Supporting Information for

Direct Comparison of the Olefin Polymerization Behavior of Ti^{III} and Ti^{IV} Tris(pyrazolyl)borate Catalysts

Kenji Michiue and Richard F. Jordan*

Department of Chemistry, The University of Chicago,
5735 South Ellis Avenue, Chicago, IL 60637

X-ray Crystallographic Analysis of compound **2**·4toluene.

X-ray Crystallographic Analysis of $K[Tp^{Ms*}TiCl_3]\cdot 4$toluene (**2**·4toluene).

Data Collection

An irregular broken fragment (0.40 x 0.20 x 0.20 mm) was selected under a stereo-microscope while immersed in Fluorolube oil to avoid possible reaction with air. The crystal was removed from the oil using a tapered glass fiber that also served to hold the crystal for data collection. The crystal was mounted and centered on a Bruker SMART APEX system at 200 K. Rotation and still images showed the diffractions to be sharp. Frames separated in reciprocal space were obtained and provided an orientation matrix and initial cell parameters. Final cell parameters were obtained from the full data set. Two attempts were made to obtain data from other crystals at 100 K, but both failed because the crystals underwent some type of phase transformation at 100 K.

Approximately ¾ of a sphere of reciprocal data was obtained to a resolution of 0.84 Å using 0.3^o steps in ω using 30 second integration times for each frame. Data collection was made at 200 K. Integration of intensities and refinement of cell parameters were done using SAINT [1]. Absorption corrections were applied using SADABS [1] based on redundant diffractions.

Structure solution and refinement

The space group was determined as P1(bar) based on systematic absences and intensity statistics. Direct methods were used to locate all Ti, Cl and K atoms as well as most C atoms from the E-map. Repeated difference Fourier maps allowed recognition of all expected non-hydrogen atoms. Four C_7H_8 (toluene) molecules are present and while the geometry was easily seen, all show various levels of disorder as shown by large anisotropic displacement parameters. Hydrogen positions were calculated following anisotropic refinement of all non-hydrogen atoms. The H atom on the B was found from the difference map. No anomalous bond lengths or thermal parameters were noted except for the toluene solvent. All ORTEP diagrams have been drawn with 50% probability ellipsoids.

Equations of interest:

$R_{int} = \Sigma \mid F_o^2 - \langle F_o^2 \rangle \mid / \Sigma \mid F_o^2 \mid$ $\quad$ $R1 = \Sigma \mid \mid F_o \mid - \mid F_c \mid \mid / \Sigma \mid F_o \mid$

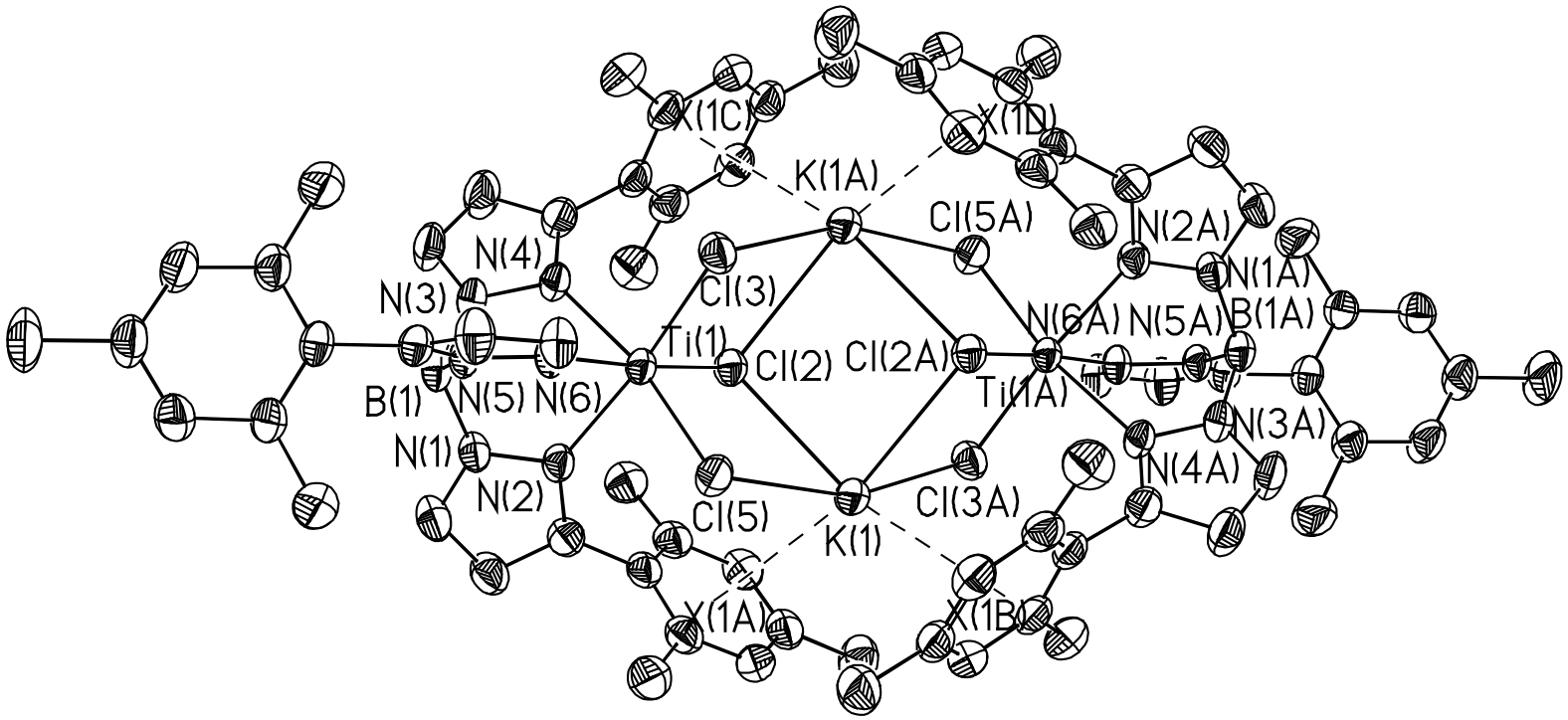
$wR2 = [\Sigma [w (F_o^2 - F_c^2)^2] / \Sigma [w (F_o^2)^2]]^{1/2}$ $\quad$ $GooF = S = [\Sigma [w (F_o^2 - F_c^2)^2] / (n-p)^{1/2}$

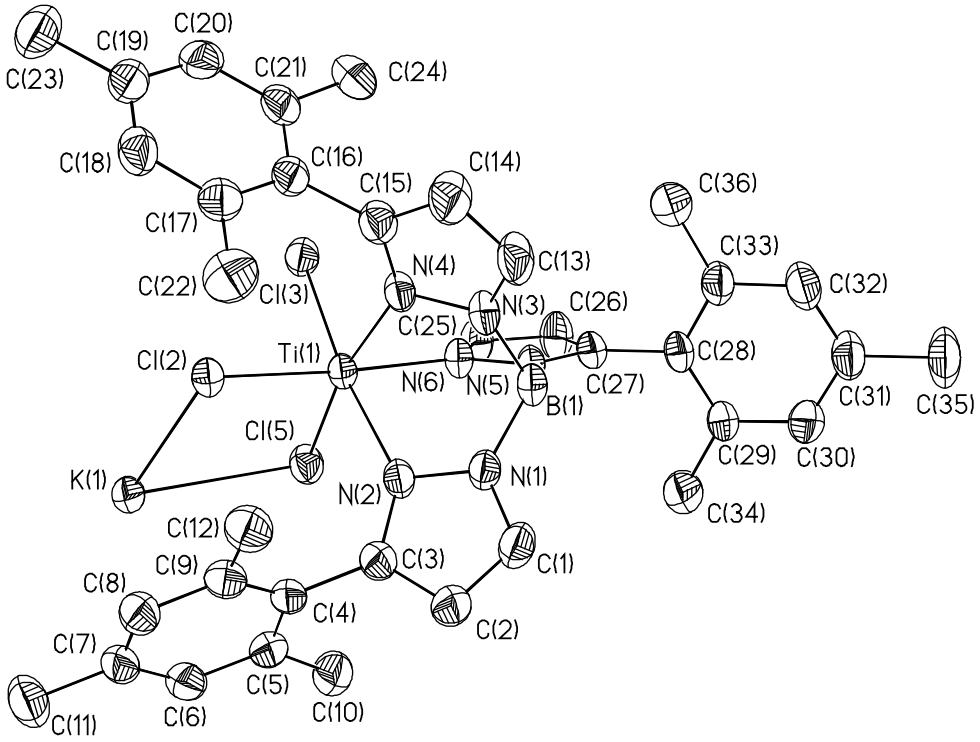
where: $w = q / \sigma^2 (F_o^2) + (aP)^2 + bP$; $\quad$ n = number of independent reflections;

