1.506 (18)	C(10A)-O(5A)	1.410 (15)
C(10A)-O(6A)	1.464 (15)	C(1B)-C(2B)	1.541 (17)
C(1B)-C(4B)	1.510 (16)	C(1B)-O(1B)	1.412 (15)
C(2B)-C(8B)	1.514 (17)	C(2B)-O(2B)	1.425 (15)
C(3B)-C(4B)	1.524 (17)	C(3B)-O(2B)	1.417 (16)
C(3B)-O(4B)	1.409 (16)	C(4B)-O(3B)	1.432 (15)
C(5B)-C(6B)	1.514 (20)	C(5B)-C(7B)	1.493 (21)
C(5B)-O(3B)	1.429 (15)	C(5B)-O(4B)	1.440 (16)
C(8B)-C(9B)	1.532 (19)	C(8B)-O(6B)	1.466 (14)
C(9B)-O(5B)	1.424 (21)	C(10B)-C(11B)	1.451 (30)
C(10B)-C(12B)	1.528 (30)	C(10B)-O(5B)	1.410 (25)
C(10B)-O(6B)	1.488 (22)	C(1C)-C(2C)	1.537 (18)
C(1C)-C(4C)	1.558 (17)	C(1C)-O(1C)	1.422 (14)
C(2C)-C(8C)	1.487 (19)	C(2C)-O(2C)	1.465 (16)
C(3C)-C(4C)	1.493 (17)	C(3C)-O(2C)	1.390 (18)
C(3C)-O(4C)	1.442 (16)	C(4C)-O(3C)	1.437 (14)
C(5C)-C(6C)	1.486 (22)	C(5C)-C(7C)	1.524 (22)
C(5C)-O(3C)	1.440 (15)	C(5C)-O(4C)	1.417 (16)
C(8C)-C(9C)	1.513 (21)	C(8C)-O(6C)	1.463 (15)
C(9C)-O(5C)	1.377 (18)	C(10C)-C(11C)	1.514 (20)
C(10C)-C(12C)	1.522 (21)	C(10C)-O(5C)	1.404 (17)
C(10C)-O(6C)	1.434 (16)	C(1D)-C(2D)	1.557 (15)
C(1D)-C(4D)	1.549 (16)	C(1D)-O(1D)	1.418 (14)
C(2D)-C(8D)	1.498 (18)	C(2D)-O(2D)	1.430 (14)
C(3D)-C(4D)	1.531 (18)	C(3D)-O(2D)	1.397 (17)
C(3D)-O(4D)	1.421 (18)	C(4D)-O(3D)	1.420 (15)
C(5D)-C(6D)	1.494 (23)	C(5D)-C(7D)	1.507 (25)
C(5D)-O(3D)	1.410 (16)	C(5D)-O(4D)	1.404 (19)
C(8D)-C(9D)	1.538 (23)	C(8D)-O(6D)	1.461 (15)
C(9D)-O(5D)	1.306 (24)	C(10D)-C(11D)	1.517 (24)
C(10D)-C(12D)	1.498 (24)	C(10D)-O(5D)	1.429 (20)
C(10D)-O(6D)	1.462 (17)	C(1E)-C(2E)	1.554 (18)
C(1E)-C(4E)	1.536 (16)	C(1E)-O(1E)	1.402 (14)
C(2E)-C(8E)	1.521 (18)	C(2E)-O(2E)	1.449 (16)

C(3E)-C(4E)	1.521 (17)	C(3E)-O(2E)	1.381 (17)
C(3E)-O(4E)	1.408 (15)	C(4E)-O(3E)	1.428 (14)
C(5E)-C(6E)	1.483 (22)	C(5E)-C(7E)	1.508 (21)
C(5E)-O(3E)	1.435 (15)	C(5E)-O(4E)	1.425 (16)
C(8E)-C(9E)	1.526 (19)	C(8E)-O(6E)	1.435 (14)
C(9E)-O(5E)	1.437 (17)	C(10E)-C(11E)	1.534 (19)
C(10E)-C(12E)	1.503 (19)	C(10E)-O(5E)	1.424 (16)
C(10E)-O(6E)	1.416 (16)	C(1F)-C(2F)	1.551 (18)
C(1F)-C(4F)	1.548 (17)	C(1F)-O(1F)	1.395 (15)
C(2F)-C(8F)	1.505 (18)	C(2F)-O(2F)	1.431 (15)
C(3F)-C(4F)	1.504 (18)	C(3F)-O(2F)	1.394 (16)
C(3F)-O(4F)	1.412 (16)	C(4F)-O(3F)	1.455 (16)
C(5F)-C(6F)	1.522 (22)	C(5F)-C(7F)	1.510 (24)
C(5F)-O(3F)	1.412 (16)	C(5F)-O(4F)	1.416 (17)
C(8F)-C(9F)	1.531 (19)	C(8F)-O(6F)	1.419 (15)
C(9F)-O(5F)	1.416 (15)	C(10F)-C(11F)	1.528 (18)
C(10F)-C(12F)	1.491 (22)	C(10F)-O(5F)	1.408 (16)
C(10F)-O(6F)	1.460 (16)	C(1)-C(2)	1.374 (26)
C(1)-C(6)	1.395 (25)	C(1)-C(7)	1.524 (27)
C(2)-C(3)	1.387 (28)	C(3)-C(4)	1.369 (29)
C(4)-C(5)	1.447 (27)	C(5)-C(6)	1.401 (25)
C(1')-C(2')	1.395 (1)	C(1')-C(6')	1.395 (1)
C(1')-C(7')	1.410 (23)	C(1')-C(2")	1.396 (28)
C(1')-C(2')	1.385 (25)	C(1')-C(4")	1.389 (22)
C(1')-C(6')	1.404 (28)	C(1')-C(6")	1.415 (26)
C(3')-C(2')	1.395 (1)	C(3')-C(2')	1.416 (22)
C(3')-C(4")	1.399 (26)	C(4')-C(4")	1.409 (23)
C(5')-C(6')	1.395 (1)	C(5')-C(4")	1.410 (28)
C(5')-C(6')	1.405 (23)		

