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Novel aspects of the transamination reaction between $Ti(NMe_2)_4$ and primary amines.

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Electronic Supplementary Information 2

X-ray data for all complexes: **1, 3-5**, **7-9**, **10**, **11** (this compound was crystallized with 3 different cell parameters), **12**, **15-17,** $[V(\mu\text{-N-1-adamantyl})(NMe_2)_2]_2$ and $[V(\mu\text{-}NAr^{Cl2})(NMe_2)(NHAr^{Cl2})]_2$ (Ar^{Cl2} = o-Cl_2-C_6H_3). Comparison of Average Interatomic Distances (Å) and Angles (deg).

1. Experimental details

Crystal Structure Determination.

Crystal data collection and processing parameters are given below. The selected crystals, sensitive to air and moisture, were mounted on a glass fiber using perfluoropolyether oil and cooled rapidly to 180 K in a stream of cold N_2. For all the structures data collection were collected at low temperature (T=180K) on a Stoe Imaging Plate Diffraction System (IPDS), or on an Oxford Diffraction Kappa CCD Excalibur diffractometer, or on a Bruker Kappa Apex II diffractometer, using a graphite-monochromated Mo-Kα radiation (λ = 0.71073Å) and equipped with an Oxford Cryosystems Cryostream Cooler Device. Final unit cell parameters were obtained by means of a least-squares refinement of a set of 8000 well measured reflections, and a crystal decay was monitored during data collection by measuring 200 reflections by image, no significant fluctuation of intensities has been observed. Structures have been solved by means of Direct Methods using the program SIR92,[1] and subsequent difference Fourier maps, models were refined by least-squares procedures on a F^2 by using SHELXL-97 [2] integrated in the package WINGX version 1.64,[3] and an empirical absorption corrections were applied on data.[4] For **15** and **17**, it was not possible to solve diffuse electron-density residuals (enclosed solvent molecules). Treatment with the SQUEEZE facility from PLATON,[5] resulted in a smooth refinement. Since a few low order reflections are missing from the data set, the electron count will be underestimated. Thus, the values given for D(calc), F(000) and the molecular weight are only valid for the ordered part of the structure. Details of the structure solution and refinements are given in the Supporting Information (CIF file). A full listing of atomic coordinates, bond lengths and angles, and displacement parameters for all structures have been deposited at the Cambridge Crystallographic Data Centre (CCDC-931095 to 931109).

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Table A Comparison of Average Interatomic Distances (Å) and Angles (deg) in Complexes **1**, **3-5**.

	1	**3**	**4**	**5**
Ti-N_{imido}	1.9121(15) [Ti1-N1] 1.9277(16) [Ti1-N1']	1.908(6) [Ti1-N1] 1.954(7) [Ti1-N1']	1.8885(17) [Ti1-N1] 1.9596(16) [Ti1-N2] 1.9267(17) [Ti2-N2] 1.9691(16) [Ti2-N1]	1.8622(14) [Ti1-N1], 2.4668(14) [Ti2-N1], 2.1024(15) [Ti3-N1], 1.9279(16) [Ti1-N2], 1.9527(15) [Ti2-N2], 2.0723(16) [Ti2-N3], 1.8702(14) [Ti3-N3], 1.8954(16) [Ti1-N4], 2.0254(15) [Ti3-N4]
N_{imido}-C/Si	1.468(2)	1.726(7)	1.7275(17) [Si1-N1] 1.7254(17) [Si2-N2]	1.408(2) [C1-N1], 1.402(2) [C17-N2], 1.402(2) [C13-N3], 1.400(2) [C19-N4]
Ti-NMe_2	1.9078(17) [Ti1-N2] 1.9087(18) [Ti1-N3]	1.892(7) [Ti1-N2] 1.892(7) [Ti1-N3]	1.8946(18) [Ti1-N5] 1.9057(19) [Ti2-N4] 1.8707(19) [Ti2-N6]	1.9071(17) [Ti1-N5], 1.9044(15) [Ti2-N6], 1.9030(16) [Ti2-N7], 1.8976(15) [Ti3-N8]
Ti-NH_{amido}	-	-	1.9124(19)	-
Ti-N_{NHMe2}	-	-	-	2.2407(16)
Ti···Ti	2.8018(7)	2.823(3)	2.8215(5)	2.8786(7) [Ti1...Ti3], 2.9796(7) [Ti1...Ti2], 3.0850(9) [Ti2...Ti3]
Ti-N_{imido}-C/Si	130.37(13) [Ti1] 131.04(12) [Ti1']	131.1(4) [Ti1] 128.3(4) [Ti1']	125.42(9) [Si1-N1-Ti1] 139.03(10) [Si1-N1-Ti2] 142.68(10) [Si2-N2-Ti1] 124.13(9) [Si2-N2-Ti2]	137.73(12) [C1-N1-Ti1], 120.26(11) [C1-N1-Ti3], 120.19(11) [C1-N1-Ti2], 126.74(12) [C7-N2-Ti1], 132.80(13) [C7-N2-Ti2], 139.14(12) [C13-N3-Ti3], 117.99(11) [C13-N3-Ti2], 123.50(12) [C19-N4-Ti1], 130.57(11) [C19-N4-Ti3]
Ti-N_{imido}-Ti	93.72(7)	93.9(3)	93.99(7) [Ti1-N1-Ti2] 93.11(7) [Ti1-N2-Ti2]	85.79(5) [Ti1-N1-Ti2], 100.31(7) [Ti1-N2-Ti2], 92.92(7) [Ti1-N1-Ti3], 94.42(7) [Ti1-N4-Ti3], 84.54(5) [Ti3-N1-Ti2], 102.86(7) [Ti3-N3-Ti2]
N_{imido}-Ti-N_{imido}	86.28(7)	86.1(3)	86.86(7) [N1-Ti1-N2] 85.56(7) [N2-Ti2-N1]	90.04(7) [N1-Ti1-N4], 93.75(6) [N1-Ti1-N2], 109.83(7) [N4-Ti1-N2], 120.35(8) [N5-Ti1-N2], 117.69(6) [N2-Ti2-N3], 76.53(6) [N2-Ti2-N1], 76.25(5) [N3-Ti2-N1], 114.35(6) [N3-Ti3-N4], 90.23(6) [N3-Ti3-N1], 80.15(6) [N4-Ti3-N1]
Ti-NH_{amido}-C/Si	-		147.80(13)	-
N_{NMe2}-Ti-N_{NMe2}	110.00(8)	111.1(3)	110.60(9)	101.00(7) [N7-Ti2-N6]
N_{NMe2}-Ti-N_{amido}	-		111.47(9)	-

Table B Comparison of Average Interatomic Distances (Å) and Angles (deg) in Complexes **7-9, 10, 11, 15**.

	7	**8**	**9**	**10**	**11**	**15**
Ti-N_{imido}	2.0211(10) [Ti1-N1] 1.8818(11) [Ti1-N2] 2.0123(11) [Ti2-N2] 1.8694(10) [Ti2-N1]	1.9626(15) [Ti1-N1] 1.8485(15) [Ti1-N2] 2.0139(15) [Ti2-N2] 1.9173(16) [Ti2-N1]	1.9602(19) [Ti1-N1] 1.9522(18) [Ti2-N1]	1.8362(19) [Ti1-N3] 2.054(2) [Ti2-N3] 1.913(2) [Ti1-N4] 1.953(2) [Ti2-N4]	2.074(4) [Ti1-N1] 1.723(6) [Ti1-N2] 1.841(4) [Ti2-N1]	2.070(3) [Ti1-N1] 2.053(3) [Ti1-N2] 1.876(3) [Ti2-N2] 1.861(3) [Ti2-N1] 1.758(3) [Ti1-N5]
N_{imido}-C	1.4085(15) [N1] 1.4099(15) [N2]	1.418(2) [N1] 1.409(2) [N2]	1.426(3)	1.404(3) [N3] 1.427(3) [N4]	1.411(6) [C1-N1] 1.362(8) [C13-N2]	1.409(5) [C1-N1] 1.422(5) [C13-N2] 1.337(5) [C25-N3]
Ti-NMe_2	1.8890(11) [Ti1-N3] 1.9197(11) [Ti1-N4] 1.8948(11) [Ti2-N5] 1.9224(12) [Ti2-N6]	1.8993(16) [Ti1-N4] 1.9115(17) [Ti2-N5] 1.8829(17) [Ti2-N6]	1.901(2) [Ti1-N2] 1.901(2) [Ti1-N3] 1.900(2) [Ti1-N4] 1.888(2) [Ti2-N5] 1.897(2) [Ti2-N6] 1.911(2) [Ti2-N7]	1.909(2) [Ti2-N5] 1.870(2) [Ti2-N6]	1.875(6) [Ti2-N3] 1.918(6) [Ti1-N5]	1.923(3) [Ti1-N6] 1.925(3) [Ti2-N7]
Ti-NH_{amido}	-	1.9442(17)	-	1.9469(19) [Ti1-N1] 1.955(2) [Ti1-N2]	-	-
Ti-N_L [a]	-	-	-	-	2.185(8) [Ti2-N4]	2.359(3) [Ti2-N3] 2.240(3) [Ti2-N4]
Ti···Ti	2.8089(3)	2.7896(5)	3.621	2.8134(6)	2.8198(17)	2.8475(10)
Ti-N_{imido}-C	111.28(8) [C1-N1-Ti1] 152.99(8) [C1-N1-Ti2] 152.28(9) [C13-N2-Ti1] 113.34(8) [C13-N2-Ti2]	130.17(12) [C1-N1-Ti1] 137.15(12) [C1-N1-Ti2] 158.65(14) [C13-N2-Ti1] 102.80(12) [C13-N2-Ti2]	111.97(14) [C1-N1-Ti1] 112.37(14) [C1-N1-Ti2]	170.07(18) [C25-N3-Ti1] 92.63(14) [C25-N3-Ti2] 134.43(17) [C37-N4-Ti1] 129.81(16) [C37-N4-Ti2]	123.4(3) [C1-N1-Ti1] 143.2(3) [C1- N1-Ti2] 168.2(5) [C13-N2-Ti1]	114.7(2) [C1-N1-Ti1] 151.0(3) [C1-N1-Ti2] 119.0(2) [C13-N2-Ti1] 147.7(3) [C13-N2-Ti2] 174.9(3) [C35-N5-Ti1]
Ti-N_{imido}-Ti	92.36(4) [Ti1-N1-Ti2] 92.27(4) [Ti1-N2-Ti2]	91.94(6) [Ti1-N1-Ti2] 92.38(6) [Ti1-N2-Ti2]	135.53(10)	92.48(9) [Ti1-N3-Ti2] 93.39(9) [Ti1-N4-Ti2]	91.97(16) [Ti1-N1-Ti2]	92.67(13) [Ti1-N1-Ti2] 92.80(13) [Ti1-N2-Ti2]
N_{imido}-Ti-N_{imido}	87.07(4) [N1-Ti1-N2] 87.67(4) [N2-Ti2-N1]	88.83(7) [N1-Ti1-N2] 85.46(6) [N2-Ti2-N1]	-	82.97(8) [N3-Ti2-N4] 90.16(9) [N3-Ti1-N4]	80.9(2) [N1-Ti1-N1'] 93.9(2) [N1-Ti2-N1'] 119.57(18) [N2-Ti1-N1]	92.67(13) [N1-Ti1-N2] 92.80(13) [N2-Ti2-N1] 123.79(14) [N5-Ti1-N1] 119.25(14) [N5-Ti1-N2]
Ti-NH_{amido}-C	-	126.45(14)	-	135.74(17) [C1-N1-Ti1] 136.48(16) [C13-N2-Ti1]	-	-
N_{NMe2}-Ti-N_{NMe2}	103.09(5) [N3-Ti1-N4] 103.44(5) [N5-Ti2-N6]	105.01(7)	103.87(9) [N3-Ti1-N4] 104.28(10) [N3-Ti1-N2] 105.19(9) [N4-Ti1-N2] 103.07(11) [N5-Ti2-N6] 104.40(10) [N5-Ti2-N7] 107.95(10) [N6-Ti2-N7]	102.44(11) [N5-Ti2-N6]	-	-
N_{NMe2}-Ti-N_{amido}	-	107.35(7)	-	113.05(8) [N1-Ti1-N2] [b]	-	-
N_L-Ti-N_L [a]	-	-	-	-	-	76.47(11) [N3-Ti2-N4]

a L = $NHMe_2$ or Py. **b** N_{NHAr*}-Ti- N_{NHAr*} angle.

Table C Comparison of Average Interatomic Distances (Å) and Angles (deg) in Monomeric Complexes **12**, **16-17**.

	12	**16**	**17**
Ti-N_{imido}	-	1.7334(14)	1.7230(17)
N_{imido}-C	-	1.380(2)	1.382(3)
Ti-NMe_2	-	1.9560(15)	
Ti-NH_{Ar*}	1.9028(17) [N1] 1.8984(17) [N2]	2.0450(13)	2.0206(16) [N1] 2.0293(17) [N3]
Ti-N_{Py}	-	2.2821(16) [N4] 2.2437(15) [N5]	2.2953(17) [N4] 2.2669(17) [N5]
Ti···Ti	-	-	-
Ti-N_{imido}-C	-	173.62(12)	175.80(15)
Ti-N_{imido}-Ti	-	-	-
N_{imido}-Ti-N_{imido}	-	-	-
Ti-NH_{amido}-C	137.54(14) [N1] 103.1 [N1]	147.60(12)	144.60(14) [N1] 154.45(14) [N3]
N_{NMe2}-Ti-N_{NMe2}	-	-	-
N_{NMe2}-Ti-N_{amido}	-	147.75(6)	-
N_{Py}-Ti-N_{Py}	-	162.78(5)	155.76(6)

Table D. Crystallographic Data, Data Collection and Refinement Parameters for Compounds **1, 3-5, 7-10.**

Compound ref.	**1**	**3**	**4**	**5**	**7**	**8**	**9**	**10**
Chemical formula	$C_{28}H_{54}N_6Ti_2$	$C_{44}H_{54}N_6Si_2Ti_2$	$C_{60}H_{64}N_6Si_3Ti_2$	$C_{34}H_{51}N_9Ti_3$	$C_{32}H_{58}N_6Ti_2$	$C_{42}H_{70}N_6Ti_2$	$C_{24}H_{53}N_7Ti_2$	$C_{52}H_{82}N_6Ti_2$
Formula weight	570.51	818.85	1049.24	729.54	622.64	754.84	535.53	887.04
Crystal system	Monoclinic	Monoclinic	Triclinic	Monoclinic	Triclinic	Orthorhombic	Orthorhombic	Monoclinic
Space group	*P* 2_1/c	*P* 2_1/c	*P* -1	*P* 2_1/n	*P* -1	*P* bca	*P* bca	*P* 2_1/n
a, Å	8.67590(10)	12.8129(18)	11.3357(4)	10.501(2)	9.7228(3)	11.1946(7)	17.0404(7)	11.5158(4)
b, Å	18.4936(4)	15.846(3)	13.4320(5)	27.443(5)	10.4433(3)	20.0122(12)	16.0775(6)	22.9429(8)
c, Å	10.1458(2)	11.4001(17)	19.7408(9)	13.322(3)	18.5184(5)	38.540(2)	23.1921(9)	19.6453(7)
α, deg	90	90	92.607(4)	90	77.236(2)	90	90	90
β, deg	109.043(3)	108.955(16)	104.677(4)	90.77(3)	75.656(2)	90	90	98.712(2)
γ, deg	90	90	106.071(3)	90	79.334(2)	90	90	90
V, Å^3	1538.79(5)	2189.1(6)	2772.34(19)	3838.8(13)	1759.70(9)	8634.0(9)	6353.9(4)	5130.5(3)
Z	2	2	2	4	2	8	8	4
D_{calc}, g cm^{-3}	1.231	1.242	1.257	1.262	1.175	1.161	1.12	1.148
μ (Mo-Kα), mm^{-1}	0.545	0.457	0.397	0.644	0.482	0.404	0.525	0.350
F(000)	616	864	1104	1536	672	3264	2320	1920
θ range (deg)	2.39 - 26.01	2.45 - 24.71	3.10 - 26.37	2.08 - 26.06	1.15 - 32.12	2.62 - 26.37	2.84 - 26.04	1.93 - 25.24
Measured reflections	11893	14897	21233	29677	50964	77764	63139	59919
Unique reflections / Rint	2994 / 0.0430	3712 / 0.2704	11316 / 0.0242	7499 / 0.0342	12229 / 0.0303	8799 / 0.0524	6262 / 0.0714	9171 / 0.0592
Parameters / restraints	167 / 0	248 / 0	631 / 1	425 / 0	377 / 0	473 / 0	314 / 0	561 / 0
Final *R* indices [I>σ2(I)]	R1 = 0.0353 *w*R2 = 0.0812	R1 = 0.0674 *w*R2 = 0.0964	R1 = 0.0446 *w*R2 = 0.1219	R1 = 0.0330 *w*R2 = 0.0862	R1 = 0.0368 *w*R2 = 0.0918	R1 = 0.0370 *w*R2 = 0.0861	R1 = 0.0402 *w*R2 = 0.0908	R1 = 0.0479 wR2 = 0.1100
Final *R* indices all data	R1 = 0.0523 *w*R2 = 0.0867	R1 = 0.2369 *w*R2 = 0.1539	R1 = 0.0578 *w*R2 = 0.1296	R1 = 0.0403 *w*R2 = 0.0906	R1 = 0.0571 *w*R2 =0.1032	R1 = 0.0654 *w*R2 = 0.0994	R1 = 0.0726 *w*R2 = 0.1052	R1 = 0.0792 wR2 = 0.1263
Goodness of fit	1.022	0.777	1.128	1.044	1.036	1.029	1.031	1.016
Δρmax - Δρmin	0.289 and -0.278	0.324 and -0.586	0.492 and -0.511	0.555 and -0.373	0.405 and -0.273	0.296 and -0.312	0.347 and -0.346	0.392 and -0.296
CCDC number	931095	931097	931098	931099	931101	931102	931103	931104

Table E. Crystallographic Data, Data Collection and Refinement Parameters for Compounds **11-12, 15-17, [V(μ-N-1-adamantyl)(NMe$_2$)$_2$]$_2$** and **[V(N-*o*-Cl$_2$C$_6$H$_3$)$_2$(NH *o*-Cl$_2$C$_6$H$_3$)$_2$(NMe$_2$)$_2$]**.

Compound ref.	**11**[a]	**12**	**15**	**16**[b]	**17**	[V(μ-N-1-adamantyl)(NMe$_2$)$_2$]$_2$	[V(N-*o*-Cl$_2$C$_6$H$_3$)$_2$(NH-*o*-Cl$_2$C$_6$H$_3$)$_2$(NMe$_2$)$_2$]
Chemical formula	$C_{42}H_{70}N_6Ti_2.2C_6H_6$	$C_{48}H_{72}N_4Ti$	$C_{50}H_{73}N_7Ti_2$	$C_{43}H_{59}N_5Ti$	$C_{46}H_{63}N_5Ti$	$C_{28}H_{54}N_6V_2$	$C_{28}H_{28}Cl_8N_6V_2$
Formula weight	911.00	753.00	867.95	693.85	733.91	576.65	834.04
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic	Orthorhombic
Space group	*P* 2$_1$/m	*C* 2/c	*P* 2$_1$/c	*C* 1/c	*P* -1	*I* 2$_1$/m	*F* dd2
a, Å	11.1210(8)	19.1831(6)	12.6101(6)	14.4789(10)	9.6975(5)	8.6878(10)	23.961(5)
b, Å	24.3670(9)	13.1110(4)	22.6800(14)	15.7622(10)	12.1115(6)	12.6566(10)	32.093(6)
c, Å	11.1710(7)	18.5082(6)	21.3541(10)	18.8740(10)	22.0445(10)	13.9992(16)	8.9451(18)
α, deg	90	90	90	90	80.776(2)	90	90
β, deg	119.258(9)	91.513(3)	99.489(5)	110.076(2)	79.744(2)	97.749(13)	90
γ, deg	90	90	90	90	73.268(2)	90	90
V, Å^3	2641.0(3)	4653.4(3)	6023.6(5)	4045.7(4)	2423.5(2)	1525.3(3)	6879(2)
Z	2	4	4	4	2	2	16
D_{calc}, g cm^{-3}	1.146	1.081	0.957	1.139	1.006	1.256	1.611
μ (Mo-Kα), mm^{-1}	0.341	0.218	0.297	0.246	0.208	0.639	1.196
F(000)	984	1656	1864	1496	792	620	3360
θ range (deg)	3.26 - 25.03	3.30 - 26.37	3.38 - 26.37	2.83 - 30.00	0.95 - 26.37	2.61 - 23.25	3.06 - 32.17
Measured reflections	17960	19596	50674	30095	56608	4442	17470
Unique reflections / Rint	4775 / 0.0337	4756 / 0.0532	12293 / 0.1365	11376 / 0.0338	9895 / 0.0353	1137 / 0.0526	5691 / 0.0404
Parameters / restraints	305 / 0	248 / 0	548 / 0	454 / 2	482 / 0	92 / 0	201 / 1
Final *R* indices [I>σ2(I)]	R1 = 0.0840 *w*R2 = 0.2023	R1 = 0.0497 *w*R2 = 0.1170	R1 = 0.0742 *w*R2 = 0.1545	R1 = 0.0407 *w*R2 = 0.0836	R1 = 0.0591 wR2 = 0.1662	R1 = 0.0441 wR2 = 0.1134	R1 = 0.0347 wR2 = 0.0789
Final *R* indices all data	R1 = R1 = 0.0992 *w*R2 = 0.2081	R1 = 0.0874 *w*R2 = 0.1243	R1 = 0.1516 *w*R2 = 0.1816	R1 = 0.0601 *w*R2 =0.0907	R1 = 0.0661 0.1721	R1 = 0.0458 wR2 = 0.1149	R1 = 0.0549 wR2 = 0.0833
Goodness of fit	1.172	0.917	0.918	1.016	1.082	1.052	0.884
Δρmax - Δρmin	1.503 and -1.441	0.322 and -0.546	0.374 and -0.337	0.244 and -0.203	1.275 and -0.480	0.322 and -0.317	0.373 and -0.512
CCDC number	931105	931106	931107	931108	931109	931096	931100

a. The compound crystallized with a molecule of C_6D_6. It was also crystallized with a toluene solvent molecule (see *Supplementary Material*: Triclinic, P -1 = 11.071(2), b = 11.263(2), c = 22.679(5), α = 88.421(8), β = 80.276(8), γ = 61.068(7), V = 2434.45(3) A^3), or without solvent (see *Supplementary Material*: Monoclinic, P 2$_1$/m a = 10.9940(10), b = 20.0818(12), c = 11.2102(8), β = 118.368(11), V = 2177.8(3) A^3). **b.** Absolute structure parameter = 0.114(14).

Data for compound 1

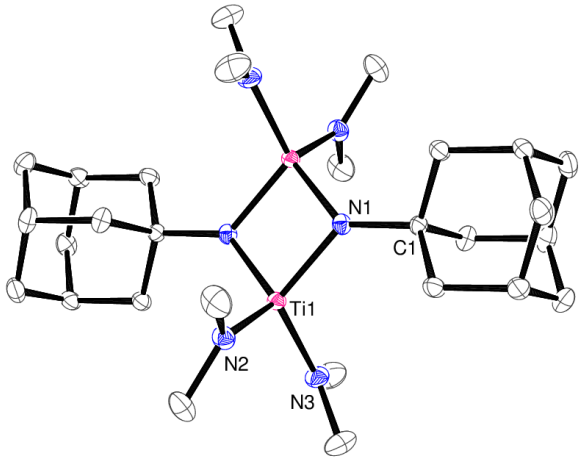


Table 1. Crystal data and structure refinement for **1**.

Identification code	cl508a
Empirical formula	C28 H54 N6 Ti2
Formula weight	570.51
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 1 21/c 1
Unit cell dimensions	a = 8.67590(10) A alpha = 90 deg. b = 18.4936(4) A beta = 109.043(3) deg. c = 10.1458(2) A gamma = 90 deg.
Volume	1538.79(5) A^3
Z, Calculated density	2, 1.231 Mg/m^3
Absorption coefficient	0.545 mm^-1
F(000)	616
Crystal size	0.28 x 0.2 x 0.08 mm
Theta range for data collection	2.39 to 26.01 deg.
Limiting indices	-10<=h<=10, -22<=k<=22, -12<=l<=12
Reflections collected / unique	11893 / 2994 [R(int) = 0.0430]
Completeness to theta = 26.01	98.8 %
Absorption correction	Empirical (SHELXA)
Max. and min. transmission	0.915 and 0.686
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2994 / 0 / 167
Goodness-of-fit on F^2	1.022
Final R indices [I>2sigma(I)]	R1 = 0.0353, wR2 = 0.0812
R indices (all data)	R1 = 0.0523, wR2 = 0.0867
Largest diff. peak and hole	0.289 and -0.278 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **1**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ti(1)	5302(1)	571(1)	5958(1)	21(1)
N(1)	3719(2)	348(1)	4194(2)	23(1)
N(2)	4398(2)	652(1)	7432(2)	31(1)
N(3)	6631(2)	1393(1)	5954(2)	33(1)
C(1)	2662(2)	825(1)	3121(2)	21(1)
C(2)	1199(2)	388(1)	2203(2)	26(1)
C(3)	55(2)	874(1)	1083(2)	31(1)
C(4)	976(3)	1187(1)	167(2)	37(1)
C(5)	2420(3)	1638(1)	1062(2)	35(1)
C(6)	3571(2)	1149(1)	2187(2)	30(1)
C(7)	2015(2)	1447(1)	3794(2)	29(1)
C(8)	874(2)	1936(1)	2674(2)	32(1)
C(9)	-571(2)	1490(1)	1769(2)	33(1)
C(10)	1807(3)	2253(1)	1762(2)	37(1)
C(21)	2790(3)	415(2)	7389(3)	50(1)
C(22)	5299(3)	959(2)	8773(2)	48(1)
C(31)	6316(3)	2099(1)	6420(3)	49(1)
C(32)	8023(3)	1408(2)	5461(3)	55(1)

Table 3. Bond lengths [A] and angles [deg] for **1**.

Ti(1)-N(2)	1.9078(17)
Ti(1)-N(3)	1.9087(18)
Ti(1)-N(1)	1.9121(15)
Ti(1)-N(1)#1	1.9277(16)
Ti(1)-Ti(1)#1	2.8018(7)
N(1)-C(1)	1.468(2)
N(1)-Ti(1)#1	1.9277(16)
N(2)-C(22)	1.446(3)
N(2)-C(21)	1.450(3)
N(3)-C(31)	1.445(3)
N(3)-C(32)	1.450(3)
C(1)-C(7)	1.534(3)
C(1)-C(2)	1.537(3)
C(1)-C(6)	1.538(3)
C(2)-C(3)	1.532(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.524(3)
C(3)-C(9)	1.525(3)
C(3)-H(3)	1.0000
C(4)-C(5)	1.532(3)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(10)	1.526(3)
C(5)-C(6)	1.540(3)
C(5)-H(5)	1.0000
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.536(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(10)	1.531(3)
C(8)-C(9)	1.531(3)
C(8)-H(8)	1.0000
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800

C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800

N(2)-Ti(1)-N(3)	110.00(8)
N(2)-Ti(1)-N(1)	113.44(7)
N(3)-Ti(1)-N(1)	114.84(7)
N(2)-Ti(1)-N(1)#1	115.85(7)
N(3)-Ti(1)-N(1)#1	114.81(7)
N(1)-Ti(1)-N(1)#1	86.28(7)
N(2)-Ti(1)-Ti(1)#1	124.85(6)
N(3)-Ti(1)-Ti(1)#1	125.13(6)
N(1)-Ti(1)-Ti(1)#1	43.36(5)
N(1)#1-Ti(1)-Ti(1)#1	42.92(5)
C(1)-N(1)-Ti(1)	130.37(13)
C(1)-N(1)-Ti(1)#1	131.04(12)
Ti(1)-N(1)-Ti(1)#1	93.72(7)
C(22)-N(2)-C(21)	111.48(18)
C(22)-N(2)-Ti(1)	122.32(15)
C(21)-N(2)-Ti(1)	126.19(15)
C(31)-N(3)-C(32)	111.34(19)
C(31)-N(3)-Ti(1)	122.69(15)
C(32)-N(3)-Ti(1)	125.94(17)
N(1)-C(1)-C(7)	110.61(15)
N(1)-C(1)-C(2)	108.94(15)
C(7)-C(1)-C(2)	108.35(14)
N(1)-C(1)-C(6)	111.62(14)
C(7)-C(1)-C(6)	108.61(16)
C(2)-C(1)-C(6)	108.63(16)
C(3)-C(2)-C(1)	110.32(16)
C(3)-C(2)-H(2A)	109.6
C(1)-C(2)-H(2A)	109.6
C(3)-C(2)-H(2B)	109.6
C(1)-C(2)-H(2B)	109.6
H(2A)-C(2)-H(2B)	108.1
C(4)-C(3)-C(9)	109.24(19)
C(4)-C(3)-C(2)	109.54(16)
C(9)-C(3)-C(2)	109.90(16)
C(4)-C(3)-H(3)	109.4
C(9)-C(3)-H(3)	109.4
C(2)-C(3)-H(3)	109.4
C(3)-C(4)-C(5)	109.59(17)
C(3)-C(4)-H(4A)	109.8
C(5)-C(4)-H(4A)	109.8
C(3)-C(4)-H(4B)	109.8
C(5)-C(4)-H(4B)	109.8
H(4A)-C(4)-H(4B)	108.2
C(10)-C(5)-C(4)	109.87(18)
C(10)-C(5)-C(6)	109.46(18)
C(4)-C(5)-C(6)	109.10(18)
C(10)-C(5)-H(5)	109.5
C(4)-C(5)-H(5)	109.5
C(6)-C(5)-H(5)	109.5
C(1)-C(6)-C(5)	110.22(16)
C(1)-C(6)-H(6A)	109.6
C(5)-C(6)-H(6A)	109.6
C(1)-C(6)-H(6B)	109.6
C(5)-C(6)-H(6B)	109.6
H(6A)-C(6)-H(6B)	108.1
C(1)-C(7)-C(8)	110.66(16)
C(1)-C(7)-H(7A)	109.5
C(8)-C(7)-H(7A)	109.5
C(1)-C(7)-H(7B)	109.5
C(8)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	108.1
C(10)-C(8)-C(9)	109.62(17)
C(10)-C(8)-C(7)	109.43(17)
C(9)-C(8)-C(7)	109.25(18)
C(10)-C(8)-H(8)	109.5
C(9)-C(8)-H(8)	109.5
C(7)-C(8)-H(8)	109.5

C(3)-C(9)-C(8)	109.43(15)
C(3)-C(9)-H(9A)	109.8
C(8)-C(9)-H(9A)	109.8
C(3)-C(9)-H(9B)	109.8
C(8)-C(9)-H(9B)	109.8
H(9A)-C(9)-H(9B)	108.2
C(5)-C(10)-C(8)	109.20(18)
C(5)-C(10)-H(10A)	109.8
C(8)-C(10)-H(10A)	109.8
C(5)-C(10)-H(10B)	109.8
C(8)-C(10)-H(10B)	109.8
H(10A)-C(10)-H(10B)	108.3
N(2)-C(21)-H(21A)	109.5
N(2)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
N(2)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(2)-C(22)-H(22A)	109.5
N(2)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
N(2)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
N(3)-C(31)-H(31A)	109.5
N(3)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
N(3)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
N(3)-C(32)-H(32A)	109.5
N(3)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
N(3)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **1**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ti(1)	20(1)	20(1)	21(1)	-1(1)	5(1)	-1(1)
N(1)	18(1)	26(1)	23(1)	2(1)	5(1)	1(1)
N(2)	34(1)	33(1)	27(1)	-1(1)	12(1)	3(1)
N(3)	29(1)	28(1)	39(1)	-1(1)	8(1)	-8(1)
C(1)	20(1)	21(1)	21(1)	1(1)	6(1)	3(1)
C(2)	25(1)	26(1)	23(1)	-2(1)	4(1)	1(1)
C(3)	29(1)	30(1)	25(1)	-3(1)	-2(1)	1(1)
C(4)	51(1)	37(1)	21(1)	4(1)	9(1)	14(1)
C(5)	42(1)	32(1)	35(1)	13(1)	19(1)	6(1)
C(6)	29(1)	29(1)	35(1)	8(1)	14(1)	5(1)
C(7)	30(1)	27(1)	25(1)	-5(1)	4(1)	4(1)
C(8)	35(1)	27(1)	29(1)	-5(1)	6(1)	11(1)
C(9)	27(1)	38(1)	32(1)	3(1)	6(1)	11(1)
C(10)	43(1)	24(1)	42(1)	5(1)	9(1)	5(1)
C(21)	48(1)	68(2)	41(1)	1(1)	24(1)	-11(1)
C(22)	52(1)	63(2)	26(1)	-3(1)	10(1)	3(1)
C(31)	43(1)	28(1)	75(2)	-5(1)	20(1)	-5(1)
C(32)	54(2)	47(2)	76(2)	-5(1)	38(1)	-16(1)

Data for compound [V(μ-N-1-adamantyl)(NMe$_2$)$_2$]$_2$

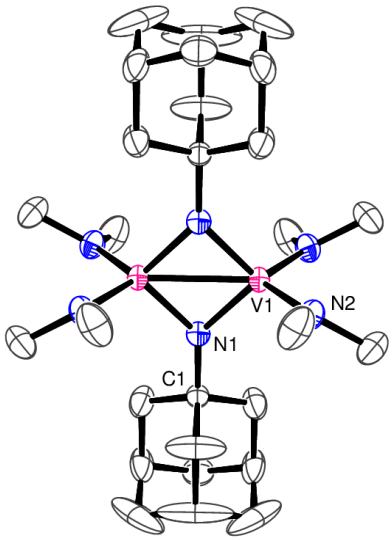


Table 1. Crystal data and structure refinement for **[V(μ-N-1-adamantyl)(NMe$_2$)$_2$]$_2$**.