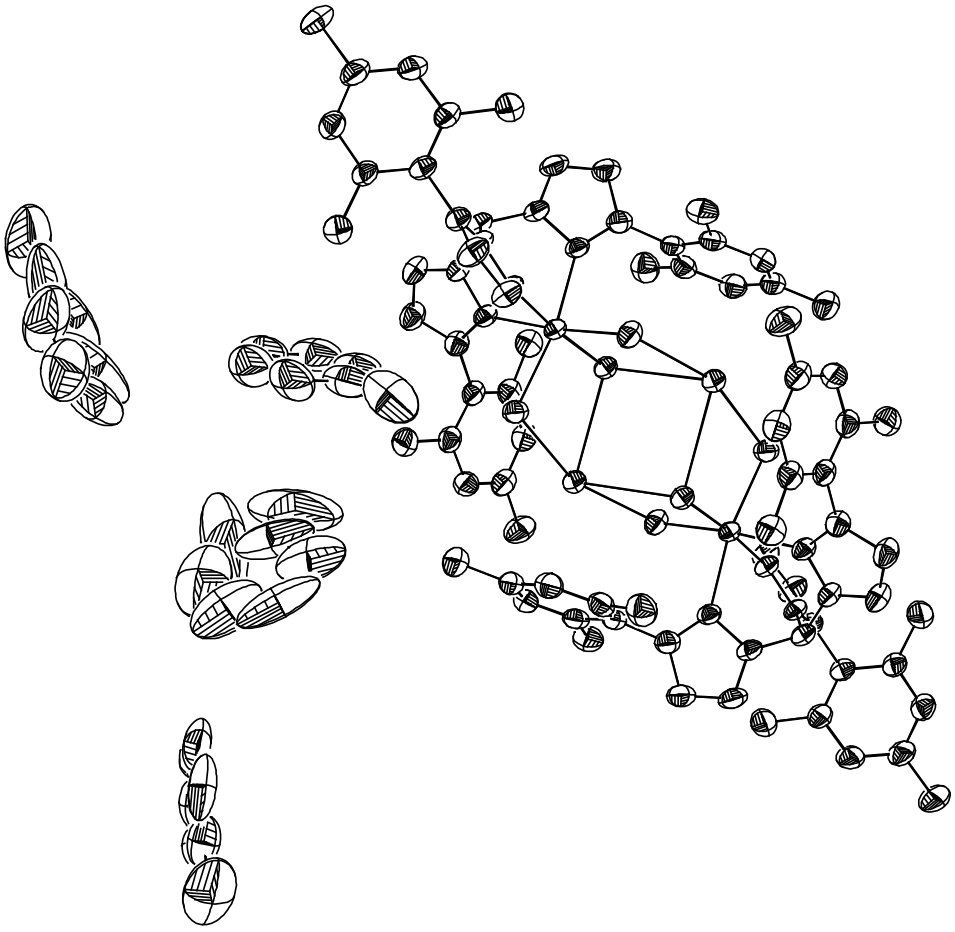
q, a, b, P as defined in [1] $\quad$ p = number of parameters refined.

References

[1] All software and sources of scattering factors are contained in the SHELXTL (version 5.1) program library (G. Sheldrick, Bruker Analytical X-ray Systems, Madison, WI).


X(1C)
X(1D)
K(1A)
Cl(5A)
N(2A)
N(4)
N(1A)
N(3)
Cl(3)
B(1A)
N(6A)
N(5A)
Ti(1)
Cl(2)
Cl(2A)
B(1)
N(5)
N(6)
Ti(1A)
N(3A)
N(1)
N(4A)
N(2)
Cl(5)
Cl(3A)
K(1)
X(1A)
X(1B)


C(20)
C(19)
C(23)
C(21)
C(24)
C(18)
C(16)
C(15)
C(14)
C(36)
C(17)
C(33)
C(22)
Cl(3)
N(4)
C(13)
C(32)
N(3)
C(26)
C(25)
Cl(2)
Ti(1)
C(28)
N(6)
N(5)
C(27)
C(31)
C(35)
B(1)
Cl(5)
C(29)
C(30)
K(1)
N(2)
N(1)
C(34)
C(12)
C(3)
C(1)
C(9)
C(8)
C(4)
C(2)
C(7)
C(5)
C(6)
C(10)
C(11)



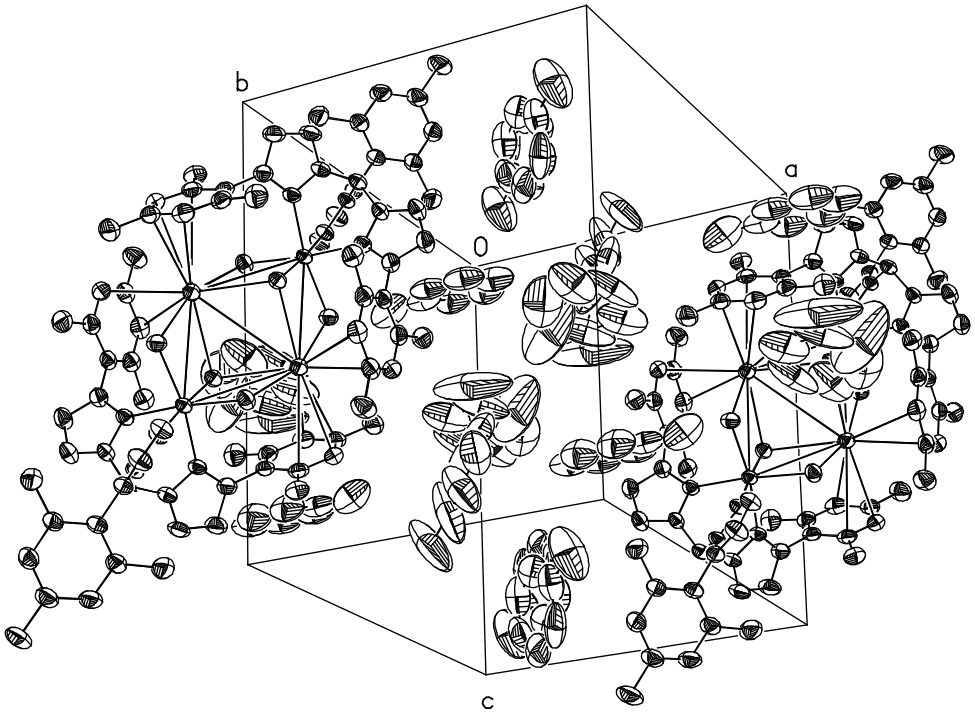

b
a
0
c

Table 1. Crystal and structure refinement for **2**·4toluene.