Table S16 Bond angles (°) for complex 6

Li(1)-Ti-Li(2)	120.2(6)	Li(1)-Ti-Li(3)	121.1(6)
Li(2)-Ti-Li(3)	118.7(6)	Li(1)-Ti-O(1A)	134.6(5)
Li(2)-Ti-O(1A)	92.6(5)	Li(3)-Ti-O(1A)	41.9(5)
Li(1)-Ti-O(1B)	40.4(5)	Li(2)-Ti-O(1B)	134.3(5)
Li(3)-Ti-O(1B)	95.4(5)	O(1A)-Ti-O(1B)	94.3(3)
Li(1)-Ti-O(1C)	92.8(5)	Li(2)-Ti-O(1C)	42.5(5)
Li(3)-Ti-O(1C)	133.8(5)	O(1A)-Ti-O(1C)	92.1(3)
O(1B)-Ti-O(1C)	92.1(3)	Li(1)-Ti-O(1D)	41.7(5)
Li(2)-Ti-O(1D)	92.9(5)	Li(3)-Ti-O(1D)	134.1(5)
O(1A)-Ti-O(1D)	174.5(3)	O(1B)-Ti-O(1D)	82.1(3)
O(1C)-Ti-O(1D)	92.1(3)	Li(1)-Ti-O(1E)	134.1(5)
Li(2)-Ti-O(1E)	42.2(5)	Li(3)-Ti-O(1E)	90.8(5)
O(1A)-Ti-O(1E)	91.3(3)	O(1B)-Ti-O(1E)	173.6(3)
O(1C)-Ti-O(1E)	84.7(3)	O(1D)-Ti-O(1E)	92.5(3)
Li(1)-Ti-O(1F)	93.1(5)	Li(2)-Ti-O(1F)	133.6(5)
Li(3)-Ti-O(1F)	41.4(5)	O(1A)-Ti-O(1F)	83.4(3)
O(1B)-Ti-O(1F)	92.1(3)	O(1C)-Ti-O(1F)	174.1(3)
O(1D)-Ti-O(1F)	92.7(3)	O(1E)-Ti-O(1F)	91.5(3)
Ti-Li(1)-C(8B)	118.1(8)	Ti-Li(1)-O(1B)	45.0(5)
C(8B)-Li(1)-O(1B)	73.1(8)	Ti-Li(1)-O(6B)	129.9(10)
C(8B)-Li(1)-O(6B)	33.2(5)	O(1B)-Li(1)-O(6B)	91.9(10)
Ti-Li(1)-C(8D)	118.3(8)	C(8B)-Li(1)-C(8D)	123.6(9)
O(1B)-Li(1)-C(8D)	163.2(12)	O(6B)-Li(1)-C(8D)	103.6(9)
Ti-Li(1)-O(1D)	44.6(5)	C(8B)-Li(1)-O(1D)	162.7(11)
O(1B)-Li(1)-O(1D)	89.6(10)	O(6B)-Li(1)-O(1D)	150.9(12)
C(8D)-Li(1)-O(1D)	73.8(8)	Ti-Li(1)-O(6D)	128.6(10)
C(8B)-Li(1)-O(6D)	103.7(9)	O(1B)-Li(1)-O(6D)	149.0(13)
O(6B)-Li(1)-O(6D)	101.5(10)	C(8D)-Li(1)-O(6D)	33.8(5)
O(1D)-Li(1)-O(6D)	91.8(10)	Ti-Li(2)-C(8C)	117.0(9)
Ti-Li(2)-O(1C)	45.2(6)	C(8C)-Li(2)-O(1C)	72.7(8)
Ti-Li(2)-O(6C)	125.5(10)	C(8C)-Li(2)-O(6C)	32.3(5)
O(1C)-Li(2)-O(6C)	91.6(10)	Ti-Li(2)-C(8E)	116.5(8)
C(8C)-Li(2)-C(8E)	126.5(10)	O(1C)-Li(2)-C(8E)	160.2(12)
O(6C)-Li(2)-C(8E)	107.6(10)	Ti-Li(2)-O(1E)	45.7(6)
C(8C)-Li(2)-O(1E)	160.4(12)	O(1C)-Li(2)-O(1E)	91.0(11)
O(6C)-Li(2)-O(1E)	142.4(13)	C(8E)-Li(2)-O(1E)	71.2(8)
Ti-Li(2)-O(6E)	128.2(10)	C(8C)-Li(2)-O(6E)	108.7(10)
O(1C)-Li(2)-O(6E)	147.4(13)	O(6C)-Li(2)-O(6E)	106.2(11)
C(8E)-Li(2)-O(6E)	30.7(5)	O(1E)-Li(2)-O(6E)	91.0(10)
Ti-Li(3)-C(8A)	118.2(8)	Ti-Li(3)-O(1A)	45.2(5)
C(8A)-Li(3)-O(1A)	73.6(8)	Ti-Li(3)-O(6A)	126.9(10)
C(8A)-Li(3)-O(6A)	31.8(5)	O(1A)-Li(3)-O(6A)	92.0(10)
Ti-Li(3)-C(8F)	118.0(8)	C(8A)-Li(3)-C(8F)	123.8(9)
O(1A)-Li(3)-C(8F)	160.8(12)	O(6A)-Li(3)-C(8F)	107.2(10)
Ti-Li(3)-O(1F)	45.4(5)	C(8A)-Li(3)-O(1F)	162.5(12)
O(1A)-Li(3)-O(1F)	90.6(10)	O(6A)-Li(3)-O(1F)	146.1(13)
C(8F)-Li(3)-O(1F)	73.1(8)	Ti-Li(3)-O(6F)	127.4(10)
C(8A)-Li(3)-O(6F)	105.6(9)	O(1A)-Li(3)-O(6F)	144.0(13)
O(6A)-Li(3)-O(6F)	105.7(10)	C(8F)-Li(3)-O(6F)	31.4(5)
O(1F)-Li(3)-O(6F)	91.5(10)	C(2A)-C(1A)-C(4A)	101.1(9)
C(2A)-C(1A)-O(1A)	114.6(10)	C(4A)-C(1A)-O(1A)	113.2(9)
C(1A)-C(2A)-C(8A)	115.5(10)	C(1A)-C(2A)-O(2A)	103.6(9)
C(8A)-C(2A)-O(2A)	103.2(9)	C(4A)-C(3A)-O(2A)	105.8(9)
C(4A)-C(3A)-O(4A)	103.5(10)	O(2A)-C(3A)-O(4A)	112.0(10)
C(1A)-C(4A)-C(3A)	105.1(9)	C(1A)-C(4A)-O(3A)	108.8(9)
C(3A)-C(4A)-O(3A)	104.8(9)	C(6A)-C(5A)-C(7A)	113.5(12)

