Table 1. Crystal data and structure refinement for [LTiCl$_2$].

Identification code	iw003m
Empirical formula	C32 H30 Cl2 N4 Ti
Formula weight	589.40
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pbca
Unit cell dimensions	a = 15.5864(7) A alpha = 90 deg. b = 16.2149(7) A beta = 90 deg. c = 23.5128(11) A gamma = 90 deg.
Volume	5942.4(5) A^3
Z, Calculated density	8, 1.318 Mg/m^3
Absorption coefficient	0.496 mm^-1
F(000)	2448
Crystal size	0.25 x 0.14 x 0.12 mm
Theta range for data collection	1.73 to 22.50 deg.
Limiting indices	-16<=h<=16, -17<=k<=12, -25<=l<=25
Reflections collected / unique	23213 / 3872 [R(int) = 0.0805]
Completeness to theta = 22.50	99.7 %
Absorption correction	SADABS
Max. and min. transmission	0.927998 and 0.803088
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3872 / 0 / 356
Goodness-of-fit on F^2	1.078
Final R indices [I>2sigma(I)]	R1 = 0.0560, wR2 = 0.1121
R indices (all data)	R1 = 0.0915, wR2 = 0.1320
Largest diff. peak and hole	0.486 and -0.345 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for [**L**$TiCl_2$].
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ti(1)	9321(1)	2469(1)	7262(1)	28(1)
Cl(1)	8921(1)	3647(1)	6803(1)	47(1)
Cl(2)	9764(1)	1323(1)	6779(1)	47(1)
N(1)	9919(2)	2985(2)	7912(2)	28(1)
N(2)	10678(2)	2934(2)	7130(2)	32(1)
N(3)	8704(2)	1898(2)	7887(2)	29(1)
N(4)	7973(2)	2024(2)	7099(2)	30(1)
C(1)	8324(3)	2773(3)	9747(2)	48(2)
C(2)	8732(3)	3255(3)	9267(2)	32(1)
C(3)	8604(3)	4106(3)	9256(2)	36(1)
C(4)	8948(3)	4581(3)	8826(2)	37(1)
C(5)	9399(3)	4217(3)	8388(2)	30(1)
C(6)	9524(3)	3367(3)	8389(2)	25(1)
C(7)	9207(3)	2874(3)	8834(2)	28(1)
C(8)	9370(3)	1961(3)	8826(2)	27(1)
C(9)	9068(3)	1490(3)	8364(2)	29(1)
C(10)	9170(3)	633(3)	8356(2)	36(1)
C(11)	9587(3)	243(3)	8799(2)	44(1)
C(12)	9915(3)	701(3)	9242(2)	41(1)
C(13)	9819(3)	1554(3)	9261(2)	35(1)
C(14)	10243(4)	2014(3)	9747(2)	51(2)
C(15)	10651(3)	3278(3)	7652(2)	26(1)
C(16)	11286(3)	3804(3)	7853(2)	34(1)
C(17)	11976(3)	3948(3)	7492(2)	41(1)
C(18)	12006(3)	3586(3)	6961(2)	46(2)
C(19)	11341(3)	3081(3)	6780(2)	39(1)
C(20)	11322(4)	2684(4)	6204(2)	61(2)
C(21)	7975(3)	1632(3)	7608(2)	28(1)
C(22)	7329(3)	1099(3)	7772(2)	36(1)
C(23)	6651(3)	999(3)	7401(2)	43(1)
C(24)	6629(3)	1414(3)	6889(2)	42(1)
C(25)	7306(3)	1929(3)	6739(2)	37(1)
C(26)	7341(4)	2386(4)	6185(2)	55(2)
C(100)	1887(7)	962(4)	4985(4)	114(4)
C(101)	2674(5)	623(5)	4748(4)	100(3)
C(102)	2609(5)	68(4)	4315(3)	68(2)
C(103)	1845(5)	-184(5)	4122(3)	78(2)
C(104)	1123(6)	94(5)	4337(3)	89(2)
C(105)	1115(5)	669(4)	4735(4)	78(2)

Table 3. Selected bond lengths [A] and angles [deg] for [**L**$TiCl_2$].