Identification Code	2a	
Empirical formula	$C_{36}H_{41}BCl_3KN_6Ti + 4C_7H_8$	
Formula weight	1127.42 (including solvent)	
Temperature	200 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space Group	P1(bar)	
Unit cell dimensions	a = 13.178(5) Å	α = 103.240(6) ^{o}
	b = 15.142(6) Å	β = 95.392(7) ^{o}
	c = 15.989(6) Å	γ = 93.562(7) ^{o}
Volume	3080(2) Å^3	
Z	2	
Density (calculated)	1.216 Mg/m^3	
Absorption coefficient	0.380 mm^{-1}	
F(000)	1172	
Crystal size, color, habit	0.40 x 0.20 x 0.20 mm, pale blue, fragment	
Theta range for data collection	1.99 – 25.03 ^{o}	
Index ranges	$-15 \le h \le 15$, $-18 \le k \le 18$, $-19 \le l \le 19$	
Reflections collected	22,428	
Independent reflections	10,801 (R_{int} = 0.0249)	
Absorption correction	SADABS based on redundant diffractions	
Max. and min. transmission	1.0, 0.794	
Refinement method	Full-matrix least squares on F^2	
Weighting scheme	$w = q [\sigma^2 (F_o^2) + (aP)^2 + bP]^{-1}$ where:	
	$P = (F_o^2 + 2 F_c^2)/3$, a = 0.0848, b = 0.0, q =1	
Data / restraints / parameters	10801 / 0 / 705	
Goodness-of-fit on F^2	1.024	
Final R indices [I > 2 sigma(I)]	R1 = 0.0558, wR2 = 0.1377	
R indices (all data)	R1 = 0.0737, wR2 = 0.1476	
Largest diff. peak and hole	0.476, -0.226 eÅ^{-3}	

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

	x	y	z	U(eq)
B(1)	2041(3)	8114(2)	1413(2)	36(1)
C(1)	3741(2)	8014(2)	2310(2)	47(1)
C(2)	4129(2)	8239(2)	3164(2)	50(1)
C(3)	3335(2)	8591(2)	3612(2)	40(1)
C(4)	3407(2)	9002(2)	4560(2)	40(1)
C(5)	3428(2)	8451(2)	5149(2)	43(1)
C(6)	3501(2)	8864(2)	6032(2)	47(1)
C(7)	3570(2)	9800(2)	6334(2)	47(1)
C(8)	3582(2)	10321(2)	5741(2)	47(1)
C(9)	3527(2)	9949(2)	4855(2)	43(1)
C(10)	3406(3)	7431(2)	4856(2)	57(1)
C(11)	3656(3)	10231(3)	7293(2)	64(1)
C(12)	3674(2)	10559(2)	4249(2)	51(1)
C(13)	1706(3)	9536(2)	844(2)	51(1)
C(14)	1203(3)	10299(2)	1074(2)	59(1)
C(15)	804(2)	10235(2)	1835(2)	43(1)
C(16)	195(2)	10926(2)	2336(2)	40(1)
C(17)	698(2)	11669(2)	2946(2)	45(1)
C(18)	114(3)	12326(2)	3373(2)	49(1)
C(19)	-928(3)	12284(2)	3196(2)	49(1)
C(20)	-1402(3)	11566(2)	2563(2)	48(1)
C(21)	-861(3)	10881(2)	2125(2)	44(1)
C(22)	1839(3)	11787(2)	3123(2)	60(1)
C(23)	-1523(3)	13018(2)	3689(2)	67(1)
C(24)	-1401(3)	10122(2)	1407(2)	59(1)
C(25)	-143(2)	6846(2)	1880(2)	45(1)
C(26)	-25(2)	6257(2)	1101(2)	49(1)
C(27)	804(2)	6630(2)	801(2)	37(1)
C(28)	1284(2)	6300(2)	-6(2)	37(1)
C(29)	1971(2)	5634(2)	-34(2)	41(1)
C(30)	2385(2)	5306(2)	-798(2)	48(1)
C(31)	2138(3)	5619(2)	-1523(2)	53(1)
C(32)	1466(3)	6284(2)	-1479(2)	59(1)
C(33)	1027(2)	6632(2)	-727(2)	47(1)
C(34)	2259(3)	5263(3)	739(2)	76(1)
C(35)	2598(4)	5223(3)	-2359(2)	88(1)
C(36)	275(3)	7343(3)	-727(2)	70(1)
C(37)	2446(6)	2373(5)	9890(7)	219(5)
C(38)	3252(4)	2835(3)	9502(5)	101(2)
C(39)	4072(5)	3313(4)	9978(4)	104(2)
C(40)	4786(5)	3738(4)	9636(6)	119(2)
C(41)	4708(6)	3696(5)	8812(7)	132(3)
C(42)	3924(8)	3229(6)	8284(5)	135(3)
C(43)	3131(5)	2772(4)	8602(6)	132(3)
C(44)	707(6)	5067(5)	2991(5)	166(3)
C(45)	1737(6)	4962(4)	2875(3)	106(2)
C(46)	2410(6)	5696(4)	2991(3)	108(2)
C(47)	3421(7)	5587(4)	2890(3)	123(2)

C(48)	3778(6)	4749(5)	2663(4)	137(2)
C(49)	3034(7)	3993(4)	2522(4)	135(2)
C(50)	2051(7)	4095(4)	2629(4)	125(2)
C(51)	5844(11)	1635(8)	296(9)	378(11)
C(52)	5277(14)	1602(12)	903(16)	373(15)
C(53)	4584(8)	1142(6)	1158(9)	217(5)
C(54)	4210(9)	1212(9)	1889(9)	204(5)
C(55)	4570(7)	1934(10)	2606(9)	196(5)
C(56)	5333(8)	2454(9)	2396(11)	268(9)
C(57)	5796(7)	2393(9)	1683(12)	220(7)
C(58)	3090(20)	4811(12)	5019(8)	482(18)
C(59)	2921(13)	4253(8)	5244(6)	207(7)
C(60)	1778(10)	4149(7)	5313(5)	182(4)
C(61)	1581(8)	3331(11)	5638(6)	206(7)
C(62)	2414(12)	2897(10)	5746(6)	208(6)
C(63)	3440(15)	3163(13)	5614(10)	253(8)
C(64)	3670(30)	3763(13)	5277(18)	460(30)
Cl(2)	1117(1)	10144(1)	4175(1)	36(1)
Cl(3)	-964(1)	8828(1)	2974(1)	42(1)
Cl(5)	843(1)	7814(1)	4109(1)	42(1)
K(1)	1092(1)	9345(1)	5763(1)	42(1)
N(1)	2774(2)	8212(2)	2244(1)	36(1)
N(2)	2498(2)	8568(2)	3052(1)	35(1)
N(3)	1619(2)	9037(2)	1421(1)	38(1)
N(4)	1056(2)	9466(1)	2054(1)	34(1)
N(5)	1156(2)	7404(2)	1392(1)	34(1)
N(6)	570(2)	7543(2)	2062(1)	35(1)
Ti(1)	842(1)	8743(1)	3102(1)	31(1)

Table 3. Bond lengths [Å] and angles [°] for **2**·4toluene.

B(1)-N(5)	1.529(4)
B(1)-N(3)	1.534(4)
B(1)-N(1)	1.538(4)
C(1)-N(1)	1.328(4)
C(1)-C(2)	1.371(4)
C(2)-C(3)	1.387(4)
C(3)-N(2)	1.348(4)
C(3)-C(4)	1.493(4)
C(4)-C(5)	1.394(4)
C(4)-C(9)	1.396(4)
C(5)-C(6)	1.398(4)
C(5)-C(10)	1.505(4)
C(6)-C(7)	1.383(5)
C(7)-C(8)	1.366(5)
C(7)-C(11)	1.514(4)
C(8)-C(9)	1.393(4)
C(9)-C(12)	1.501(4)
C(13)-N(3)	1.328(4)
C(13)-C(14)	1.363(4)
C(14)-C(15)	1.390(4)
C(15)-N(4)	1.343(4)
C(15)-C(16)	1.491(4)
C(16)-C(17)	1.393(4)
C(16)-C(21)	1.394(4)
C(17)-C(18)	1.390(4)
C(17)-C(22)	1.496(5)
C(18)-C(19)	1.371(5)
C(18)-K(1)#1	3.516(4)
C(19)-C(20)	1.375(5)
C(19)-C(23)	1.514(4)
C(19)-K(1)#1	3.284(3)
C(20)-C(21)	1.388(4)
C(20)-K(1)#1	3.285(3)
C(21)-C(24)	1.511(4)
C(21)-K(1)#1	3.511(3)
C(25)-N(6)	1.329(4)
C(25)-C(26)	1.384(4)
C(26)-C(27)	1.374(4)
C(27)-N(5)	1.351(3)
C(27)-C(28)	1.487(4)
C(28)-C(33)	1.381(4)
C(28)-C(29)	1.393(4)
C(29)-C(30)	1.385(4)
C(29)-C(34)	1.498(4)
C(30)-C(31)	1.369(4)
C(31)-C(32)	1.376(5)
C(31)-C(35)	1.532(4)
C(32)-C(33)	1.393(4)
C(33)-C(36)	1.507(4)
C(37)-C(38)	1.495(8)
C(38)-C(39)	1.329(7)
C(38)-C(43)	1.414(9)
C(39)-C(40)	1.335(8)
C(40)-C(41)	1.299(9)