Table 3.6 (cont.)

C(6A)-C(5A)-O(3A)	109.9(10)	C(7A)-C(5A)-O(3A)	110.1(11)
C(6A)-C(5A)-O(4A)	108.5(11)	C(7A)-C(5A)-O(4A)	110.6(11)
O(3A)-C(5A)-O(4A)	103.7(10)	Li(3)-C(8A)-C(2A)	100.5(8)
Li(3)-C(8A)-C(9A)	143.4(10)	C(2A)-C(8A)-C(9A)	114.1(11)
Li(3)-C(8A)-O(6A)	49.2(7)	C(2A)-C(8A)-O(6A)	110.9(10)
C(9A)-C(8A)-O(6A)	104.5(10)	C(8A)-C(9A)-O(5A)	105.6(10)
C(11A)-C(10A)-C(12A)	114.9(11)	C(11A)-C(10A)-O(5A)	113.3(11)
C(12A)-C(10A)-O(5A)	106.1(10)	C(11A)-C(10A)-O(6A)	107.6(11)
C(12A)-C(10A)-O(6A)	109.9(10)	O(5A)-C(10A)-O(6A)	104.5(9)
Ti-O(1A)-Li(3)	92.8(7)	Ti-O(1A)-C(1A)	126.8(7)
Li(3)-O(1A)-C(1A)	123.4(9)	C(2A)-O(2A)-C(3A)	111.6(9)
C(4A)-O(3A)-C(5A)	106.1(9)	C(3A)-O(4A)-C(5A)	111.0(9)
C(9A)-O(5A)-C(10A)	105.2(10)	Li(3)-O(6A)-C(8A)	99.0(9)
Li(3)-O(6A)-C(10A)	143.7(9)	C(8A)-O(6A)-C(10A)	107.7(8)
C(2B)-C(1B)-C(4B)	99.5(9)	C(2B)-C(1B)-O(1B)	110.7(10)
C(4B)-C(1B)-O(1B)	115.2(10)	C(1B)-C(2B)-C(8B)	115.9(10)
C(1B)-C(2B)-O(2B)	106.4(10)	C(8B)-C(2B)-O(2B)	104.7(9)
C(4B)-C(3B)-O(2B)	106.0(10)	C(4B)-C(3B)-O(4B)	106.6(10)
O(2B)-C(3B)-O(4B)	111.7(11)	C(1B)-C(4B)-C(3B)	107.4(10)
C(1B)-C(4B)-O(3B)	108.5(10)	C(3B)-C(4B)-O(3B)	103.6(10)
C(6B)-C(5B)-C(7B)	115.1(12)	C(6B)-C(5B)-O(3B)	110.1(11)
C(7B)-C(5B)-O(3B)	107.6(11)	C(6B)-C(5B)-O(4B)	108.4(11)
C(7B)-C(5B)-O(4B)	109.7(11)	O(3B)-C(5B)-O(4B)	105.5(9)
Li(1)-C(8B)-C(2B)	100.1(9)	Li(1)-C(8B)-C(9B)	142.2(9)
C(2B)-C(8B)-C(9B)	114.6(11)	Li(1)-C(8B)-O(6B)	50.2(7)
C(2B)-C(8B)-O(6B)	109.9(9)	C(9B)-C(8B)-O(6B)	101.5(10)
C(8B)-C(9B)-O(5B)	101.7(11)	C(11B)-C(10B)-C(12B)	116.8(18)
C(11B)-C(10B)-O(5B)	106.6(17)	C(12B)-C(10B)-O(5B)	114.4(17)
C(11B)-C(10B)-O(6B)	112.1(16)	C(12B)-C(10B)-O(6B)	103.0(16)