Identification code	cl413
Empirical formula	C28 H54 N6 V2
Formula weight	576.65
Temperature	190(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, I 1 2/m 1
Unit cell dimensions	a = 8.6878(10) A alpha = 90 deg.
	b = 12.6566(10) A beta = 97.749(13) deg.
	c = 13.9992(16) A gamma = 90 deg.
Volume	1525.3(3) A^3
Z, Calculated density	2, 1.256 Mg/m^3
Absorption coefficient	0.639 mm^-1
F(000)	620
Crystal size	0.3 x 0.18 x 0.12 mm
Theta range for data collection	2.61 to 23.25 deg.
Limiting indices	-9<=h<=9, -14<=k<=14, -15<=l<=15
Reflections collected / unique	4442 / 1137 [R(int) = 0.0526]
Completeness to theta = 23.25	98.9 %
Absorption correction	Empirical (SHELXA)
Max. and min. transmission	0.821 and 0.454
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1137 / 0 / 92
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0441, wR2 = 0.1134
R indices (all data)	R1 = 0.0458, wR2 = 0.1149
Largest diff. peak and hole	0.322 and -0.317 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **[V(μ-N-1-adamantyl)(NMe$_2$)$_2$]$_2$** U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
V(1)	5000	9012(1)	0	25(1)
N(1)	4282(3)	10000	816(2)	26(1)
N(2)	6669(3)	8185(2)	551(2)	34(1)
C(1)	3731(4)	10000	1761(3)	26(1)
C(2)	5126(6)	10000	2534(3)	78(2)
C(3)	4567(7)	10000	3533(4)	117(4)
C(4)	3582(6)	9015(5)	3632(3)	102(2)
C(5)	2192(5)	9033(2)	2873(3)	57(1)
C(6)	2724(5)	9034(2)	1867(3)	51(1)
C(7)	1232(5)	10000	2992(3)	46(1)
C(21)	8295(4)	8461(3)	775(3)	56(1)
C(22)	6341(4)	7198(3)	1014(2)	47(1)

Table 3. Bond lengths [A] and angles [deg] for **[V(μ-N-1-adamantyl)(NMe$_2$)$_2$]$_2$**.

V(1)-N(1)	1.857(2)
V(1)-N(1)#1	1.857(2)
V(1)-N(2)#2	1.868(2)
V(1)-N(2)	1.868(2)
V(1)-V(1)#1	2.5006(12)
N(1)-C(1)	1.467(5)
N(1)-V(1)#1	1.857(2)
N(2)-C(21)	1.448(4)
N(2)-C(22)	1.454(4)
C(1)-C(2)	1.512(6)
C(1)-C(6)	1.522(4)
C(1)-C(6)#3	1.522(4)
C(2)-C(3)	1.541(7)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.528(7)
C(3)-C(4)#3	1.528(7)
C(3)-H(3)	1.0000
C(4)-C(5)	1.498(7)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(7)	1.503(4)
C(5)-C(6)	1.541(4)
C(5)-H(5)	1.0000
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(5)#3	1.503(4)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
N(1)-V(1)-N(1)#1	95.35(13)
N(1)-V(1)-N(2)#2	108.95(11)
N(1)#1-V(1)-N(2)#2	115.45(11)
N(1)-V(1)-N(2)	115.45(11)
N(1)#1-V(1)-N(2)	108.95(11)
N(2)#2-V(1)-N(2)	111.84(15)
N(1)-V(1)-V(1)#1	47.68(6)
N(1)#1-V(1)-V(1)#1	47.68(6)
N(2)#2-V(1)-V(1)#1	124.08(7)
N(2)-V(1)-V(1)#1	124.08(7)

C(1)-N(1)-V(1)#1	137.09(7)
C(1)-N(1)-V(1)	137.09(7)
V(1)#1-N(1)-V(1)	84.65(13)
C(21)-N(2)-C(22)	110.8(2)
C(21)-N(2)-V(1)	129.4(2)
C(22)-N(2)-V(1)	118.54(19)
N(1)-C(1)-C(2)	108.5(3)
N(1)-C(1)-C(6)	110.5(2)
C(2)-C(1)-C(6)	110.3(3)
N(1)-C(1)-C(6)#3	110.5(2)
C(2)-C(1)-C(6)#3	110.3(3)
C(6)-C(1)-C(6)#3	106.9(3)
C(1)-C(2)-C(3)	109.2(4)
C(1)-C(2)-H(2A)	109.8
C(3)-C(2)-H(2A)	109.8
C(1)-C(2)-H(2B)	109.8
C(3)-C(2)-H(2B)	109.8
H(2A)-C(2)-H(2B)	108.3
C(4)-C(3)-C(4)#3	109.3(5)
C(4)-C(3)-C(2)	109.3(3)
C(4)#3-C(3)-C(2)	109.3(3)
C(4)-C(3)-H(3)	109.6
C(4)#3-C(3)-H(3)	109.6
C(2)-C(3)-H(3)	109.6
C(5)-C(4)-C(3)	109.3(3)
C(5)-C(4)-H(4A)	109.8
C(3)-C(4)-H(4A)	109.8
C(5)-C(4)-H(4B)	109.8
C(3)-C(4)-H(4B)	109.8
H(4A)-C(4)-H(4B)	108.3
C(4)-C(5)-C(7)	109.9(4)
C(4)-C(5)-C(6)	109.6(3)
C(7)-C(5)-C(6)	109.9(3)
C(4)-C(5)-H(5)	109.1
C(7)-C(5)-H(5)	109.1
C(6)-C(5)-H(5)	109.1
C(1)-C(6)-C(5)	109.7(3)
C(1)-C(6)-H(6A)	109.7
C(5)-C(6)-H(6A)	109.7
C(1)-C(6)-H(6B)	109.7
C(5)-C(6)-H(6B)	109.7
H(6A)-C(6)-H(6B)	108.2
C(5)#3-C(7)-C(5)	109.0(4)
C(5)#3-C(7)-H(7A)	109.9
C(5)-C(7)-H(7A)	109.9
C(5)#3-C(7)-H(7B)	109.9
C(5)-C(7)-H(7B)	109.9
H(7A)-C(7)-H(7B)	108.3
N(2)-C(21)-H(21A)	109.5
N(2)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
N(2)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(2)-C(22)-H(22A)	109.5
N(2)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
N(2)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+2,-z #2 -x+1,y,-z #3 x,-y+2,z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **[V(μ-N-1-adamantyl)(NMe$_2$)$_2$]$_2$.**

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
V(1)	24(1)	23(1)	28(1)	0	4(1)	0
N(1)	23(2)	28(2)	28(2)	0	4(1)	0
N(2)	32(1)	31(1)	39(1)	5(1)	5(1)	2(1)
C(1)	26(2)	26(2)	27(2)	0	5(2)	0
C(2)	35(3)	168(7)	28(2)	0	1(2)	0
C(3)	46(3)	282(13)	20(2)	0	-1(2)	0
C(4)	120(4)	144(5)	56(2)	62(3)	57(3)	87(4)
C(5)	91(3)	30(2)	60(2)	6(2)	47(2)	-3(2)
C(6)	78(2)	31(2)	52(2)	-5(1)	39(2)	-9(2)
C(7)	47(3)	54(3)	40(2)	0	19(2)	0
C(21)	36(2)	55(2)	75(2)	21(2)	-7(2)	1(2)
C(22)	51(2)	43(2)	48(2)	15(2)	10(1)	5(2)

Data for compound 3

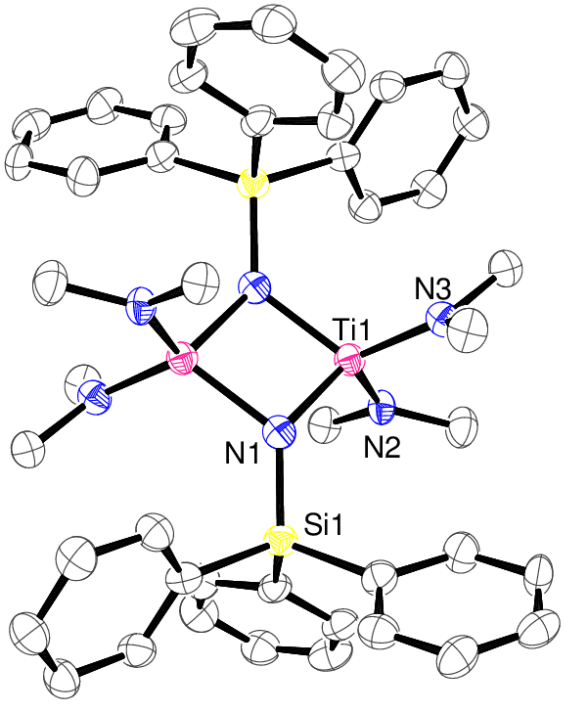


Table 1. Crystal data and structure refinement for **3**.

Identification code	cl848b
Empirical formula	C44 H54 N6 Si2 Ti2
Formula weight	818.85
Temperature	180 K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 1 21/c 1
Unit cell dimensions	a = 12.8129(18) A alpha = 90 deg.
	b = 15.846(3) A beta = 108.955(16) deg.
	c = 11.4001(17) A gamma = 90 deg.
Volume	2189.1(6) A^3
Z, Calculated density	2, 1.242 Mg/m^3
Absorption coefficient	0.457 mm^-1
F(000)	864
Crystal size	0.17 x 0.125 x 0.025 mm
Theta range for data collection	2.45 to 24.71 deg.
Limiting indices	-14<=h<=15, -18<=k<=18, -13<=l<=13
Reflections collected / unique	14897 / 3712 [R(int) = 0.2704]
Completeness to theta = 24.71	99.7 %
Absorption correction	Empirical (DIFABS)
Max. and min. transmission	0.985 and 0.927
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3712 / 0 / 248
Goodness-of-fit on F^2	0.777
Final R indices [I>2sigma(I)]	R1 = 0.0674, wR2 = 0.0964
R indices (all data)	R1 = 0.2369, wR2 = 0.1539
Largest diff. peak and hole	0.324 and -0.586 e.A^-3

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

	x	y	z	U(eq)
C(1)	8037(7)	-333(6)	5192(7)	53(2)
C(2)	7950(9)	-1213(6)	5213(9)	58(3)
C(3)	8385(10)	-1714(7)	4457(9)	69(3)
C(4)	8891(9)	-1358(8)	3710(9)	69(3)
C(5)	8958(9)	-500(9)	3645(8)	71(3)
C(6)	8542(8)	29(6)	4392(8)	58(2)
C(7)	7908(8)	1434(6)	6289(8)	56(2)
C(8)	7577(9)	1983(6)	5261(8)	63(3)
C(9)	7873(10)	2842(6)	5379(11)	74(3)
C(10)	8533(9)	3169(7)	6492(10)	65(3)
C(11)	8871(10)	2647(7)	7478(10)	67(3)
C(12)	8570(8)	1796(6)	7393(9)	58(3)
C(13)	7912(7)	-146(6)	7792(7)	49(2)
C(14)	7346(8)	43(6)	8639(8)	57(2)
C(15)	7678(9)	-305(6)	9827(7)	62(3)
C(16)	8600(9)	-812(6)	10240(7)	64(3)
C(17)	9182(9)	-987(6)	9437(7)	61(3)
C(18)	8838(7)	-650(6)	8245(7)	56(2)
C(19)	5793(10)	882(6)	1872(9)	70(3)
C(20)	5731(8)	-575(6)	2459(7)	59(2)
C(21)	3795(8)	2066(6)	2782(8)	56(2)
C(22)	4769(10)	2347(6)	4937(8)	65(3)
N(1)	5998(6)	274(4)	5624(5)	46(2)
N(2)	5535(6)	302(4)	2740(6)	49(2)
N(3)	4520(6)	1710(4)	3949(6)	51(2)
Si(1)	7421(2)	313(2)	6188(2)	47(1)
Ti(1)	4981(1)	571(1)	4043(1)	45(1)

Table 3. Bond lengths [A] and angles [deg] for **3**.

C(1)-C(2)	1.400(14)
C(1)-C(6)	1.401(13)
C(1)-Si(1)	1.883(10)
C(2)-C(3)	1.413(14)
C(3)-C(4)	1.350(16)
C(4)-C(5)	1.366(16)
C(5)-C(6)	1.417(14)
C(7)-C(12)	1.393(13)
C(7)-C(8)	1.409(13)
C(7)-Si(1)	1.873(10)
C(8)-C(9)	1.409(13)
C(9)-C(10)	1.377(14)
C(10)-C(11)	1.349(14)
C(11)-C(12)	1.396(14)
C(13)-C(18)	1.384(12)
C(13)-C(14)	1.414(13)
C(13)-Si(1)	1.876(8)
C(14)-C(15)	1.395(11)
C(15)-C(16)	1.378(13)
C(16)-C(17)	1.384(13)
C(17)-C(18)	1.392(11)
C(19)-N(2)	1.465(11)
C(20)-N(2)	1.465(11)
C(21)-N(3)	1.465(10)
C(22)-N(3)	1.467(11)
N(1)-Si(1)	1.726(7)
N(1)-Ti(1)	1.908(6)
N(1)-Ti(1)#1	1.954(7)
N(2)-Ti(1)	1.892(7)
N(3)-Ti(1)	1.892(7)
Ti(1)-N(1)#1	1.954(7)
Ti(1)-Ti(1)#1	2.823(3)
C(2)-C(1)-C(6)	118.4(9)
C(2)-C(1)-Si(1)	118.7(8)

C(6)-C(1)-Si(1)	122.9(7)
C(1)-C(2)-C(3)	120.0(10)
C(4)-C(3)-C(2)	121.0(10)
C(3)-C(4)-C(5)	120.1(11)
C(4)-C(5)-C(6)	120.9(10)
C(1)-C(6)-C(5)	119.5(10)
C(12)-C(7)-C(8)	115.3(9)
C(12)-C(7)-Si(1)	122.6(7)
C(8)-C(7)-Si(1)	122.0(7)
C(9)-C(8)-C(7)	121.2(9)
C(10)-C(9)-C(8)	121.1(10)
C(11)-C(10)-C(9)	118.2(9)
C(10)-C(11)-C(12)	121.8(9)
C(7)-C(12)-C(11)	122.3(9)
C(18)-C(13)-C(14)	115.7(7)
C(18)-C(13)-Si(1)	124.3(7)
C(14)-C(13)-Si(1)	120.0(7)
C(15)-C(14)-C(13)	121.2(9)
C(16)-C(15)-C(14)	121.3(9)
C(15)-C(16)-C(17)	118.5(8)
C(16)-C(17)-C(18)	120.1(9)
C(13)-C(18)-C(17)	123.2(9)
Si(1)-N(1)-Ti(1)	131.1(4)
Si(1)-N(1)-Ti(1)#1	128.3(4)
Ti(1)-N(1)-Ti(1)#1	93.9(3)
C(20)-N(2)-C(19)	110.8(7)
C(20)-N(2)-Ti(1)	121.3(5)
C(19)-N(2)-Ti(1)	127.8(6)
C(21)-N(3)-C(22)	110.4(7)
C(21)-N(3)-Ti(1)	120.8(5)
C(22)-N(3)-Ti(1)	128.7(6)
N(1)-Si(1)-C(7)	110.3(4)
N(1)-Si(1)-C(13)	109.2(4)
C(7)-Si(1)-C(13)	108.0(4)
N(1)-Si(1)-C(1)	110.7(3)
C(7)-Si(1)-C(1)	110.9(4)
C(13)-Si(1)-C(1)	107.7(4)
N(2)-Ti(1)-N(3)	111.1(3)
N(2)-Ti(1)-N(1)	111.8(3)
N(3)-Ti(1)-N(1)	113.2(3)
N(2)-Ti(1)-N(1)#1	115.3(3)
N(3)-Ti(1)-N(1)#1	117.1(3)
N(1)-Ti(1)-N(1)#1	86.1(3)
N(2)-Ti(1)-Ti(1)#1	123.1(2)
N(3)-Ti(1)-Ti(1)#1	125.6(2)
N(1)-Ti(1)-Ti(1)#1	43.7(2)
N(1)#1-Ti(1)-Ti(1)#1	42.41(17)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **3**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	42(5)	72(7)	43(4)	7(4)	9(4)	-10(5)
C(2)	65(7)	57(6)	56(5)	-3(5)	25(5)	-2(5)
C(3)	81(8)	57(6)	70(6)	-14(5)	27(6)	10(6)
C(4)	63(7)	80(8)	69(6)	-3(5)	30(5)	9(6)
C(5)	63(7)	101(10)	60(5)	-17(6)	35(5)	-10(7)
C(6)	49(6)	72(6)	56(5)	0(5)	21(4)	-9(5)
C(7)	54(6)	58(6)	61(6)	3(5)	25(5)	0(5)
C(8)	73(8)	66(6)	44(5)	2(4)	9(5)	-11(5)
C(9)	73(8)	48(6)	108(9)	29(6)	41(7)	2(5)
C(10)	59(7)	59(6)	80(7)	-17(6)	28(6)	-17(5)
C(11)	71(7)	55(6)	77(6)	-15(5)	25(5)	-18(5)
C(12)	51(6)	67(7)	59(6)	-2(5)	21(5)	6(5)
C(13)	43(5)	55(5)	51(4)	-4(4)	16(4)	-2(4)
C(14)	58(7)	59(6)	51(5)	1(4)	16(4)	5(5)
C(15)	75(7)	73(6)	39(4)	-7(4)	20(4)	-5(6)
C(16)	71(8)	74(7)	42(5)	3(4)	10(5)	4(6)

C(17)	64(7)	66(6)	45(4)	7(4)	10(5)	2(5)
C(18)	48(6)	68(6)	50(4)	0(4)	14(4)	0(5)
C(19)	87(8)	65(7)	70(6)	14(5)	42(6)	3(6)
C(20)	70(6)	53(5)	55(4)	-5(5)	21(4)	-5(5)
C(21)	61(7)	54(5)	52(5)	3(4)	17(5)	2(5)
C(22)	81(8)	63(6)	49(5)	-12(4)	21(5)	-9(6)
N(1)	51(4)	50(4)	41(3)	-1(3)	18(3)	4(3)
N(2)	59(5)	36(4)	53(4)	3(3)	20(3)	1(3)
N(3)	55(5)	59(4)	40(4)	1(3)	16(4)	6(4)
Si(1)	44(2)	52(2)	44(1)	-1(1)	12(1)	-2(1)
Ti(1)	47(1)	46(1)	42(1)	1(1)	15(1)	1(1)

Data for compound 4

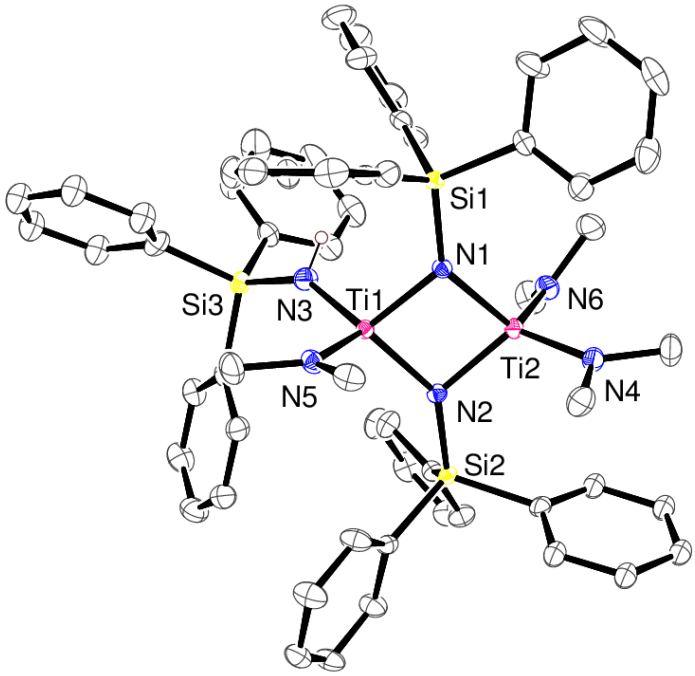


Table 1. Crystal data and structure refinement for **4**.

Identification code	cl848
Empirical formula	C60 H64 N6 Si3 Ti2
Formula weight	1049.24
Temperature	180 K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 11.3357(4) A alpha = 92.607(4) deg.
	b = 13.4320(5) A beta = 104.677(4) deg.
	c = 19.7408(9) A gamma = 106.071(3) deg.
Volume	2772.34(19) A^3
Z, Calculated density	2, 1.257 Mg/m^3
Absorption coefficient	0.397 mm^-1
F(000)	1104
Crystal size	0.45 x 0.3 x 0.2 mm
Theta range for data collection	3.10 to 26.37 deg.
Limiting indices	-14<=h<=14, -16<=k<=16, -19<=l<=24
Reflections collected / unique	21233 / 11316 [R(int) = 0.0242]
Completeness to theta = 26.37	99.7 %
Absorption correction	Empirical (DIFABS)
Max. and min. transmission	0.921 and 0.838
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11316 / 1 / 631
Goodness-of-fit on F^2	1.128
Final R indices [I>2sigma(I)]	R1 = 0.0446, wR2 = 0.1219
R indices (all data)	R1 = 0.0578, wR2 = 0.1296
Largest diff. peak and hole	0.492 and -0.511 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **4**.

	x	y	z	U(eq)
C(1)	8426(2)	3401(2)	1582(1)	30(1)
C(2)	8318(3)	4396(2)	1719(2)	56(1)
C(3)	7220(3)	4645(3)	1395(2)	70(1)
C(4)	6213(3)	3912(3)	945(2)	57(1)
C(5)	6289(3)	2928(3)	799(2)	55(1)
C(6)	7402(2)	2677(2)	1114(2)	45(1)
C(7)	11023(2)	3743(2)	1372(1)	28(1)
C(8)	12360(2)	4036(2)	1610(1)	40(1)
C(9)	13113(3)	4429(2)	1175(2)	49(1)
C(10)	12561(3)	4539(2)	489(2)	47(1)
C(11)	11255(3)	4255(2)	237(1)	46(1)
C(12)	10496(2)	3870(2)	676(1)	36(1)
C(13)	10775(2)	3911(2)	2871(1)	31(1)
C(14)	10652(2)	3414(2)	3469(1)	37(1)
C(15)	11215(3)	3946(2)	4147(1)	49(1)
C(56)	5828(2)	-167(2)	1331(2)	53(1)
C(16)	11904(3)	4978(3)	4238(2)	60(1)
C(17)	12044(3)	5491(2)	3662(2)	64(1)
C(57)	11129(3)	1278(2)	652(1)	42(1)
C(18)	11487(3)	4957(2)	2985(1)	46(1)
C(19)	10778(2)	-1856(2)	1709(1)	27(1)
C(20)	11064(2)	-2787(2)	1825(1)	39(1)
C(21)	11730(3)	-3183(2)	1434(1)	44(1)
C(22)	12123(2)	-2661(2)	917(1)	40(1)
C(23)	11860(3)	-1738(2)	785(1)	48(1)
C(24)	11181(3)	-1348(2)	1172(1)	41(1)
C(25)	10298(2)	-1671(2)	3156(1)	28(1)
C(26)	9784(3)	-2649(2)	3344(1)	39(1)
C(27)	10174(3)	-2883(2)	4031(1)	49(1)
C(28)	11087(3)	-2134(2)	4540(1)	47(1)
C(29)	11612(3)	-1168(2)	4369(1)	50(1)
C(30)	11225(2)	-936(2)	3683(1)	40(1)
C(31)	8097(2)	-2121(2)	1828(1)	32(1)
C(32A)	7180(7)	-2256(5)	2155(4)	39(1)
C(33A)	5883(4)	-2769(4)	1796(2)	39(1)
C(34A)	5533(5)	-3151(4)	1101(2)	39(1)
C(35A)	6461(4)	-3011(4)	741(2)	39(1)
C(36A)	7736(5)	-2518(5)	1081(3)	39(1)
C(32B)	7224(12)	-2096(8)	2283(6)	39(1)
C(33B)	5960(7)	-2600(6)	2072(4)	39(1)
C(34B)	5449(8)	-3135(6)	1379(4)	39(1)
C(35B)	6184(7)	-3164(6)	946(4)	39(1)
C(36B)	7523(8)	-2655(8)	1200(6)	39(1)
C(58)	13283(3)	1657(2)	1389(2)	52(1)
C(37)	14193(2)	771(2)	3557(1)	32(1)
C(38)	13741(2)	119(2)	2910(1)	40(1)
C(39)	14003(3)	-817(2)	2827(2)	47(1)
C(40)	14739(3)	-1135(2)	3393(2)	51(1)
C(41)	15205(3)	-518(2)	4040(2)	51(1)
C(42)	14944(2)	420(2)	4120(1)	40(1)
C(43)	13638(2)	2367(2)	4531(1)	35(1)
C(44)	12553(3)	1792(2)	4708(2)	46(1)
C(45)	12303(3)	2048(3)	5337(2)	60(1)
C(46)	13123(3)	2887(3)	5796(2)	68(1)
C(47)	14198(4)	3475(3)	5638(2)	77(1)
C(48)	14449(3)	3215(3)	5012(2)	59(1)
C(55)	7288(3)	-154(2)	640(1)	46(1)
C(49)	15309(2)	3091(2)	3554(1)	39(1)
C(50A)	16562(8)	3147(7)	4019(3)	51(1)
C(51A)	17677(6)	3845(5)	3961(3)	51(1)
C(52A)	17610(5)	4451(4)	3414(3)	51(1)
C(53A)	16453(5)	4419(4)	2955(3)	51(1)
C(54A)	15331(5)	3690(4)	3020(3)	51(1)
C(50B)	16505(13)	3189(11)	3854(5)	51(1)
C(51B)	17540(9)	4001(8)	3751(5)	51(1)
C(52B)	17232(8)	4736(7)	3328(5)	51(1)
C(53B)	16007(7)	4746(6)	3071(4)	51(1)
C(54B)	14977(8)	3972(6)	3189(4)	51(1)
C(59)	7413(3)	1387(2)	2957(2)	55(1)

C(60)	8580(3)	341(3)	3653(2)	60(1)
N(1)	9877(2)	1862(1)	1995(1)	23(1)
N(2)	10009(2)	-44(1)	2194(1)	23(1)
N(3)	12512(2)	2007(2)	3004(1)	35(1)
N(4)	7165(2)	69(2)	1339(1)	33(1)
N(5)	11935(2)	1376(1)	1372(1)	31(1)
N(6)	8185(2)	683(2)	2962(1)	37(1)
Si(1)	10010(1)	3170(1)	1961(1)	23(1)
Si(2)	9827(1)	-1358(1)	2224(1)	23(1)
Si(3)	13875(1)	2055(1)	3648(1)	29(1)
Ti(1)	11250(1)	1284(1)	2157(1)	21(1)
Ti(2)	8647(1)	576(1)	2123(1)	24(1)

Table 3. Bond lengths [A] and angles [deg] for **4**.