Ti(1)-N(1)	1.975(4)
Ti(1)-N(3)	1.985(4)
Ti(1)-N(4)	2.254(4)
Ti(1)-N(2)	2.267(4)
Ti(1)-Cl(1)	2.2803(15)
Ti(1)-Cl(2)	2.2835(15)
N(1)-C(15)	1.380(5)
N(2)-C(15)	1.349(6)
N(3)-C(21)	1.381(6)
N(4)-C(21)	1.354(5)
N(1)-Ti(1)-N(3)	81.57(14)
N(1)-Ti(1)-N(4)	134.93(14)
N(3)-Ti(1)-N(4)	61.61(14)
N(1)-Ti(1)-N(2)	61.65(14)
N(3)-Ti(1)-N(2)	135.14(15)
N(4)-Ti(1)-N(2)	162.34(13)
N(1)-Ti(1)-Cl(1)	98.03(12)
N(3)-Ti(1)-Cl(1)	127.41(12)
N(4)-Ti(1)-Cl(1)	86.15(11)
N(2)-Ti(1)-Cl(1)	84.92(10)
N(1)-Ti(1)-Cl(2)	125.92(12)
N(3)-Ti(1)-Cl(2)	97.81(12)
N(4)-Ti(1)-Cl(2)	86.40(10)
N(2)-Ti(1)-Cl(2)	85.44(11)
Cl(1)-Ti(1)-Cl(2)	121.92(6)
N(2)-C(15)-N(1)	106.6(4)
N(4)-C(21)-N(3)	105.9(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [A] and angles [deg] for [**L**TiCl$_2$].

Ti(1)-N(1)	1.975(4)
Ti(1)-N(3)	1.985(4)
Ti(1)-N(4)	2.254(4)
Ti(1)-N(2)	2.267(4)
Ti(1)-Cl(1)	2.2803(15)
Ti(1)-Cl(2)	2.2835(15)
Ti(1)-C(15)	2.620(5)
Ti(1)-C(21)	2.628(5)
N(1)-C(15)	1.380(5)
N(1)-C(6)	1.423(5)
N(2)-C(19)	1.342(6)
N(2)-C(15)	1.349(6)
N(3)-C(21)	1.381(6)
N(3)-C(9)	1.421(6)
N(4)-C(25)	1.349(6)
N(4)-C(21)	1.354(5)
C(1)-C(2)	1.514(6)
C(2)-C(3)	1.394(7)
C(2)-C(7)	1.402(6)
C(3)-C(4)	1.378(7)
C(4)-C(5)	1.380(6)
C(5)-C(6)	1.392(6)
C(6)-C(7)	1.407(6)
C(7)-C(8)	1.502(6)
C(8)-C(13)	1.405(6)
C(8)-C(9)	1.409(6)
C(9)-C(10)	1.399(6)
C(10)-C(11)	1.381(7)
C(11)-C(12)	1.377(7)
C(12)-C(13)	1.392(7)
C(13)-C(14)	1.517(7)
C(15)-C(16)	1.389(6)
C(16)-C(17)	1.390(7)
C(17)-C(18)	1.381(7)
C(18)-C(19)	1.387(7)
C(19)-C(20)	1.499(7)
C(21)-C(22)	1.382(6)
C(22)-C(23)	1.381(7)
C(23)-C(24)	1.379(7)
C(24)-C(25)	1.392(7)
C(25)-C(26)	1.500(7)
C(100)-C(105)	1.421(11)
C(100)-C(101)	1.455(11)
C(101)-C(102)	1.364(9)
C(102)-C(103)	1.337(9)
C(103)-C(104)	1.313(9)
C(104)-C(105)	1.321(10)
N(1)-Ti(1)-N(3)	81.57(14)
N(1)-Ti(1)-N(4)	134.93(14)
N(3)-Ti(1)-N(4)	61.61(14)
N(1)-Ti(1)-N(2)	61.65(14)
N(3)-Ti(1)-N(2)	135.14(15)
N(4)-Ti(1)-N(2)	162.34(13)
N(1)-Ti(1)-Cl(1)	98.03(12)
N(3)-Ti(1)-Cl(1)	127.41(12)