O(5B)-C(10B)-O(6B)	103.1(14)	Ti-O(1B)-Li(1)	94.6(7)
Ti-O(1B)-C(1B)	127.6(7)	Li(1)-O(1B)-C(1B)	123.9(10)
C(2B)-O(2B)-C(3B)	108.9(9)	C(4B)-O(3B)-C(5B)	109.0(9)
C(3B)-O(4B)-C(5B)	109.5(9)	C(9B)-O(5B)-C(10B)	112.5(15)
Li(1)-O(6B)-C(8B)	96.5(9)	Li(1)-O(6B)-C(10B)	154.7(11)
C(8B)-O(6B)-C(10B)	108.8(11)	C(2C)-C(1C)-C(4C)	101.7(9)
C(2C)-C(1C)-O(1C)	112.7(10)	C(4C)-C(1C)-O(1C)	111.3(9)
C(1C)-C(2C)-C(8C)	117.3(11)	C(1C)-C(2C)-O(2C)	104.7(10)
C(8C)-C(2C)-O(2C)	105.3(10)	C(4C)-C(3C)-O(2C)	107.5(10)
C(4C)-C(3C)-O(4C)	104.4(10)	O(2C)-C(3C)-O(4C)	111.9(11)
C(1C)-C(4C)-C(3C)	105.4(10)	C(1C)-C(4C)-O(3C)	106.4(9)
C(3C)-C(4C)-O(3C)	103.7(9)	C(6C)-C(5C)-C(7C)	114.9(13)
C(6C)-C(5C)-O(3C)	108.5(11)	C(7C)-C(5C)-O(3C)	108.0(11)
C(6C)-C(5C)-O(4C)	112.6(12)	C(7C)-C(5C)-O(4C)	106.3(11)
O(3C)-C(5C)-O(4C)	106.1(10)	Li(2)-C(8C)-C(2C)	100.3(10)
Li(2)-C(8C)-C(9C)	140.1(11)	C(2C)-C(8C)-C(9C)	117.0(12)
Li(2)-C(8C)-O(6C)	48.0(7)	C(2C)-C(8C)-O(6C)	109.6(11)
C(9C)-C(8C)-O(6C)	102.9(11)	C(8C)-C(9C)-O(5C)	105.8(12)
C(11C)-C(10C)-C(12C)	112.1(12)	C(11C)-C(10C)-O(5C)	109.6(12)
C(12C)-C(10C)-O(5C)	112.1(12)	C(11C)-C(10C)-O(6C)	108.3(11)
C(12C)-C(10C)-O(6C)	110.0(11)	O(5C)-C(10C)-O(6C)	104.3(10)
Ti-O(1C)-Li(2)	92.2(8)	Ti-O(1C)-C(1C)	124.2(7)
Li(2)-O(1C)-C(1C)	123.2(10)	C(2C)-O(2C)-C(3C)	112.5(10)
C(4C)-O(3C)-C(5C)	109.4(9)	C(3C)-O(4C)-C(5C)	109.5(10)
C(9C)-O(5C)-C(10C)	107.0(11)	Li(2)-O(6C)-C(8C)	99.8(9)
Li(2)-O(6C)-C(10C)	144.6(10)	C(8C)-O(6C)-C(10C)	107.2(9)
C(2D)-C(1D)-C(4D)	99.0(8)	C(2D)-C(1D)-O(1D)	112.6(9)
C(4D)-C(1D)-O(1D)	113.6(9)	C(1D)-C(2D)-C(8D)	113.7(9)
C(1D)-C(2D)-O(2D)	105.8(9)	C(8D)-C(2D)-O(2D)	105.7(10)
C(4D)-C(3D)-O(2D)	106.9(10)	C(4D)-C(3D)-O(4D)	104.5(11)