C(41)-C(42)	1.323(9)
C(42)-C(43)	1.413(10)
C(44)-C(45)	1.401(8)
C(45)-C(46)	1.344(7)
C(45)-C(50)	1.382(8)
C(46)-C(47)	1.372(8)
C(47)-C(48)	1.364(8)
C(48)-C(49)	1.423(9)
C(49)-C(50)	1.336(8)
C(51)-C(52)	1.286(13)
C(52)-C(53)	1.268(14)
C(52)-C(57)	1.58(3)
C(53)-C(54)	1.296(12)
C(54)-C(55)	1.412(13)
C(55)-C(56)	1.353(13)
C(56)-C(57)	1.330(19)
C(58)-C(59)	1.012(15)
C(59)-C(64)	1.28(3)
C(59)-C(60)	1.522(16)
C(60)-C(61)	1.467(15)
C(61)-C(62)	1.332(19)
C(62)-C(63)	1.43(2)
C(63)-C(64)	1.20(4)
Cl(2)-Ti(1)	2.3866(10)
Cl(2)-K(1)	3.0540(13)
Cl(2)-K(1)#1	3.0639(14)
Cl(3)-Ti(1)	2.3831(12)
Cl(3)-K(1)#1	3.0536(13)
Cl(5)-Ti(1)	2.3685(10)
Cl(5)-K(1)	3.0670(13)
K(1)-Cl(3)#1	3.0536(13)
K(1)-Cl(2)#1	3.0639(14)
K(1)-C(19)#1	3.284(3)
K(1)-C(20)#1	3.285(3)
K(1)-C(21)#1	3.511(3)
K(1)-C(18)#1	3.516(4)
K(1)-Ti(1)#1	4.1898(13)
K(1)-K(1)#1	4.4469(16)
N(1)-N(2)	1.373(3)
N(2)-Ti(1)	2.221(2)
N(3)-N(4)	1.377(3)
N(4)-Ti(1)	2.231(2)
N(5)-N(6)	1.364(3)
N(6)-Ti(1)	2.149(2)
Ti(1)-K(1)#1	4.1898(13)
K(1)-X(1A)	3.262
K(1)-X(1B)	3.230

N(5)-B(1)-N(3)	109.3(2)
N(5)-B(1)-N(1)	109.4(2)
N(3)-B(1)-N(1)	108.5(2)
N(1)-C(1)-C(2)	109.0(3)
C(1)-C(2)-C(3)	105.5(3)
N(2)-C(3)-C(2)	109.7(3)
N(2)-C(3)-C(4)	124.3(2)
C(2)-C(3)-C(4)	125.8(3)
C(5)-C(4)-C(9)	120.1(3)

C(5)-C(4)-C(3)	120.5(3)
C(9)-C(4)-C(3)	119.2(3)
C(4)-C(5)-C(6)	118.7(3)
C(4)-C(5)-C(10)	121.5(3)
C(6)-C(5)-C(10)	119.7(3)
C(7)-C(6)-C(5)	121.9(3)
C(8)-C(7)-C(6)	117.9(3)
C(8)-C(7)-C(11)	121.2(3)
C(6)-C(7)-C(11)	120.9(3)
C(7)-C(8)-C(9)	122.8(3)
C(8)-C(9)-C(4)	118.4(3)
C(8)-C(9)-C(12)	119.9(3)
C(4)-C(9)-C(12)	121.5(3)
N(3)-C(13)-C(14)	109.4(3)
C(13)-C(14)-C(15)	105.2(3)
N(4)-C(15)-C(14)	110.1(3)
N(4)-C(15)-C(16)	125.1(3)
C(14)-C(15)-C(16)	124.8(3)
C(17)-C(16)-C(21)	120.3(3)
C(17)-C(16)-C(15)	119.5(3)
C(21)-C(16)-C(15)	119.8(3)
C(18)-C(17)-C(16)	118.3(3)
C(18)-C(17)-C(22)	120.0(3)
C(16)-C(17)-C(22)	121.7(3)
C(19)-C(18)-C(17)	122.5(3)
C(19)-C(18)-K(1)#1	69.00(18)
C(17)-C(18)-K(1)#1	88.94(19)
C(18)-C(19)-C(20)	118.0(3)
C(18)-C(19)-C(23)	120.0(3)
C(20)-C(19)-C(23)	121.9(3)
C(18)-C(19)-K(1)#1	88.07(19)
C(20)-C(19)-K(1)#1	77.97(18)
C(23)-C(19)-K(1)#1	104.0(2)
C(19)-C(20)-C(21)	122.0(3)
C(19)-C(20)-K(1)#1	77.87(18)
C(21)-C(20)-K(1)#1	87.55(18)
C(20)-C(21)-C(16)	118.7(3)
C(20)-C(21)-C(24)	120.6(3)
C(16)-C(21)-C(24)	120.6(3)
C(20)-C(21)-K(1)#1	69.18(17)
C(16)-C(21)-K(1)#1	86.86(17)
C(24)-C(21)-K(1)#1	115.8(2)
N(6)-C(25)-C(26)	110.7(3)
C(27)-C(26)-C(25)	105.8(3)
N(5)-C(27)-C(26)	107.2(2)
N(5)-C(27)-C(28)	122.8(3)
C(26)-C(27)-C(28)	130.0(3)
C(33)-C(28)-C(29)	120.5(3)
C(33)-C(28)-C(27)	120.3(3)
C(29)-C(28)-C(27)	119.2(3)
C(30)-C(29)-C(28)	118.8(3)
C(30)-C(29)-C(34)	119.7(3)
C(28)-C(29)-C(34)	121.5(3)
C(31)-C(30)-C(29)	121.9(3)
C(30)-C(31)-C(32)	118.4(3)
C(30)-C(31)-C(35)	120.1(3)
C(32)-C(31)-C(35)	121.5(3)

C(31)-C(32)-C(33)	121.8(3)
C(28)-C(33)-C(32)	118.6(3)
C(28)-C(33)-C(36)	122.1(3)
C(32)-C(33)-C(36)	119.3(3)
C(39)-C(38)-C(43)	119.0(6)
C(39)-C(38)-C(37)	122.1(8)
C(43)-C(38)-C(37)	118.9(7)
C(38)-C(39)-C(40)	122.3(6)
C(41)-C(40)-C(39)	120.8(7)
C(40)-C(41)-C(42)	121.3(8)
C(41)-C(42)-C(43)	121.0(8)
C(42)-C(43)-C(38)	115.6(6)
C(46)-C(45)-C(50)	120.4(7)
C(46)-C(45)-C(44)	120.3(7)
C(50)-C(45)-C(44)	119.3(7)
C(45)-C(46)-C(47)	120.0(6)
C(48)-C(47)-C(46)	122.2(7)
C(47)-C(48)-C(49)	115.8(8)
C(50)-C(49)-C(48)	122.2(7)
C(49)-C(50)-C(45)	119.3(7)
C(53)-C(52)-C(51)	146(3)
C(53)-C(52)-C(57)	109.9(17)
C(51)-C(52)-C(57)	103.4(19)
C(52)-C(53)-C(54)	133.7(18)
C(53)-C(54)-C(55)	120.6(14)
C(56)-C(55)-C(54)	109.8(14)
C(57)-C(56)-C(55)	132.9(18)
C(56)-C(57)-C(52)	112.8(11)
C(58)-C(59)-C(64)	113(3)
C(58)-C(59)-C(60)	109(3)
C(64)-C(59)-C(60)	136.6(18)
C(61)-C(60)-C(59)	106.9(11)
C(62)-C(61)-C(60)	113.3(9)
C(61)-C(62)-C(63)	127.4(17)
C(64)-C(63)-C(62)	125(2)
C(63)-C(64)-C(59)	109(3)
Ti(1)-Cl(2)-K(1)	97.63(4)
Ti(1)-Cl(2)-K(1)#1	99.73(3)
K(1)-Cl(2)-K(1)#1	93.25(3)
Ti(1)-Cl(3)-K(1)#1	100.09(3)
Ti(1)-Cl(5)-K(1)	97.69(4)
Cl(3)#1-K(1)-Cl(2)	94.79(4)
Cl(3)#1-K(1)-Cl(2)#1	68.18(2)
Cl(2)-K(1)-Cl(2)#1	86.75(3)
Cl(3)#1-K(1)-Cl(5)	161.84(3)
Cl(2)-K(1)-Cl(5)	69.77(4)
Cl(2)#1-K(1)-Cl(5)	100.46(3)
Cl(3)#1-K(1)-C(19)#1	108.96(7)
Cl(2)-K(1)-C(19)#1	155.80(6)
Cl(2)#1-K(1)-C(19)#1	97.60(6)
Cl(5)-K(1)-C(19)#1	86.04(7)
Cl(3)#1-K(1)-C(20)#1	88.01(7)
Cl(2)-K(1)-C(20)#1	171.95(7)
Cl(2)#1-K(1)-C(20)#1	101.29(6)
Cl(5)-K(1)-C(20)#1	108.59(7)
C(19)#1-K(1)-C(20)#1	24.16(8)
Cl(3)#1-K(1)-C(21)#1	67.47(6)