C(1)-C(6)	1.378(3)
C(1)-C(2)	1.396(3)
C(1)-Si(1)	1.878(2)
C(2)-C(3)	1.384(4)
C(3)-C(4)	1.359(5)
C(4)-C(5)	1.371(4)
C(5)-C(6)	1.396(4)
C(7)-C(12)	1.391(3)
C(7)-C(8)	1.402(3)
C(7)-Si(1)	1.880(2)
C(8)-C(9)	1.382(3)
C(9)-C(10)	1.374(4)
C(10)-C(11)	1.372(4)
C(11)-C(12)	1.389(3)
C(13)-C(18)	1.388(3)
C(13)-C(14)	1.400(3)
C(13)-Si(1)	1.882(2)
C(14)-C(15)	1.392(3)
C(15)-C(16)	1.367(4)
C(56)-N(4)	1.457(3)
C(16)-C(17)	1.377(5)
C(17)-C(18)	1.391(4)
C(57)-N(5)	1.460(3)
C(19)-C(20)	1.390(3)
C(19)-C(24)	1.392(3)
C(19)-Si(2)	1.880(2)
C(20)-C(21)	1.390(3)
C(21)-C(22)	1.361(4)
C(22)-C(23)	1.374(4)
C(23)-C(24)	1.391(3)
C(25)-C(26)	1.390(3)
C(25)-C(30)	1.392(3)
C(25)-Si(2)	1.883(2)
C(26)-C(27)	1.395(3)
C(27)-C(28)	1.378(4)
C(28)-C(29)	1.367(4)
C(29)-C(30)	1.391(3)
C(31)-C(36B)	1.314(12)
C(31)-C(32A)	1.333(8)
C(31)-C(36A)	1.459(7)
C(31)-C(32B)	1.500(14)
C(31)-Si(2)	1.882(2)
C(32A)-C(33A)	1.416(7)
C(33A)-C(34A)	1.361(6)
C(34A)-C(35A)	1.387(6)
C(35A)-C(36A)	1.385(6)
C(32B)-C(33B)	1.349(13)
C(33B)-C(34B)	1.414(10)
C(34B)-C(35B)	1.343(10)
C(35B)-C(36B)	1.426(11)
C(58)-N(5)	1.460(3)
C(37)-C(42)	1.404(3)
C(37)-C(38)	1.406(3)
C(37)-Si(3)	1.867(2)
C(38)-C(39)	1.381(4)
C(39)-C(40)	1.377(4)
C(40)-C(41)	1.384(4)
C(41)-C(42)	1.383(4)
C(43)-C(48)	1.386(4)

C(43)-C(44)	1.395(4)
C(43)-Si(3)	1.878(2)
C(44)-C(45)	1.392(4)
C(45)-C(46)	1.362(5)
C(46)-C(47)	1.374(5)
C(47)-C(48)	1.389(4)
C(55)-N(4)	1.447(3)
C(49)-C(50B)	1.301(14)
C(49)-C(54A)	1.355(5)
C(49)-C(50A)	1.463(8)
C(49)-C(54B)	1.500(8)
C(49)-Si(3)	1.881(2)
C(50A)-C(51A)	1.384(9)
C(51A)-C(52A)	1.381(7)
C(52A)-C(53A)	1.381(7)
C(53A)-C(54A)	1.413(6)
C(50B)-C(51B)	1.428(14)
C(51B)-C(52B)	1.383(11)
C(52B)-C(53B)	1.357(11)
C(53B)-C(54B)	1.409(10)
C(59)-N(6)	1.454(3)
C(60)-N(6)	1.460(3)
N(1)-Si(1)	1.7275(17)
N(1)-Ti(1)	1.8885(17)
N(1)-Ti(2)	1.9691(16)
N(2)-Si(2)	1.7254(17)
N(2)-Ti(2)	1.9267(17)
N(2)-Ti(1)	1.9596(16)
N(3)-Si(3)	1.717(2)
N(3)-Ti(1)	1.9124(19)
N(4)-Ti(2)	1.9057(19)
N(5)-Ti(1)	1.8946(18)
N(6)-Ti(2)	1.8707(19)
Ti(1)-Ti(2)	2.8215(5)

C(6)-C(1)-C(2)	117.6(2)
C(6)-C(1)-Si(1)	123.54(18)
C(2)-C(1)-Si(1)	118.46(19)
C(3)-C(2)-C(1)	121.1(3)
C(4)-C(3)-C(2)	120.2(3)
C(3)-C(4)-C(5)	120.1(3)
C(4)-C(5)-C(6)	119.9(3)
C(1)-C(6)-C(5)	121.0(3)
C(12)-C(7)-C(8)	116.6(2)
C(12)-C(7)-Si(1)	122.30(17)
C(8)-C(7)-Si(1)	121.11(18)
C(9)-C(8)-C(7)	121.6(2)
C(10)-C(9)-C(8)	120.3(3)
C(11)-C(10)-C(9)	119.6(2)
C(10)-C(11)-C(12)	120.2(2)
C(11)-C(12)-C(7)	121.7(2)
C(18)-C(13)-C(14)	117.1(2)
C(18)-C(13)-Si(1)	122.39(19)
C(14)-C(13)-Si(1)	120.54(17)
C(15)-C(14)-C(13)	121.5(2)
C(16)-C(15)-C(14)	119.8(3)
C(15)-C(16)-C(17)	120.3(3)
C(16)-C(17)-C(18)	119.9(3)
C(13)-C(18)-C(17)	121.5(3)
C(20)-C(19)-C(24)	116.4(2)
C(20)-C(19)-Si(2)	121.23(17)
C(24)-C(19)-Si(2)	122.30(17)
C(21)-C(20)-C(19)	121.9(2)
C(22)-C(21)-C(20)	120.2(2)
C(21)-C(22)-C(23)	119.7(2)
C(22)-C(23)-C(24)	120.1(2)
C(23)-C(24)-C(19)	121.6(2)
C(26)-C(25)-C(30)	117.1(2)
C(26)-C(25)-Si(2)	122.01(17)
C(30)-C(25)-Si(2)	120.83(16)
C(25)-C(26)-C(27)	121.5(2)
C(28)-C(27)-C(26)	119.8(2)
C(29)-C(28)-C(27)	119.9(2)
C(28)-C(29)-C(30)	120.3(3)
C(29)-C(30)-C(25)	121.4(2)
C(36B)-C(31)-C(32A)	104.6(4)
C(36B)-C(31)-C(36A)	15.2(4)

C(32A)-C(31)-C(36A)	118.3(3)
C(36B)-C(31)-C(32B)	114.4(5)
C(32A)-C(31)-C(32B)	10.5(5)
C(36A)-C(31)-C(32B)	127.5(4)
C(36B)-C(31)-Si(2)	129.6(4)
C(32A)-C(31)-Si(2)	125.8(3)
C(36A)-C(31)-Si(2)	115.7(2)
C(32B)-C(31)-Si(2)	116.0(4)
C(31)-C(32A)-C(33A)	121.7(5)
C(34A)-C(33A)-C(32A)	120.6(4)
C(33A)-C(34A)-C(35A)	119.2(4)
C(36A)-C(35A)-C(34A)	121.3(4)
C(35A)-C(36A)-C(31)	118.8(4)
C(33B)-C(32B)-C(31)	122.9(7)
C(32B)-C(33B)-C(34B)	117.4(7)
C(35B)-C(34B)-C(33B)	122.0(7)
C(34B)-C(35B)-C(36B)	118.6(7)
C(31)-C(36B)-C(35B)	124.5(7)
C(42)-C(37)-C(38)	116.0(2)
C(42)-C(37)-Si(3)	122.11(19)
C(38)-C(37)-Si(3)	121.82(17)
C(39)-C(38)-C(37)	122.7(2)
C(40)-C(39)-C(38)	119.5(3)
C(39)-C(40)-C(41)	119.9(3)
C(42)-C(41)-C(40)	120.4(2)
C(41)-C(42)-C(37)	121.6(2)
C(48)-C(43)-C(44)	116.6(2)
C(48)-C(43)-Si(3)	122.9(2)
C(44)-C(43)-Si(3)	120.3(2)
C(45)-C(44)-C(43)	121.8(3)
C(46)-C(45)-C(44)	119.9(3)
C(45)-C(46)-C(47)	119.9(3)
C(46)-C(47)-C(48)	120.0(3)
C(43)-C(48)-C(47)	121.7(3)
C(50B)-C(49)-C(54A)	104.6(5)
C(50B)-C(49)-C(50A)	11.8(6)
C(54A)-C(49)-C(50A)	115.2(4)
C(50B)-C(49)-C(54B)	118.6(6)
C(54A)-C(49)-C(54B)	29.7(3)
C(50A)-C(49)-C(54B)	125.2(5)
C(50B)-C(49)-Si(3)	127.2(5)
C(54A)-C(49)-Si(3)	125.8(3)
C(50A)-C(49)-Si(3)	118.1(3)
C(54B)-C(49)-Si(3)	113.3(3)
C(51A)-C(50A)-C(49)	122.1(5)
C(52A)-C(51A)-C(50A)	118.7(5)
C(51A)-C(52A)-C(53A)	121.4(5)
C(52A)-C(53A)-C(54A)	118.5(5)
C(49)-C(54A)-C(53A)	123.5(4)
C(49)-C(50B)-C(51B)	123.6(9)
C(52B)-C(51B)-C(50B)	117.2(8)
C(53B)-C(52B)-C(51B)	121.8(8)
C(52B)-C(53B)-C(54B)	121.6(8)
C(53B)-C(54B)-C(49)	115.9(6)
Si(1)-N(1)-Ti(1)	125.42(9)
Si(1)-N(1)-Ti(2)	139.03(10)
Ti(1)-N(1)-Ti(2)	93.99(7)
Si(2)-N(2)-Ti(2)	124.13(9)
Si(2)-N(2)-Ti(1)	142.68(10)
Ti(2)-N(2)-Ti(1)	93.11(7)
Si(3)-N(3)-Ti(1)	147.80(13)
C(55)-N(4)-C(56)	111.1(2)
C(55)-N(4)-Ti(2)	120.40(16)
C(56)-N(4)-Ti(2)	128.51(18)
C(57)-N(5)-C(58)	110.8(2)
C(57)-N(5)-Ti(1)	121.78(15)
C(58)-N(5)-Ti(1)	127.05(17)
C(59)-N(6)-C(60)	112.9(2)
C(59)-N(6)-Ti(2)	112.55(17)
C(60)-N(6)-Ti(2)	133.84(18)
N(1)-Si(1)-C(1)	112.58(9)
N(1)-Si(1)-C(7)	111.16(9)
C(1)-Si(1)-C(7)	105.41(10)
N(1)-Si(1)-C(13)	109.80(9)
C(1)-Si(1)-C(13)	109.50(10)
C(7)-Si(1)-C(13)	108.23(10)
N(2)-Si(2)-C(19)	112.46(9)

N(2)-Si(2)-C(31)	109.40(9)
C(19)-Si(2)-C(31)	107.38(10)
N(2)-Si(2)-C(25)	111.91(9)
C(19)-Si(2)-C(25)	108.40(9)
C(31)-Si(2)-C(25)	107.05(10)
N(3)-Si(3)-C(37)	108.28(10)
N(3)-Si(3)-C(43)	108.56(11)
C(37)-Si(3)-C(43)	112.38(11)
N(3)-Si(3)-C(49)	112.03(11)
C(37)-Si(3)-C(49)	107.50(11)
C(43)-Si(3)-C(49)	108.14(11)
N(1)-Ti(1)-N(5)	109.92(8)
N(1)-Ti(1)-N(3)	108.82(8)
N(5)-Ti(1)-N(3)	111.47(9)
N(1)-Ti(1)-N(2)	86.86(7)
N(5)-Ti(1)-N(2)	117.04(8)
N(3)-Ti(1)-N(2)	119.35(8)
N(1)-Ti(1)-Ti(2)	44.12(5)
N(5)-Ti(1)-Ti(2)	126.90(6)
N(3)-Ti(1)-Ti(2)	120.48(7)
N(2)-Ti(1)-Ti(2)	42.99(5)
N(6)-Ti(2)-N(4)	110.60(9)
N(6)-Ti(2)-N(2)	113.64(8)
N(4)-Ti(2)-N(2)	118.07(8)
N(6)-Ti(2)-N(1)	113.27(8)
N(4)-Ti(2)-N(1)	113.71(8)
N(2)-Ti(2)-N(1)	85.56(7)
N(6)-Ti(2)-Ti(1)	119.25(7)
N(4)-Ti(2)-Ti(1)	129.97(6)
N(2)-Ti(2)-Ti(1)	43.91(5)
N(1)-Ti(2)-Ti(1)	41.89(5)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **4**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	29(1)	37(1)	31(1)	11(1)	12(1)	15(1)
C(2)	60(2)	56(2)	55(2)	-5(1)	-2(2)	39(2)
C(3)	70(2)	78(2)	66(2)	-6(2)	-4(2)	56(2)
C(4)	44(2)	88(2)	55(2)	21(2)	17(1)	42(2)
C(5)	35(1)	64(2)	56(2)	19(2)	-3(1)	9(1)
C(6)	36(1)	37(1)	57(2)	11(1)	3(1)	12(1)
C(7)	31(1)	20(1)	35(1)	4(1)	13(1)	8(1)
C(8)	34(1)	41(1)	51(2)	19(1)	15(1)	14(1)
C(9)	36(1)	48(2)	68(2)	14(1)	27(1)	9(1)
C(10)	56(2)	35(1)	60(2)	11(1)	39(2)	10(1)
C(11)	67(2)	42(1)	33(1)	8(1)	21(1)	15(1)
C(12)	38(1)	35(1)	35(1)	3(1)	12(1)	8(1)
C(13)	31(1)	30(1)	36(1)	1(1)	8(1)	15(1)
C(14)	39(1)	41(1)	34(1)	0(1)	14(1)	15(1)
C(15)	54(2)	65(2)	32(1)	-3(1)	10(1)	26(2)
C(56)	29(1)	58(2)	67(2)	7(2)	8(1)	9(1)
C(16)	64(2)	65(2)	41(2)	-20(1)	0(1)	19(2)
C(17)	69(2)	38(2)	67(2)	-19(1)	3(2)	9(2)
C(57)	58(2)	48(2)	27(1)	5(1)	18(1)	21(1)
C(18)	56(2)	31(1)	45(2)	0(1)	5(1)	12(1)
C(19)	28(1)	23(1)	26(1)	0(1)	4(1)	7(1)
C(20)	51(2)	32(1)	45(1)	15(1)	22(1)	19(1)
C(21)	59(2)	33(1)	53(2)	10(1)	21(1)	27(1)
C(22)	45(1)	44(1)	38(1)	0(1)	14(1)	22(1)
C(23)	72(2)	45(2)	43(2)	15(1)	32(1)	28(1)
C(24)	62(2)	34(1)	37(1)	11(1)	20(1)	25(1)
C(25)	29(1)	28(1)	29(1)	8(1)	10(1)	10(1)
C(26)	49(2)	30(1)	36(1)	7(1)	11(1)	7(1)
C(27)	67(2)	43(2)	42(2)	22(1)	20(1)	19(1)
C(28)	50(2)	64(2)	33(1)	21(1)	10(1)	24(1)
C(29)	43(2)	61(2)	34(1)	10(1)	-1(1)	6(1)
C(30)	37(1)	40(1)	33(1)	9(1)	5(1)	2(1)
C(31)	31(1)	20(1)	41(1)	4(1)	2(1)	7(1)
C(32A)	30(1)	40(1)	42(2)	-3(1)	7(1)	4(1)
C(33A)	30(1)	40(1)	42(2)	-3(1)	7(1)	4(1)

C(34A)	30(1)	40(1)	42(2)	-3(1)	7(1)	4(1)
C(35A)	30(1)	40(1)	42(2)	-3(1)	7(1)	4(1)
C(36A)	30(1)	40(1)	42(2)	-3(1)	7(1)	4(1)
C(32B)	30(1)	40(1)	42(2)	-3(1)	7(1)	4(1)
C(33B)	30(1)	40(1)	42(2)	-3(1)	7(1)	4(1)
C(34B)	30(1)	40(1)	42(2)	-3(1)	7(1)	4(1)
C(35B)	30(1)	40(1)	42(2)	-3(1)	7(1)	4(1)
C(36B)	30(1)	40(1)	42(2)	-3(1)	7(1)	4(1)
C(58)	42(2)	60(2)	64(2)	11(2)	29(1)	16(1)
C(37)	22(1)	38(1)	36(1)	9(1)	8(1)	8(1)
C(38)	32(1)	39(1)	42(1)	3(1)	0(1)	12(1)
C(39)	44(2)	41(1)	53(2)	-3(1)	8(1)	14(1)
C(40)	57(2)	44(2)	62(2)	12(1)	21(2)	26(1)
C(41)	52(2)	62(2)	50(2)	26(1)	16(1)	32(2)
C(42)	38(1)	53(2)	33(1)	13(1)	9(1)	17(1)
C(43)	32(1)	46(1)	30(1)	7(1)	6(1)	17(1)
C(44)	49(2)	49(2)	47(2)	15(1)	19(1)	19(1)
C(45)	64(2)	77(2)	59(2)	35(2)	35(2)	34(2)
C(46)	74(2)	111(3)	36(2)	16(2)	24(2)	46(2)
C(47)	66(2)	112(3)	45(2)	-19(2)	16(2)	16(2)
C(48)	43(2)	82(2)	44(2)	-10(2)	15(1)	7(2)
C(55)	44(2)	50(2)	35(1)	0(1)	4(1)	6(1)
C(49)	42(1)	38(1)	27(1)	-4(1)	8(1)	0(1)
C(50A)	43(1)	51(1)	55(1)	10(1)	15(1)	6(1)
C(51A)	43(1)	51(1)	55(1)	10(1)	15(1)	6(1)
C(52A)	43(1)	51(1)	55(1)	10(1)	15(1)	6(1)
C(53A)	43(1)	51(1)	55(1)	10(1)	15(1)	6(1)
C(54A)	43(1)	51(1)	55(1)	10(1)	15(1)	6(1)
C(50B)	43(1)	51(1)	55(1)	10(1)	15(1)	6(1)
C(51B)	43(1)	51(1)	55(1)	10(1)	15(1)	6(1)
C(52B)	43(1)	51(1)	55(1)	10(1)	15(1)	6(1)
C(53B)	43(1)	51(1)	55(1)	10(1)	15(1)	6(1)
C(54B)	43(1)	51(1)	55(1)	10(1)	15(1)	6(1)
C(59)	56(2)	49(2)	69(2)	2(1)	35(2)	16(1)
C(60)	67(2)	81(2)	41(2)	15(2)	26(2)	27(2)
N(1)	24(1)	22(1)	24(1)	5(1)	8(1)	8(1)
N(2)	25(1)	21(1)	23(1)	4(1)	8(1)	6(1)
N(3)	34(1)	33(1)	32(1)	0(1)	-2(1)	12(1)
N(4)	27(1)	31(1)	38(1)	5(1)	7(1)	7(1)
N(5)	32(1)	33(1)	33(1)	8(1)	16(1)	13(1)
N(6)	38(1)	40(1)	37(1)	3(1)	21(1)	11(1)
Si(1)	24(1)	21(1)	27(1)	3(1)	8(1)	9(1)
Si(2)	24(1)	19(1)	23(1)	3(1)	5(1)	5(1)
Si(3)	24(1)	32(1)	26(1)	3(1)	2(1)	6(1)
Ti(1)	20(1)	21(1)	21(1)	3(1)	5(1)	6(1)
Ti(2)	23(1)	24(1)	27(1)	3(1)	10(1)	6(1)

Data for compound 5

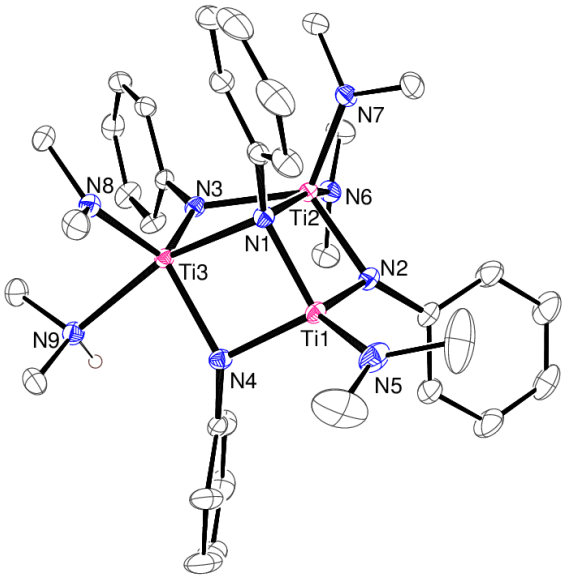


Table 1. Crystal data and structure refinement for **5**.

Identification code	cl549
Empirical formula	C34 H51 N9 Ti3
Formula weight	729.54
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 1 21/n 1
Unit cell dimensions	a = 10.501(2) A alpha = 90 deg. b = 27.443(5) A beta = 90.77(3) deg. c = 13.322(3) A gamma = 90 deg.
Volume	3838.8(13) A^3
Z, Calculated density	4, 1.262 Mg/m^3
Absorption coefficient	0.644 mm^-1
F(000)	1536
Crystal size	0.25 x 0.15 x 0.1 mm
Theta range for data collection	2.08 to 26.06 deg.
Limiting indices	-12<=h<=12, -33<=k<=33, -16<=l<=15
Reflections collected / unique	29677 / 7499 [R(int) = 0.0342]
Completeness to theta = 26.06	99.0 %
Absorption correction	Empirical (SHELXA)
Max. and min. transmission	0.834 and 0.483
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7499 / 0 / 425
Goodness-of-fit on F^2	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0330, wR2 = 0.0862
R indices (all data)	R1 = 0.0403, wR2 = 0.0906
Largest diff. peak and hole	0.555 and -0.373 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	8961(2)	1373(1)	6177(1)	26(1)
C(2)	9264(2)	960(1)	5614(1)	35(1)
C(3)	10053(2)	999(1)	4791(2)	49(1)
C(4)	10547(2)	1442(1)	4513(2)	57(1)
C(5)	10285(2)	1848(1)	5076(2)	53(1)
C(6)	9505(2)	1817(1)	5906(2)	38(1)
C(7)	8208(2)	1392(1)	10069(1)	29(1)
C(8)	9285(3)	1235(1)	10605(2)	48(1)
C(9)	9427(3)	1332(1)	11623(2)	59(1)
C(10)	8511(3)	1593(1)	12122(2)	55(1)
C(11)	7453(3)	1753(1)	11602(2)	58(1)
C(12)	7299(2)	1656(1)	10583(2)	43(1)
C(13)	6320(2)	5(1)	7392(1)	23(1)
C(14)	5324(2)	-154(1)	7995(1)	32(1)
C(15)	4998(2)	-643(1)	8047(2)	38(1)
C(16)	5652(2)	-985(1)	7501(2)	36(1)
C(17)	6610(2)	-835(1)	6878(2)	35(1)
C(18)	6941(2)	-347(1)	6817(1)	28(1)
C(19)	4810(2)	1696(1)	8297(1)	25(1)
C(20)	4110(2)	2131(1)	8279(2)	42(1)
C(21)	3096(3)	2200(1)	8920(2)	59(1)
C(22)	2755(2)	1844(1)	9592(2)	57(1)
C(23)	3431(2)	1413(1)	9623(2)	48(1)
C(24)	4444(2)	1336(1)	8982(1)	34(1)
C(25)	7569(4)	2813(1)	7488(3)	90(1)
C(26)	9262(4)	2545(2)	8575(3)	104(2)
C(27)	8684(2)	-234(1)	9394(2)	42(1)
C(28)	6991(2)	266(1)	9971(2)	40(1)
C(29)	10970(2)	888(1)	7935(2)	37(1)
C(30)	10312(2)	113(1)	7279(2)	37(1)
C(31)	6481(2)	1519(1)	4711(2)	37(1)
C(32)	6485(2)	639(1)	4667(2)	37(1)
C(33)	3564(2)	1425(1)	6045(2)	37(1)
C(34)	3680(2)	546(1)	6121(2)	38(1)
N(1)	8082(1)	1352(1)	6964(1)	22(1)
N(2)	8084(2)	1297(1)	9038(1)	27(1)
N(3)	6699(1)	494(1)	7361(1)	23(1)
N(4)	5828(1)	1632(1)	7643(1)	24(1)
N(5)	8134(2)	2408(1)	8042(1)	41(1)
N(6)	8028(2)	229(1)	9268(1)	28(1)
N(7)	9917(2)	551(1)	7803(1)	27(1)
N(8)	6367(2)	1073(1)	5288(1)	26(1)
N(9)	4119(2)	1004(1)	6593(1)	27(1)
Ti(1)	7550(1)	1750(1)	8010(1)	22(1)
Ti(2)	8247(1)	703(1)	8241(1)	21(1)
Ti(3)	6242(1)	1073(1)	6708(1)	19(1)

Table 3. Bond lengths [A] and angles [deg] for **5**.

C(1)-C(6)	1.396(3)
C(1)-C(2)	1.397(3)
C(1)-N(1)	1.408(2)
C(2)-C(3)	1.387(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.375(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.374(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.387(3)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-C(12)	1.387(3)
C(7)-C(8)	1.398(3)

C(7)-N(2)	1.402(2)
C(8)-C(9)	1.388(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.379(4)
C(9)-H(9)	0.9500
C(10)-C(11)	1.373(4)
C(10)-H(10)	0.9500
C(11)-C(12)	1.390(3)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(13)-C(14)	1.397(3)
C(13)-C(18)	1.399(2)
C(13)-N(3)	1.402(2)
C(14)-C(15)	1.387(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.377(3)
C(15)-H(15)	0.9500
C(16)-C(17)	1.376(3)
C(16)-H(16)	0.9500
C(17)-C(18)	1.385(3)
C(17)-H(17)	0.9500
C(18)-H(18)	0.9500
C(19)-N(4)	1.400(2)
C(19)-C(20)	1.401(3)
C(19)-C(24)	1.402(3)
C(20)-C(21)	1.387(3)
C(20)-H(20)	0.9500
C(21)-C(22)	1.376(4)
C(21)-H(21)	0.9500
C(22)-C(23)	1.380(4)
C(22)-H(22)	0.9500
C(23)-C(24)	1.389(3)
C(23)-H(23)	0.9500
C(24)-H(24)	0.9500
C(25)-N(5)	1.455(4)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-N(5)	1.424(4)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-N(6)	1.455(2)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-N(6)	1.450(3)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-N(7)	1.450(3)
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-N(7)	1.455(2)
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-N(8)	1.451(2)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-N(8)	1.457(2)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-N(9)	1.482(2)
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-N(9)	1.476(2)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
N(1)-Ti(1)	1.8622(14)
N(1)-Ti(3)	2.1024(15)
N(1)-Ti(2)	2.4668(14)

N(2)-Ti(1)	1.9279(16)
N(2)-Ti(2)	1.9527(15)
N(3)-Ti(3)	1.8702(14)
N(3)-Ti(2)	2.0723(16)
N(4)-Ti(1)	1.8954(16)
N(4)-Ti(3)	2.0254(15)
N(5)-Ti(1)	1.9071(17)
N(6)-Ti(2)	1.9044(15)
N(7)-Ti(2)	1.9030(16)
N(8)-Ti(3)	1.8976(15)
N(9)-Ti(3)	2.2407(16)
N(9)-H(9A)	0.9300
Ti(1)-Ti(3)	2.8786(7)
Ti(1)-Ti(2)	2.9796(7)
Ti(2)-Ti(3)	3.0850(9)

C(6)-C(1)-C(2)	118.17(18)
C(6)-C(1)-N(1)	120.18(17)
C(2)-C(1)-N(1)	121.56(17)
C(3)-C(2)-C(1)	120.3(2)
C(3)-C(2)-H(2)	119.8
C(1)-C(2)-H(2)	119.8
C(4)-C(3)-C(2)	120.8(2)
C(4)-C(3)-H(3)	119.6
C(2)-C(3)-H(3)	119.6
C(5)-C(4)-C(3)	119.4(2)
C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
C(4)-C(5)-C(6)	120.7(2)
C(4)-C(5)-H(5)	119.7
C(6)-C(5)-H(5)	119.7
C(5)-C(6)-C(1)	120.5(2)
C(5)-C(6)-H(6)	119.7
C(1)-C(6)-H(6)	119.7
C(12)-C(7)-C(8)	117.81(18)
C(12)-C(7)-N(2)	121.68(18)
C(8)-C(7)-N(2)	120.48(18)
C(9)-C(8)-C(7)	121.0(2)
C(9)-C(8)-H(8)	119.5
C(7)-C(8)-H(8)	119.5
C(10)-C(9)-C(8)	120.3(2)
C(10)-C(9)-H(9)	119.8
C(8)-C(9)-H(9)	119.8
C(11)-C(10)-C(9)	119.2(2)
C(11)-C(10)-H(10)	120.4
C(9)-C(10)-H(10)	120.4
C(10)-C(11)-C(12)	121.0(2)
C(10)-C(11)-H(11)	119.5
C(12)-C(11)-H(11)	119.5
C(7)-C(12)-C(11)	120.6(2)
C(7)-C(12)-H(12)	119.7
C(11)-C(12)-H(12)	119.7
C(14)-C(13)-C(18)	117.23(16)
C(14)-C(13)-N(3)	122.04(15)
C(18)-C(13)-N(3)	120.72(16)
C(15)-C(14)-C(13)	121.18(18)
C(15)-C(14)-H(14)	119.4
C(13)-C(14)-H(14)	119.4
C(16)-C(15)-C(14)	120.5(2)
C(16)-C(15)-H(15)	119.7
C(14)-C(15)-H(15)	119.7
C(17)-C(16)-C(15)	119.23(18)
C(17)-C(16)-H(16)	120.4
C(15)-C(16)-H(16)	120.4
C(16)-C(17)-C(18)	120.71(18)
C(16)-C(17)-H(17)	119.6
C(18)-C(17)-H(17)	119.6
C(17)-C(18)-C(13)	121.06(18)
C(17)-C(18)-H(18)	119.5
C(13)-C(18)-H(18)	119.5
N(4)-C(19)-C(20)	120.11(17)
N(4)-C(19)-C(24)	122.35(17)
C(20)-C(19)-C(24)	117.54(18)
C(21)-C(20)-C(19)	120.8(2)
C(21)-C(20)-H(20)	119.6
C(19)-C(20)-H(20)	119.6
C(22)-C(21)-C(20)	120.9(2)

C(22)-C(21)-H(21)	119.6
C(20)-C(21)-H(21)	119.6
C(21)-C(22)-C(23)	119.3(2)
C(21)-C(22)-H(22)	120.4
C(23)-C(22)-H(22)	120.4
C(22)-C(23)-C(24)	120.6(2)
C(22)-C(23)-H(23)	119.7
C(24)-C(23)-H(23)	119.7
C(23)-C(24)-C(19)	120.9(2)
C(23)-C(24)-H(24)	119.6
C(19)-C(24)-H(24)	119.6
N(5)-C(25)-H(25A)	109.5
N(5)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
N(5)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
N(5)-C(26)-H(26A)	109.5
N(5)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
N(5)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
N(6)-C(27)-H(27A)	109.5
N(6)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
N(6)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
N(6)-C(28)-H(28A)	109.5
N(6)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
N(6)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
N(7)-C(29)-H(29A)	109.5
N(7)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
N(7)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
N(7)-C(30)-H(30A)	109.5
N(7)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
N(7)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
N(8)-C(31)-H(31A)	109.5
N(8)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
N(8)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
N(8)-C(32)-H(32A)	109.5
N(8)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
N(8)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
N(9)-C(33)-H(33A)	109.5
N(9)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
N(9)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
N(9)-C(34)-H(34A)	109.5
N(9)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
N(9)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(1)-N(1)-Ti(1)	137.73(12)
C(1)-N(1)-Ti(3)	120.26(11)
Ti(1)-N(1)-Ti(3)	92.92(7)
C(1)-N(1)-Ti(2)	120.19(11)
Ti(1)-N(1)-Ti(2)	85.79(5)
Ti(3)-N(1)-Ti(2)	84.54(5)

C(7)-N(2)-Ti(1)	126.74(12)
C(7)-N(2)-Ti(2)	132.80(13)
Ti(1)-N(2)-Ti(2)	100.31(7)
C(13)-N(3)-Ti(3)	139.14(12)
C(13)-N(3)-Ti(2)	117.99(11)
Ti(3)-N(3)-Ti(2)	102.86(7)
C(19)-N(4)-Ti(1)	123.50(12)
C(19)-N(4)-Ti(3)	130.57(11)
Ti(1)-N(4)-Ti(3)	94.42(7)
C(26)-N(5)-C(25)	112.5(3)
C(26)-N(5)-Ti(1)	121.7(2)
C(25)-N(5)-Ti(1)	125.67(19)
C(28)-N(6)-C(27)	110.22(16)
C(28)-N(6)-Ti(2)	121.00(13)
C(27)-N(6)-Ti(2)	128.23(13)
C(29)-N(7)-C(30)	111.38(16)
C(29)-N(7)-Ti(2)	121.82(13)
C(30)-N(7)-Ti(2)	126.76(13)
C(31)-N(8)-C(32)	112.41(16)
C(31)-N(8)-Ti(3)	122.30(12)
C(32)-N(8)-Ti(3)	125.04(13)
C(34)-N(9)-C(33)	109.58(15)
C(34)-N(9)-Ti(3)	113.93(12)
C(33)-N(9)-Ti(3)	110.59(12)
C(34)-N(9)-H(9A)	107.5
C(33)-N(9)-H(9A)	107.5
Ti(3)-N(9)-H(9A)	107.5
N(1)-Ti(1)-N(4)	90.04(7)
N(1)-Ti(1)-N(5)	118.22(7)
N(4)-Ti(1)-N(5)	118.28(8)
N(1)-Ti(1)-N(2)	93.75(6)
N(4)-Ti(1)-N(2)	109.83(7)
N(5)-Ti(1)-N(2)	120.35(8)
N(1)-Ti(1)-Ti(3)	46.84(5)
N(4)-Ti(1)-Ti(3)	44.55(5)
N(5)-Ti(1)-Ti(3)	140.83(6)
N(2)-Ti(1)-Ti(3)	98.22(5)
N(1)-Ti(1)-Ti(2)	55.66(4)
N(4)-Ti(1)-Ti(2)	95.31(4)
N(5)-Ti(1)-Ti(2)	146.35(6)
N(2)-Ti(1)-Ti(2)	40.15(4)
Ti(3)-Ti(1)-Ti(2)	63.528(18)
N(7)-Ti(2)-N(6)	101.00(7)
N(7)-Ti(2)-N(2)	115.95(7)
N(6)-Ti(2)-N(2)	99.65(7)
N(7)-Ti(2)-N(3)	119.01(6)
N(6)-Ti(2)-N(3)	96.66(7)
N(2)-Ti(2)-N(3)	117.69(6)
N(7)-Ti(2)-N(1)	90.18(6)
N(6)-Ti(2)-N(1)	168.71(6)
N(2)-Ti(2)-N(1)	76.53(6)
N(3)-Ti(2)-N(1)	76.25(5)
N(7)-Ti(2)-Ti(1)	113.95(5)
N(6)-Ti(2)-Ti(1)	134.56(5)
N(2)-Ti(2)-Ti(1)	39.54(5)
N(3)-Ti(2)-Ti(1)	91.08(4)
N(1)-Ti(2)-Ti(1)	38.56(3)
N(7)-Ti(2)-Ti(3)	119.53(5)
N(6)-Ti(2)-Ti(3)	127.77(5)
N(2)-Ti(2)-Ti(3)	91.24(5)
N(3)-Ti(2)-Ti(3)	36.23(4)
N(1)-Ti(2)-Ti(3)	42.72(4)
Ti(1)-Ti(2)-Ti(3)	56.641(10)
N(3)-Ti(3)-N(8)	116.25(6)
N(3)-Ti(3)-N(4)	114.35(6)
N(8)-Ti(3)-N(4)	129.17(6)
N(3)-Ti(3)-N(1)	90.23(6)
N(8)-Ti(3)-N(1)	94.97(7)
N(4)-Ti(3)-N(1)	80.15(6)
N(3)-Ti(3)-N(9)	102.03(6)
N(8)-Ti(3)-N(9)	90.81(7)
N(4)-Ti(3)-N(9)	83.37(6)
N(1)-Ti(3)-N(9)	162.47(6)
N(3)-Ti(3)-Ti(1)	98.66(5)
N(8)-Ti(3)-Ti(1)	124.21(5)
N(4)-Ti(3)-Ti(1)	41.03(4)
N(1)-Ti(3)-Ti(1)	40.25(4)