O(2D)-C(3D)-O(4D)	110.3(11)	C(1D)-C(4D)-C(3D)	104.9(10)
C(1D)-C(4D)-O(3D)	107.7(9)	C(3D)-C(4D)-O(3D)	103.0(9)
C(6D)-C(5D)-C(7D)	111.2(14)	C(6D)-C(5D)-O(3D)	112.5(12)
C(7D)-C(5D)-O(3D)	109.1(13)	C(6D)-C(5D)-O(4D)	108.3(12)
C(7D)-C(5D)-O(4D)	107.9(13)	O(3D)-C(5D)-O(4D)	107.8(11)
Li(1)-C(8D)-C(2D)	103.1(9)	Li(1)-C(8D)-C(9D)	141.1(12)
C(2D)-C(8D)-C(9D)	114.1(12)	Li(1)-C(8D)-O(6D)	50.6(7)
C(2D)-C(8D)-O(6D)	110.8(10)	C(9D)-C(8D)-O(6D)	103.2(11)
C(8D)-C(9D)-O(5D)	105.0(15)	C(11D)-C(10D)-C(12D)	110.1(13)
C(11D)-C(10D)-O(5D)	113.1(13)	C(12D)-C(10D)-O(5D)	113.1(13)
C(11D)-C(10D)-O(6D)	107.9(12)	C(12D)-C(10D)-O(6D)	108.9(12)
O(5D)-C(10D)-O(6D)	103.4(11)	Ti-O(1D)-Li(1)	93.8(7)
Ti-O(1D)-C(1D)	130.9(7)	Li(1)-O(1D)-C(1D)	121.6(9)
C(2D)-O(2D)-C(3D)	111.1(10)	C(4D)-O(3D)-C(5D)	108.7(10)
C(3D)-O(4D)-C(5D)	109.5(11)	C(9D)-O(5D)-C(10D)	115.9(14)
Li(1)-O(6D)-C(8D)	95.6(9)	Li(1)-O(6D)-C(10D)	153.7(10)
C(8D)-O(6D)-C(10D)	107.7(9)	C(2E)-C(1E)-C(4E)	98.8(9)
C(2E)-C(1E)-O(1E)	112.1(10)	C(4E)-C(1E)-O(1E)	112.5(9)
C(1E)-C(2E)-C(8E)	116.0(10)	C(1E)-C(2E)-O(2E)	108.5(10)
C(8E)-C(2E)-O(2E)	104.9(10)	C(4E)-C(3E)-O(2E)	106.4(10)
C(4E)-C(3E)-O(4E)	104.6(10)	O(2E)-C(3E)-O(4E)	113.1(10)
C(1E)-C(4E)-C(3E)	107.5(10)	C(1E)-C(4E)-O(3E)	109.7(9)
C(3E)-C(4E)-O(3E)	102.7(9)	C(6E)-C(5E)-C(7E)	114.6(12)
C(6E)-C(5E)-O(3E)	108.5(11)	C(7E)-C(5E)-O(3E)	110.4(11)
C(6E)-C(5E)-O(4E)	110.0(12)	C(7E)-C(5E)-O(4E)	107.0(11)
O(3E)-C(5E)-O(4E)	106.0(10)	Li(2)-C(8E)-C(2E)	100.4(9)
Li(2)-C(8E)-C(9E)	142.7(10)	C(2E)-C(8E)-C(9E)	114.4(11)
Li(2)-C(8E)-O(6E)	46.7(7)	C(2E)-C(8E)-O(6E)	113.2(10)
C(9E)-C(8E)-O(6E)	104.0(10)	C(8E)-C(9E)-O(5E)	104.3(10)
C(11E)-C(10E)-C(12E)	113.3(11)	C(11E)-C(10E)-O(5E)	111.4(11)
C(12E)-C(10E)-O(5E)	107.1(11)	C(11E)-C(10E)-O(6E)	110.2(11)
C(12E)-C(10E)-O(6E)	109.2(11)	O(5E)-C(10E)-O(6E)	105.3(9)
Ti-O(1E)-Li(2)	92.1(8)	Ti-O(1E)-C(1E)	123.9(7)
Li(2)-O(1E)-C(1E)	127.1(10)	C(2E)-O(2E)-C(3E)	111.2(10)
C(4E)-O(3E)-C(5E)	109.7(9)	C(3E)-O(4E)-C(5E)	109.7(9)
C(9E)-O(5E)-C(10E)	105.5(10)	Li(2)-O(6E)-C(8E)	102.5(9)
Li(2)-O(6E)-C(10E)	142.8(10)	C(8E)-O(6E)-C(10E)	109.0(9)
C(2F)-C(1F)-C(4F)	100.5(9)	C(2F)-C(1F)-O(1F)	112.9(10)
C(4F)-C(1F)-O(1F)	113.4(10)	C(1F)-C(2F)-C(8F)	115.9(11)
C(1F)-C(2F)-O(2F)	105.2(10)	C(8F)-C(2F)-O(2F)	106.4(10)
C(4F)-C(3F)-O(2F)	106.9(10)	C(4F)-C(3F)-O(4F)	104.8(10)
O(2F)-C(3F)-O(4F)	111.9(11)	C(1F)-C(4F)-C(3F)	106.5(10)
C(1F)-C(4F)-O(3F)	107.7(10)	C(3F)-C(4F)-O(3F)	104.6(10)
C(6F)-C(5F)-C(7F)	113.8(13)	C(6F)-C(5F)-O(3F)	110.9(12)
C(7F)-C(5F)-O(3F)	108.8(12)	C(6F)-C(5F)-O(4F)	107.5(12)
C(7F)-C(5F)-O(4F)	109.0(12)	O(3F)-C(5F)-O(4F)	106.6(10)
Li(3)-C(8F)-C(2F)	100.3(9)	Li(3)-C(8F)-C(9F)	144.7(9)
C(2F)-C(8F)-C(9F)	112.8(11)	Li(3)-C(8F)-O(6F)	49.7(7)
C(2F)-C(8F)-O(6F)	112.0(10)	C(9F)-C(8F)-O(6F)	104.0(10)
C(8F)-C(9F)-O(5F)	104.2(10)	C(11F)-C(10F)-C(12F)	112.4(11)
C(11F)-C(10F)-O(5F)	109.5(10)	C(12F)-C(10F)-O(5F)	113.8(12)
C(11F)-C(10F)-O(6F)	108.8(11)	C(12F)-C(10F)-O(6F)	107.7(11)
O(5F)-C(10F)-O(6F)	104.2(10)	Ti-O(1F)-Li(3)	93.2(7)
Ti-O(1F)-C(1F)	125.7(7)	Li(3)-O(1F)-C(1F)	124.7(10)
C(2F)-O(2F)-C(3F)	112.2(9)	C(4F)-O(3F)-C(5F)	108.5(9)
C(3F)-O(4F)-C(5F)	111.6(10)	C(9F)-O(5F)-C(10F)	105.7(10)
Li(3)-O(6F)-C(8F)	98.8(9)	Li(3)-O(6F)-C(10F)	144.9(9)
C(8F)-O(6F)-C(10F)	108.3(9)	C(2)-C(1)-C(6)	120.0(17)
C(2)-C(1)-C(7)	119.1(17)	C(6)-C(1)-C(7)	120.9(17)