Cl(2)-K(1)-C(21)#1	161.91(6)
Cl(2)#1-K(1)-C(21)#1	83.33(6)
Cl(5)-K(1)-C(21)#1	126.95(6)
C(19)#1-K(1)-C(21)#1	41.50(7)
C(20)#1-K(1)-C(21)#1	23.27(7)
Cl(3)#1-K(1)-C(18)#1	106.64(6)
Cl(2)-K(1)-C(18)#1	144.47(7)
Cl(2)#1-K(1)-C(18)#1	75.85(6)
Cl(5)-K(1)-C(18)#1	83.06(7)
C(19)#1-K(1)-C(18)#1	22.93(8)
C(20)#1-K(1)-C(18)#1	40.32(9)
C(21)#1-K(1)-C(18)#1	46.18(8)
Cl(3)#1-K(1)-Ti(1)#1	34.056(19)
Cl(2)-K(1)-Ti(1)#1	91.96(3)
Cl(2)#1-K(1)-Ti(1)#1	34.156(17)
Cl(5)-K(1)-Ti(1)#1	133.50(3)
C(19)#1-K(1)-Ti(1)#1	105.01(6)
C(20)#1-K(1)-Ti(1)#1	94.56(6)
C(21)#1-K(1)-Ti(1)#1	71.44(5)
C(18)#1-K(1)-Ti(1)#1	90.56(6)
Cl(3)#1-K(1)-K(1)#1	78.54(3)
Cl(2)-K(1)-K(1)#1	43.46(2)
Cl(2)#1-K(1)-K(1)#1	43.29(2)
Cl(5)-K(1)-K(1)#1	83.55(3)
C(19)#1-K(1)-K(1)#1	135.85(7)
C(20)#1-K(1)-K(1)#1	144.58(7)
C(21)#1-K(1)-K(1)#1	124.95(6)
C(18)#1-K(1)-K(1)#1	112.98(7)
Ti(1)#1-K(1)-K(1)#1	56.86(3)
C(1)-N(1)-N(2)	109.7(2)
C(1)-N(1)-B(1)	127.7(2)
N(2)-N(1)-B(1)	122.5(2)
C(3)-N(2)-N(1)	106.1(2)
C(3)-N(2)-Ti(1)	137.91(19)
N(1)-N(2)-Ti(1)	115.18(16)
C(13)-N(3)-N(4)	109.5(2)
C(13)-N(3)-B(1)	127.5(2)
N(4)-N(3)-B(1)	122.9(2)
C(15)-N(4)-N(3)	105.9(2)
C(15)-N(4)-Ti(1)	139.05(19)
N(3)-N(4)-Ti(1)	115.09(16)
C(27)-N(5)-N(6)	110.3(2)
C(27)-N(5)-B(1)	131.6(2)
N(6)-N(5)-B(1)	118.1(2)
C(25)-N(6)-N(5)	106.0(2)
C(25)-N(6)-Ti(1)	132.48(19)
N(5)-N(6)-Ti(1)	121.42(16)
N(6)-Ti(1)-N(2)	86.67(8)
N(6)-Ti(1)-N(4)	84.49(9)
N(2)-Ti(1)-N(4)	83.26(8)
N(6)-Ti(1)-Cl(5)	89.62(7)
N(2)-Ti(1)-Cl(5)	88.03(6)
N(4)-Ti(1)-Cl(5)	169.74(6)
N(6)-Ti(1)-Cl(3)	86.90(7)
N(2)-Ti(1)-Cl(3)	172.93(6)
N(4)-Ti(1)-Cl(3)	93.19(6)
Cl(5)-Ti(1)-Cl(3)	94.87(3)

N(6)-Ti(1)-Cl(2)	175.49(7)
N(2)-Ti(1)-Cl(2)	94.25(6)
N(4)-Ti(1)-Cl(2)	91.24(7)
Cl(5)-Ti(1)-Cl(2)	94.82(4)
Cl(3)-Ti(1)-Cl(2)	91.93(3)
N(6)-Ti(1)-K(1)#1	132.39(7)
N(2)-Ti(1)-K(1)#1	140.06(6)
N(4)-Ti(1)-K(1)#1	91.61(6)
Cl(5)-Ti(1)-K(1)#1	98.55(3)
Cl(3)-Ti(1)-K(1)#1	45.85(2)
Cl(2)-Ti(1)-K(1)#1	46.12(3)
X(1A)-K(1)-X(1B)	118.6

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for **2**·4toluene. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+ ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
B(1)	41(2)	38(2)	28(2)	0(1)	10(2)	3(1)
C(1)	40(2)	50(2)	47(2)	-2(2)	12(2)	7(1)
C(2)	36(2)	62(2)	46(2)	-1(2)	2(2)	10(2)
C(3)	37(2)	42(2)	37(2)	2(1)	1(1)	3(1)
C(4)	29(2)	52(2)	34(2)	2(1)	0(1)	8(1)
C(5)	35(2)	50(2)	43(2)	5(2)	2(1)	9(1)
C(6)	43(2)	59(2)	38(2)	12(2)	2(2)	11(2)
C(7)	33(2)	62(2)	39(2)	-2(2)	-1(1)	6(1)
C(8)	39(2)	46(2)	47(2)	-2(2)	-1(2)	1(2)
C(9)	32(2)	49(2)	43(2)	5(2)	-2(1)	3(1)
C(10)	69(2)	52(2)	50(2)	7(2)	7(2)	17(2)
C(11)	63(2)	78(2)	40(2)	-4(2)	4(2)	0(2)
C(12)	45(2)	52(2)	52(2)	9(2)	1(2)	-1(2)
C(13)	73(2)	52(2)	34(2)	13(2)	25(2)	11(2)
C(14)	89(3)	54(2)	46(2)	25(2)	30(2)	22(2)
C(15)	53(2)	41(2)	34(2)	10(1)	9(1)	7(1)
C(16)	57(2)	39(2)	30(2)	14(1)	11(1)	13(1)
C(17)	57(2)	40(2)	41(2)	16(1)	6(2)	8(2)
C(18)	73(3)	34(2)	38(2)	6(2)	7(2)	6(2)
C(19)	69(2)	46(2)	38(2)	17(2)	16(2)	20(2)
C(20)	51(2)	57(2)	42(2)	21(2)	9(2)	17(2)
C(21)	61(2)	47(2)	29(2)	16(1)	8(2)	10(2)
C(22)	61(2)	50(2)	71(3)	18(2)	8(2)	3(2)
C(23)	90(3)	59(2)	62(2)	18(2)	29(2)	31(2)
C(24)	65(2)	72(2)	38(2)	13(2)	-2(2)	8(2)
C(25)	46(2)	45(2)	39(2)	3(1)	14(1)	-2(1)
C(26)	54(2)	40(2)	45(2)	-6(1)	14(2)	-8(2)
C(27)	44(2)	37(2)	27(2)	0(1)	3(1)	5(1)
C(28)	44(2)	34(1)	27(2)	-3(1)	5(1)	-1(1)
C(29)	49(2)	40(2)	31(2)	-2(1)	4(1)	6(1)
C(30)	54(2)	43(2)	44(2)	0(1)	7(2)	9(2)
C(31)	70(2)	50(2)	38(2)	1(2)	17(2)	11(2)
C(32)	90(3)	57(2)	33(2)	9(2)	15(2)	22(2)
C(33)	61(2)	43(2)	35(2)	1(1)	11(2)	12(2)
C(34)	98(3)	91(3)	47(2)	18(2)	13(2)	50(2)
C(35)	132(4)	92(3)	48(2)	11(2)	44(3)	49(3)
C(36)	94(3)	72(2)	47(2)	14(2)	10(2)	38(2)
C(37)	157(7)	146(7)	365(14)	50(8)	126(8)	-13(5)
C(38)	76(3)	66(3)	143(5)	-11(3)	10(4)	4(2)
C(39)	104(4)	87(4)	106(4)	-2(3)	-5(4)	9(3)
C(40)	76(4)	85(4)	187(8)	13(5)	8(4)	10(3)
C(41)	127(6)	121(5)	172(8)	45(6)	74(6)	66(5)
C(42)	155(7)	131(6)	105(5)	-17(4)	4(5)	94(6)
C(43)	82(4)	85(4)	181(8)	-52(4)	-35(4)	37(3)
C(44)	195(8)	139(6)	164(7)	59(5)	-27(6)	2(6)
C(45)	160(6)	95(4)	66(3)	34(3)	0(4)	-3(4)
C(46)	198(7)	70(3)	48(3)	9(2)	1(4)	-8(4)
C(47)	216(8)	83(4)	58(3)	9(3)	-2(4)	-22(5)