N(9)-Ti(3)-Ti(1)	124.20(4)
N(3)-Ti(3)-Ti(2)	40.91(4)
N(8)-Ti(3)-Ti(2)	127.17(5)
N(4)-Ti(3)-Ti(2)	89.53(5)
N(1)-Ti(3)-Ti(2)	52.75(4)
N(9)-Ti(3)-Ti(2)	133.36(4)
Ti(1)-Ti(3)-Ti(2)	59.831(19)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **5**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	22(1)	38(1)	19(1)	2(1)	0(1)	2(1)
C(2)	32(1)	48(1)	24(1)	-4(1)	0(1)	8(1)
C(3)	35(1)	86(2)	25(1)	-7(1)	2(1)	20(1)
C(4)	31(1)	111(2)	30(1)	20(1)	11(1)	14(1)
C(5)	34(1)	76(2)	49(1)	30(1)	9(1)	-1(1)
C(6)	30(1)	44(1)	40(1)	13(1)	4(1)	-1(1)
C(7)	40(1)	26(1)	20(1)	-3(1)	0(1)	-5(1)
C(8)	65(2)	50(1)	29(1)	-9(1)	-11(1)	19(1)
C(9)	87(2)	58(2)	30(1)	-5(1)	-22(1)	13(1)
C(10)	86(2)	58(2)	22(1)	-9(1)	-4(1)	-14(1)
C(11)	58(2)	77(2)	39(1)	-28(1)	16(1)	-7(1)
C(12)	40(1)	56(1)	34(1)	-16(1)	1(1)	0(1)
C(13)	28(1)	18(1)	22(1)	0(1)	-4(1)	0(1)
C(14)	45(1)	23(1)	28(1)	-3(1)	8(1)	-2(1)
C(15)	53(1)	28(1)	32(1)	3(1)	7(1)	-10(1)
C(16)	50(1)	19(1)	40(1)	2(1)	-9(1)	-3(1)
C(17)	37(1)	23(1)	45(1)	-8(1)	-7(1)	7(1)
C(18)	26(1)	25(1)	33(1)	-3(1)	-2(1)	3(1)
C(19)	25(1)	25(1)	26(1)	-9(1)	0(1)	-2(1)
C(20)	40(1)	29(1)	58(1)	-8(1)	12(1)	4(1)
C(21)	48(2)	47(1)	83(2)	-24(1)	21(1)	8(1)
C(22)	41(1)	75(2)	55(2)	-28(1)	21(1)	-7(1)
C(23)	44(1)	68(2)	32(1)	-3(1)	9(1)	-18(1)
C(24)	34(1)	37(1)	30(1)	0(1)	1(1)	-4(1)
C(25)	79(2)	26(1)	164(4)	19(2)	26(2)	-1(1)
C(26)	117(3)	108(3)	86(2)	9(2)	-29(2)	-83(3)
C(27)	47(1)	36(1)	43(1)	11(1)	4(1)	8(1)
C(28)	42(1)	48(1)	30(1)	10(1)	7(1)	5(1)
C(29)	26(1)	46(1)	38(1)	-2(1)	0(1)	-6(1)
C(30)	30(1)	38(1)	41(1)	-6(1)	2(1)	6(1)
C(31)	43(1)	40(1)	28(1)	8(1)	-2(1)	2(1)
C(32)	43(1)	41(1)	27(1)	-11(1)	-8(1)	7(1)
C(33)	30(1)	40(1)	39(1)	1(1)	-8(1)	4(1)
C(34)	34(1)	36(1)	42(1)	-7(1)	-5(1)	-9(1)
N(1)	24(1)	22(1)	20(1)	0(1)	1(1)	-2(1)
N(2)	32(1)	28(1)	20(1)	-4(1)	0(1)	-1(1)
N(3)	27(1)	19(1)	22(1)	-1(1)	0(1)	-1(1)
N(4)	27(1)	19(1)	26(1)	-1(1)	2(1)	0(1)
N(5)	50(1)	27(1)	46(1)	-10(1)	8(1)	-13(1)
N(6)	29(1)	31(1)	25(1)	4(1)	-1(1)	2(1)
N(7)	24(1)	30(1)	26(1)	0(1)	-1(1)	0(1)
N(8)	29(1)	27(1)	22(1)	-1(1)	-2(1)	1(1)
N(9)	26(1)	29(1)	26(1)	-2(1)	-1(1)	-3(1)
Ti(1)	27(1)	18(1)	22(1)	-3(1)	1(1)	-3(1)
Ti(2)	23(1)	22(1)	19(1)	-1(1)	0(1)	1(1)
Ti(3)	23(1)	17(1)	18(1)	-1(1)	-1(1)	0(1)

Data for compound 7

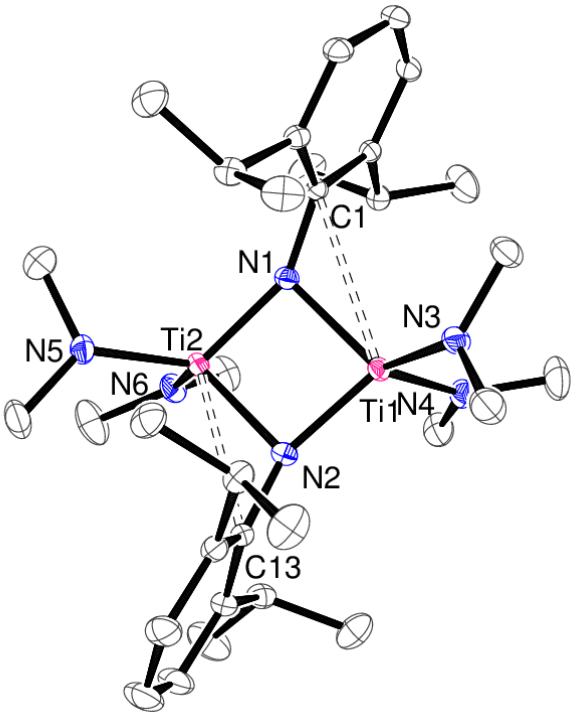


Table 1. Crystal data and structure refinement for **7**.

Identification code	cl1211
Empirical formula	C32 H58 N6 Ti2
Formula weight	622.64
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 9.7228(3) A alpha = 77.236(2) deg. b = 10.4433(3) A beta = 75.656(2) deg. c = 18.5184(5) A gamma = 79.334(2) deg.
Volume	1759.70(9) A^3
Z, Calculated density	2, 1.175 Mg/m^3
Absorption coefficient	0.482 mm^-1
F(000)	672
Crystal size	0.3 x 0.18 x 0.08 mm
Theta range for data collection	1.15 to 32.12 deg.
Limiting indices	-14<=h<=14, -15<=k<=15, -27<=l<=27
Reflections collected / unique	50964 / 12229 [R(int) = 0.0303]
Completeness to theta = 32.12	98.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.993 and 0.858
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12229 / 0 / 377
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0368, wR2 = 0.0918
R indices (all data)	R1 = 0.0571, wR2 = 0.1032
Largest diff. peak and hole	0.405 and -0.273 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **7**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	985(1)	937(1)	1969(1)	20(1)
C(2)	1398(1)	1081(1)	1167(1)	23(1)
C(3)	969(2)	222(1)	814(1)	30(1)
C(4)	143(2)	-750(1)	1221(1)	32(1)
C(5)	-319(1)	-848(1)	1997(1)	28(1)
C(6)	59(1)	-10(1)	2383(1)	21(1)
C(7)	2296(1)	2133(2)	680(1)	29(1)
C(8)	1565(2)	2988(2)	54(1)	46(1)
C(9)	3793(2)	1518(2)	322(1)	42(1)
C(10)	-568(1)	-41(1)	3220(1)	25(1)
C(11)	-1963(2)	917(2)	3320(1)	49(1)
C(12)	-800(2)	-1421(2)	3672(1)	54(1)
C(13)	4664(1)	3187(1)	2790(1)	22(1)
C(14)	5701(1)	3577(1)	2125(1)	27(1)
C(15)	6540(2)	4524(2)	2128(1)	41(1)
C(16)	6415(2)	5061(2)	2760(1)	50(1)
C(17)	5453(2)	4635(2)	3419(1)	42(1)
C(18)	4577(1)	3700(1)	3453(1)	28(1)
C(19)	5945(1)	3001(2)	1414(1)	31(1)
C(20)	5407(2)	4003(2)	775(1)	40(1)
C(21)	7533(2)	2493(2)	1134(1)	51(1)
C(22)	3628(2)	3166(2)	4200(1)	30(1)
C(23)	4451(2)	1905(2)	4580(1)	48(1)
C(24)	3092(2)	4144(2)	4739(1)	61(1)
C(25)	4077(2)	-1397(2)	1776(1)	40(1)
C(26)	6125(2)	-566(2)	1896(2)	62(1)
C(27)	3296(3)	-1946(2)	3775(1)	57(1)
C(28)	2164(2)	-107(2)	4362(1)	42(1)
C(29)	627(2)	5163(2)	1448(1)	58(1)
C(30)	2549(2)	5959(2)	1748(1)	50(1)
C(31)	-379(2)	2953(2)	4075(1)	45(1)
C(32)	122(2)	5138(2)	3548(1)	60(1)
N(1)	1518(1)	1674(1)	2364(1)	22(1)
N(2)	3711(1)	2318(1)	2794(1)	23(1)
N(3)	4574(1)	-421(1)	2060(1)	29(1)
N(4)	2905(1)	-511(1)	3652(1)	31(1)
N(5)	1795(1)	4843(1)	1837(1)	31(1)
N(6)	466(1)	3762(1)	3448(1)	32(1)
Ti(1)	3312(1)	676(1)	2697(1)	21(1)
Ti(2)	1819(1)	3261(1)	2572(1)	22(1)

Table 3. Bond lengths [A] and angles [deg] for **7**.

C(1)-N(1)	1.4085(15)
C(1)-C(2)	1.4191(16)
C(1)-C(6)	1.4248(16)
C(2)-C(3)	1.3930(18)
C(2)-C(7)	1.5201(18)
C(3)-C(4)	1.381(2)
C(3)-H(3)	0.9500
C(4)-C(5)	1.382(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.3915(17)
C(5)-H(5)	0.9500
C(6)-C(10)	1.5131(17)
C(7)-C(9)	1.528(2)
C(7)-C(8)	1.536(2)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(12)	1.524(2)
C(10)-C(11)	1.527(2)
C(10)-H(10)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-N(2)	1.4099(15)
C(13)-C(14)	1.4190(17)
C(13)-C(18)	1.4227(18)
C(14)-C(15)	1.395(2)
C(14)-C(19)	1.515(2)
C(15)-C(16)	1.375(2)
C(15)-H(15)	0.9500
C(16)-C(17)	1.382(2)
C(16)-H(16)	0.9500
C(17)-C(18)	1.3905(19)
C(17)-H(17)	0.9500
C(18)-C(22)	1.5140(19)
C(19)-C(20)	1.5257(19)
C(19)-C(21)	1.535(2)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(24)	1.519(2)
C(22)-C(23)	1.532(2)
C(22)-H(22)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800

C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-N(3)	1.4476(18)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-N(3)	1.448(2)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-N(4)	1.457(2)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-N(4)	1.445(2)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-N(5)	1.442(2)
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-N(5)	1.4472(19)
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-N(6)	1.446(2)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-N(6)	1.456(2)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
N(1)-Ti(2)	1.8694(10)
N(1)-Ti(1)	2.0211(10)
N(2)-Ti(1)	1.8818(11)
N(2)-Ti(2)	2.0123(11)
N(3)-Ti(1)	1.8890(11)
N(4)-Ti(1)	1.9197(11)
N(5)-Ti(2)	1.8948(11)
N(6)-Ti(2)	1.9224(12)
Ti(1)-Ti(2)	2.8089(3)

N(1)-C(1)-C(2)	121.26(10)
N(1)-C(1)-C(6)	119.36(10)
C(2)-C(1)-C(6)	119.33(11)
C(3)-C(2)-C(1)	118.75(12)
C(3)-C(2)-C(7)	118.69(11)
C(1)-C(2)-C(7)	122.56(11)
C(4)-C(3)-C(2)	121.82(12)
C(4)-C(3)-H(3)	119.1
C(2)-C(3)-H(3)	119.1
C(3)-C(4)-C(5)	119.40(12)
C(3)-C(4)-H(4)	120.3
C(5)-C(4)-H(4)	120.3
C(4)-C(5)-C(6)	121.56(12)
C(4)-C(5)-H(5)	119.2
C(6)-C(5)-H(5)	119.2
C(5)-C(6)-C(1)	118.90(11)

C(5)-C(6)-C(10)	120.91(11)
C(1)-C(6)-C(10)	120.10(11)
C(2)-C(7)-C(9)	111.63(12)
C(2)-C(7)-C(8)	111.47(11)
C(9)-C(7)-C(8)	109.47(12)
C(2)-C(7)-H(7)	108.0
C(9)-C(7)-H(7)	108.0
C(8)-C(7)-H(7)	108.0
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(6)-C(10)-C(12)	113.90(12)
C(6)-C(10)-C(11)	109.47(11)
C(12)-C(10)-C(11)	110.78(14)
C(6)-C(10)-H(10)	107.5
C(12)-C(10)-H(10)	107.5
C(11)-C(10)-H(10)	107.5
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
N(2)-C(13)-C(14)	120.62(11)
N(2)-C(13)-C(18)	120.09(11)
C(14)-C(13)-C(18)	119.29(11)
C(15)-C(14)-C(13)	118.63(13)
C(15)-C(14)-C(19)	118.55(12)
C(13)-C(14)-C(19)	122.82(12)
C(16)-C(15)-C(14)	121.98(15)
C(16)-C(15)-H(15)	119.0
C(14)-C(15)-H(15)	119.0
C(15)-C(16)-C(17)	119.40(14)
C(15)-C(16)-H(16)	120.3
C(17)-C(16)-H(16)	120.3
C(16)-C(17)-C(18)	121.55(15)
C(16)-C(17)-H(17)	119.2
C(18)-C(17)-H(17)	119.2
C(17)-C(18)-C(13)	119.00(13)
C(17)-C(18)-C(22)	120.28(13)
C(13)-C(18)-C(22)	120.57(11)
C(14)-C(19)-C(20)	111.99(13)
C(14)-C(19)-C(21)	111.80(13)
C(20)-C(19)-C(21)	109.06(12)
C(14)-C(19)-H(19)	107.9
C(20)-C(19)-H(19)	107.9

C(21)-C(19)-H(19)	107.9
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(18)-C(22)-C(24)	114.46(14)
C(18)-C(22)-C(23)	108.50(12)
C(24)-C(22)-C(23)	110.25(14)
C(18)-C(22)-H(22)	107.8
C(24)-C(22)-H(22)	107.8
C(23)-C(22)-H(22)	107.8
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
N(3)-C(25)-H(25A)	109.5
N(3)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
N(3)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
N(3)-C(26)-H(26A)	109.5
N(3)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
N(3)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
N(4)-C(27)-H(27A)	109.5
N(4)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
N(4)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
N(4)-C(28)-H(28A)	109.5
N(4)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
N(4)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
N(5)-C(29)-H(29A)	109.5
N(5)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
N(5)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5

N(5)-C(30)-H(30A)	109.5
N(5)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
N(5)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
N(6)-C(31)-H(31A)	109.5
N(6)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
N(6)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
N(6)-C(32)-H(32A)	109.5
N(6)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
N(6)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(1)-N(1)-Ti(2)	152.99(8)
C(1)-N(1)-Ti(1)	111.28(8)
Ti(2)-N(1)-Ti(1)	92.36(4)
C(13)-N(2)-Ti(1)	152.28(9)
C(13)-N(2)-Ti(2)	113.34(8)
Ti(1)-N(2)-Ti(2)	92.27(4)
C(25)-N(3)-C(26)	111.23(13)
C(25)-N(3)-Ti(1)	121.92(10)
C(26)-N(3)-Ti(1)	126.12(11)
C(28)-N(4)-C(27)	109.64(13)
C(28)-N(4)-Ti(1)	124.73(10)
C(27)-N(4)-Ti(1)	125.62(11)
C(29)-N(5)-C(30)	112.67(13)
C(29)-N(5)-Ti(2)	116.87(11)
C(30)-N(5)-Ti(2)	128.22(11)
C(31)-N(6)-C(32)	109.15(13)
C(31)-N(6)-Ti(2)	129.58(10)
C(32)-N(6)-Ti(2)	121.24(11)
N(2)-Ti(1)-N(3)	123.11(5)
N(2)-Ti(1)-N(4)	112.91(5)
N(3)-Ti(1)-N(4)	103.09(5)
N(2)-Ti(1)-N(1)	87.07(4)
N(3)-Ti(1)-N(1)	118.01(5)
N(4)-Ti(1)-N(1)	112.69(5)
N(2)-Ti(1)-Ti(2)	45.71(3)
N(3)-Ti(1)-Ti(2)	138.42(4)
N(4)-Ti(1)-Ti(2)	118.13(4)
N(1)-Ti(1)-Ti(2)	41.68(3)
N(1)-Ti(2)-N(5)	121.12(5)
N(1)-Ti(2)-N(6)	112.28(5)
N(5)-Ti(2)-N(6)	103.44(5)
N(1)-Ti(2)-N(2)	87.67(4)
N(5)-Ti(2)-N(2)	118.81(5)
N(6)-Ti(2)-N(2)	113.65(5)
N(1)-Ti(2)-Ti(1)	45.96(3)
N(5)-Ti(2)-Ti(1)	137.90(4)
N(6)-Ti(2)-Ti(1)	118.56(4)
N(2)-Ti(2)-Ti(1)	42.02(3)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **7**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	18(1)	20(1)	22(1)	-5(1)	-6(1)	-1(1)
C(2)	22(1)	27(1)	21(1)	-6(1)	-5(1)	-2(1)
C(3)	34(1)	34(1)	24(1)	-11(1)	-9(1)	-3(1)
C(4)	35(1)	31(1)	36(1)	-13(1)	-15(1)	-4(1)
C(5)	26(1)	24(1)	36(1)	-5(1)	-10(1)	-6(1)
C(6)	19(1)	20(1)	25(1)	-4(1)	-6(1)	-2(1)
C(7)	30(1)	37(1)	20(1)	-6(1)	-1(1)	-10(1)
C(8)	48(1)	50(1)	36(1)	9(1)	-12(1)	-16(1)
C(9)	32(1)	61(1)	34(1)	-16(1)	4(1)	-12(1)
C(10)	24(1)	25(1)	25(1)	-2(1)	-3(1)	-6(1)
C(11)	34(1)	73(1)	35(1)	-19(1)	-5(1)	13(1)
C(12)	86(1)	38(1)	35(1)	3(1)	-3(1)	-28(1)
C(13)	21(1)	21(1)	26(1)	-3(1)	-8(1)	-3(1)
C(14)	24(1)	30(1)	27(1)	2(1)	-8(1)	-6(1)
C(15)	36(1)	47(1)	42(1)	4(1)	-10(1)	-21(1)
C(16)	56(1)	50(1)	55(1)	-6(1)	-17(1)	-33(1)
C(17)	50(1)	44(1)	43(1)	-14(1)	-16(1)	-19(1)
C(18)	29(1)	27(1)	30(1)	-7(1)	-10(1)	-5(1)
C(19)	28(1)	35(1)	25(1)	1(1)	-2(1)	-6(1)
C(20)	42(1)	47(1)	29(1)	4(1)	-10(1)	-9(1)
C(21)	36(1)	63(1)	44(1)	-6(1)	1(1)	3(1)
C(22)	30(1)	36(1)	27(1)	-14(1)	-6(1)	-3(1)
C(23)	39(1)	64(1)	34(1)	4(1)	-9(1)	-2(1)
C(24)	67(1)	67(1)	57(1)	-41(1)	10(1)	-19(1)
C(25)	38(1)	34(1)	53(1)	-20(1)	-11(1)	-4(1)
C(26)	33(1)	45(1)	120(2)	-32(1)	-30(1)	5(1)
C(27)	90(2)	28(1)	47(1)	2(1)	-17(1)	0(1)
C(28)	56(1)	39(1)	26(1)	-1(1)	-6(1)	-8(1)
C(29)	58(1)	44(1)	79(1)	-8(1)	-40(1)	2(1)
C(30)	43(1)	23(1)	83(1)	-3(1)	-15(1)	-6(1)
C(31)	53(1)	41(1)	36(1)	-13(1)	5(1)	-8(1)
C(32)	78(1)	37(1)	59(1)	-26(1)	12(1)	-7(1)
N(1)	24(1)	22(1)	20(1)	-4(1)	-5(1)	-6(1)
N(2)	23(1)	25(1)	22(1)	-7(1)	-4(1)	-6(1)
N(3)	28(1)	29(1)	35(1)	-15(1)	-7(1)	1(1)
N(4)	41(1)	24(1)	28(1)	-1(1)	-11(1)	-3(1)
N(5)	32(1)	23(1)	37(1)	1(1)	-10(1)	-5(1)
N(6)	31(1)	28(1)	36(1)	-13(1)	-3(1)	-1(1)
Ti(1)	24(1)	19(1)	21(1)	-6(1)	-5(1)	-2(1)
Ti(2)	23(1)	18(1)	24(1)	-5(1)	-6(1)	-3(1)

Data for compound 8

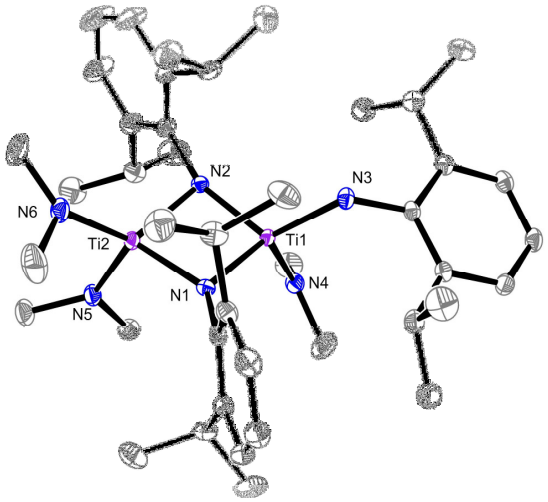


Table 1. Crystal data and structure refinement for **8**.

Identification code	cl1628
Empirical formula	C42 H70 N6 Ti2
Formula weight	754.84
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P b c a
Unit cell dimensions	a = 11.1946(7) A alpha = 90 deg. b = 20.0122(12) A beta = 90 deg. c = 38.540(2) A gamma = 90 deg.
Volume	8634.0(9) A^3
Z, Calculated density	8, 1.161 Mg/m^3
Absorption coefficient	0.404 mm^-1
F(000)	3264
Crystal size	0.15 x 0.1 x 0.02 mm
Theta range for data collection	2.62 to 26.37 deg.
Limiting indices	-10<=h<=13, -25<=k<=25, -47<=l<=48
Reflections collected / unique	77764 / 8799 [R(int) = 0.0524]
Completeness to theta = 26.37	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.975 and 0.883
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8799 / 0 / 473
Goodness-of-fit on F^2	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0370, wR2 = 0.0861
R indices (all data)	R1 = 0.0654, wR2 = 0.0994
Largest diff. peak and hole	0.296 and -0.312 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **8**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	5179(2)	4550(1)	1238(1)	23(1)
C(2)	4513(2)	4825(1)	959(1)	29(1)
C(3)	4898(2)	5420(1)	811(1)	38(1)
C(4)	5883(2)	5758(1)	935(1)	40(1)
C(5)	6475(2)	5513(1)	1220(1)	36(1)
C(6)	6146(2)	4916(1)	1376(1)	26(1)
C(7)	3383(2)	4504(1)	821(1)	37(1)
C(8)	2328(2)	5000(1)	805(1)	55(1)
C(9)	3574(2)	4205(1)	465(1)	53(1)
C(10)	6781(2)	4703(1)	1705(1)	32(1)
C(11)	6233(2)	5060(1)	2016(1)	49(1)
C(12)	8137(2)	4827(1)	1694(1)	53(1)
C(13)	3103(2)	2273(1)	1522(1)	26(1)
C(14)	2168(2)	2253(1)	1273(1)	32(1)
C(15)	1146(2)	1888(1)	1348(1)	54(1)
C(16)	1029(2)	1543(2)	1655(1)	70(1)
C(17)	1946(2)	1546(2)	1893(1)	59(1)
C(18)	2989(2)	1906(1)	1837(1)	35(1)
C(19)	2256(2)	2587(1)	922(1)	33(1)
C(20)	2297(2)	2066(1)	634(1)	53(1)
C(21)	1243(2)	3081(1)	856(1)	48(1)
C(22)	4001(2)	1853(1)	2093(1)	36(1)
C(23)	4589(3)	1165(1)	2068(1)	60(1)
C(24)	3609(3)	1991(2)	2466(1)	61(1)
C(25)	6544(2)	2648(1)	535(1)	23(1)
C(26)	6651(2)	1980(1)	421(1)	25(1)
C(27)	7722(2)	1780(1)	270(1)	30(1)
C(28)	8658(2)	2216(1)	223(1)	33(1)
C(29)	8523(2)	2875(1)	319(1)	31(1)
C(30)	7478(2)	3107(1)	472(1)	27(1)
C(31)	5624(2)	1491(1)	469(1)	31(1)
C(32)	5566(2)	1222(1)	842(1)	42(1)
C(33)	5645(2)	908(1)	215(1)	42(1)
C(34)	7312(2)	3849(1)	538(1)	36(1)
C(35)	8460(2)	4211(1)	647(1)	49(1)
C(36)	6797(3)	4174(1)	212(1)	58(1)
C(37)	7927(2)	3140(1)	1394(1)	51(1)
C(38)	7094(2)	2126(1)	1615(1)	49(1)
C(39)	5577(2)	3372(1)	2236(1)	34(1)
C(40)	3778(2)	3880(1)	2446(1)	45(1)
C(41)	2269(3)	4635(1)	1747(1)	72(1)
C(42)	1006(2)	3654(2)	1755(1)	66(1)
N(1)	4889(1)	3909(1)	1370(1)	21(1)
N(2)	4137(1)	2656(1)	1460(1)	22(1)
N(3)	5515(2)	2862(1)	720(1)	26(1)
N(4)	6864(1)	2728(1)	1418(1)	28(1)
N(5)	4368(2)	3581(1)	2146(1)	30(1)
N(6)	2208(2)	3916(1)	1715(1)	35(1)
Ti(1)	5405(1)	3019(1)	1217(1)	19(1)
Ti(2)	3744(1)	3536(1)	1685(1)	22(1)

Table 3. Bond lengths [A] and angles [deg] for **8**.