Table S10 (cont.)

C(1)-C(2)-C(3)	122.5(19)	C(2)-C(3)-C(4)	118.3(20)
C(3)-C(4)-C(5)	120.6(17)	C(4)-C(5)-C(6)	118.8(17)
C(1)-C(6)-C(5)	119.3(17)	C(2')-C(1')-C(6')	120.0
C(2')-C(1')-C(7')	120.6	C(6')-C(1')-C(7')	119.2
C(2')-C(1')-C(2")	61.0	C(6')-C(1')-C(2")	177.5
C(7')-C(1')-C(2")	59.6	C(2')-C(1')-C(2')	2.1
C(6')-C(1')-C(2')	120.7	C(7')-C(1')-C(2')	119.6
C(2")-C(1')-C(2')	60.2	C(2')-C(1')-C(4")	59.8
C(6')-C(1')-C(4")	60.4	C(7')-C(1')-C(4")	170.6
C(2")-C(1')-C(4")	120.4	C(2')-C(1')-C(4")	60.4
C(2')-C(1')-C(6')	119.7	C(6')-C(1')-C(6')	7.1
C(7')-C(1')-C(6')	118.3	C(2")-C(1')-C(6')	170.5
C(2')-C(1')-C(6')	120.1	C(4")-C(1')-C(6')	59.9
C(2')-C(1')-C(6")	172.6	C(6')-C(1')-C(6")	60.1
C(7')-C(1')-C(6")	59.2	C(2")-C(1')-C(6")	118.6
C(2')-C(1')-C(6")	170.6	C(4")-C(1')-C(6")	119.0
C(6')-C(1')-C(6")	59.3	C(1')-C(2')-C(3')	120.0
C(1')-C(2')-C(2")	59.5	C(3')-C(2')-C(2")	177.7
C(1')-C(2')-C(4")	59.9	C(3')-C(2')-C(4")	60.3
C(2')-C(3')-C(4')	120.0	C(2')-C(3')-C(2')	2.0
C(4')-C(3')-C(2')	119.9	C(2')-C(3')-C(4")	59.6
C(4')-C(3')-C(4")	60.6	C(2')-C(3')-C(4")	59.4
C(3')-C(4')-C(4")	59.8	C(5')-C(4')-C(4")	60.4
C(4')-C(5')-C(6')	120.0	C(4')-C(5')-C(4")	60.3
C(6')-C(5')-C(4")	59.9	C(4')-C(5')-C(6')	119.7
C(6')-C(5')-C(6')	7.1	C(4")-C(5')-C(6')	59.4
C(1')-C(6')-C(5')	120.0	C(1')-C(6')-C(4")	59.6
C(5')-C(6')-C(4")	60.6	C(1')-C(6')-C(6')	89.4
C(5')-C(6')-C(6')	89.9	C(1')-C(6')-C(6")	60.7
C(5')-C(6')-C(6")	172.6	C(1')-C(7')-C(2")	59.7
C(1')-C(7')-C(6")	60.6	C(1')-C(2")-C(2')	59.5
C(1')-C(2")-C(7')	60.7	C(1')-C(2")-C(2')	59.5
C(1')-C(2')-C(3')	119.2	C(1')-C(2')-C(2")	60.3
C(3')-C(2')-C(2")	178.3	C(1')-C(2')-C(4")	60.0
C(3')-C(2')-C(4")	59.7	C(1')-C(4")-C(2')	60.3
C(1')-C(4")-C(3')	120.2	C(2')-C(4")-C(3')	60.1
C(1')-C(4")-C(4')	171.2	C(2')-C(4")-C(4')	119.5
C(3')-C(4")-C(4')	59.6	C(1')-C(4")-C(5')	119.4
C(2')-C(4")-C(5')	171.2	C(3')-C(4")-C(5')	118.7
C(4')-C(4")-C(5')	59.3	C(1')-C(4")-C(6')	60.0
C(3')-C(4")-C(6')	171.2	C(4')-C(4")-C(6')	118.7
C(5')-C(4")-C(6')	59.5	C(1')-C(4")-C(2')	59.7
C(3')-C(4")-C(2')	60.9	C(4')-C(4")-C(2')	120.4