C(48)	238(8)	94(4)	77(4)	24(3)	13(4)	0(5)
C(49)	212(8)	86(4)	115(5)	34(4)	26(6)	20(5)
C(50)	203(7)	64(3)	117(5)	41(3)	21(5)	10(4)
C(51)	480(20)	315(14)	540(20)	294(15)	450(20)	270(14)
C(52)	332(19)	303(17)	700(40)	360(20)	410(20)	242(15)
C(53)	226(10)	153(7)	326(14)	89(8)	194(11)	59(7)
C(54)	159(10)	234(13)	250(14)	82(11)	71(10)	91(9)
C(55)	99(6)	308(14)	252(13)	202(12)	20(7)	59(8)
C(56)	95(7)	352(18)	450(20)	320(20)	-36(9)	10(8)
C(57)	90(6)	240(12)	420(20)	243(14)	37(9)	54(7)
C(58)	1060(60)	310(20)	102(8)	67(12)	101(17)	80(30)
C(59)	327(15)	151(8)	105(7)	-27(5)	92(9)	-146(10)
C(60)	246(11)	178(8)	67(4)	-53(5)	8(6)	-67(8)
C(61)	150(7)	302(15)	89(5)	-87(7)	55(6)	-145(9)
C(62)	177(10)	262(14)	119(7)	-71(7)	17(8)	-61(11)
C(63)	240(16)	273(19)	180(12)	-64(13)	-58(11)	78(14)
C(64)	670(50)	223(18)	390(30)	-95(18)	-160(30)	270(30)
Cl(2)	41(1)	34(1)	30(1)	2(1)	5(1)	5(1)
Cl(3)	37(1)	47(1)	39(1)	0(1)	5(1)	6(1)
Cl(5)	55(1)	39(1)	34(1)	10(1)	9(1)	7(1)
K(1)	50(1)	47(1)	30(1)	6(1)	5(1)	16(1)
N(1)	33(1)	39(1)	32(1)	0(1)	8(1)	3(1)
N(2)	38(1)	37(1)	27(1)	1(1)	5(1)	3(1)
N(3)	46(1)	39(1)	27(1)	3(1)	11(1)	3(1)
N(4)	43(1)	35(1)	25(1)	4(1)	8(1)	4(1)
N(5)	37(1)	37(1)	24(1)	-1(1)	7(1)	3(1)
N(6)	40(1)	35(1)	28(1)	0(1)	10(1)	2(1)
Ti(1)	36(1)	32(1)	24(1)	3(1)	5(1)	4(1)

Table 5. Hydrogen coordinates [x 10^4] and isotropic displacement parameters [$Å^2$ x 10^3] for **2**·4toluene.

H(1)	4098	7764	1850	57
H(2)	4785	8170	3396	60
H(10A)	2770	7195	4510	85
H(10B)	3470	7174	5352	85
H(10C)	3963	7275	4520	85
H(11A)	4311	10571	7473	95
H(11B)	3589	9764	7606	95
H(11C)	3124	10632	7410	95
H(12A)	3444	11144	4487	76
H(12B)	3286	10294	3700	76
H(12C)	4386	10630	4172	76
H(13)	2056	9388	359	61
H(14)	1139	10763	784	71
H(22A)	2089	11225	3199	90
H(22B)	2036	12257	3639	90
H(22C)	2125	11954	2644	90
H(23A)	-1554	12941	4266	101
H(23B)	-2204	12971	3402	101
H(23C)	-1188	13605	3711	101
H(24A)	-1332	9549	1559	88
H(24B)	-1100	10117	882	88
H(24C)	-2113	10219	1325	88
H(25)	-652	6765	2228	53
H(26)	-424	5720	836	59
H(30)	2843	4860	-819	57
H(32)	1300	6507	-1966	71
H(34A)	2753	4826	603	114
H(34B)	1661	4973	897	114
H(34C)	2549	5751	1214	114
H(35A)	2341	4597	-2577	132
H(35B)	3330	5263	-2244	132
H(35C)	2412	5562	-2781	132
H(36A)	-401	7077	-711	105
H(36B)	295	7565	-1242	105
H(36C)	453	7838	-228	105
H(37A)	2668	1808	9983	329
H(37B)	1823	2256	9505	329
H(37C)	2328	2759	10433	329
H(39)	4151	3352	10570	125
H(40)	5346	4069	9992	143
H(41)	5212	4001	8588	158
H(42)	3894	3200	7695	162
H(43)	2568	2452	8242	158
H(44A)	611	5704	3169	248
H(44B)	516	4765	3426	248
H(44C)	288	4805	2456	248
H(46)	2190	6277	3140	129
H(47)	3877	6103	2980	148
H(48)	4465	4677	2603	164
H(49)	3239	3408	2350	162
H(50)	1583	3587	2539	150
H(51A)	5426	1501	-250	567
H(51B)	6340	1196	287	567

H(51C)	6190	2234	399	567
H(53)	4280	649	729	261
H(54)	3699	782	1942	245
H(55)	4321	2036	3142	235
H(56)	5584	2955	2839	322
H(57)	6364	2773	1647	264
H(58A)	3622	4700	4651	723
H(58B)	3304	5320	5496	723
H(58C)	2486	4943	4695	723
H(60)	1296	4531	5175	218
H(61)	939	3136	5757	248
H(63)	3961	2845	5803	304
H(6)	3460(20)	8470(20)	6390(20)	50(9)
H(8)	3640(20)	10930(20)	5910(20)	56(10)
H(18)	420(20)	12760(20)	3718(19)	35(8)
H(20)	-2120(20)	11549(18)	2434(18)	38(8)
H(70)	2443(18)	7902(16)	842(17)	30(7)

Table 6. Torsion angles [°] for **2**·4toluene.