C(1)-C(6)	1.413(3)
C(1)-N(1)	1.418(2)
C(1)-C(2)	1.418(3)
C(2)-C(3)	1.389(3)
C(2)-C(7)	1.516(3)
C(3)-C(4)	1.379(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.374(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.388(3)
C(5)-H(5)	0.9500
C(6)-C(10)	1.515(3)
C(7)-C(9)	1.513(3)
C(7)-C(8)	1.543(3)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.525(3)
C(10)-C(12)	1.539(3)
C(10)-H(10)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-N(2)	1.409(2)
C(13)-C(14)	1.421(3)
C(13)-C(18)	1.425(3)
C(13)-Ti(2)	2.7014(19)
C(14)-C(15)	1.388(3)
C(14)-C(19)	1.511(3)
C(15)-C(16)	1.376(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.378(4)
C(16)-H(16)	0.9500
C(17)-C(18)	1.388(3)
C(17)-H(17)	0.9500
C(18)-C(22)	1.507(3)
C(19)-C(20)	1.522(3)
C(19)-C(21)	1.525(3)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.528(3)
C(22)-C(24)	1.529(3)
C(22)-H(22)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(26)	1.413(3)
C(25)-C(30)	1.414(3)
C(25)-N(3)	1.421(2)
C(26)-C(27)	1.392(3)
C(26)-C(31)	1.520(3)
C(27)-C(28)	1.375(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.378(3)
C(28)-H(28)	0.9500
C(29)-C(30)	1.390(3)
C(29)-H(29)	0.9500
C(30)-C(34)	1.518(3)

C(31)-C(33)	1.522(3)
C(31)-C(32)	1.537(3)
C(31)-H(31)	1.0000
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(36)	1.529(3)
C(34)-C(35)	1.533(3)
C(34)-H(34)	1.0000
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-N(4)	1.451(3)
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-N(4)	1.445(3)
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-N(5)	1.458(3)
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-N(5)	1.458(3)
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-N(6)	1.445(3)
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-N(6)	1.452(3)
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
N(1)-Ti(2)	1.9173(16)
N(1)-Ti(1)	1.9626(15)
N(2)-Ti(1)	1.8485(15)
N(2)-Ti(2)	2.0139(15)
N(3)-Ti(1)	1.9442(17)
N(3)-H(3A)	0.75(3)
N(4)-Ti(1)	1.8993(16)
N(5)-Ti(2)	1.9115(17)
N(6)-Ti(2)	1.8829(17)
Ti(1)-Ti(2)	2.7896(5)

C(6)-C(1)-N(1)	120.52(17)
C(6)-C(1)-C(2)	119.21(17)
N(1)-C(1)-C(2)	120.27(17)
C(3)-C(2)-C(1)	118.79(19)
C(3)-C(2)-C(7)	118.46(19)
C(1)-C(2)-C(7)	122.73(18)
C(4)-C(3)-C(2)	121.7(2)
C(4)-C(3)-H(3)	119.1
C(2)-C(3)-H(3)	119.1
C(5)-C(4)-C(3)	119.2(2)
C(5)-C(4)-H(4)	120.4
C(3)-C(4)-H(4)	120.4
C(4)-C(5)-C(6)	121.8(2)
C(4)-C(5)-H(5)	119.1
C(6)-C(5)-H(5)	119.1
C(5)-C(6)-C(1)	119.02(19)
C(5)-C(6)-C(10)	118.81(18)
C(1)-C(6)-C(10)	122.03(17)
C(9)-C(7)-C(2)	111.7(2)
C(9)-C(7)-C(8)	109.2(2)
C(2)-C(7)-C(8)	112.31(19)
C(9)-C(7)-H(7)	107.8
C(2)-C(7)-H(7)	107.8
C(8)-C(7)-H(7)	107.8

C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(6)-C(10)-C(11)	109.66(18)
C(6)-C(10)-C(12)	113.09(19)
C(11)-C(10)-C(12)	110.2(2)
C(6)-C(10)-H(10)	107.9
C(11)-C(10)-H(10)	107.9
C(12)-C(10)-H(10)	107.9
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
N(2)-C(13)-C(14)	120.39(18)
N(2)-C(13)-C(18)	119.96(18)
C(14)-C(13)-C(18)	119.65(18)
N(2)-C(13)-Ti(2)	46.63(8)
C(14)-C(13)-Ti(2)	112.32(14)
C(18)-C(13)-Ti(2)	107.98(14)
C(15)-C(14)-C(13)	118.7(2)
C(15)-C(14)-C(19)	118.2(2)
C(13)-C(14)-C(19)	122.97(18)
C(16)-C(15)-C(14)	121.5(2)
C(16)-C(15)-H(15)	119.2
C(14)-C(15)-H(15)	119.2
C(15)-C(16)-C(17)	119.9(2)
C(15)-C(16)-H(16)	120.0
C(17)-C(16)-H(16)	120.0
C(16)-C(17)-C(18)	121.7(2)
C(16)-C(17)-H(17)	119.2
C(18)-C(17)-H(17)	119.2
C(17)-C(18)-C(13)	118.4(2)
C(17)-C(18)-C(22)	119.6(2)
C(13)-C(18)-C(22)	121.81(18)
C(14)-C(19)-C(20)	110.54(19)
C(14)-C(19)-C(21)	112.72(19)
C(20)-C(19)-C(21)	110.24(19)
C(14)-C(19)-H(19)	107.7
C(20)-C(19)-H(19)	107.7
C(21)-C(19)-H(19)	107.7
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(18)-C(22)-C(23)	110.3(2)
C(18)-C(22)-C(24)	112.8(2)
C(23)-C(22)-C(24)	110.2(2)
C(18)-C(22)-H(22)	107.8
C(23)-C(22)-H(22)	107.8
C(24)-C(22)-H(22)	107.8
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5

H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(26)-C(25)-C(30)	119.87(17)
C(26)-C(25)-N(3)	120.71(18)
C(30)-C(25)-N(3)	119.41(17)
C(27)-C(26)-C(25)	118.43(18)
C(27)-C(26)-C(31)	121.11(18)
C(25)-C(26)-C(31)	120.45(17)
C(28)-C(27)-C(26)	121.93(19)
C(28)-C(27)-H(27)	119.0
C(26)-C(27)-H(27)	119.0
C(27)-C(28)-C(29)	119.22(19)
C(27)-C(28)-H(28)	120.4
C(29)-C(28)-H(28)	120.4
C(28)-C(29)-C(30)	121.7(2)
C(28)-C(29)-H(29)	119.1
C(30)-C(29)-H(29)	119.1
C(29)-C(30)-C(25)	118.63(18)
C(29)-C(30)-C(34)	120.06(18)
C(25)-C(30)-C(34)	121.06(18)
C(26)-C(31)-C(33)	113.84(18)
C(26)-C(31)-C(32)	111.74(17)
C(33)-C(31)-C(32)	109.40(18)
C(26)-C(31)-H(31)	107.2
C(33)-C(31)-H(31)	107.2
C(32)-C(31)-H(31)	107.2
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(30)-C(34)-C(36)	109.00(19)
C(30)-C(34)-C(35)	113.89(19)
C(36)-C(34)-C(35)	109.9(2)
C(30)-C(34)-H(34)	108.0
C(36)-C(34)-H(34)	108.0
C(35)-C(34)-H(34)	108.0
C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
N(4)-C(37)-H(37A)	109.5
N(4)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
N(4)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
N(4)-C(38)-H(38A)	109.5
N(4)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
N(4)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
N(5)-C(39)-H(39A)	109.5

N(5)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
N(5)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
N(5)-C(40)-H(40A)	109.5
N(5)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
N(5)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
N(6)-C(41)-H(41A)	109.5
N(6)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
N(6)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
N(6)-C(42)-H(42A)	109.5
N(6)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
N(6)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(1)-N(1)-Ti(2)	137.15(12)
C(1)-N(1)-Ti(1)	130.17(12)
Ti(2)-N(1)-Ti(1)	91.94(6)
C(13)-N(2)-Ti(1)	158.65(14)
C(13)-N(2)-Ti(2)	102.80(12)
Ti(1)-N(2)-Ti(2)	92.38(6)
C(25)-N(3)-Ti(1)	126.45(14)
C(25)-N(3)-H(3A)	115(2)
Ti(1)-N(3)-H(3A)	111(2)
C(38)-N(4)-C(37)	111.21(18)
C(38)-N(4)-Ti(1)	128.54(15)
C(37)-N(4)-Ti(1)	120.23(15)
C(39)-N(5)-C(40)	110.50(17)
C(39)-N(5)-Ti(2)	123.12(13)
C(40)-N(5)-Ti(2)	126.11(14)
C(41)-N(6)-C(42)	113.2(2)
C(41)-N(6)-Ti(2)	111.34(17)
C(42)-N(6)-Ti(2)	134.92(18)
N(2)-Ti(1)-N(4)	109.42(7)
N(2)-Ti(1)-N(3)	118.81(7)
N(4)-Ti(1)-N(3)	107.35(7)
N(2)-Ti(1)-N(1)	88.83(7)
N(4)-Ti(1)-N(1)	114.15(7)
N(3)-Ti(1)-N(1)	117.48(7)
N(2)-Ti(1)-Ti(2)	46.16(5)
N(4)-Ti(1)-Ti(2)	115.02(5)
N(3)-Ti(1)-Ti(2)	137.62(5)
N(1)-Ti(1)-Ti(2)	43.38(5)
N(6)-Ti(2)-N(5)	105.01(7)
N(6)-Ti(2)-N(1)	119.44(7)
N(5)-Ti(2)-N(1)	109.02(7)
N(6)-Ti(2)-N(2)	125.40(7)
N(5)-Ti(2)-N(2)	111.22(7)
N(1)-Ti(2)-N(2)	85.46(6)
N(6)-Ti(2)-C(13)	98.60(7)
N(5)-Ti(2)-C(13)	110.92(7)
N(1)-Ti(2)-C(13)	113.23(6)
N(2)-Ti(2)-C(13)	30.57(6)
N(6)-Ti(2)-Ti(1)	142.88(6)
N(5)-Ti(2)-Ti(1)	111.98(5)
N(1)-Ti(2)-Ti(1)	44.68(4)
N(2)-Ti(2)-Ti(1)	41.46(4)
C(13)-Ti(2)-Ti(1)	71.32(4)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **8**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12

C(1)	26(1)	19(1)	22(1)	-2(1)	5(1)	2(1)
C(2)	35(1)	25(1)	27(1)	-1(1)	-1(1)	4(1)
C(3)	53(1)	30(1)	31(1)	6(1)	0(1)	4(1)
C(4)	56(2)	24(1)	39(1)	6(1)	11(1)	-4(1)
C(5)	38(1)	28(1)	41(1)	-3(1)	4(1)	-9(1)
C(6)	27(1)	23(1)	29(1)	-4(1)	3(1)	0(1)
C(7)	41(1)	38(1)	32(1)	6(1)	-12(1)	1(1)
C(8)	44(2)	61(2)	60(2)	3(1)	-7(1)	12(1)
C(9)	61(2)	54(2)	45(2)	-9(1)	-18(1)	2(1)
C(10)	31(1)	28(1)	38(1)	-2(1)	-6(1)	-5(1)
C(11)	69(2)	43(1)	34(1)	-6(1)	-10(1)	-1(1)
C(12)	37(1)	56(2)	68(2)	5(1)	-18(1)	-14(1)
C(13)	24(1)	25(1)	30(1)	-1(1)	4(1)	-4(1)
C(14)	25(1)	36(1)	36(1)	2(1)	-1(1)	-7(1)
C(15)	34(1)	73(2)	56(2)	15(1)	-8(1)	-23(1)
C(16)	43(2)	93(2)	75(2)	27(2)	1(2)	-37(2)
C(17)	49(2)	74(2)	53(2)	26(2)	3(1)	-25(1)
C(18)	36(1)	36(1)	33(1)	5(1)	4(1)	-6(1)
C(19)	24(1)	44(1)	32(1)	3(1)	-4(1)	-10(1)
C(20)	54(2)	58(2)	47(2)	-9(1)	12(1)	-7(1)
C(21)	38(1)	60(2)	47(2)	7(1)	-7(1)	5(1)
C(22)	45(1)	31(1)	33(1)	7(1)	0(1)	-7(1)
C(23)	65(2)	38(1)	78(2)	7(1)	-14(2)	1(1)
C(24)	81(2)	66(2)	35(1)	8(1)	5(1)	-18(2)
C(25)	25(1)	28(1)	16(1)	2(1)	-1(1)	4(1)
C(26)	28(1)	29(1)	20(1)	4(1)	-2(1)	3(1)
C(27)	33(1)	29(1)	28(1)	-4(1)	1(1)	8(1)
C(28)	25(1)	44(1)	30(1)	-4(1)	4(1)	9(1)
C(29)	27(1)	39(1)	27(1)	0(1)	2(1)	-2(1)
C(30)	31(1)	30(1)	20(1)	-1(1)	2(1)	1(1)
C(31)	31(1)	30(1)	33(1)	2(1)	-3(1)	1(1)
C(32)	50(2)	38(1)	39(1)	6(1)	4(1)	-8(1)
C(33)	49(2)	34(1)	44(1)	-4(1)	-8(1)	-3(1)
C(34)	41(1)	30(1)	37(1)	-4(1)	12(1)	-2(1)
C(35)	56(2)	36(1)	54(2)	-9(1)	15(1)	-14(1)
C(36)	73(2)	38(1)	63(2)	11(1)	0(2)	10(1)
C(37)	27(1)	57(2)	68(2)	3(1)	7(1)	-1(1)
C(38)	45(1)	36(1)	64(2)	5(1)	-11(1)	14(1)
C(39)	32(1)	39(1)	30(1)	1(1)	-4(1)	-1(1)
C(40)	43(1)	65(2)	28(1)	-11(1)	5(1)	3(1)
C(41)	89(2)	52(2)	75(2)	-5(2)	21(2)	29(2)
C(42)	27(1)	110(3)	61(2)	-21(2)	13(1)	2(1)
N(1)	22(1)	19(1)	23(1)	-1(1)	-2(1)	-1(1)
N(2)	22(1)	21(1)	22(1)	0(1)	0(1)	-2(1)
N(3)	22(1)	33(1)	24(1)	-1(1)	2(1)	2(1)
N(4)	24(1)	30(1)	30(1)	-3(1)	-1(1)	5(1)
N(5)	28(1)	38(1)	24(1)	-5(1)	2(1)	3(1)
N(6)	25(1)	45(1)	35(1)	-6(1)	2(1)	10(1)
Ti(1)	18(1)	20(1)	20(1)	-1(1)	2(1)	0(1)
Ti(2)	18(1)	25(1)	22(1)	-3(1)	1(1)	2(1)

Data for compound 9

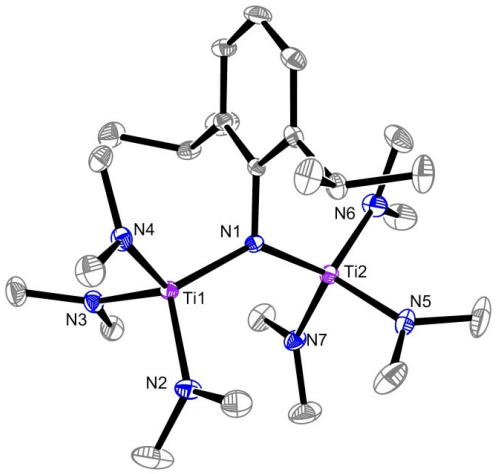


Table 1. Crystal data and structure refinement for **9**.

Identification code	cl1640
Empirical formula	C24 H53 N7 Ti2
Formula weight	535.53
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P b c a
Unit cell dimensions	a = 17.0404(7) A alpha = 90 deg.
	b = 16.0775(6) A beta = 90 deg.
	c = 23.1921(9) A gamma = 90 deg.
Volume	6353.9(4) A^3
Z, Calculated density	8, 1.12 Mg/m^3
Absorption coefficient	0.525 mm^-1
F(000)	2320
Crystal size	0.18 x 0.1 x 0.03 mm
Theta range for data collection	2.84 to 26.04 deg.
Limiting indices	-21<=h<=20, -19<=k<=15, -28<=l<=28
Reflections collected / unique	63139 / 6262 [R(int) = 0.0714]
Completeness to theta = 26.04	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.975 and 0.883
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6262 / 0 / 314
Goodness-of-fit on F^2	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0402, wR2 = 0.0908
R indices (all data)	R1 = 0.0726, wR2 = 0.1052
Largest diff. peak and hole	0.347 and -0.346 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **9**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	86(1)	2919(1)	1271(1)	25(1)
C(2)	-582(1)	2415(2)	1372(1)	34(1)
C(3)	-1305(2)	2789(2)	1441(1)	45(1)
C(4)	-1390(2)	3642(2)	1418(1)	50(1)
C(5)	-739(2)	4134(2)	1328(1)	42(1)
C(6)	4(1)	3797(1)	1258(1)	30(1)
C(7)	-516(2)	1471(2)	1411(1)	40(1)
C(8)	-687(2)	1150(2)	2014(1)	69(1)
C(9)	-1029(2)	1032(2)	975(1)	61(1)
C(10)	701(2)	4366(1)	1172(1)	38(1)
C(11)	814(2)	4955(2)	1680(2)	68(1)
C(12)	625(2)	4854(2)	610(2)	63(1)
C(13)	2356(2)	1191(2)	-39(2)	94(1)
C(14)	1250(2)	492(2)	376(1)	63(1)
C(15)	1520(2)	3467(2)	-580(1)	62(1)
C(16)	2313(2)	3438(2)	272(1)	52(1)
C(17)	-485(2)	2802(2)	-118(1)	46(1)
C(18)	-33(2)	1539(2)	-543(1)	62(1)
C(19)	1423(3)	1125(3)	2782(2)	102(2)
C(20)	1610(3)	707(2)	1810(2)	86(1)
C(21)	284(2)	3207(2)	2702(1)	72(1)
C(22)	1616(2)	3469(3)	2962(2)	81(1)
C(23)	2792(2)	3600(2)	1751(2)	62(1)
C(24)	3186(2)	2187(2)	1713(2)	85(1)
N(1)	835(1)	2545(1)	1182(1)	26(1)
N(2)	1609(1)	1295(1)	254(1)	45(1)
N(3)	1619(1)	3119(1)	-9(1)	38(1)
N(4)	120(1)	2168(1)	-107(1)	36(1)
N(5)	1470(2)	1387(1)	2191(1)	49(1)
N(6)	1098(1)	3121(2)	2526(1)	51(1)
N(7)	2528(1)	2743(1)	1757(1)	42(1)
Ti(1)	1022(1)	2287(1)	367(1)	27(1)
Ti(2)	1450(1)	2478(1)	1891(1)	31(1)

Table 3. Bond lengths [A] and angles [deg] for **9**.

C(1)-C(2)	1.416(3)
C(1)-C(6)	1.420(3)
C(1)-N(1)	1.426(3)
C(2)-C(3)	1.381(4)
C(2)-C(7)	1.525(3)
C(3)-C(4)	1.380(4)
C(3)-H(3)	0.93
C(4)-C(5)	1.379(4)
C(4)-H(4)	0.93
C(5)-C(6)	1.385(3)
C(5)-H(5)	0.93
C(6)-C(10)	1.512(3)
C(7)-C(9)	1.513(4)
C(7)-C(8)	1.519(4)
C(7)-H(7)	0.98
C(8)-H(8A)	0.96
C(8)-H(8B)	0.96
C(8)-H(8C)	0.96
C(9)-H(9A)	0.96
C(9)-H(9B)	0.96
C(9)-H(9C)	0.96
C(10)-C(11)	1.524(4)
C(10)-C(12)	1.527(4)
C(10)-H(10)	0.98
C(11)-H(11A)	0.96
C(11)-H(11B)	0.96
C(11)-H(11C)	0.96
C(12)-H(12A)	0.96
C(12)-H(12B)	0.96
C(12)-H(12C)	0.96
C(13)-N(2)	1.452(4)
C(13)-H(13A)	0.96
C(13)-H(13B)	0.96
C(13)-H(13C)	0.96
C(14)-N(2)	1.457(4)
C(14)-H(14A)	0.96
C(14)-H(14B)	0.96
C(14)-H(14C)	0.96
C(15)-N(3)	1.448(3)
C(15)-H(15A)	0.96
C(15)-H(15B)	0.96
C(15)-H(15C)	0.96
C(16)-N(3)	1.445(3)
C(16)-H(16A)	0.96
C(16)-H(16B)	0.96
C(16)-H(16C)	0.96
C(17)-N(4)	1.451(3)
C(17)-H(17A)	0.96
C(17)-H(17B)	0.96
C(17)-H(17C)	0.96
C(18)-N(4)	1.453(3)
C(18)-H(18A)	0.96
C(18)-H(18B)	0.96
C(18)-H(18C)	0.96
C(19)-N(5)	1.436(4)
C(19)-H(19A)	0.96
C(19)-H(19B)	0.96
C(19)-H(19C)	0.96
C(20)-N(5)	1.424(4)
C(20)-H(20A)	0.96
C(20)-H(20B)	0.96
C(20)-H(20C)	0.96
C(21)-N(6)	1.452(4)
C(21)-H(21A)	0.96
C(21)-H(21B)	0.96
C(21)-H(21C)	0.96
C(22)-N(6)	1.454(4)
C(22)-H(22A)	0.96
C(22)-H(22B)	0.96
C(22)-H(22C)	0.96
C(23)-N(7)	1.450(3)
C(23)-H(23A)	0.96
C(23)-H(23B)	0.96

C(23)-H(23C)	0.96
C(24)-N(7)	1.438(4)
C(24)-H(24A)	0.96
C(24)-H(24B)	0.96
C(24)-H(24C)	0.96
N(1)-Ti(2)	1.9522(18)
N(1)-Ti(1)	1.9602(19)
N(2)-Ti(1)	1.901(2)
N(3)-Ti(1)	1.893(2)
N(4)-Ti(1)	1.900(2)
N(5)-Ti(2)	1.888(2)
N(6)-Ti(2)	1.897(2)
N(7)-Ti(2)	1.911(2)

C(2)-C(1)-C(6)	119.5(2)
C(2)-C(1)-N(1)	120.18(19)
C(6)-C(1)-N(1)	120.34(19)
C(3)-C(2)-C(1)	119.2(2)
C(3)-C(2)-C(7)	119.4(2)
C(1)-C(2)-C(7)	121.3(2)
C(4)-C(3)-C(2)	121.5(2)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
C(5)-C(4)-C(3)	119.4(2)
C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
C(4)-C(5)-C(6)	121.9(2)
C(4)-C(5)-H(5)	119
C(6)-C(5)-H(5)	119
C(5)-C(6)-C(1)	118.5(2)
C(5)-C(6)-C(10)	119.8(2)
C(1)-C(6)-C(10)	121.7(2)
C(9)-C(7)-C(8)	110.3(2)
C(9)-C(7)-C(2)	112.5(2)
C(8)-C(7)-C(2)	112.3(2)
C(9)-C(7)-H(7)	107.1
C(8)-C(7)-H(7)	107.1
C(2)-C(7)-H(7)	107.1
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(6)-C(10)-C(11)	111.9(2)
C(6)-C(10)-C(12)	110.9(2)
C(11)-C(10)-C(12)	110.5(2)
C(6)-C(10)-H(10)	107.8
C(11)-C(10)-H(10)	107.8
C(12)-C(10)-H(10)	107.8
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
N(2)-C(13)-H(13A)	109.5
N(2)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
N(2)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
N(2)-C(14)-H(14A)	109.5
N(2)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5

N(2)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
N(3)-C(15)-H(15A)	109.5
N(3)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
N(3)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
N(3)-C(16)-H(16A)	109.5
N(3)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
N(3)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
N(4)-C(17)-H(17A)	109.5
N(4)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
N(4)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
N(4)-C(18)-H(18A)	109.5
N(4)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
N(4)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
N(5)-C(19)-H(19A)	109.5
N(5)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
N(5)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
N(5)-C(20)-H(20A)	109.5
N(5)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
N(5)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
N(6)-C(21)-H(21A)	109.5
N(6)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
N(6)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(6)-C(22)-H(22A)	109.5
N(6)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
N(6)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
N(7)-C(23)-H(23A)	109.5
N(7)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
N(7)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
N(7)-C(24)-H(24A)	109.5
N(7)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
N(7)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(1)-N(1)-Ti(2)	112.37(14)
C(1)-N(1)-Ti(1)	111.97(14)
Ti(2)-N(1)-Ti(1)	135.53(10)
C(13)-N(2)-C(14)	110.9(2)
C(13)-N(2)-Ti(1)	128.5(2)
C(14)-N(2)-Ti(1)	119.68(19)
C(16)-N(3)-C(15)	111.7(2)
C(16)-N(3)-Ti(1)	118.88(17)
C(15)-N(3)-Ti(1)	129.21(19)
C(17)-N(4)-C(18)	110.4(2)
C(17)-N(4)-Ti(1)	120.95(16)
C(18)-N(4)-Ti(1)	128.18(19)
C(20)-N(5)-C(19)	112.1(3)
C(20)-N(5)-Ti(2)	119.2(2)

C(19)-N(5)-Ti(2)	128.5(2)
C(21)-N(6)-C(22)	110.4(2)
C(21)-N(6)-Ti(2)	124.88(19)
C(22)-N(6)-Ti(2)	123.9(2)
C(24)-N(7)-C(23)	110.3(2)
C(24)-N(7)-Ti(2)	128.6(2)
C(23)-N(7)-Ti(2)	120.76(18)
N(3)-Ti(1)-N(4)	103.87(9)
N(3)-Ti(1)-N(2)	104.28(10)
N(4)-Ti(1)-N(2)	105.19(9)
N(3)-Ti(1)-N(1)	112.43(8)
N(4)-Ti(1)-N(1)	116.61(8)
N(2)-Ti(1)-N(1)	113.27(9)
N(5)-Ti(2)-N(6)	103.07(11)
N(5)-Ti(2)-N(7)	104.40(10)
N(6)-Ti(2)-N(7)	107.95(10)
N(5)-Ti(2)-N(1)	111.79(9)
N(6)-Ti(2)-N(1)	117.07(9)
N(7)-Ti(2)-N(1)	111.52(9)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **9**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	26(1)	30(1)	21(1)	-4(1)	-1(1)	-1(1)
C(2)	34(1)	40(1)	26(1)	-2(1)	2(1)	-7(1)
C(3)	32(1)	57(2)	47(2)	-4(1)	7(1)	-6(1)
C(4)	28(1)	67(2)	56(2)	-7(2)	7(1)	12(1)
C(5)	39(2)	39(1)	48(2)	-9(1)	0(1)	11(1)
C(6)	33(1)	31(1)	27(1)	-6(1)	-3(1)	5(1)
C(7)	43(2)	36(1)	41(2)	4(1)	4(1)	-12(1)
C(8)	98(3)	58(2)	52(2)	16(2)	-1(2)	-23(2)
C(9)	78(2)	48(2)	58(2)	0(1)	-17(2)	-19(2)
C(10)	35(1)	23(1)	56(2)	-5(1)	-2(1)	1(1)
C(11)	63(2)	43(2)	97(3)	-33(2)	-16(2)	-1(2)
C(12)	62(2)	39(2)	88(2)	19(2)	5(2)	-3(1)
C(13)	66(3)	75(2)	141(4)	-20(3)	37(3)	17(2)
C(14)	86(2)	36(2)	67(2)	-14(2)	5(2)	8(2)
C(15)	53(2)	86(2)	47(2)	22(2)	7(2)	-9(2)
C(16)	35(2)	62(2)	58(2)	12(2)	3(1)	-10(1)
C(17)	48(2)	51(2)	40(2)	2(1)	-15(1)	1(1)
C(18)	72(2)	69(2)	45(2)	-20(2)	-14(2)	0(2)
C(19)	127(4)	110(3)	69(3)	57(2)	-17(3)	-6(3)
C(20)	111(3)	45(2)	100(3)	5(2)	-30(3)	14(2)
C(21)	54(2)	125(3)	37(2)	-21(2)	0(2)	0(2)
C(22)	65(2)	121(3)	59(2)	-39(2)	-25(2)	14(2)
C(23)	47(2)	58(2)	82(2)	6(2)	-21(2)	-17(2)
C(24)	41(2)	75(2)	139(4)	24(2)	13(2)	16(2)
N(1)	26(1)	22(1)	30(1)	-1(1)	-2(1)	0(1)
N(2)	44(1)	39(1)	51(1)	-10(1)	6(1)	8(1)
N(3)	34(1)	43(1)	37(1)	5(1)	4(1)	-4(1)
N(4)	37(1)	43(1)	28(1)	-3(1)	-4(1)	-5(1)
N(5)	55(2)	47(1)	45(1)	16(1)	-6(1)	-2(1)
N(6)	47(1)	71(2)	35(1)	-15(1)	-10(1)	6(1)
N(7)	31(1)	43(1)	51(1)	7(1)	-6(1)	1(1)
Ti(1)	27(1)	26(1)	28(1)	-2(1)	0(1)	0(1)
Ti(2)	31(1)	34(1)	29(1)	0(1)	-3(1)	1(1)

Data for compound 10

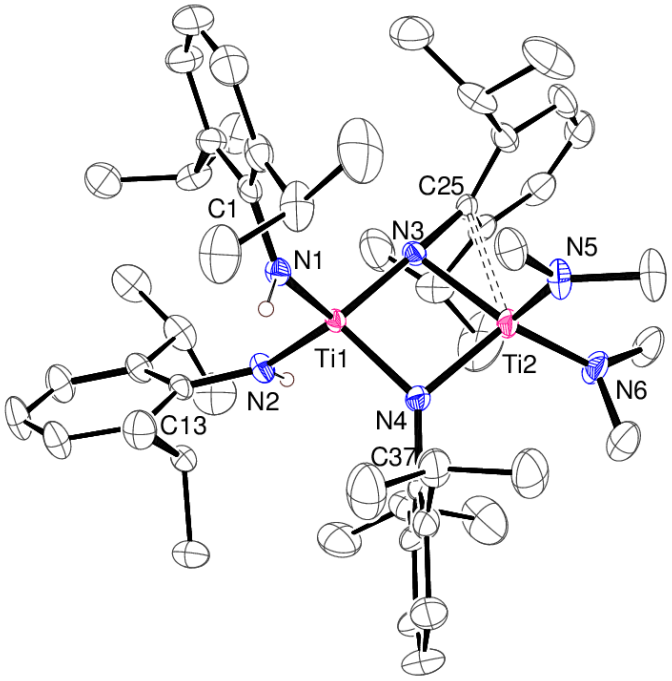


Table 1. Crystal data and structure refinement for **10**.

Identification code	cl19532a
Empirical formula	C52 H82 N6 Ti2
Formula weight	887.04
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 1 21/n 1
Unit cell dimensions	a = 11.5158(4) A alpha = 90 deg. b = 22.9429(8) A beta = 98.712(2) deg. c = 19.6453(7) A gamma = 90 deg.
Volume	5130.5(3) A^3
Z, Calculated density	4, 1.148 Mg/m^3
Absorption coefficient	0.350 mm^-1
F(000)	1920
Crystal size	0.18 x 0.1 x 0.04 mm
Theta range for data collection	1.93 to 25.24 deg.
Limiting indices	-11<=h<=13, -27<=k<=24, -23<=l<=23
Reflections collected / unique	59919 / 9171 [R(int) = 0.0592]
Completeness to theta = 25.24	98.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9873 and 0.9125
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9171 / 0 / 561
Goodness-of-fit on F^2	1.016
Final R indices [I>2sigma(I)]	R1 = 0.0479, wR2 = 0.1100
R indices (all data)	R1 = 0.0792, wR2 = 0.1263
Largest diff. peak and hole	0.392 and -0.296 e.A^-3

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

	x	y	z	U(eq)
C(1)	7647(2)	348(1)	2351(1)	34(1)
C(2)	8153(2)	-75(1)	2833(2)	47(1)
C(3)	8749(3)	-546(1)	2586(2)	67(1)
C(4)	8847(3)	-601(2)	1906(2)	72(1)
C(5)	8383(3)	-186(1)	1444(2)	58(1)
C(6)	7782(2)	293(1)	1650(2)	42(1)
C(7)	8116(3)	-21(2)	3598(2)	60(1)
C(8)	9219(3)	288(2)	3964(2)	82(1)
C(9)	7932(4)	-602(2)	3958(2)	103(2)
C(10)	7368(3)	757(1)	1116(2)	48(1)
C(11)	8400(3)	1037(2)	833(2)	61(1)
C(12)	6451(3)	547(2)	525(2)	67(1)
C(13)	6809(2)	2257(1)	1535(1)	32(1)
C(14)	7698(2)	2396(1)	2084(1)	33(1)
C(15)	8691(3)	2692(1)	1940(2)	52(1)
C(16)	8803(3)	2860(2)	1288(2)	63(1)
C(17)	7916(3)	2743(1)	753(2)	55(1)
C(18)	6913(2)	2444(1)	861(1)	40(1)
C(19)	5941(3)	2329(1)	260(2)	54(1)
C(20)	6353(3)	2263(2)	-433(2)	70(1)
C(21)	5006(4)	2800(2)	220(2)	86(1)
C(22)	7612(2)	2263(1)	2831(1)	36(1)
C(23)	8703(3)	1949(1)	3191(2)	51(1)
C(24)	7373(3)	2818(1)	3218(2)	61(1)
C(25)	3500(2)	404(1)	1450(1)	30(1)
C(26)	3445(2)	-213(1)	1536(1)	43(1)
C(27)	2440(3)	-500(2)	1218(2)	62(1)
C(28)	1545(3)	-208(2)	820(2)	71(1)
C(29)	1648(3)	373(2)	687(2)	60(1)
C(30)	2613(2)	691(1)	988(1)	41(1)
C(31)	4477(3)	-550(1)	1894(2)	57(1)
C(32)	5252(3)	-756(2)	1371(2)	76(1)
C(33)	4133(5)	-1072(2)	2299(2)	99(2)
C(34)	2754(3)	1316(1)	785(2)	56(1)
C(35)	3183(4)	1353(2)	106(2)	103(2)
C(36)	1655(5)	1676(2)	781(4)	174(3)
C(37)	4641(2)	1913(1)	3360(2)	42(1)
C(38)	5128(3)	1872(1)	4062(2)	52(1)
C(39)	5043(4)	2358(2)	4481(2)	80(1)
C(40)	4523(4)	2869(2)	4229(3)	100(2)
C(41)	4068(3)	2899(2)	3553(3)	82(1)
C(42)	4099(3)	2438(1)	3100(2)	55(1)
C(43)	5690(3)	1320(2)	4367(2)	57(1)
C(44)	6929(3)	1406(2)	4762(2)	93(1)
C(45)	4913(4)	1027(2)	4838(2)	80(1)
C(46)	3533(3)	2523(1)	2358(2)	67(1)
C(47)	4008(4)	3055(2)	2027(2)	83(1)
C(48)	2175(3)	2552(2)	2299(3)	124(2)
C(49)	4955(3)	-45(1)	3548(2)	55(1)
C(50)	2899(3)	-116(2)	3630(2)	82(1)
C(51)	1892(3)	1260(2)	3355(2)	69(1)
C(52)	795(3)	889(2)	2291(2)	74(1)
N(1)	7021(2)	828(1)	2559(1)	30(1)
N(2)	5832(2)	1926(1)	1663(1)	34(1)
N(3)	4416(2)	725(1)	1829(1)	28(1)
N(4)	4691(2)	1421(1)	2921(1)	33(1)
N(5)	3794(2)	177(1)	3290(1)	49(1)
N(6)	1955(2)	996(1)	2681(1)	50(1)
Ti(1)	5572(1)	1233(1)	2200(1)	24(1)
Ti(2)	3529(1)	810(1)	2655(1)	35(1)

Table 3. Bond lengths [A] and angles [deg] for **10**.