C(5')-C(4")-C(2')	173.2	C(1')-C(4")-C(6')	60.6
C(3')-C(4")-C(6')	178.1	C(4')-C(4")-C(6')	119.4
C(5')-C(4")-C(6')	60.1	C(1')-C(6')-C(5')	118.6
C(1')-C(6')-C(6')	83.5	C(5')-C(6')-C(6')	83.0
C(1')-C(6')-C(4")	59.5	C(5')-C(6')-C(4")	60.4
C(1')-C(6')-C(6")	60.7	C(5')-C(6')-C(6")	173.2
C(1')-C(6")-C(6')	59.3	C(1')-C(6")-C(7')	60.3
C(1')-C(6")-C(6')	60.0		

Table S17. Anisotropic displacement coefficients ($Å^2 x 10^3$) for complex 6.

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ti	8(1)	12(1)	11(1)	-1(1)	-1(1)	1(1)

The anisotropic displacement factor exponent takes the form:
$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table S18 H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$) for complex 6

	x	y	z	U
H(1AA)	555	2502	7916	80
H(2AA)	-1050	2653	8070	80
H(3AA)	-886	3221	6145	80
H(4AA)	568	2730	6474	80
H(6AA)	-1643	1172	7143	80
H(6AB)	-2026	989	6334	80
H(6AC)	-1053	661	6638	80
H(7AA)	-282	2034	5418	80
H(7AB)	-196	1209	5549	80
H(7AC)	-1170	1538	5245	80
H(8AA)	-698	4128	8097	80
H(9AA)	-2087	3316	8739	80
H(9AB)	-2157	4118	8505	80
H(11A)	-1076	2624	9507	80
H(11B)	-108	2665	9981	80
H(11C)	-1089	2832	10354	80
H(12A)	-119	4589	10077	80
H(12B)	-482	4099	10719	80
H(12C)	499	3932	10346	80
H(1BA)	1918	5109	7153	80
H(2BA)	1938	5784	6104	80
H(3BA)	480	4313	5458	80
H(4BA)	576	4250	6708	80
H(6BA)	-1312	4584	6360	80
H(6BB)	-1607	5210	6885	80
H(6BC)	-1896	5235	6033	80
H(7BA)	60	6484	6166	80
H(7BB)	-1028	6445	5909	80
H(7BC)	-739	6420	6760	80
H(8BA)	3205	4791	5517	80
H(9BA)	2935	6027	4957	80
H(9BB)	3986	5725	4992	80
H(11D)	3847	6892	7156	80
H(11E)	2949	6399	7012	80
H(11F)	3788	6152	7558	80
H(12D)	5490	6459	6609	80
H(12E)	5372	5704	6971	80
H(12F)	5417	5779	6102	80
H(1CA)	3445	2796	6160	80
H(2CA)	3334	1859	5392	80
H(3CA)	976	2750	5159	80
H(4CA)	1996	3561	5685	80
H(6CA)	3440	2386	4005	80
H(6CB)	3112	2782	3270	80
H(6CC)	3961	3089	3770	80
H(7CA)	1982	4254	4194	80
H(7CB)	3030	4270	3895	80
H(7CC)	2182	3963	3395	80
H(8CA)	1903	1307	6264	80
H(9CA)	3123	627	5319	80
H(9CB)	2165	330	5631	80
H(11G)	3362	249	7712	80
H(11H)	4375	-41	7499	80
H(11I)	4277	733	7817	80