N(1)-C(1)-C(2)-C(3)	-0.3(4)
C(1)-C(2)-C(3)-N(2)	0.9(4)
C(1)-C(2)-C(3)-C(4)	-174.7(3)
N(2)-C(3)-C(4)-C(5)	108.7(3)
C(2)-C(3)-C(4)-C(5)	-76.4(4)
N(2)-C(3)-C(4)-C(9)	-76.0(4)
C(2)-C(3)-C(4)-C(9)	98.9(4)
C(9)-C(4)-C(5)-C(6)	4.3(4)
C(3)-C(4)-C(5)-C(6)	179.6(3)
C(9)-C(4)-C(5)-C(10)	-173.8(3)
C(3)-C(4)-C(5)-C(10)	1.5(4)
C(4)-C(5)-C(6)-C(7)	-1.1(5)
C(10)-C(5)-C(6)-C(7)	177.0(3)
C(5)-C(6)-C(7)-C(8)	-1.0(5)
C(5)-C(6)-C(7)-C(11)	-179.6(3)
C(6)-C(7)-C(8)-C(9)	0.0(5)
C(11)-C(7)-C(8)-C(9)	178.5(3)
C(7)-C(8)-C(9)-C(4)	3.2(5)
C(7)-C(8)-C(9)-C(12)	-172.4(3)
C(5)-C(4)-C(9)-C(8)	-5.3(4)
C(3)-C(4)-C(9)-C(8)	179.3(3)
C(5)-C(4)-C(9)-C(12)	170.3(3)
C(3)-C(4)-C(9)-C(12)	-5.1(4)
N(3)-C(13)-C(14)-C(15)	0.3(4)
C(13)-C(14)-C(15)-N(4)	0.0(4)
C(13)-C(14)-C(15)-C(16)	179.4(3)
N(4)-C(15)-C(16)-C(17)	93.3(4)
C(14)-C(15)-C(16)-C(17)	-86.0(4)
N(4)-C(15)-C(16)-C(21)	-94.0(4)
C(14)-C(15)-C(16)-C(21)	86.6(4)
C(21)-C(16)-C(17)-C(18)	4.2(4)
C(15)-C(16)-C(17)-C(18)	176.8(3)
C(21)-C(16)-C(17)-C(22)	-173.7(3)
C(15)-C(16)-C(17)-C(22)	-1.1(4)
C(16)-C(17)-C(18)-C(19)	-2.2(5)
C(22)-C(17)-C(18)-C(19)	175.7(3)
C(16)-C(17)-C(18)-K(1)#1	61.9(3)
C(22)-C(17)-C(18)-K(1)#1	-120.2(3)
C(17)-C(18)-C(19)-C(20)	-0.8(5)
K(1)#1-C(18)-C(19)-C(20)	-75.3(3)
C(17)-C(18)-C(19)-C(23)	179.5(3)
K(1)#1-C(18)-C(19)-C(23)	105.1(3)
C(17)-C(18)-C(19)-K(1)#1	74.4(3)
C(18)-C(19)-C(20)-C(21)	1.9(5)
C(23)-C(19)-C(20)-C(21)	-178.4(3)
K(1)#1-C(19)-C(20)-C(21)	-79.3(3)
C(18)-C(19)-C(20)-K(1)#1	81.2(3)
C(23)-C(19)-C(20)-K(1)#1	-99.2(3)
C(19)-C(20)-C(21)-C(16)	0.0(5)
K(1)#1-C(20)-C(21)-C(16)	-74.0(3)
C(19)-C(20)-C(21)-C(24)	-177.5(3)
K(1)#1-C(20)-C(21)-C(24)	108.5(3)
C(19)-C(20)-C(21)-K(1)#1	74.0(3)

C(17)-C(16)-C(21)-C(20)	-3.2(4)
C(15)-C(16)-C(21)-C(20)	-175.8(3)
C(17)-C(16)-C(21)-C(24)	174.3(3)
C(15)-C(16)-C(21)-C(24)	1.7(4)
C(17)-C(16)-C(21)-K(1)#1	-67.3(3)
C(15)-C(16)-C(21)-K(1)#1	120.1(2)
N(6)-C(25)-C(26)-C(27)	-0.4(4)
C(25)-C(26)-C(27)-N(5)	0.5(3)
C(25)-C(26)-C(27)-C(28)	-179.7(3)
N(5)-C(27)-C(28)-C(33)	-83.8(4)
C(26)-C(27)-C(28)-C(33)	96.4(4)
N(5)-C(27)-C(28)-C(29)	98.0(3)
C(26)-C(27)-C(28)-C(29)	-81.8(4)
C(33)-C(28)-C(29)-C(30)	-0.6(4)
C(27)-C(28)-C(29)-C(30)	177.6(3)
C(33)-C(28)-C(29)-C(34)	-179.9(3)
C(27)-C(28)-C(29)-C(34)	-1.7(4)
C(28)-C(29)-C(30)-C(31)	0.1(5)
C(34)-C(29)-C(30)-C(31)	179.5(3)
C(29)-C(30)-C(31)-C(32)	0.5(5)
C(29)-C(30)-C(31)-C(35)	-178.8(3)
C(30)-C(31)-C(32)-C(33)	-0.8(6)
C(35)-C(31)-C(32)-C(33)	178.5(4)
C(29)-C(28)-C(33)-C(32)	0.4(5)
C(27)-C(28)-C(33)-C(32)	-177.8(3)
C(29)-C(28)-C(33)-C(36)	179.1(3)
C(27)-C(28)-C(33)-C(36)	0.9(5)
C(31)-C(32)-C(33)-C(28)	0.3(5)
C(31)-C(32)-C(33)-C(36)	-178.4(3)
C(43)-C(38)-C(39)-C(40)	0.1(8)
C(37)-C(38)-C(39)-C(40)	-178.9(6)
C(38)-C(39)-C(40)-C(41)	-0.4(9)
C(39)-C(40)-C(41)-C(42)	-0.4(10)
C(40)-C(41)-C(42)-C(43)	1.3(9)
C(41)-C(42)-C(43)-C(38)	-1.5(8)
C(39)-C(38)-C(43)-C(42)	0.7(7)
C(37)-C(38)-C(43)-C(42)	179.8(5)
C(50)-C(45)-C(46)-C(47)	-1.9(8)
C(44)-C(45)-C(46)-C(47)	178.9(6)
C(45)-C(46)-C(47)-C(48)	0.8(9)
C(46)-C(47)-C(48)-C(49)	1.0(9)
C(47)-C(48)-C(49)-C(50)	-1.8(10)
C(48)-C(49)-C(50)-C(45)	0.8(10)
C(46)-C(45)-C(50)-C(49)	1.1(9)
C(44)-C(45)-C(50)-C(49)	-179.7(6)
C(51)-C(52)-C(53)-C(54)	169(2)
C(57)-C(52)-C(53)-C(54)	3(2)
C(52)-C(53)-C(54)-C(55)	1(2)
C(53)-C(54)-C(55)-C(56)	-2.3(15)
C(54)-C(55)-C(56)-C(57)	-2.2(15)
C(55)-C(56)-C(57)-C(52)	6.5(16)
C(53)-C(52)-C(57)-C(56)	-6.2(15)
C(51)-C(52)-C(57)-C(56)	-178.1(9)
C(58)-C(59)-C(60)-C(61)	179.8(12)
C(64)-C(59)-C(60)-C(61)	12(2)
C(59)-C(60)-C(61)-C(62)	-2.6(9)
C(60)-C(61)-C(62)-C(63)	2.6(14)