C(1)-N(1)	1.409(3)
C(1)-C(6)	1.416(4)
C(1)-C(2)	1.419(4)
C(2)-C(3)	1.405(5)
C(2)-C(7)	1.515(5)
C(3)-C(4)	1.363(5)
C(4)-C(5)	1.368(5)
C(5)-C(6)	1.390(4)
C(6)-C(10)	1.519(4)
C(7)-C(8)	1.535(5)
C(7)-C(9)	1.538(5)
C(10)-C(12)	1.525(4)
C(10)-C(11)	1.527(4)
C(13)-C(14)	1.407(4)
C(13)-N(2)	1.411(3)
C(13)-C(18)	1.414(4)
C(14)-C(15)	1.396(4)
C(14)-C(22)	1.516(4)
C(15)-C(16)	1.362(4)
C(16)-C(17)	1.377(4)
C(17)-C(18)	1.386(4)
C(18)-C(19)	1.522(4)
C(19)-C(20)	1.514(5)
C(19)-C(21)	1.520(5)
C(22)-C(23)	1.526(4)
C(22)-C(24)	1.530(4)
C(25)-N(3)	1.404(3)
C(25)-C(30)	1.420(4)
C(25)-C(26)	1.428(4)
C(25)-Ti(2)	2.541(2)
C(26)-C(27)	1.395(4)
C(26)-C(31)	1.500(4)
C(27)-C(28)	1.369(5)
C(28)-C(29)	1.367(5)
C(29)-C(30)	1.384(4)
C(30)-C(34)	1.503(4)
C(31)-C(33)	1.523(5)
C(31)-C(32)	1.535(5)
C(34)-C(35)	1.495(5)
C(34)-C(36)	1.511(5)
C(37)-C(38)	1.410(4)
C(37)-C(42)	1.415(4)
C(37)-N(4)	1.427(3)
C(38)-C(39)	1.399(5)
C(38)-C(43)	1.507(5)
C(39)-C(40)	1.374(6)
C(40)-C(41)	1.353(6)
C(41)-C(42)	1.386(5)
C(42)-C(46)	1.516(5)
C(43)-C(44)	1.531(5)
C(43)-C(45)	1.535(4)
C(46)-C(47)	1.524(5)
C(46)-C(48)	1.552(5)
C(49)-N(5)	1.449(4)
C(50)-N(5)	1.473(4)
C(51)-Ti(2)	2.701(3)
C(52)-N(6)	1.457(4)
N(1)-Ti(1)	1.9469(19)
N(2)-Ti(1)	1.955(2)
N(3)-Ti(1)	1.8362(19)
N(3)-Ti(2)	2.054(2)
N(4)-Ti(1)	1.913(2)
N(4)-Ti(2)	1.953(2)
N(5)-Ti(2)	1.909(2)
N(6)-Ti(2)	1.870(2)

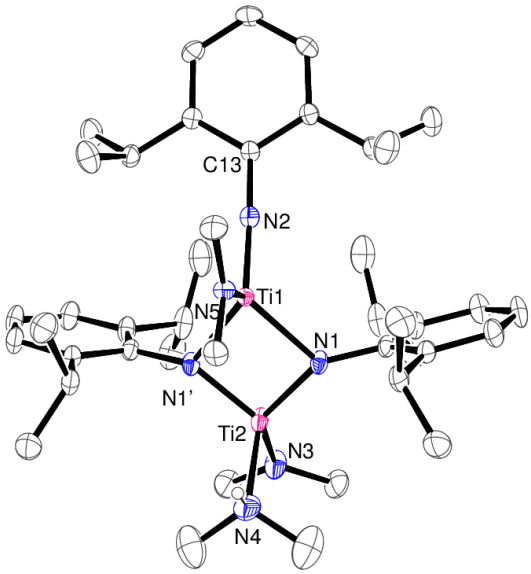
Ti(1)-Ti(2)	2.8134(6)
N(1)-C(1)-C(6)	119.2(2)
N(1)-C(1)-C(2)	121.2(3)
C(6)-C(1)-C(2)	119.6(2)
C(3)-C(2)-C(1)	118.0(3)
C(3)-C(2)-C(7)	119.6(3)
C(1)-C(2)-C(7)	122.3(3)
C(4)-C(3)-C(2)	121.7(3)
C(3)-C(4)-C(5)	120.3(3)
C(4)-C(5)-C(6)	121.3(3)
C(5)-C(6)-C(1)	119.1(3)
C(5)-C(6)-C(10)	118.1(3)
C(1)-C(6)-C(10)	122.7(2)
C(2)-C(7)-C(8)	110.9(3)
C(2)-C(7)-C(9)	114.3(3)
C(8)-C(7)-C(9)	110.3(3)
C(6)-C(10)-C(12)	114.4(3)
C(6)-C(10)-C(11)	111.4(2)
C(12)-C(10)-C(11)	110.1(3)
C(14)-C(13)-N(2)	119.5(2)
C(14)-C(13)-C(18)	119.6(2)
N(2)-C(13)-C(18)	120.9(2)
C(15)-C(14)-C(13)	118.5(2)
C(15)-C(14)-C(22)	118.0(2)
C(13)-C(14)-C(22)	123.4(2)
C(16)-C(15)-C(14)	121.7(3)
C(15)-C(16)-C(17)	119.9(3)
C(16)-C(17)-C(18)	121.2(3)
C(17)-C(18)-C(13)	118.9(3)
C(17)-C(18)-C(19)	120.0(3)
C(13)-C(18)-C(19)	121.1(2)
C(20)-C(19)-C(21)	110.0(3)
C(20)-C(19)-C(18)	114.9(3)
C(21)-C(19)-C(18)	110.3(3)
C(14)-C(22)-C(23)	111.9(2)
C(14)-C(22)-C(24)	110.9(2)
C(23)-C(22)-C(24)	111.2(2)
N(3)-C(25)-C(30)	120.4(2)
N(3)-C(25)-C(26)	120.0(2)
C(30)-C(25)-C(26)	119.7(2)
N(3)-C(25)-Ti(2)	53.85(11)
C(30)-C(25)-Ti(2)	109.41(16)
C(26)-C(25)-Ti(2)	104.35(17)
C(27)-C(26)-C(25)	117.6(3)
C(27)-C(26)-C(31)	120.8(3)
C(25)-C(26)-C(31)	121.4(2)
C(28)-C(27)-C(26)	121.8(3)
C(29)-C(28)-C(27)	120.4(3)
C(28)-C(29)-C(30)	121.2(3)
C(29)-C(30)-C(25)	118.8(3)
C(29)-C(30)-C(34)	120.0(3)
C(25)-C(30)-C(34)	121.0(2)
C(26)-C(31)-C(33)	113.6(3)
C(26)-C(31)-C(32)	110.2(3)
C(33)-C(31)-C(32)	109.4(3)
C(35)-C(34)-C(30)	110.7(3)
C(35)-C(34)-C(36)	110.7(4)
C(30)-C(34)-C(36)	113.6(3)
C(38)-C(37)-C(42)	119.8(3)
C(38)-C(37)-N(4)	119.4(3)
C(42)-C(37)-N(4)	120.8(3)
C(39)-C(38)-C(37)	118.0(4)
C(39)-C(38)-C(43)	120.0(3)
C(37)-C(38)-C(43)	121.9(3)
C(40)-C(39)-C(38)	122.2(4)
C(41)-C(40)-C(39)	118.6(4)
C(40)-C(41)-C(42)	123.2(4)

C(41)-C(42)-C(37)	118.1(4)
C(41)-C(42)-C(46)	118.0(3)
C(37)-C(42)-C(46)	123.9(3)
C(38)-C(43)-C(44)	113.9(3)
C(38)-C(43)-C(45)	110.7(3)
C(44)-C(43)-C(45)	109.6(3)
C(42)-C(46)-C(47)	112.6(3)
C(42)-C(46)-C(48)	111.0(4)
C(47)-C(46)-C(48)	110.9(3)
C(1)-N(1)-Ti(1)	135.74(17)
C(13)-N(2)-Ti(1)	136.48(16)
C(25)-N(3)-Ti(1)	170.07(18)
C(25)-N(3)-Ti(2)	92.63(14)
Ti(1)-N(3)-Ti(2)	92.48(9)
C(37)-N(4)-Ti(1)	134.43(17)
C(37)-N(4)-Ti(2)	129.81(16)
Ti(1)-N(4)-Ti(2)	93.39(9)
C(49)-N(5)-C(50)	110.6(3)
C(49)-N(5)-Ti(2)	122.95(18)
C(50)-N(5)-Ti(2)	126.2(2)
C(52)-N(6)-Ti(2)	139.8(2)
N(3)-Ti(1)-N(4)	90.16(9)
N(3)-Ti(1)-N(1)	111.71(9)
N(4)-Ti(1)-N(1)	111.12(9)
N(3)-Ti(1)-N(2)	117.60(9)
N(4)-Ti(1)-N(2)	111.03(9)
N(1)-Ti(1)-N(2)	113.05(8)
N(3)-Ti(1)-Ti(2)	46.82(6)
N(4)-Ti(1)-Ti(2)	43.87(6)
N(1)-Ti(1)-Ti(2)	115.57(6)
N(2)-Ti(1)-Ti(2)	130.96(6)
N(6)-Ti(2)-N(5)	102.44(11)
N(6)-Ti(2)-N(4)	117.22(10)
N(5)-Ti(2)-N(4)	109.60(10)
N(6)-Ti(2)-N(3)	130.01(10)
N(5)-Ti(2)-N(3)	113.22(10)
N(4)-Ti(2)-N(3)	82.97(8)
N(6)-Ti(2)-C(25)	103.43(9)
N(5)-Ti(2)-C(25)	107.94(10)
N(4)-Ti(2)-C(25)	115.13(8)
N(3)-Ti(2)-C(25)	33.52(7)
N(6)-Ti(2)-C(51)	31.27(10)
N(5)-Ti(2)-C(51)	90.71(12)
N(4)-Ti(2)-C(51)	95.33(9)
N(3)-Ti(2)-C(51)	155.23(10)
C(25)-Ti(2)-C(51)	134.67(9)
N(6)-Ti(2)-Ti(1)	142.25(9)
N(5)-Ti(2)-Ti(1)	114.31(7)
N(4)-Ti(2)-Ti(1)	42.74(6)
N(3)-Ti(2)-Ti(1)	40.70(5)
C(25)-Ti(2)-Ti(1)	73.98(5)
C(51)-Ti(2)-Ti(1)	135.41(8)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **10**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	20(1)	28(1)	53(2)	1(1)	1(1)	-2(1)
C(2)	30(2)	40(2)	72(2)	16(2)	4(1)	1(1)
C(3)	49(2)	40(2)	111(3)	25(2)	8(2)	14(2)
C(4)	65(2)	40(2)	114(3)	-8(2)	22(2)	15(2)
C(5)	54(2)	44(2)	74(2)	-15(2)	12(2)	9(2)
C(6)	35(2)	35(2)	54(2)	-11(1)	4(1)	1(1)
C(7)	39(2)	69(2)	70(2)	37(2)	3(2)	6(2)
C(8)	52(2)	116(3)	72(3)	23(2)	-5(2)	-1(2)
C(9)	91(3)	97(3)	122(4)	72(3)	19(3)	6(3)
C(10)	52(2)	51(2)	40(2)	-8(1)	6(1)	14(2)
C(11)	65(2)	59(2)	57(2)	-1(2)	2(2)	-5(2)
C(12)	57(2)	89(3)	53(2)	1(2)	0(2)	-2(2)
C(13)	29(1)	23(1)	41(2)	4(1)	3(1)	-1(1)
C(14)	33(1)	27(1)	40(2)	-2(1)	5(1)	-5(1)
C(15)	45(2)	60(2)	50(2)	2(2)	1(1)	-23(2)
C(16)	53(2)	77(2)	59(2)	13(2)	9(2)	-35(2)
C(17)	60(2)	60(2)	46(2)	15(2)	10(2)	-19(2)
C(18)	43(2)	33(2)	44(2)	8(1)	2(1)	-5(1)
C(19)	58(2)	50(2)	48(2)	16(2)	-8(2)	-9(2)
C(20)	89(3)	70(2)	46(2)	10(2)	-6(2)	-10(2)
C(21)	80(3)	94(3)	75(3)	15(2)	-17(2)	20(2)
C(22)	33(2)	35(2)	39(2)	-7(1)	6(1)	-8(1)
C(23)	43(2)	65(2)	43(2)	3(2)	-1(1)	-5(2)
C(24)	74(2)	47(2)	64(2)	-21(2)	22(2)	-10(2)
C(25)	24(1)	38(2)	29(1)	-8(1)	7(1)	-7(1)
C(26)	49(2)	41(2)	39(2)	-6(1)	8(1)	-16(1)
C(27)	65(2)	57(2)	64(2)	-18(2)	15(2)	-37(2)
C(28)	37(2)	104(3)	70(2)	-42(2)	9(2)	-29(2)
C(29)	35(2)	93(3)	47(2)	-29(2)	-5(1)	4(2)
C(30)	28(1)	59(2)	35(2)	-15(1)	2(1)	3(1)
C(31)	74(2)	29(2)	63(2)	3(1)	-4(2)	-9(2)
C(32)	70(2)	56(2)	100(3)	-11(2)	3(2)	11(2)
C(33)	148(4)	46(2)	100(3)	16(2)	8(3)	-18(2)
C(34)	55(2)	58(2)	47(2)	-1(2)	-17(2)	14(2)
C(35)	123(4)	97(3)	98(3)	-6(3)	44(3)	-45(3)
C(36)	135(5)	125(5)	281(9)	103(5)	99(5)	85(4)
C(37)	27(1)	51(2)	53(2)	-23(1)	19(1)	-11(1)
C(38)	48(2)	67(2)	47(2)	-24(2)	24(2)	-24(2)
C(39)	96(3)	92(3)	62(2)	-44(2)	40(2)	-40(3)
C(40)	122(4)	76(3)	117(4)	-59(3)	68(3)	-19(3)
C(41)	73(3)	60(2)	124(4)	-39(2)	50(3)	2(2)
C(42)	35(2)	48(2)	87(3)	-25(2)	24(2)	2(1)
C(43)	57(2)	84(3)	33(2)	-15(2)	13(2)	-24(2)
C(44)	68(3)	139(4)	71(3)	-6(3)	7(2)	-32(3)
C(45)	86(3)	108(3)	51(2)	0(2)	24(2)	-29(2)
C(46)	42(2)	45(2)	111(3)	-16(2)	-3(2)	16(2)
C(47)	82(3)	48(2)	117(3)	-4(2)	3(2)	15(2)
C(48)	46(2)	85(3)	232(7)	-4(4)	-7(3)	19(2)
C(49)	53(2)	61(2)	48(2)	16(2)	3(2)	-11(2)
C(50)	66(2)	95(3)	91(3)	25(2)	34(2)	-24(2)
C(51)	37(2)	116(3)	54(2)	-32(2)	6(2)	-15(2)
C(52)	30(2)	130(3)	63(2)	-39(2)	9(2)	-16(2)
N(1)	22(1)	34(1)	31(1)	-2(1)	-2(1)	-2(1)
N(2)	25(1)	30(1)	46(1)	9(1)	-2(1)	0(1)
N(3)	25(1)	26(1)	34(1)	-1(1)	3(1)	-1(1)
N(4)	26(1)	37(1)	36(1)	-8(1)	6(1)	-3(1)
N(5)	38(1)	61(2)	51(2)	10(1)	14(1)	-14(1)
N(6)	26(1)	74(2)	53(2)	-21(1)	13(1)	-7(1)
Ti(1)	19(1)	24(1)	28(1)	0(1)	3(1)	-1(1)
Ti(2)	23(1)	43(1)	39(1)	-6(1)	9(1)	-8(1)

Data for compound 11



This compound was crystallized with 3 different cell parameters

1. From C_6D_6 solutions (contains one molecule of C_6D_6)

Table 1. Crystal data and structure refinement for **11**.

Identification code	CL1609b
Empirical formula	C54 H82 N6 Ti2
Formula weight	911
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/m
Unit cell dimensions	a = 11.1210(8) A alpha = 90 deg.
	b = 24.3670(9) A beta = 119.258(9) deg.
	c = 11.1710(7) A gamma = 90 deg.
Volume	2641.0(3) A^3
Z, Calculated density	2, 1.146 Mg/m^3
Absorption coefficient	0.341 mm^-1
F(000)	984
Crystal size	0.22 x 0.13 x 0.05 mm
Theta range for data collection	3.26 to 25.03 deg.
Limiting indices	-12<=h<=13, -24<=k<=29, -13<=l<=13
Reflections collected / unique	17960 / 4775 [R(int) = 0.0337]
Completeness to theta = 25.03	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.998 and 0.971
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4775 / 0 / 305
Goodness-of-fit on F^2	1.172
Final R indices [I>2sigma(I)]	R1 = 0.084, wR2 = 0.2023
R indices (all data)	R1 = 0.0992, wR2 = 0.2081
Largest diff. peak and hole	1.503 and -1.441 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **11**.

	x	y	z	U(eq)
C(1)	9883(5)	1392(2)	7967(5)	30(1)
C(2)	11205(6)	1219(2)	8238(6)	38(1)
C(3)	11573(6)	674(2)	8546(6)	47(1)
C(4)	10677(7)	299(2)	8581(7)	51(2)
C(5)	9391(6)	460(2)	8305(6)	43(1)
C(6)	8952(5)	1000(2)	7977(5)	34(1)
C(7)	7503(5)	1147(2)	7641(6)	38(1)
C(8)	6435(7)	831(3)	6406(7)	59(2)
C(9)	7272(7)	1065(3)	8872(6)	53(2)
C(10)	12264(7)	1615(2)	8233(7)	52(2)
C(11)	12956(8)	1379(3)	7433(9)	72(2)
C(12)	13331(7)	1760(3)	9652(8)	68(2)
C(13)	12018(6)	2500	12119(7)	25(1)
C(14)	12515(5)	1995(2)	12856(5)	28(1)
C(15)	13382(5)	2010(2)	14252(5)	36(1)
C(16)	13802(7)	2500	14955(8)	40(2)
C(17)	12015(5)	1460(2)	12104(5)	34(1)
C(18)	13108(6)	1012(2)	12592(7)	50(2)
C(19)	10750(6)	1254(3)	12165(7)	54(2)
C(20)	10094(8)	2994(3)	4651(7)	60(2)
C(21)	6567(9)	2007(3)	4022(10)	86(3)
C(22)	6682(7)	2500	8373(8)	37(2)
C(23)	8104(8)	2500	10793(8)	40(2)
C(25)	8445(12)	574(5)	3771(15)	103(4)
C(26)	7931(16)	220(5)	4369(11)	117(4)
C(27)	6600(18)	36(4)	3594(18)	114(4)
C(28)	5852(10)	208(5)	2321(17)	110(4)
C(29)	6371(14)	567(5)	1776(11)	104(3)
C(30)	7661(15)	749(4)	2530(17)	104(4)
N(1)	9488(4)	1948(2)	7684(4)	30(1)
N(2)	11067(6)	2500	10759(6)	30(1)
N(3)	9817(8)	2500	5198(7)	50(2)
N(4)	6950(9)	2500	4861(7)	57(2)
N(5)	8093(6)	2500	9499(5)	28(1)
Ti(1)	9624(1)	2500	9157(1)	23(1)
Ti(2)	9124(2)	2500	6428(1)	37(1)

Table 3. Bond lengths [A] and angles [deg] for **11**.

C(1)-N(1)	1.411(6)
C(1)-C(6)	1.412(7)
C(1)-C(2)	1.413(7)
C(2)-C(3)	1.384(7)
C(2)-C(10)	1.524(7)
C(3)-C(4)	1.367(8)
C(3)-H(3)	0.95
C(4)-C(5)	1.365(8)
C(4)-H(4)	0.95
C(5)-C(6)	1.390(7)
C(5)-H(5)	0.95
C(6)-C(7)	1.508(7)
C(7)-C(8)	1.518(8)
C(7)-C(9)	1.531(8)
C(7)-H(7)	1
C(8)-H(8A)	0.98
C(8)-H(8B)	0.98
C(8)-H(8C)	0.98
C(9)-H(9A)	0.98
C(9)-H(9B)	0.98
C(9)-H(9C)	0.98
C(10)-C(12)	1.485(10)
C(10)-C(11)	1.548(8)
C(10)-H(10)	1
C(11)-H(11A)	0.98
C(11)-H(11B)	0.98
C(11)-H(11C)	0.98
C(12)-H(12A)	0.98

C(12)-H(12B)	0.98
C(12)-H(12C)	0.98
C(13)-N(2)	1.362(8)
C(13)-C(14)#1	1.433(6)
C(13)-C(14)	1.433(6)
C(14)-C(15)	1.377(7)
C(14)-C(17)	1.502(7)
C(15)-C(16)	1.379(6)
C(15)-H(15)	0.95
C(16)-C(15)#1	1.379(6)
C(16)-H(16)	0.95
C(17)-C(18)	1.523(7)
C(17)-C(19)	1.526(7)
C(17)-H(17)	1
C(18)-H(18A)	0.98
C(18)-H(18B)	0.98
C(18)-H(18C)	0.98
C(19)-H(19A)	0.98
C(19)-H(19B)	0.98
C(19)-H(19C)	0.98
C(20)-N(3)	1.449(6)
C(20)-H(20A)	0.98
C(20)-H(20B)	0.98
C(20)-H(20C)	0.98
C(21)-N(4)	1.454(8)
C(21)-H(21A)	0.98
C(21)-H(21B)	0.98
C(21)-H(21C)	0.98
C(22)-N(5)	1.454(9)
C(22)-H(22A)	0.98
C(22)-H(22B)	0.98
C(22)-H(22C)	0.98
C(23)-N(5)	1.439(9)
C(23)-H(23A)	0.98
C(23)-H(23B)	0.98
C(23)-H(23C)	0.98
C(25)-C(30)	1.297(15)
C(25)-C(26)	1.376(15)
C(25)-H(25)	0.95
C(26)-C(27)	1.374(16)
C(26)-H(26)	0.95
C(27)-C(28)	1.317(16)
C(27)-H(27)	0.95
C(28)-C(29)	1.347(16)
C(28)-H(28)	0.95
C(29)-C(30)	1.336(15)
C(29)-H(29)	0.95
C(30)-H(30)	0.95
N(1)-Ti(2)	1.841(4)
N(1)-Ti(1)	2.074(4)
N(2)-Ti(1)	1.723(6)
N(3)-C(20)#1	1.449(6)
N(3)-Ti(2)	1.875(6)
N(4)-C(21)#1	1.454(8)
N(4)-Ti(2)	2.185(8)
N(4)-H(4A)	0.93
N(5)-Ti(1)	1.918(6)
Ti(1)-N(1)#1	2.074(4)
Ti(1)-Ti(2)	2.8198(17)
Ti(2)-N(1)#1	1.841(4)

N(1)-C(1)-C(6)	120.1(4)
N(1)-C(1)-C(2)	120.7(4)
C(6)-C(1)-C(2)	119.1(4)
C(3)-C(2)-C(1)	119.3(5)
C(3)-C(2)-C(10)	118.3(5)
C(1)-C(2)-C(10)	122.4(5)
C(4)-C(3)-C(2)	121.2(5)
C(4)-C(3)-H(3)	119.4
C(2)-C(3)-H(3)	119.4
C(5)-C(4)-C(3)	119.9(5)
C(5)-C(4)-H(4)	120
C(3)-C(4)-H(4)	120
C(4)-C(5)-C(6)	121.7(5)
C(4)-C(5)-H(5)	119.1
C(6)-C(5)-H(5)	119.1
C(5)-C(6)-C(1)	118.6(5)

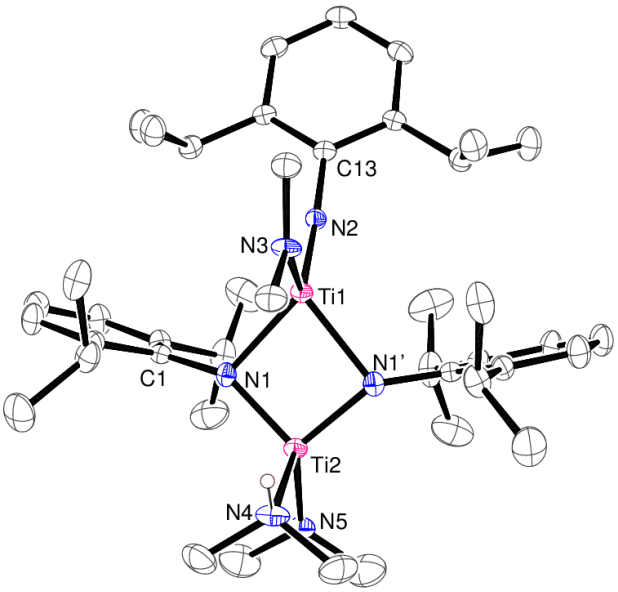
C(5)-C(6)-C(7)	119.0(5)
C(1)-C(6)-C(7)	122.4(4)
C(6)-C(7)-C(8)	111.9(5)
C(6)-C(7)-C(9)	112.0(5)
C(8)-C(7)-C(9)	110.5(5)
C(6)-C(7)-H(7)	107.4
C(8)-C(7)-H(7)	107.4
C(9)-C(7)-H(7)	107.4
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(12)-C(10)-C(2)	111.3(5)
C(12)-C(10)-C(11)	110.0(6)
C(2)-C(10)-C(11)	111.7(5)
C(12)-C(10)-H(10)	107.9
C(2)-C(10)-H(10)	107.9
C(11)-C(10)-H(10)	107.9
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
N(2)-C(13)-C(14)#1	120.8(3)
N(2)-C(13)-C(14)	120.8(3)
C(14)#1-C(13)-C(14)	118.4(6)
C(15)-C(14)-C(13)	119.2(5)
C(15)-C(14)-C(17)	121.3(4)
C(13)-C(14)-C(17)	119.4(4)
C(14)-C(15)-C(16)	121.5(5)
C(14)-C(15)-H(15)	119.2
C(16)-C(15)-H(15)	119.2
C(15)#1-C(16)-C(15)	120.0(7)
C(15)#1-C(16)-H(16)	120
C(15)-C(16)-H(16)	120
C(14)-C(17)-C(18)	114.2(4)
C(14)-C(17)-C(19)	111.0(4)
C(18)-C(17)-C(19)	109.9(5)
C(14)-C(17)-H(17)	107.2
C(18)-C(17)-H(17)	107.2
C(19)-C(17)-H(17)	107.2
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
N(3)-C(20)-H(20A)	109.5
N(3)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
N(3)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
N(4)-C(21)-H(21A)	109.5
N(4)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5

N(4)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(5)-C(22)-H(22A)	109.5
N(5)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
N(5)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
N(5)-C(23)-H(23A)	109.5
N(5)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
N(5)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(30)-C(25)-C(26)	120.2(11)
C(30)-C(25)-H(25)	119.9
C(26)-C(25)-H(25)	119.9
C(27)-C(26)-C(25)	118.3(11)
C(27)-C(26)-H(26)	120.9
C(25)-C(26)-H(26)	120.9
C(28)-C(27)-C(26)	119.7(11)
C(28)-C(27)-H(27)	120.2
C(26)-C(27)-H(27)	120.2
C(27)-C(28)-C(29)	120.7(11)
C(27)-C(28)-H(28)	119.6
C(29)-C(28)-H(28)	119.6
C(30)-C(29)-C(28)	119.7(11)
C(30)-C(29)-H(29)	120.1
C(28)-C(29)-H(29)	120.1
C(25)-C(30)-C(29)	121.3(11)
C(25)-C(30)-H(30)	119.4
C(29)-C(30)-H(30)	119.4
C(1)-N(1)-Ti(2)	143.2(3)
C(1)-N(1)-Ti(1)	123.4(3)
Ti(2)-N(1)-Ti(1)	91.97(16)
C(13)-N(2)-Ti(1)	168.2(5)
C(20)-N(3)-C(20)#1	112.3(6)
C(20)-N(3)-Ti(2)	123.9(3)
C(20)#1-N(3)-Ti(2)	123.9(3)
C(21)#1-N(4)-C(21)	111.5(9)
C(21)#1-N(4)-Ti(2)	112.2(5)
C(21)-N(4)-Ti(2)	112.2(5)
C(21)#1-N(4)-H(4A)	106.9
C(21)-N(4)-H(4A)	106.9
Ti(2)-N(4)-H(4A)	106.9
C(23)-N(5)-C(22)	110.2(6)
C(23)-N(5)-Ti(1)	128.8(5)
C(22)-N(5)-Ti(1)	121.0(4)
N(2)-Ti(1)-N(5)	105.1(3)
N(2)-Ti(1)-N(1)#1	119.57(18)
N(5)-Ti(1)-N(1)#1	115.52(16)
N(2)-Ti(1)-N(1)	119.57(18)
N(5)-Ti(1)-N(1)	115.52(16)
N(1)#1-Ti(1)-N(1)	80.9(2)
N(2)-Ti(1)-Ti(2)	135.5(2)
N(5)-Ti(1)-Ti(2)	119.36(17)
N(1)#1-Ti(1)-Ti(2)	40.72(11)
N(1)-Ti(1)-Ti(2)	40.72(11)
N(1)#1-Ti(2)-N(1)	93.9(2)
N(1)#1-Ti(2)-N(3)	122.85(18)
N(1)-Ti(2)-N(3)	122.85(18)
N(1)#1-Ti(2)-N(4)	110.83(18)
N(1)-Ti(2)-N(4)	110.83(19)
N(3)-Ti(2)-N(4)	95.9(3)
N(1)#1-Ti(2)-Ti(1)	47.31(12)
N(1)-Ti(2)-Ti(1)	47.31(12)
N(3)-Ti(2)-Ti(1)	149.1(3)
N(4)-Ti(2)-Ti(1)	115.0(2)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **11**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	46(3)	22(2)	32(3)	-1(2)	27(2)	0(2)
C(2)	50(3)	25(3)	55(3)	0(2)	37(3)	2(2)
C(3)	53(4)	32(3)	67(4)	7(3)	37(3)	7(3)
C(4)	67(4)	21(3)	71(4)	10(3)	38(4)	8(3)
C(5)	49(3)	26(3)	56(4)	7(2)	27(3)	-4(2)
C(6)	40(3)	24(2)	35(3)	0(2)	18(2)	-4(2)
C(7)	43(3)	24(3)	47(3)	5(2)	23(3)	-3(2)
C(8)	51(4)	48(4)	55(4)	5(3)	9(3)	-4(3)
C(9)	54(4)	54(4)	60(4)	7(3)	36(3)	0(3)
C(10)	55(4)	31(3)	92(5)	10(3)	53(4)	6(3)
C(11)	79(5)	67(5)	110(6)	15(4)	76(5)	8(4)
C(12)	65(5)	46(4)	116(6)	-2(4)	62(5)	-5(3)
C(13)	16(3)	27(3)	32(4)	0	12(3)	0
C(14)	23(2)	29(3)	34(3)	2(2)	15(2)	4(2)
C(15)	30(3)	39(3)	34(3)	10(2)	11(2)	8(2)
C(16)	21(4)	56(5)	29(4)	0	1(3)	0
C(17)	36(3)	26(3)	38(3)	4(2)	16(2)	2(2)
C(18)	46(3)	34(3)	66(4)	0(3)	24(3)	6(3)
C(19)	44(3)	44(3)	75(4)	-12(3)	31(3)	-10(3)
C(20)	90(5)	52(4)	56(4)	7(3)	50(4)	-10(4)
C(21)	107(7)	68(5)	121(7)	-24(5)	85(6)	-24(5)
C(22)	22(4)	39(4)	46(4)	0	13(3)	0
C(23)	45(5)	50(5)	37(4)	0	29(4)	0
C(25)	90(7)	75(7)	151(11)	-51(7)	65(8)	-19(6)
C(26)	164(12)	104(9)	91(8)	1(6)	70(8)	49(9)
C(27)	160(13)	74(7)	180(13)	-26(8)	140(12)	-29(8)
C(28)	61(6)	115(9)	175(12)	-66(9)	73(8)	-20(6)
C(29)	112(9)	109(8)	100(8)	4(6)	59(7)	55(7)
C(30)	123(10)	63(6)	183(13)	11(7)	119(10)	9(6)
N(1)	43(2)	22(2)	38(2)	-1(2)	29(2)	-1(2)
N(2)	30(3)	27(3)	34(3)	0	17(3)	0
N(3)	85(5)	37(4)	54(4)	0	56(4)	0
N(4)	92(6)	51(4)	36(4)	0	36(4)	0
N(5)	26(3)	32(3)	25(3)	0	12(2)	0
Ti(1)	26(1)	22(1)	23(1)	0	14(1)	0
Ti(2)	70(1)	21(1)	39(1)	0	42(1)	0



2. From toluene solutions (contains no solvent)

Table 1. Crystal data and structure refinement for **11**.