H(12G)	4605	1041	5871	80
H(12H)	5056	1230	6659	80
H(12I)	5155	455	6341	80
H(1DA)	4399	2594	7025	80
H(2DA)	6006	2890	7064	80
H(3DA)	5279	3271	8956	80
H(4DA)	4181	2489	8440	80
H(6DA)	5178	1484	9400	80
H(6DB)	5564	839	8940	80
H(6DC)	6254	1241	9507	80
H(7DA)	7042	1875	7771	80
H(7DB)	7404	1496	8507	80
H(7DC)	6714	1093	7940	80
H(8DA)	5391	4297	7194	80
H(9DA)	7109	3864	6840	80
H(9DB)	6728	4622	6615	80
H(11J)	5363	4772	5149	80
H(11K)	5688	4242	4530	80
H(11L)	4638	4202	4824	80
H(12J)	5727	2710	5689	80
H(12K)	4849	2921	5164	80
H(12L)	5899	2961	4870	80
H(1EA)	1400	2705	8895	80
H(2EA)	1562	1708	9590	80
H(3EA)	3940	2537	9783	80
H(4EA)	2904	3404	9361	80
H(6EA)	1634	2184	11053	80
H(6EB)	2100	2528	11775	80
H(6EC)	1184	2875	11391	80
H(7EA)	3079	4044	10868	80
H(7EB)	2100	4052	11280	80
H(7EC)	3015	3706	11665	80
H(8EA)	2986	1219	8662	80
H(9EA)	1775	491	9580	80
H(9EB)	2765	227	9293	80
H(11M)	262	889	8983	80
H(11N)	-172	1065	8186	80
H(11O)	-203	281	8490	80
H(12M)	1689	199	7173	80
H(12N)	698	-156	7343	80
H(12O)	729	627	7039	80
H(1FA)	2925	5014	7984	80
H(2FA)	2831	5738	8981	80
H(3FA)	4273	4265	9738	80
H(4FA)	4251	4144	8495	80
H(6FA)	6249	4592	8769	80
H(6FB)	6484	5259	8279	80
H(6FC)	6738	5265	9137	80
H(7FA)	4638	6389	8993	80
H(7FB)	5718	6402	9275	80
H(7FC)	5464	6395	8417	80
H(8FA)	1637	4740	9636	80
H(9FA)	1806	6208	9787	80
H(9FB)	1425	5678	10383	80
H(11P)	-868	5243	8934	80
H(11Q)	-1061	6021	8647	80
H(11R)	-640	5448	8110	80
H(12P)	1420	6522	8571	80
H(12Q)	796	6245	7886	80

H(12R)	375	6818	8423	80
H(2A)	1424	7383	6889	80
H(3A)	2407	7348	5850	80
H(4A)	2318	8286	4991	80
H(5A)	1129	9206	5108	80
H(6A)	65	9160	6114	80
H(7A)	-483	8585	7208	80
H(7B)	-355	7755	7247	80
H(7C)	365	8253	7692	80

Table S19. Data collection and refinement parameters for complex 7.

Empirical Formula	$C_{69}\ H_{100}\ Cl_2\ Li_4\ Mn\ O_{24}$
Color; Habit	Colorless ; Prismatic
Crystal Size (mm)	0.30 x 0.45 x 1.00
Crystal System	Monoclinic
Space Group	$P2_1$
Unit Cell Dimensions	$\underline{a}$ = 13.306(7) Å
	$\underline{b}$ = 21.311(11) Å
	$\underline{c}$ = 13.376(6) Å
	β = 95.01(2)°
Volume	3779(3) $Å^3$
Z	2
Formula Weight	1467.1
Density(calc.)	1.289 g/cm^3
Absorption Coefficient	0.319 mm^{-1}
F(000)	1554
Diffractometer Used	Siemens P4
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	120
Monochromator	Highly oriented graphite crystal
2θ Range	2.0 to 55.0°
Scan Type	$\theta - 2\theta$
Scan Speed	Variable; 4.00 to 20.00°/min. in ω
Scan Range (ω)	1.10°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 35.0% of total scan time
Standard Reflections	2 measured every 50 reflections
Index Ranges	$-15 \leq h \leq 15$, $-6 \leq k \leq 27$
	$-17 \leq \ell \leq 17$
Reflections Collected	7284
Independent Reflections	6923 (R_{int} = 9.60%)
Observed Reflections	4939 ($F > 4.0\sigma(F)$)
System Used	Siemens SHELXTL IRIS
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Hydrogen Atoms	Riding model, fixed isotropic U