C(61)-C(62)-C(63)-C(64)	-10(3)
C(62)-C(63)-C(64)-C(59)	15(3)
C(58)-C(59)-C(64)-C(63)	175(2)
C(60)-C(59)-C(64)-C(63)	-18(3)
Ti(1)-Cl(2)-K(1)-Cl(3)#1	-168.04(3)
K(1)#1-Cl(2)-K(1)-Cl(3)#1	-67.77(2)
Ti(1)-Cl(2)-K(1)-Cl(2)#1	-100.27(3)
K(1)#1-Cl(2)-K(1)-Cl(2)#1	0.0
Ti(1)-Cl(2)-K(1)-Cl(5)	2.13(3)
K(1)#1-Cl(2)-K(1)-Cl(5)	102.40(3)
Ti(1)-Cl(2)-K(1)-C(19)#1	1.07(16)
K(1)#1-Cl(2)-K(1)-C(19)#1	101.35(16)
Ti(1)-Cl(2)-K(1)-C(20)#1	81.8(5)
K(1)#1-Cl(2)-K(1)-C(20)#1	-177.9(5)
Ti(1)-Cl(2)-K(1)-C(21)#1	-157.04(19)
K(1)#1-Cl(2)-K(1)-C(21)#1	-56.8(2)
Ti(1)-Cl(2)-K(1)-C(18)#1	-40.33(11)
K(1)#1-Cl(2)-K(1)-C(18)#1	59.95(10)
Ti(1)-Cl(2)-K(1)-Ti(1)#1	-134.04(3)
K(1)#1-Cl(2)-K(1)-Ti(1)#1	-33.771(17)
Ti(1)-Cl(2)-K(1)-K(1)#1	-100.27(3)
Ti(1)-Cl(5)-K(1)-Cl(3)#1	30.93(11)
Ti(1)-Cl(5)-K(1)-Cl(2)	-2.15(3)
Ti(1)-Cl(5)-K(1)-Cl(2)#1	80.42(3)
Ti(1)-Cl(5)-K(1)-C(19)#1	177.42(7)
Ti(1)-Cl(5)-K(1)-C(20)#1	-173.78(7)
Ti(1)-Cl(5)-K(1)-C(21)#1	169.91(7)
Ti(1)-Cl(5)-K(1)-C(18)#1	154.58(7)
Ti(1)-Cl(5)-K(1)-Ti(1)#1	70.43(4)
Ti(1)-Cl(5)-K(1)-K(1)#1	40.40(3)
C(2)-C(1)-N(1)-N(2)	-0.3(3)
C(2)-C(1)-N(1)-B(1)	177.4(3)
N(5)-B(1)-N(1)-C(1)	115.6(3)
N(3)-B(1)-N(1)-C(1)	-125.3(3)
N(5)-B(1)-N(1)-N(2)	-67.0(3)
N(3)-B(1)-N(1)-N(2)	52.1(3)
C(2)-C(3)-N(2)-N(1)	-1.0(3)
C(4)-C(3)-N(2)-N(1)	174.6(3)
C(2)-C(3)-N(2)-Ti(1)	167.6(2)
C(4)-C(3)-N(2)-Ti(1)	-16.7(5)
C(1)-N(1)-N(2)-C(3)	0.8(3)
B(1)-N(1)-N(2)-C(3)	-177.1(2)
C(1)-N(1)-N(2)-Ti(1)	-170.82(19)
B(1)-N(1)-N(2)-Ti(1)	11.3(3)
C(14)-C(13)-N(3)-N(4)	-0.4(4)
C(14)-C(13)-N(3)-B(1)	178.5(3)
N(5)-B(1)-N(3)-C(13)	-120.3(3)
N(1)-B(1)-N(3)-C(13)	120.6(3)
N(5)-B(1)-N(3)-N(4)	58.6(3)
N(1)-B(1)-N(3)-N(4)	-60.6(3)
C(14)-C(15)-N(4)-N(3)	-0.2(4)
C(16)-C(15)-N(4)-N(3)	-179.7(3)
C(14)-C(15)-N(4)-Ti(1)	179.0(2)
C(16)-C(15)-N(4)-Ti(1)	-0.4(5)
C(13)-N(3)-N(4)-C(15)	0.4(3)
B(1)-N(3)-N(4)-C(15)	-178.6(3)
C(13)-N(3)-N(4)-Ti(1)	-179.1(2)

B(1)-N(3)-N(4)-Ti(1)	1.9(3)
C(26)-C(27)-N(5)-N(6)	-0.4(3)
C(28)-C(27)-N(5)-N(6)	179.7(2)
C(26)-C(27)-N(5)-B(1)	-179.1(3)
C(28)-C(27)-N(5)-B(1)	1.1(5)
N(3)-B(1)-N(5)-C(27)	117.8(3)
N(1)-B(1)-N(5)-C(27)	-123.6(3)
N(3)-B(1)-N(5)-N(6)	-60.8(3)
N(1)-B(1)-N(5)-N(6)	57.8(3)
C(26)-C(25)-N(6)-N(5)	0.2(3)
C(26)-C(25)-N(6)-Ti(1)	176.7(2)
C(27)-N(5)-N(6)-C(25)	0.2(3)
B(1)-N(5)-N(6)-C(25)	179.0(2)
C(27)-N(5)-N(6)-Ti(1)	-176.82(17)
B(1)-N(5)-N(6)-Ti(1)	2.0(3)
C(25)-N(6)-Ti(1)-N(2)	142.4(3)
N(5)-N(6)-Ti(1)-N(2)	-41.55(19)
C(25)-N(6)-Ti(1)-N(4)	-134.1(3)
N(5)-N(6)-Ti(1)-N(4)	41.99(19)
C(25)-N(6)-Ti(1)-Cl(5)	54.3(3)
N(5)-N(6)-Ti(1)-Cl(5)	-129.60(19)
C(25)-N(6)-Ti(1)-Cl(3)	-40.6(3)
N(5)-N(6)-Ti(1)-Cl(3)	135.50(19)
C(25)-N(6)-Ti(1)-Cl(2)	-115.6(8)
N(5)-N(6)-Ti(1)-Cl(2)	60.5(9)
C(25)-N(6)-Ti(1)-K(1)#1	-47.0(3)
N(5)-N(6)-Ti(1)-K(1)#1	129.14(17)
C(3)-N(2)-Ti(1)-N(6)	-134.5(3)
N(1)-N(2)-Ti(1)-N(6)	33.47(18)
C(3)-N(2)-Ti(1)-N(4)	140.7(3)
N(1)-N(2)-Ti(1)-N(4)	-51.36(17)
C(3)-N(2)-Ti(1)-Cl(5)	-44.7(3)
N(1)-N(2)-Ti(1)-Cl(5)	123.21(17)
C(3)-N(2)-Ti(1)-Cl(3)	-159.1(4)
N(1)-N(2)-Ti(1)-Cl(3)	8.8(6)
C(3)-N(2)-Ti(1)-Cl(2)	50.0(3)
N(1)-N(2)-Ti(1)-Cl(2)	-142.11(16)
C(3)-N(2)-Ti(1)-K(1)#1	56.3(3)
N(1)-N(2)-Ti(1)-K(1)#1	-135.79(14)
C(15)-N(4)-Ti(1)-N(6)	138.1(3)
N(3)-N(4)-Ti(1)-N(6)	-42.69(18)
C(15)-N(4)-Ti(1)-N(2)	-134.6(3)
N(3)-N(4)-Ti(1)-N(2)	44.60(18)
C(15)-N(4)-Ti(1)-Cl(5)	-166.7(3)
N(3)-N(4)-Ti(1)-Cl(5)	12.5(5)
C(15)-N(4)-Ti(1)-Cl(3)	51.5(3)
N(3)-N(4)-Ti(1)-Cl(3)	-129.26(17)
C(15)-N(4)-Ti(1)-Cl(2)	-40.5(3)
N(3)-N(4)-Ti(1)-Cl(2)	138.74(17)
C(15)-N(4)-Ti(1)-K(1)#1	5.6(3)
N(3)-N(4)-Ti(1)-K(1)#1	-175.13(17)
K(1)-Cl(5)-Ti(1)-N(6)	-176.62(6)
K(1)-Cl(5)-Ti(1)-N(2)	96.69(6)
K(1)-Cl(5)-Ti(1)-N(4)	128.5(4)
K(1)-Cl(5)-Ti(1)-Cl(3)	-89.77(3)
K(1)-Cl(5)-Ti(1)-Cl(2)	2.59(3)
K(1)-Cl(5)-Ti(1)-K(1)#1	-43.72(3)

K(1)#1-Cl(3)-Ti(1)-N(6)	-173.45(6)
K(1)#1-Cl(3)-Ti(1)-N(2)	-148.8(5)
K(1)#1-Cl(3)-Ti(1)-N(4)	-89.15(7)
K(1)#1-Cl(3)-Ti(1)-Cl(5)	97.20(4)
K(1)#1-Cl(3)-Ti(1)-Cl(2)	2.20(3)
K(1)-Cl(2)-Ti(1)-N(6)	167.3(8)
K(1)#1-Cl(2)-Ti(1)-N(6)	72.7(8)
K(1)-Cl(2)-Ti(1)-N(2)	-90.98(6)
K(1)#1-Cl(2)-Ti(1)-N(2)	174.38(6)
K(1)-Cl(2)-Ti(1)-N(4)	-174.31(6)
K(1)#1-Cl(2)-Ti(1)-N(4)	91.05(6)
K(1)-Cl(2)-Ti(1)-Cl(5)	-2.60(3)
K(1)#1-Cl(2)-Ti(1)-Cl(5)	-97.24(3)
K(1)-Cl(2)-Ti(1)-Cl(3)	92.46(3)
K(1)#1-Cl(2)-Ti(1)-Cl(3)	-2.19(3)
K(1)-Cl(2)-Ti(1)-K(1)#1	94.64(3)