Identification code	cl166911
Empirical formula	C42 H70 N6 Ti2
Formula weight	754.84
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 1 21/m 1
Unit cell dimensions	a = 10.9940(10) A alpha = 90 deg.
	b = 20.0818(12) A beta = 118.368(11) deg.
	c = 11.2102(8) A gamma = 90 deg.
Volume	2177.8(3) A^3
Z, Calculated density	2, 1.151 Mg/m^3
Absorption coefficient	0.401 mm^-1
F(000)	816
Crystal size	0.18 x 0.1 x 0.03 mm
Theta range for data collection	3.64 to 26.37 deg.
Limiting indices	-12<=h<=13, -25<=k<=25, -10<=l<=14
Reflections collected / unique	10254 / 4426 [R(int) = 0.0697]
Completeness to theta = 26.37	96.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.998 and 0.862
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4426 / 0 / 249
Goodness-of-fit on F^2	0.729
Final R indices [I>2sigma(I)]	R1 = 0.0466, wR2 = 0.0705
R indices (all data)	R1 = 0.1266, wR2 = 0.0795
Largest diff. peak and hole	0.382 and -0.377 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **11**.

	x	y	z	U(eq)
C(1)	8877(3)	1164(2)	2785(2)	25(1)
C(2)	9796(3)	992(2)	2268(3)	32(1)
C(3)	9780(3)	348(2)	1833(3)	41(1)
C(4)	8921(4)	-137(2)	1893(3)	47(1)
C(5)	8069(3)	23(2)	2433(3)	42(1)
C(6)	8027(3)	663(2)	2879(3)	30(1)
C(7)	10788(4)	1493(2)	2199(3)	47(1)
C(8)	12288(4)	1299(2)	3141(3)	80(1)
C(9)	10628(4)	1578(2)	776(3)	84(2)
C(10)	7053(3)	807(2)	3459(3)	40(1)
C(11)	5548(4)	781(2)	2359(3)	52(1)
C(12)	7291(4)	317(2)	4608(3)	67(1)
C(13)	6826(4)	2500	-1294(4)	25(1)
C(14)	6578(3)	1888(2)	-1996(2)	26(1)
C(15)	6016(3)	1902(2)	-3400(3)	35(1)
C(16)	5739(5)	2500	-4096(4)	38(1)
C(19)	6824(3)	1238(2)	-1239(3)	33(1)
C(20)	5585(3)	1049(2)	-1039(3)	46(1)
C(21)	7214(4)	659(2)	-1868(3)	52(1)
C(25)	5329(4)	2500	2575(4)	37(1)
C(26)	4279(5)	2500	183(4)	37(1)
C(27)	9399(4)	1896(2)	6755(3)	59(1)
C(28)	12381(4)	3096(2)	6243(3)	77(1)
N(1)	8787(2)	1828(1)	3165(2)	25(1)
N(2)	7312(3)	2500	107(3)	26(1)
N(3)	5595(4)	2500	1426(3)	28(1)
N(4)	8931(4)	2500	5908(3)	38(1)
N(5)	11561(4)	2500	5621(3)	38(1)
Ti(1)	7456(1)	2500	1710(1)	24(1)
Ti(2)	9651(1)	2500	4393(1)	26(1)

Table 3. Bond lengths [A] and angles [deg] for **11**.

C(1)-C(6)	1.411(4)
C(1)-N(1)	1.416(3)
C(1)-C(2)	1.426(4)
C(2)-C(3)	1.379(4)
C(2)-C(7)	1.512(4)
C(3)-C(4)	1.381(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.373(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.388(4)
C(5)-H(5)	0.9500
C(6)-C(10)	1.521(4)
C(7)-C(8)	1.527(4)
C(7)-C(9)	1.529(4)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.524(4)
C(10)-C(12)	1.541(4)
C(10)-H(10)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-N(2)	1.398(4)
C(13)-C(14)	1.415(3)
C(13)-C(14)#1	1.415(3)
C(14)-C(15)	1.391(3)
C(14)-C(19)	1.509(4)

C(15)-C(16)	1.385(3)
C(15)-H(15)	0.9500
C(16)-C(15)#1	1.385(3)
C(16)-H(16)	0.9500
C(19)-C(21)	1.523(4)
C(19)-C(20)	1.529(4)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(25)-N(3)	1.450(4)
C(25)-H(25A)	0.9784
C(25)-H(25B)	0.9786
C(25)-H(25C)	0.9819
C(26)-N(3)	1.455(5)
C(26)-H(26A)	0.9802
C(26)-H(26B)	0.9799
C(26)-H(26C)	0.9803
C(27)-N(4)	1.474(3)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-N(5)	1.461(4)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
N(1)-Ti(2)	1.837(2)
N(1)-Ti(1)	2.088(2)
N(2)-Ti(1)	1.727(3)
N(3)-Ti(1)	1.915(3)
N(4)-C(27)#1	1.474(3)
N(4)-Ti(2)	2.189(3)
N(4)-H(4A)	0.9300
N(5)-C(28)#1	1.461(4)
N(5)-Ti(2)	1.886(4)
Ti(1)-N(1)#1	2.088(2)
Ti(1)-Ti(2)	2.8235(11)
Ti(2)-N(1)#1	1.837(2)

C(6)-C(1)-N(1)	120.3(3)
C(6)-C(1)-C(2)	118.6(3)
N(1)-C(1)-C(2)	121.0(3)
C(3)-C(2)-C(1)	118.6(3)
C(3)-C(2)-C(7)	119.6(3)
C(1)-C(2)-C(7)	121.8(3)
C(2)-C(3)-C(4)	122.6(3)
C(2)-C(3)-H(3)	118.7
C(4)-C(3)-H(3)	118.7
C(5)-C(4)-C(3)	118.8(3)
C(5)-C(4)-H(4)	120.6
C(3)-C(4)-H(4)	120.6
C(4)-C(5)-C(6)	121.6(3)
C(4)-C(5)-H(5)	119.2
C(6)-C(5)-H(5)	119.2
C(5)-C(6)-C(1)	119.8(3)
C(5)-C(6)-C(10)	118.8(3)
C(1)-C(6)-C(10)	121.5(3)
C(2)-C(7)-C(8)	111.3(3)
C(2)-C(7)-C(9)	113.6(3)
C(8)-C(7)-C(9)	107.5(3)
C(2)-C(7)-H(7)	108.1
C(8)-C(7)-H(7)	108.1
C(9)-C(7)-H(7)	108.1
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5

H(9B)-C(9)-H(9C)	109.5
C(6)-C(10)-C(11)	111.2(2)
C(6)-C(10)-C(12)	111.2(3)
C(11)-C(10)-C(12)	110.0(3)
C(6)-C(10)-H(10)	108.1
C(11)-C(10)-H(10)	108.1
C(12)-C(10)-H(10)	108.1
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
N(2)-C(13)-C(14)	119.66(16)
N(2)-C(13)-C(14)#1	119.66(16)
C(14)-C(13)-C(14)#1	120.7(3)
C(15)-C(14)-C(13)	118.5(3)
C(15)-C(14)-C(19)	121.2(3)
C(13)-C(14)-C(19)	120.2(2)
C(16)-C(15)-C(14)	121.0(3)
C(16)-C(15)-H(15)	119.5
C(14)-C(15)-H(15)	119.5
C(15)#1-C(16)-C(15)	120.3(4)
C(15)#1-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(14)-C(19)-C(21)	114.5(2)
C(14)-C(19)-C(20)	111.3(3)
C(21)-C(19)-C(20)	110.2(3)
C(14)-C(19)-H(19)	106.8
C(21)-C(19)-H(19)	106.8
C(20)-C(19)-H(19)	106.8
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(3)-C(25)-H(25A)	109.5
N(3)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.7
N(3)-C(25)-H(25C)	109.3
H(25A)-C(25)-H(25C)	111.1
H(25B)-C(25)-H(25C)	107.6
N(3)-C(26)-H(26A)	109.5
N(3)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
N(3)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.4
H(26B)-C(26)-H(26C)	109.5
N(4)-C(27)-H(27A)	109.5
N(4)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
N(4)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
N(5)-C(28)-H(28A)	109.5
N(5)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
N(5)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(1)-N(1)-Ti(2)	146.2(2)
C(1)-N(1)-Ti(1)	119.74(16)
Ti(2)-N(1)-Ti(1)	91.78(9)
C(13)-N(2)-Ti(1)	165.0(3)

C(25)-N(3)-C(26)	108.8(3)
C(25)-N(3)-Ti(1)	120.2(2)
C(26)-N(3)-Ti(1)	131.0(2)
C(27)-N(4)-C(27)#1	110.7(3)
C(27)-N(4)-Ti(2)	110.8(2)
C(27)#1-N(4)-Ti(2)	110.8(2)
C(27)-N(4)-H(4A)	108.1
C(27)#1-N(4)-H(4A)	108.1
Ti(2)-N(4)-H(4A)	108.1
C(28)-N(5)-C(28)#1	110.0(4)
C(28)-N(5)-Ti(2)	124.7(2)
C(28)#1-N(5)-Ti(2)	124.7(2)
N(2)-Ti(1)-N(3)	105.33(14)
N(2)-Ti(1)-N(1)#1	119.80(10)
N(3)-Ti(1)-N(1)#1	115.25(9)
N(2)-Ti(1)-N(1)	119.80(10)
N(3)-Ti(1)-N(1)	115.25(9)
N(1)#1-Ti(1)-N(1)	80.59(12)
N(2)-Ti(1)-Ti(2)	135.86(12)
N(3)-Ti(1)-Ti(2)	118.81(9)
N(1)#1-Ti(1)-Ti(2)	40.57(6)
N(1)-Ti(1)-Ti(2)	40.57(6)
N(1)-Ti(2)-N(1)#1	94.59(13)
N(1)-Ti(2)-N(5)	123.14(9)
N(1)#1-Ti(2)-N(5)	123.14(9)
N(1)-Ti(2)-N(4)	109.40(9)
N(1)#1-Ti(2)-N(4)	109.40(9)
N(5)-Ti(2)-N(4)	96.97(13)
N(1)-Ti(2)-Ti(1)	47.65(7)
N(1)#1-Ti(2)-Ti(1)	47.65(7)
N(5)-Ti(2)-Ti(1)	150.35(10)
N(4)-Ti(2)-Ti(1)	112.68(9)

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1/2,z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **11**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	22(2)	30(2)	21(2)	2(1)	10(2)	1(2)
C(2)	29(2)	30(2)	41(2)	3(2)	19(2)	5(2)
C(3)	45(3)	31(2)	60(2)	2(2)	36(2)	11(2)
C(4)	59(3)	32(2)	55(2)	-6(2)	32(2)	8(2)
C(5)	52(3)	31(2)	55(2)	-2(2)	36(2)	-7(2)
C(6)	36(2)	28(2)	30(2)	0(1)	19(2)	-3(2)
C(7)	41(3)	38(2)	82(3)	-5(2)	46(2)	2(2)
C(8)	67(4)	113(4)	64(2)	-11(2)	33(3)	-31(3)
C(9)	56(3)	122(4)	79(3)	40(3)	37(2)	-12(3)
C(10)	48(3)	36(2)	50(2)	-5(2)	33(2)	-10(2)
C(11)	57(3)	39(2)	81(2)	-13(2)	50(2)	-9(2)
C(12)	111(4)	56(3)	61(2)	4(2)	63(2)	-5(3)
C(13)	20(3)	33(3)	25(2)	0	12(2)	0
C(14)	22(2)	35(2)	24(2)	-3(1)	13(1)	-2(2)
C(15)	33(2)	44(2)	30(2)	-10(2)	16(2)	-3(2)
C(16)	36(3)	60(4)	24(2)	0	19(2)	0
C(19)	34(2)	33(2)	33(2)	-5(2)	17(2)	1(2)
C(20)	61(3)	40(2)	47(2)	0(2)	35(2)	-5(2)
C(21)	65(3)	40(2)	65(2)	-5(2)	41(2)	9(2)
C(25)	25(3)	51(3)	37(2)	0	16(2)	0
C(26)	30(3)	45(3)	35(2)	0	15(2)	0
C(27)	66(3)	71(3)	41(2)	18(2)	26(2)	-3(2)
C(28)	53(3)	101(4)	68(2)	-9(2)	22(2)	-22(3)
N(1)	29(2)	24(1)	31(1)	0(1)	21(1)	-3(1)
N(2)	33(2)	24(2)	23(2)	0	15(2)	0
N(3)	27(2)	49(3)	14(2)	0	14(2)	0
N(4)	28(2)	61(3)	22(2)	0	9(2)	0
N(5)	34(3)	46(3)	29(2)	0	11(2)	0
Ti(1)	25(1)	28(1)	21(1)	0	13(1)	0
Ti(2)	22(1)	32(1)	23(1)	0	10(1)	0

3. From toluene solutions (contains toluene)

Table 1. Crystal data and structure refinement for **11**.

Identification code	cl1752
Empirical formula	C42 H70 N6 Ti2, C7 H8
Formula weight	846.97
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 11.071(2) A alpha = 88.421(8) deg.
	b = 11.263(2) A beta = 80.276(8) deg.
	c = 22.679(5) A gamma = 61.068(7) deg.
Volume	2434.5(8) A^3
Z, Calculated density	2, 1.155 Mg/m^3
Absorption coefficient	0.366 mm^-1
F(000)	916
Crystal size	0.18 x 0.12 x 0.03 mm
Theta range for data collection	0.91 to 25.35 deg.
Limiting indices	-13<=h<=13, -13<=k<=13, -26<=l<=27
Reflections collected / unique	37710 / 8816 [R(int) = 0.0466]
Completeness to theta = 25.35	98.7 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8816 / 0 / 533
Goodness-of-fit on F^2	1.165
Final R indices [I>2sigma(I)]	R1 = 0.1532, wR2 = 0.3960
R indices (all data)	R1 = 0.1678, wR2 = 0.4029
Largest diff. peak and hole	2.360 and -2.217 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **11**.

	x	y	z	U(eq)
Ti(1)	1594(2)	3620(2)	2243(1)	14(1)
C(100)	3710(30)	8700(20)	4809(10)	85(6)
Ti(2)	3796(2)	923(2)	2215(1)	15(1)
C(53)	5200(30)	6260(30)	4155(17)	140(15)
C(49)	5590(30)	7200(60)	4045(11)	170(20)
C(52)	4100(30)	6480(20)	4633(17)	123(12)
C(50)	4800(30)	8450(30)	4359(11)	99(8)
C(51)	3450(20)	7580(20)	4898(9)	75(5)
C(21)	6667(16)	-1008(15)	1613(8)	62(5)
C(47)	6789(15)	2021(17)	1143(9)	63(5)
C(35)	6190(17)	2183(17)	3375(8)	61(4)
C(22)	6402(16)	-792(15)	2683(8)	59(4)
C(48)	5017(16)	4508(15)	1348(8)	56(4)
C(18)	3705(16)	-1506(14)	1700(7)	54(4)
C(31)	537(17)	1085(15)	4104(7)	54(4)
C(19)	3392(15)	-1333(14)	2777(7)	51(4)
C(44)	2212(19)	438(14)	291(6)	53(4)
C(34)	4528(15)	4298(16)	2951(7)	52(4)
C(12)	1094(17)	7237(15)	3877(6)	49(4)
C(13)	-762(15)	6768(16)	3645(6)	49(3)
C(27)	2325(15)	3530(14)	4623(6)	43(3)
C(32)	-1021(14)	3484(14)	3839(6)	46(3)
C(45)	267(15)	2749(16)	711(6)	48(3)
C(26)	3429(15)	3379(14)	4187(6)	41(3)
C(33)	4874(14)	2806(16)	3156(5)	46(4)
C(15)	1927(16)	7005(14)	592(6)	46(3)
C(40)	3946(14)	3107(13)	-143(5)	39(3)
C(28)	1391(15)	3182(14)	4454(5)	41(3)
C(39)	4616(14)	3230(13)	279(5)	36(3)

C(46)	5211(13)	3057(14)	1313(5)	39(3)
C(41)	3031(13)	2587(12)	-5(5)	34(3)
C(16)	192(13)	6208(13)	960(5)	35(3)
C(43)	1750(13)	1680(12)	714(5)	33(3)
C(2)	-1589(11)	5211(11)	2310(6)	35(3)
C(25)	3603(13)	2945(12)	3597(5)	30(2)
C(8)	-104(12)	9423(10)	2257(6)	30(2)
C(38)	4415(12)	2899(12)	864(5)	32(3)
C(11)	618(12)	6702(11)	3397(5)	30(2)
C(30)	468(12)	2279(12)	3734(5)	29(2)
C(3)	-578(11)	2827(11)	2247(5)	24(2)
C(7)	372(11)	8648(10)	1717(5)	26(2)
C(9)	34(11)	8754(11)	2789(5)	29(2)
C(14)	1386(12)	6404(11)	1116(5)	25(2)
C(29)	1521(11)	2682(10)	3878(5)	24(2)
C(42)	2783(11)	2230(10)	579(4)	23(2)
C(10)	554(10)	7401(10)	2806(4)	20(2)
N(6)	5723(9)	-307(9)	2187(5)	29(2)
C(5)	1021(10)	6601(9)	2250(4)	17(2)
C(24)	2611(11)	2617(9)	3431(4)	19(2)
C(6)	909(10)	7259(10)	1702(4)	19(2)
C(37)	3464(10)	2405(10)	1022(4)	20(2)
N(5)	3072(9)	-573(8)	2237(4)	25(2)
N(4)	-278(8)	3932(8)	2263(4)	22(2)
N(1)	3148(8)	2099(8)	1621(3)	16(2)
N(3)	1440(8)	5234(8)	2248(3)	16(2)
N(2)	2705(8)	2219(8)	2835(4)	18(2)
C(101)	3010(40)	9900(30)	5172(14)	178(18)

Table 3. Bond lengths [A] and angles [deg] for **11**.

Ti(1)-N(3)	1.742(8)
Ti(1)-N(4)	1.920(8)
Ti(1)-N(1)	2.085(8)
Ti(1)-N(2)	2.089(8)
Ti(1)-Ti(2)	2.823(2)
C(100)-C(50)	1.36(3)
C(100)-C(101)	1.39(3)
C(100)-C(51)	1.43(3)
Ti(2)-N(1)	1.842(8)
Ti(2)-N(2)	1.843(8)
Ti(2)-N(6)	1.891(9)
Ti(2)-N(5)	2.185(9)
C(53)-C(49)	1.31(5)
C(53)-C(52)	1.42(5)
C(53)-H(53)	0.9500
C(49)-C(50)	1.38(5)
C(49)-H(49)	0.9500
C(52)-C(51)	1.20(3)
C(52)-H(52)	0.9500
C(50)-H(50)	0.9500
C(51)-H(51)	0.9500
C(21)-N(6)	1.486(17)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(47)-C(46)	1.54(2)
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(35)-C(33)	1.45(2)
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(22)-N(6)	1.407(18)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(48)-C(46)	1.545(19)
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(18)-N(5)	1.465(16)
C(18)-H(18A)	0.9800

C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(31)-C(30)	1.543(17)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(19)-N(5)	1.466(16)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(44)-C(43)	1.534(17)
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(34)-C(33)	1.61(2)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(12)-C(11)	1.538(16)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(11)	1.502(17)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(27)-C(26)	1.378(19)
C(27)-C(28)	1.379(18)
C(27)-H(27)	0.9500
C(32)-C(30)	1.529(17)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(45)-C(43)	1.495(19)
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(26)-C(25)	1.388(16)
C(26)-H(26)	0.9500
C(33)-C(25)	1.524(15)
C(33)-H(33)	1.0000
C(15)-C(14)	1.529(15)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(40)-C(39)	1.355(18)
C(40)-C(41)	1.386(17)
C(40)-H(40)	0.9500
C(28)-C(29)	1.395(16)
C(28)-H(28)	0.9500
C(39)-C(38)	1.378(16)
C(39)-H(39)	0.9500
C(46)-C(38)	1.519(16)
C(46)-H(46)	1.0000
C(41)-C(42)	1.395(15)
C(41)-H(41)	0.9500
C(16)-C(14)	1.538(15)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(43)-C(42)	1.530(15)
C(43)-H(43)	1.0000
C(2)-N(4)	1.458(13)
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800
C(25)-C(24)	1.423(14)
C(8)-C(7)	1.392(16)
C(8)-C(9)	1.395(16)
C(8)-H(8)	0.9500
C(38)-C(37)	1.406(15)
C(11)-C(10)	1.530(15)
C(11)-H(11)	1.0000
C(30)-C(29)	1.523(15)
C(30)-H(30)	1.0000
C(3)-N(4)	1.437(12)
C(3)-H(3A)	0.9800

C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(7)-C(6)	1.378(14)
C(7)-H(7)	0.9500
C(9)-C(10)	1.346(15)
C(9)-H(9)	0.9500
C(14)-C(6)	1.521(14)
C(14)-H(14)	1.0000
C(29)-C(24)	1.413(14)
C(42)-C(37)	1.423(14)
C(10)-C(5)	1.436(13)
C(5)-N(3)	1.376(12)
C(5)-C(6)	1.422(13)
C(24)-N(2)	1.408(12)
C(37)-N(1)	1.420(12)
N(5)-H(5)	0.9300
C(101)-H(10A)	0.9800
C(101)-H(10B)	0.9800
C(101)-H(10C)	0.9800

N(3)-Ti(1)-N(4)	104.9(4)
N(3)-Ti(1)-N(1)	119.6(3)
N(4)-Ti(1)-N(1)	115.6(3)
N(3)-Ti(1)-N(2)	120.1(3)
N(4)-Ti(1)-N(2)	115.1(3)
N(1)-Ti(1)-N(2)	80.9(3)
N(3)-Ti(1)-Ti(2)	136.1(3)
N(4)-Ti(1)-Ti(2)	119.0(2)
N(1)-Ti(1)-Ti(2)	40.7(2)
N(2)-Ti(1)-Ti(2)	40.8(2)
C(50)-C(100)-C(101)	122(3)
C(50)-C(100)-C(51)	113(2)
C(101)-C(100)-C(51)	124(3)
N(1)-Ti(2)-N(2)	94.6(4)
N(1)-Ti(2)-N(6)	122.3(4)
N(2)-Ti(2)-N(6)	123.2(4)
N(1)-Ti(2)-N(5)	110.6(3)
N(2)-Ti(2)-N(5)	108.3(3)
N(6)-Ti(2)-N(5)	97.7(4)
N(1)-Ti(2)-Ti(1)	47.6(2)
N(2)-Ti(2)-Ti(1)	47.7(3)
N(6)-Ti(2)-Ti(1)	149.6(3)
N(5)-Ti(2)-Ti(1)	112.7(2)
C(49)-C(53)-C(52)	120(3)
C(49)-C(53)-H(53)	119.8
C(52)-C(53)-H(53)	119.8
C(53)-C(49)-C(50)	119(3)
C(53)-C(49)-H(49)	120.4
C(50)-C(49)-H(49)	120.4
C(51)-C(52)-C(53)	118(3)
C(51)-C(52)-H(52)	121.0
C(53)-C(52)-H(52)	121.0
C(100)-C(50)-C(49)	121(2)
C(100)-C(50)-H(50)	119.3
C(49)-C(50)-H(50)	119.3
C(52)-C(51)-C(100)	127(3)
C(52)-C(51)-H(51)	116.4
C(100)-C(51)-H(51)	116.4
N(6)-C(21)-H(21A)	109.5
N(6)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
N(6)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(46)-C(47)-H(47A)	109.5
C(46)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(46)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
N(6)-C(22)-H(22A)	109.5

N(6)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
N(6)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(46)-C(48)-H(48A)	109.5
C(46)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(46)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
N(5)-C(18)-H(18A)	109.5
N(5)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
N(5)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
N(5)-C(19)-H(19A)	109.5
N(5)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
N(5)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(43)-C(44)-H(44A)	109.5
C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(26)-C(27)-C(28)	116.9(12)
C(26)-C(27)-H(27)	121.5
C(28)-C(27)-H(27)	121.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(43)-C(45)-H(45A)	109.5
C(43)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(43)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(27)-C(26)-C(25)	123.2(11)
C(27)-C(26)-H(26)	118.4
C(25)-C(26)-H(26)	118.4
C(35)-C(33)-C(25)	115.9(12)
C(35)-C(33)-C(34)	109.2(10)
C(25)-C(33)-C(34)	107.7(11)
C(35)-C(33)-H(33)	107.9
C(25)-C(33)-H(33)	107.9
C(34)-C(33)-H(33)	107.9

C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(39)-C(40)-C(41)	120.4(11)
C(39)-C(40)-H(40)	119.8
C(41)-C(40)-H(40)	119.8
C(27)-C(28)-C(29)	123.6(12)
C(27)-C(28)-H(28)	118.2
C(29)-C(28)-H(28)	118.2
C(40)-C(39)-C(38)	123.4(11)
C(40)-C(39)-H(39)	118.3
C(38)-C(39)-H(39)	118.3
C(38)-C(46)-C(47)	109.9(11)
C(38)-C(46)-C(48)	112.0(11)
C(47)-C(46)-C(48)	109.4(11)
C(38)-C(46)-H(46)	108.5
C(47)-C(46)-H(46)	108.5
C(48)-C(46)-H(46)	108.5
C(40)-C(41)-C(42)	119.0(10)
C(40)-C(41)-H(41)	120.5
C(42)-C(41)-H(41)	120.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(45)-C(43)-C(42)	112.7(10)
C(45)-C(43)-C(44)	112.4(11)
C(42)-C(43)-C(44)	110.6(10)
C(45)-C(43)-H(43)	106.9
C(42)-C(43)-H(43)	106.9
C(44)-C(43)-H(43)	106.9
N(4)-C(2)-H(2A)	109.5
N(4)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
N(4)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(26)-C(25)-C(24)	118.9(11)
C(26)-C(25)-C(33)	118.4(10)
C(24)-C(25)-C(33)	122.7(9)
C(7)-C(8)-C(9)	118.4(9)
C(7)-C(8)-H(8)	120.8
C(9)-C(8)-H(8)	120.8
C(39)-C(38)-C(37)	117.5(11)
C(39)-C(38)-C(46)	120.6(11)
C(37)-C(38)-C(46)	121.9(10)
C(13)-C(11)-C(10)	111.0(10)
C(13)-C(11)-C(12)	110.1(11)
C(10)-C(11)-C(12)	114.4(9)
C(13)-C(11)-H(11)	107.0
C(10)-C(11)-H(11)	107.0
C(12)-C(11)-H(11)	107.0
C(29)-C(30)-C(32)	111.5(10)
C(29)-C(30)-C(31)	110.4(10)
C(32)-C(30)-C(31)	110.8(10)
C(29)-C(30)-H(30)	108.0
C(32)-C(30)-H(30)	108.0
C(31)-C(30)-H(30)	108.0
N(4)-C(3)-H(3A)	109.5
N(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
N(4)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(6)-C(7)-C(8)	121.4(10)
C(6)-C(7)-H(7)	119.3
C(8)-C(7)-H(7)	119.3
C(10)-C(9)-C(8)	123.2(10)
C(10)-C(9)-H(9)	118.4
C(8)-C(9)-H(9)	118.4
C(6)-C(14)-C(15)	112.9(9)
C(6)-C(14)-C(16)	110.7(9)

C(15)-C(14)-C(16)	109.6(10)
C(6)-C(14)-H(14)	107.8
C(15)-C(14)-H(14)	107.8
C(16)-C(14)-H(14)	107.8
C(28)-C(29)-C(24)	118.2(10)
C(28)-C(29)-C(30)	120.3(10)
C(24)-C(29)-C(30)	121.4(9)
C(41)-C(42)-C(37)	119.9(10)
C(41)-C(42)-C(43)	117.2(9)
C(37)-C(42)-C(43)	122.9(9)
C(9)-C(10)-C(5)	118.5(9)
C(9)-C(10)-C(11)	122.2(9)
C(5)-C(10)-C(11)	119.3(9)
C(22)-N(6)-C(21)	111.9(12)
C(22)-N(6)-Ti(2)	126.4(9)
C(21)-N(6)-Ti(2)	121.3(10)
N(3)-C(5)-C(6)	120.0(8)
N(3)-C(5)-C(10)	120.4(8)
C(6)-C(5)-C(10)	119.3(8)
N(2)-C(24)-C(29)	119.7(9)
N(2)-C(24)-C(25)	121.4(9)
C(29)-C(24)-C(25)	118.9(9)
C(7)-C(6)-C(5)	119.2(9)
C(7)-C(6)-C(14)	122.0(9)
C(5)-C(6)-C(14)	118.9(8)
C(38)-C(37)-N(1)	121.1(9)
C(38)-C(37)-C(42)	119.7(9)
N(1)-C(37)-C(42)	119.2(9)
C(18)-N(5)-C(19)	110.4(10)
C(18)-N(5)-Ti(2)	112.1(8)
C(19)-N(5)-Ti(2)	109.0(8)
C(18)-N(5)-H(5)	108.4
C(19)-N(5)-H(5)	108.4
Ti(2)-N(5)-H(5)	108.4
C(3)-N(4)-C(2)	108.8(8)
C(3)-N(4)-Ti(1)	121.6(6)
C(2)-N(4)-Ti(1)	129.6(7)
C(37)-N(1)-Ti(2)	145.7(7)
C(37)-N(1)-Ti(1)	120.4(6)
Ti(2)-N(1)-Ti(1)	91.7(3)
C(5)-N(3)-Ti(1)	167.7(7)
C(24)-N(2)-Ti(2)	144.7(7)
C(24)-N(2)-Ti(1)	121.5(6)
Ti(2)-N(2)-Ti(1)	91.5(3)
C(100)-C(101)-H(10A)	109.5
C(100)-C(101)-H(10B)	109.5
H(10A)-C(101)-H(10B)	109.5
C(100)-C(101)-H(10C)	109.5
H(10A)-C(101)-H(10C)	109.5
H(10B)-C(101)-H(10C)	109.5