N(4)-Ti(1)-Cl(1)	86.15(11)
N(2)-Ti(1)-Cl(1)	84.92(10)
N(1)-Ti(1)-Cl(2)	125.92(12)
N(3)-Ti(1)-Cl(2)	97.81(12)
N(4)-Ti(1)-Cl(2)	86.40(10)
N(2)-Ti(1)-Cl(2)	85.44(11)
Cl(1)-Ti(1)-Cl(2)	121.92(6)
N(1)-Ti(1)-C(15)	31.11(14)
N(3)-Ti(1)-C(15)	110.98(14)
N(4)-Ti(1)-C(15)	163.21(13)
N(2)-Ti(1)-C(15)	31.00(13)
Cl(1)-Ti(1)-C(15)	87.83(10)
Cl(2)-Ti(1)-C(15)	110.02(11)
N(1)-Ti(1)-C(21)	110.84(14)
N(3)-Ti(1)-C(21)	31.05(14)
N(4)-Ti(1)-C(21)	31.01(13)
N(2)-Ti(1)-C(21)	163.61(14)
Cl(1)-Ti(1)-C(21)	111.11(11)
Cl(2)-Ti(1)-C(21)	88.61(10)
C(15)-Ti(1)-C(21)	141.48(13)
C(15)-N(1)-C(6)	123.8(4)
C(15)-N(1)-Ti(1)	101.2(3)
C(6)-N(1)-Ti(1)	126.3(3)
C(19)-N(2)-C(15)	120.6(4)
C(19)-N(2)-Ti(1)	149.5(3)
C(15)-N(2)-Ti(1)	89.1(3)
C(21)-N(3)-C(9)	123.9(4)
C(21)-N(3)-Ti(1)	101.1(3)
C(9)-N(3)-Ti(1)	127.4(3)
C(25)-N(4)-C(21)	120.1(4)
C(25)-N(4)-Ti(1)	149.4(3)
C(21)-N(4)-Ti(1)	89.9(3)
C(3)-C(2)-C(7)	119.8(4)
C(3)-C(2)-C(1)	117.7(4)
C(7)-C(2)-C(1)	122.4(5)
C(4)-C(3)-C(2)	120.8(5)
C(3)-C(4)-C(5)	120.4(5)
C(4)-C(5)-C(6)	119.5(5)
C(5)-C(6)-C(7)	121.1(4)
C(5)-C(6)-N(1)	119.4(4)
C(7)-C(6)-N(1)	119.4(4)
C(2)-C(7)-C(6)	118.3(4)
C(2)-C(7)-C(8)	122.2(4)
C(6)-C(7)-C(8)	119.5(4)
C(13)-C(8)-C(9)	118.3(4)
C(13)-C(8)-C(7)	122.6(4)
C(9)-C(8)-C(7)	119.1(4)
C(10)-C(9)-C(8)	120.7(4)
C(10)-C(9)-N(3)	119.9(4)
C(8)-C(9)-N(3)	119.4(4)
C(11)-C(10)-C(9)	119.9(5)
C(12)-C(11)-C(10)	119.8(5)
C(11)-C(12)-C(13)	121.4(5)
C(12)-C(13)-C(8)	119.8(5)
C(12)-C(13)-C(14)	117.8(5)
C(8)-C(13)-C(14)	122.3(5)
N(2)-C(15)-N(1)	106.6(4)
N(2)-C(15)-C(16)	122.8(4)
N(1)-C(15)-C(16)	130.6(4)
N(2)-C(15)-Ti(1)	59.9(2)
N(1)-C(15)-Ti(1)	47.7(2)

C(16)-C(15)-Ti(1)	172.1(3)
C(15)-C(16)-C(17)	116.5(5)
C(18)-C(17)-C(16)	120.5(5)
C(17)-C(18)-C(19)	120.2(5)
N(2)-C(19)-C(18)	119.5(5)
N(2)-C(19)-C(20)	117.5(5)
C(18)-C(19)-C(20)	123.1(5)
N(4)-C(21)-N(3)	105.9(4)
N(4)-C(21)-C(22)	122.7(4)
N(3)-C(21)-C(22)	131.4(4)
N(4)-C(21)-Ti(1)	59.1(2)
N(3)-C(21)-Ti(1)	47.8(2)
C(22)-C(21)-Ti(1)	172.4(3)
C(23)-C(22)-C(21)	117.0(5)
C(24)-C(23)-C(22)	120.8(5)
C(23)-C(24)-C(25)	119.7(5)
N(4)-C(25)-C(24)	119.6(5)
N(4)-C(25)-C(26)	117.4(5)
C(24)-C(25)-C(26)	123.0(5)
C(105)-C(100)-C(101)	115.4(7)
C(102)-C(101)-C(100)	118.2(7)
C(103)-C(102)-C(101)	121.3(7)
C(104)-C(103)-C(102)	122.0(8)
C(103)-C(104)-C(105)	121.5(9)
C(104)-C(105)-C(100)	121.4(7)

Symmetry transformations used to generate equivalent atoms:

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [**L**$TiCl_2$].

	x	y	z	U(eq)
H(1A)	7746	2987	9820	72
H(1B)	8673	2831	10092	72
H(1C)	8288	2189	9642	72
H(3A)	8277	4361	9548	44
H(4A)	8873	5162	8832	45
H(5A)	9622	4545	8087	36
H(10A)	8952	320	8047	44
H(11A)	9648	-340	8798	53
H(12A)	10213	429	9540	49
H(14A)	10814	1781	9818	76
H(14B)	9892	1960	10091	76
H(14C)	10299	2599	9647	76
H(16A)	11251	4051	8219	40
H(17A)	12430	4298	7612	50
H(18A)	12483	3684	6718	56
H(20A)	10780	2819	6014	91
H(20B)	11368	2084	6247	91
H(20C)	11803	2887	5976	91
H(22A)	7350	815	8125	43
H(23A)	6193	639	7499	52
H(24A)	6153	1349	6640	50
H(26A)	7415	2977	6259	83
H(26B)	6805	2298	5976	83
H(26C)	7825	2183	5959	83
H(100)	1888	1352	5287	136
H(10D)	3218	784	4892	120
H(10E)	3116	-145	4146	81
H(10F)	1824	-575	3822	93
H(10G)	594	-123	4202	107
H(10H)	581	891	4857	94