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **11**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ti(1)	15(1)	10(1)	18(1)	1(1)	-3(1)	-7(1)
C(100)	116(18)	69(12)	85(14)	23(11)	-62(14)	-43(13)
Ti(2)	12(1)	10(1)	21(1)	0(1)	-4(1)	-4(1)
C(53)	81(19)	110(20)	180(30)	-50(20)	-90(20)	9(16)
C(49)	90(20)	390(70)	57(14)	-40(30)	12(13)	-130(30)
C(52)	81(17)	59(14)	230(40)	-13(18)	-70(20)	-26(13)
C(50)	114(19)	160(20)	66(14)	23(15)	-14(13)	-100(20)
C(51)	57(11)	91(15)	85(14)	32(12)	-20(10)	-42(11)
C(21)	44(8)	45(8)	82(12)	-22(8)	26(8)	-19(7)
C(47)	38(8)	65(10)	96(13)	14(9)	-32(8)	-26(8)
C(35)	56(10)	59(10)	70(11)	-8(8)	5(8)	-33(8)
C(22)	47(9)	39(8)	91(12)	3(8)	-38(9)	-13(7)
C(48)	47(8)	46(8)	73(11)	-13(7)	-24(8)	-16(7)
C(18)	55(9)	31(7)	74(10)	-20(7)	-17(8)	-16(7)
C(31)	69(10)	53(9)	67(10)	2(7)	-5(8)	-53(8)
C(19)	46(8)	39(7)	66(10)	23(7)	-3(7)	-23(7)

C(44)	96(12)	44(8)	41(8)	5(6)	-8(8)	-52(9)
C(34)	46(8)	68(10)	52(9)	12(7)	-5(7)	-38(8)
C(12)	83(11)	49(8)	32(7)	2(6)	-18(7)	-44(8)
C(13)	49(8)	61(9)	45(8)	11(7)	-3(6)	-34(7)
C(27)	61(9)	54(8)	30(7)	1(6)	-7(6)	-40(7)
C(32)	37(7)	50(8)	50(8)	-5(6)	7(6)	-24(6)
C(45)	51(8)	72(10)	36(7)	18(7)	-19(6)	-40(8)
C(26)	53(8)	51(8)	35(7)	4(6)	-22(6)	-34(7)
C(33)	57(8)	90(11)	23(6)	-29(6)	15(6)	-66(9)
C(15)	70(10)	48(8)	28(7)	10(6)	2(6)	-39(8)
C(40)	54(8)	47(7)	22(6)	-2(5)	9(5)	-33(7)
C(28)	53(8)	58(8)	25(6)	5(6)	-4(6)	-37(7)
C(39)	47(7)	46(7)	20(6)	-7(5)	4(5)	-29(6)
C(46)	40(7)	67(9)	28(6)	-1(6)	-3(5)	-40(7)
C(41)	49(7)	39(7)	26(6)	6(5)	-16(5)	-27(6)
C(16)	38(7)	38(7)	33(6)	-1(5)	-6(5)	-20(6)
C(43)	49(7)	43(7)	24(6)	8(5)	-11(5)	-32(6)
C(2)	13(5)	22(6)	60(8)	5(5)	-2(5)	-2(4)
C(25)	39(7)	40(7)	23(6)	1(5)	-5(5)	-27(6)
C(8)	31(6)	13(5)	49(7)	4(5)	-8(5)	-12(5)
C(38)	35(6)	31(6)	33(6)	-4(5)	-1(5)	-20(5)
C(11)	36(6)	22(5)	28(6)	-3(4)	0(5)	-14(5)
C(30)	32(6)	38(6)	22(5)	1(5)	2(4)	-22(5)
C(3)	21(5)	38(6)	27(5)	0(5)	-7(4)	-25(5)
C(7)	26(5)	18(5)	36(6)	8(4)	-5(5)	-12(4)
C(9)	28(6)	33(6)	28(6)	-11(5)	3(4)	-19(5)
C(14)	35(6)	21(5)	25(5)	4(4)	-3(5)	-19(5)
C(29)	28(6)	18(5)	25(5)	2(4)	0(4)	-12(4)
C(42)	28(5)	20(5)	20(5)	-1(4)	-4(4)	-12(4)
C(10)	19(5)	20(5)	21(5)	-3(4)	0(4)	-9(4)
N(6)	14(4)	18(4)	50(6)	4(4)	-7(4)	-3(4)
C(5)	14(4)	13(4)	21(5)	0(4)	-4(4)	-4(4)
C(24)	29(5)	7(4)	21(5)	0(4)	-6(4)	-9(4)
C(6)	17(5)	21(5)	22(5)	5(4)	-8(4)	-11(4)
C(37)	19(5)	16(5)	19(5)	0(4)	4(4)	-7(4)
N(5)	15(4)	15(4)	41(5)	0(4)	-3(4)	-5(3)
N(4)	14(4)	11(4)	39(5)	2(3)	-3(4)	-5(3)
N(1)	19(4)	12(4)	19(4)	1(3)	-5(3)	-8(3)
N(3)	18(4)	14(4)	17(4)	1(3)	-6(3)	-9(3)
N(2)	16(4)	17(4)	19(4)	-3(3)	0(3)	-10(3)
C(101)	270(50)	81(18)	150(30)	-19(18)	-100(30)	-30(20)

Data for compound 12

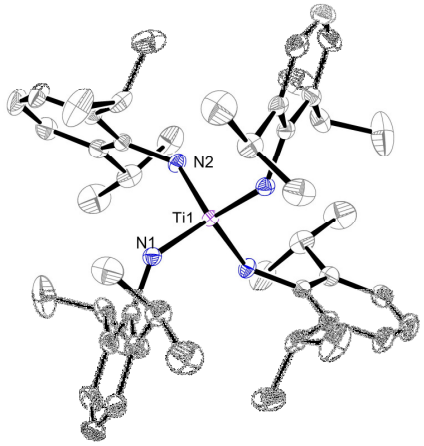


Table 1. Crystal data and structure refinement for **12**.

Empirical formula	C48 H76 N4 Ti
Formula weight	757.03
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C 1 2/c 1
Unit cell dimensions	a = 19.1831(6) A alpha = 90 deg. b = 13.1110(4) A beta = 91.513(3) deg. c = 18.5082(6) A gamma = 90 deg.
Volume	4653.4(3) A^3
Z, Calculated density	4, 1.081 Mg/m^3
Absorption coefficient	0.218 mm^-1
F(000)	1656
Crystal size	0.22 x 0.14 x 0.04 mm
Theta range for data collection	3.30 to 26.37 deg.
Limiting indices	-23<=h<=23, -16<=k<=14, -23<=l<=23
Reflections collected / unique	19596 / 4756 [R(int) = 0.0532]
Completeness to theta = 26.37	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.978 and 0.922
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4756 / 0 / 248
Goodness-of-fit on F^2	0.917
Final R indices [I>2sigma(I)]	R1 = 0.0497, wR2 = 0.1170
R indices (all data)	R1 = 0.0874, wR2 = 0.1243
Largest diff. peak and hole	0.322 and -0.546 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **12**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	10987(1)	2736(2)	6446(1)	32(1)
C(2)	10916(1)	3723(2)	6148(1)	37(1)
C(3)	11172(1)	3887(2)	5460(1)	48(1)
C(4)	11500(1)	3122(2)	5088(1)	56(1)
C(5)	11570(1)	2174(2)	5393(2)	54(1)
C(6)	11317(1)	1955(2)	6070(1)	42(1)
C(7)	10576(1)	4565(2)	6571(1)	47(1)
C(8)	10279(2)	5437(2)	6105(2)	79(1)
C(9)	11082(2)	5011(2)	7147(2)	63(1)
C(10)	11420(1)	896(2)	6390(2)	48(1)
C(11)	11171(2)	55(2)	5868(2)	96(1)
C(12)	12176(2)	743(3)	6643(3)	108(2)
C(13)	8935(1)	655(2)	6447(1)	32(1)
C(14)	8642(1)	1475(2)	6059(1)	37(1)
C(15)	7981(1)	1356(2)	5750(2)	54(1)
C(16)	7625(1)	449(2)	5805(2)	60(1)
C(17)	7914(1)	-348(2)	6184(1)	51(1)
C(18)	8573(1)	-270(2)	6516(1)	40(1)
C(19)	9044(1)	2450(2)	5927(1)	45(1)
C(20)	9427(2)	2361(2)	5218(2)	73(1)
C(21)	8597(2)	3406(2)	5954(2)	86(1)
C(22)	8898(2)	-1145(2)	6947(2)	54(1)
C(23)	9447(2)	-1707(2)	6510(2)	73(1)
C(24)	8360(2)	-1900(2)	7233(2)	91(1)
N(1)	10694(1)	2529(1)	7124(1)	31(1)
N(2)	9597(1)	778(1)	6787(1)	33(1)
Ti(1)	10000	1655(1)	7500	25(1)

Table 3. Bond lengths [A] and angles [deg] for **12**.

C(1)-C(6)	1.399(3)
C(1)-C(2)	1.412(3)
C(1)-N(1)	1.414(3)
C(2)-C(3)	1.394(3)
C(2)-C(7)	1.512(3)
C(3)-C(4)	1.378(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.370(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.386(3)
C(5)-H(5)	0.9500
C(6)-C(10)	1.521(3)
C(7)-C(8)	1.533(3)
C(7)-C(9)	1.537(4)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(12)	1.525(4)
C(10)-C(11)	1.534(4)
C(10)-H(10)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.403(3)
C(13)-C(18)	1.406(3)
C(13)-N(2)	1.412(3)
C(14)-C(15)	1.385(3)

C(14)-C(19)	1.517(3)
C(15)-C(16)	1.376(4)
C(15)-H(15)	0.9500
C(16)-C(17)	1.368(4)
C(16)-H(16)	0.9500
C(17)-C(18)	1.394(3)
C(17)-H(17)	0.9500
C(18)-C(22)	1.521(3)
C(19)-C(21)	1.521(4)
C(19)-C(20)	1.526(4)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.533(4)
C(22)-C(24)	1.534(4)
C(22)-H(22)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
N(1)-Ti(1)	1.9028(17)
N(1)-H(1A)	0.9200
N(1)-H(1B)	0.9200
N(2)-Ti(1)	1.8984(17)
N(2)-H(2A)	0.9200
N(2)-H(2B)	0.9200
Ti(1)-N(2)#1	1.8984(17)
Ti(1)-N(1)#1	1.9028(17)

C(6)-C(1)-C(2)	121.1(2)
C(6)-C(1)-N(1)	119.79(19)
C(2)-C(1)-N(1)	119.1(2)
C(3)-C(2)-C(1)	117.8(2)
C(3)-C(2)-C(7)	121.8(2)
C(1)-C(2)-C(7)	120.4(2)
C(4)-C(3)-C(2)	121.4(2)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
C(5)-C(4)-C(3)	119.7(2)
C(5)-C(4)-H(4)	120.1
C(3)-C(4)-H(4)	120.1
C(4)-C(5)-C(6)	121.8(3)
C(4)-C(5)-H(5)	119.1
C(6)-C(5)-H(5)	119.1
C(5)-C(6)-C(1)	118.2(2)
C(5)-C(6)-C(10)	119.8(2)
C(1)-C(6)-C(10)	122.0(2)
C(2)-C(7)-C(8)	114.4(2)
C(2)-C(7)-C(9)	111.3(2)
C(8)-C(7)-C(9)	109.0(2)
C(2)-C(7)-H(7)	107.3
C(8)-C(7)-H(7)	107.3
C(9)-C(7)-H(7)	107.3
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(6)-C(10)-C(12)	110.7(2)
C(6)-C(10)-C(11)	112.0(2)
C(12)-C(10)-C(11)	112.1(3)
C(6)-C(10)-H(10)	107.2
C(12)-C(10)-H(10)	107.2
C(11)-C(10)-H(10)	107.2

C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	121.0(2)
C(14)-C(13)-N(2)	118.97(18)
C(18)-C(13)-N(2)	120.0(2)
C(15)-C(14)-C(13)	118.3(2)
C(15)-C(14)-C(19)	119.5(2)
C(13)-C(14)-C(19)	122.0(2)
C(16)-C(15)-C(14)	121.2(2)
C(16)-C(15)-H(15)	119.4
C(14)-C(15)-H(15)	119.4
C(17)-C(16)-C(15)	120.1(2)
C(17)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
C(16)-C(17)-C(18)	121.4(2)
C(16)-C(17)-H(17)	119.3
C(18)-C(17)-H(17)	119.3
C(17)-C(18)-C(13)	117.9(2)
C(17)-C(18)-C(22)	122.1(2)
C(13)-C(18)-C(22)	120.1(2)
C(14)-C(19)-C(21)	113.5(2)
C(14)-C(19)-C(20)	109.5(2)
C(21)-C(19)-C(20)	112.1(2)
C(14)-C(19)-H(19)	107.1
C(21)-C(19)-H(19)	107.1
C(20)-C(19)-H(19)	107.1
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(18)-C(22)-C(23)	111.3(2)
C(18)-C(22)-C(24)	113.4(3)
C(23)-C(22)-C(24)	110.5(2)
C(18)-C(22)-H(22)	107.1
C(23)-C(22)-H(22)	107.1
C(24)-C(22)-H(22)	107.1
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(1)-N(1)-Ti(1)	137.54(14)
C(1)-N(1)-H(1A)	102.7
Ti(1)-N(1)-H(1A)	102.7
C(1)-N(1)-H(1B)	102.7
Ti(1)-N(1)-H(1B)	102.7
H(1A)-N(1)-H(1B)	105.0
C(13)-N(2)-Ti(1)	136.37(14)
C(13)-N(2)-H(2A)	103.1
Ti(1)-N(2)-H(2A)	103.1
C(13)-N(2)-H(2B)	103.1
Ti(1)-N(2)-H(2B)	103.1

H(2A)-N(2)-H(2B)	105.1
N(2)-Ti(1)-N(2)#1	105.49(11)
N(2)-Ti(1)-N(1)	112.74(8)
N(2)#1-Ti(1)-N(1)	110.04(8)
N(2)-Ti(1)-N(1)#1	110.04(8)
N(2)#1-Ti(1)-N(1)#1	112.74(8)
N(1)-Ti(1)-N(1)#1	105.92(11)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y,-z+3/2

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **12**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	30(1)	35(1)	30(1)	-2(1)	-2(1)	-13(1)
C(2)	34(1)	41(1)	34(1)	2(1)	-5(1)	-17(1)
C(3)	46(2)	56(2)	41(2)	10(1)	-7(1)	-28(1)
C(4)	55(2)	84(2)	31(1)	-3(1)	7(1)	-31(2)
C(5)	48(2)	65(2)	49(2)	-19(1)	15(1)	-20(1)
C(6)	34(1)	50(2)	41(1)	-12(1)	6(1)	-16(1)
C(7)	54(2)	34(1)	52(2)	6(1)	1(1)	-7(1)
C(8)	97(3)	53(2)	87(2)	24(2)	0(2)	8(2)
C(9)	83(2)	46(2)	59(2)	-12(1)	8(2)	-23(2)
C(10)	42(2)	38(1)	65(2)	-12(1)	15(1)	-7(1)
C(11)	148(4)	55(2)	88(3)	-33(2)	39(3)	-28(2)
C(12)	50(2)	72(2)	203(5)	53(3)	7(3)	1(2)
C(13)	31(1)	37(1)	29(1)	-8(1)	-1(1)	-7(1)
C(14)	34(1)	44(1)	32(1)	-2(1)	-7(1)	-8(1)
C(15)	44(2)	59(2)	56(2)	7(1)	-19(1)	-8(1)
C(16)	36(2)	76(2)	67(2)	7(2)	-16(1)	-16(2)
C(17)	45(2)	54(2)	54(2)	-7(1)	4(1)	-24(1)
C(18)	44(2)	38(1)	38(1)	-8(1)	2(1)	-10(1)
C(19)	54(2)	40(1)	39(1)	7(1)	-19(1)	-10(1)
C(20)	97(3)	77(2)	45(2)	10(2)	-4(2)	-48(2)
C(21)	90(3)	45(2)	119(3)	3(2)	-48(2)	-1(2)
C(22)	71(2)	33(1)	57(2)	-4(1)	-9(2)	-11(1)
C(23)	83(2)	45(2)	91(2)	-23(2)	-20(2)	5(2)
C(24)	122(3)	54(2)	97(3)	18(2)	-6(2)	-35(2)
N(1)	32(1)	29(1)	32(1)	-1(1)	-5(1)	0(1)
N(2)	34(1)	31(1)	34(1)	0(1)	-2(1)	-3(1)
Ti(1)	28(1)	22(1)	25(1)	0	-4(1)	0

Data for compound 15

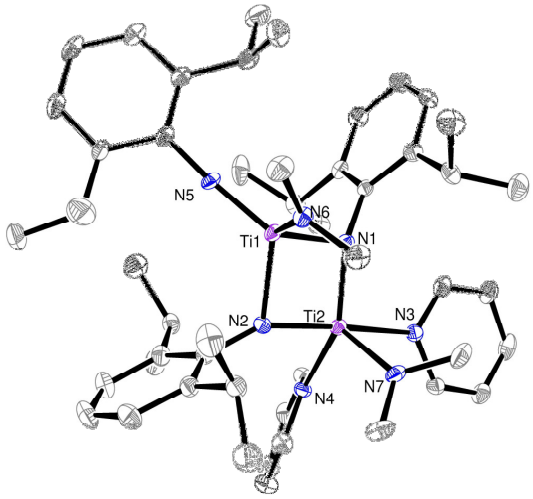


Table 1. Crystal data and structure refinement for **15**.

Identification code	cl1732
Empirical formula	C50 H73 N7 Ti2
Formula weight	867.95
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 1 21/c 1
Unit cell dimensions	a = 12.6101(6) A alpha = 90 deg.
	b = 22.6800(14) A beta = 99.489(5) deg.
	c = 21.3541(10) A gamma = 90 deg.
Volume	6023.6(5) A^3
Z, Calculated density	4, 0.957 Mg/m^3
Absorption coefficient	0.297 mm^-1
F(000)	1864
Crystal size	0.2 x 0.05 x 0.04 mm
Theta range for data collection	3.38 to 26.37 deg.
Limiting indices	-15<=h<=15, -28<=k<=28, -26<=l<=26
Reflections collected / unique	50674 / 12293 [R(int) = 0.1365]
Completeness to theta = 26.37	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9987 and 0.9359
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12293 / 0 / 548
Goodness-of-fit on F^2	0.918
Final R indices [I>2sigma(I)]	R1 = 0.0742, wR2 = 0.1545
R indices (all data)	R1 = 0.1516, wR2 = 0.1816
Largest diff. peak and hole	0.374 and -0.337 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **15**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	2648(3)	1252(2)	6672(2)	23(1)
C(2)	3313(3)	1562(2)	7169(2)	27(1)
C(3)	4348(3)	1349(2)	7390(2)	33(1)
C(4)	4730(3)	855(2)	7140(2)	37(1)
C(5)	4112(3)	572(2)	6645(2)	37(1)
C(6)	3077(3)	757(2)	6391(2)	30(1)
C(7)	2949(3)	2112(2)	7459(2)	34(1)
C(8)	3631(3)	2650(2)	7333(2)	43(1)
C(9)	2991(4)	2040(2)	8176(2)	58(2)
C(10)	2469(3)	446(2)	5813(2)	34(1)
C(11)	3036(4)	543(2)	5237(2)	51(1)
C(12)	2338(4)	-212(2)	5936(2)	49(1)
C(13)	-1307(3)	1985(2)	6820(2)	27(1)
C(14)	-1189(3)	2398(2)	7323(2)	32(1)
C(15)	-2096(3)	2565(2)	7570(2)	43(1)
C(16)	-3091(4)	2334(2)	7349(2)	52(1)
C(17)	-3208(3)	1935(2)	6857(2)	44(1)
C(18)	-2333(3)	1756(2)	6586(2)	32(1)
C(19)	-117(3)	2653(2)	7632(2)	32(1)
C(20)	-159(4)	3317(2)	7721(2)	49(1)
C(21)	277(4)	2372(2)	8279(2)	48(1)
C(22)	-2514(3)	1290(2)	6065(2)	36(1)
C(23)	-3434(4)	1450(3)	5532(2)	58(2)
C(24)	-2769(4)	681(2)	6336(2)	53(1)
C(25)	1680(3)	2839(2)	5095(2)	32(1)
C(26)	2370(4)	3082(2)	4731(2)	37(1)
C(27)	3409(4)	2905(2)	4827(2)	44(1)
C(28)	3745(4)	2487(2)	5291(2)	39(1)
C(29)	3006(3)	2272(2)	5643(2)	32(1)
C(30)	-605(3)	3206(2)	5981(2)	33(1)
C(31)	-806(4)	3801(2)	5990(2)	41(1)
C(32)	20(4)	4174(2)	6234(2)	43(1)
C(33)	1014(4)	3940(2)	6454(2)	38(1)
C(34)	1161(3)	3345(2)	6412(2)	34(1)
C(35)	778(3)	743(2)	8350(2)	26(1)
C(36)	1771(3)	483(2)	8626(2)	28(1)
C(37)	1933(4)	331(2)	9264(2)	35(1)
C(38)	1158(4)	433(2)	9639(2)	40(1)
C(39)	188(4)	681(2)	9370(2)	39(1)
C(40)	-25(3)	836(2)	8737(2)	30(1)
C(41)	2624(3)	346(2)	8217(2)	35(1)
C(42)	3777(3)	379(2)	8574(2)	54(1)
C(43)	2415(4)	-254(2)	7893(2)	56(2)
C(44)	-1130(4)	1054(2)	8439(2)	40(1)
C(45)	-1836(4)	544(3)	8162(2)	58(2)
C(46)	-1709(4)	1402(3)	8895(2)	68(2)
C(47)	-380(3)	319(2)	5791(2)	37(1)
C(48)	-318(4)	-222(2)	6753(2)	45(1)
C(49)	-1126(3)	1882(2)	4913(2)	46(1)
C(50)	572(4)	1514(2)	4736(2)	45(1)
N(1)	1591(2)	1447(2)	6454(1)	26(1)
N(2)	-388(2)	1810(1)	6560(1)	23(1)
N(3)	1978(3)	2445(2)	5557(1)	28(1)
N(4)	375(2)	2969(2)	6174(1)	26(1)
N(5)	608(2)	911(1)	7720(1)	26(1)
N(6)	-107(2)	345(2)	6485(1)	28(1)
N(7)	3(3)	1814(2)	5184(1)	30(1)
Ti(1)	428(1)	1063(1)	6902(1)	23(1)
Ti(2)	631(1)	2002(1)	6045(1)	23(1)

Table 3. Bond lengths [A] and angles [deg] for **15**.

C(1)-N(1)	1.409(5)

C(1)-C(6)	1.423(6)
C(1)-C(2)	1.423(5)
C(2)-C(3)	1.400(5)
C(2)-C(7)	1.499(6)
C(3)-C(4)	1.363(6)
C(3)-H(3)	0.9500
C(4)-C(5)	1.365(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.393(5)
C(5)-H(5)	0.9500
C(6)-C(10)	1.516(5)
C(7)-C(9)	1.531(6)
C(7)-C(8)	1.542(6)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(12)	1.529(6)
C(10)-C(11)	1.536(6)
C(10)-H(10)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(18)	1.407(5)
C(13)-C(14)	1.415(5)
C(13)-N(2)	1.422(5)
C(14)-C(15)	1.390(5)
C(14)-C(19)	1.518(6)
C(15)-C(16)	1.370(6)
C(15)-H(15)	0.9500
C(16)-C(17)	1.378(6)
C(16)-H(16)	0.9500
C(17)-C(18)	1.389(6)
C(17)-H(17)	0.9500
C(18)-C(22)	1.524(6)
C(19)-C(20)	1.521(6)
C(19)-C(21)	1.528(6)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.528(6)
C(22)-C(24)	1.550(6)
C(22)-H(22)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-N(3)	1.337(5)
C(25)-C(26)	1.375(5)
C(25)-H(25)	0.9500
C(26)-C(27)	1.353(6)
C(26)-H(26)	0.9500
C(27)-C(28)	1.387(6)
C(27)-H(27)	0.9500
C(28)-C(29)	1.379(5)
C(28)-H(28)	0.9500
C(29)-N(3)	1.338(5)
C(29)-H(29)	0.9500
C(30)-N(4)	1.348(5)
C(30)-C(31)	1.372(6)
C(30)-H(30)	0.9500
C(31)-C(32)	1.377(6)
C(31)-H(31)	0.9500
C(32)-C(33)	1.372(6)
C(32)-H(32)	0.9500

C(33)-C(34)	1.368(6)
C(33)-H(33)	0.9500
C(34)-N(4)	1.342(5)
C(34)-H(34)	0.9500
C(35)-N(5)	1.382(4)
C(35)-C(36)	1.420(5)
C(35)-C(40)	1.425(5)
C(36)-C(37)	1.389(5)
C(36)-C(41)	1.524(5)
C(37)-C(38)	1.381(6)
C(37)-H(37)	0.9500
C(38)-C(39)	1.382(6)
C(38)-H(38)	0.9500
C(39)-C(40)	1.379(5)
C(39)-H(39)	0.9500
C(40)-C(44)	1.516(6)
C(41)-C(42)	1.529(6)
C(41)-C(43)	1.530(6)
C(41)-H(41)	1.0000
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-C(45)	1.520(6)
C(44)-C(46)	1.529(6)
C(44)-H(44)	1.0000
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
C(47)-N(6)	1.466(5)
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-N(6)	1.449(5)
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-N(7)	1.454(5)
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(50)-N(7)	1.457(5)
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
N(1)-Ti(2)	1.861(3)
N(1)-Ti(1)	2.070(3)
N(2)-Ti(2)	1.876(3)
N(2)-Ti(1)	2.053(3)
N(3)-Ti(2)	2.359(3)
N(4)-Ti(2)	2.240(3)
N(5)-Ti(1)	1.758(3)
N(6)-Ti(1)	1.923(3)
N(7)-Ti(2)	1.925(3)
Ti(1)-Ti(2)	2.8475(10)

N(1)-C(1)-C(6)	120.9(3)
N(1)-C(1)-C(2)	120.0(3)
C(6)-C(1)-C(2)	119.1(3)
C(3)-C(2)-C(1)	118.9(4)
C(3)-C(2)-C(7)	118.7(4)
C(1)-C(2)-C(7)	122.4(4)
C(4)-C(3)-C(2)	121.4(4)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
C(3)-C(4)-C(5)	119.8(4)
C(3)-C(4)-H(4)	120.1
C(5)-C(4)-H(4)	120.1
C(4)-C(5)-C(6)	122.6(4)
C(4)-C(5)-H(5)	118.7
C(6)-C(5)-H(5)	118.7
C(5)-C(6)-C(1)	118.0(4)

C(5)-C(6)-C(10)	119.6(4)
C(1)-C(6)-C(10)	122.4(4)
C(2)-C(7)-C(9)	111.3(4)
C(2)-C(7)-C(8)	111.6(3)
C(9)-C(7)-C(8)	109.3(4)
C(2)-C(7)-H(7)	108.2
C(9)-C(7)-H(7)	108.2
C(8)-C(7)-H(7)	108.2
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(6)-C(10)-C(12)	111.6(4)
C(6)-C(10)-C(11)	110.1(3)
C(12)-C(10)-C(11)	110.9(4)
C(6)-C(10)-H(10)	108.0
C(12)-C(10)-H(10)	108.0
C(11)-C(10)-H(10)	108.0
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(18)-C(13)-C(14)	119.3(4)
C(18)-C(13)-N(2)	121.3(4)
C(14)-C(13)-N(2)	119.4(4)
C(15)-C(14)-C(13)	118.6(4)
C(15)-C(14)-C(19)	117.4(4)
C(13)-C(14)-C(19)	123.9(4)
C(16)-C(15)-C(14)	122.0(4)
C(16)-C(15)-H(15)	119.0
C(14)-C(15)-H(15)	119.0
C(15)-C(16)-C(17)	119.4(4)
C(15)-C(16)-H(16)	120.3
C(17)-C(16)-H(16)	120.3
C(16)-C(17)-C(18)	121.2(4)
C(16)-C(17)-H(17)	119.4
C(18)-C(17)-H(17)	119.4
C(17)-C(18)-C(13)	119.4(4)
C(17)-C(18)-C(22)	118.3(4)
C(13)-C(18)-C(22)	122.2(4)
C(14)-C(19)-C(20)	112.6(4)
C(14)-C(19)-C(21)	111.6(4)
C(20)-C(19)-C(21)	108.2(4)
C(14)-C(19)-H(19)	108.1
C(20)-C(19)-H(19)	108.1
C(21)-C(19)-H(19)	108.1
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(18)-C(22)-C(23)	112.5(4)
C(18)-C(22)-C(24)	111.1(4)
C(23)-C(22)-C(24)	108.1(4)

C(18)-C(22)-H(22)	108.3
C(23)-C(22)-H(22)	108.3
C(24)-C(22)-H(22)	108.3
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
N(3)-C(25)-C(26)	123.9(4)
N(3)-C(25)-H(25)	118.0
C(26)-C(25)-H(25)	118.0
C(27)-C(26)-C(25)	118.8(4)
C(27)-C(26)-H(26)	120.6
C(25)-C(26)-H(26)	120.6
C(26)-C(27)-C(28)	119.1(4)
C(26)-C(27)-H(27)	120.5
C(28)-C(27)-H(27)	120.5
C(29)-C(28)-C(27)	118.5(4)
C(29)-C(28)-H(28)	120.8
C(27)-C(28)-H(28)	120.8
N(3)-C(29)-C(28)	123.2(4)
N(3)-C(29)-H(29)	118.4
C(28)-C(29)-H(29)	118.4
N(4)-C(30)-C(31)	123.4(4)
N(4)-C(30)-H(30)	118.3
C(31)-C(30)-H(30)	118.3
C(30)-C(31)-C(32)	118.7(4)
C(30)-C(31)-H(31)	120.7
C(32)-C(31)-H(31)	120.7
C(33)-C(32)-C(31)	118.9(4)
C(33)-C(32)-H(32)	120.6
C(31)-C(32)-H(32)	120.6
C(34)-C(33)-C(32)	119.1(4)
C(34)-C(33)-H(33)	120.5
C(32)-C(33)-H(33)	120.5
N(4)-C(34)-C(33)	123.5(4)
N(4)-C(34)-H(34)	118.2
C(33)-C(34)-H(34)	118.2
N(5)-C(35)-C(36)	120.2(3)
N(5)-C(35)-C(40)	120.9(4)
C(36)-C(35)-C(40)	118.9(3)
C(37)-C(36)-C(35)	119.2(4)
C(37)-C(36)-C(41)	120.5(4)
C(35)-C(36)-C(41)	120.3(3)
C(38)-C(37)-C(36)	121.5(4)
C(38)-C(37)-H(37)	119.2
C(36)-C(37)-H(37)	119.2
C(37)-C(38)-C(39)	119.4(4)
C(37)-C(38)-H(38)	120.3
C(39)-C(38)-H(38)	120.3
C(40)-C(39)-C(38)	121.8(4)
C(40)-C(39)-H(39)	119.1
C(38)-C(39)-H(39)	119.1
C(39)-C(40)-C(35)	119.2(4)
C(39)-C(40)-C(44)	120.7(4)
C(35)-C(40)-C(44)	119.8(3)
C(36)-C(41)-C(42)	114.1(4)
C(36)-C(41)-C(43)	110.8(4)
C(42)-C(41)-C(43)	110.3(4)
C(36)-C(41)-H(41)	107.1
C(42)-C(41)-H(41)	107.1
C(43)-C(41)-H(41)	107.1
C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(41)-C(43)-H(43A)	109.5
C(41)-C(43)-H(43B)	109.5

H(43A)-C(43)-H(43B)	109.5
C(41)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(40)-C(44)-C(45)	110.7(4)
C(40)-C(44)-C(46)	113.8(4)
C(45)-C(44)-C(46)	109.3(4)
C(40)-C(44)-H(44)	107.6
C(45)-C(44)-H(44)	107.6
C(46)-C(44)-H(44)	107.6
C(44)-C(45)-H(45A)	109.5
C(44)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(44)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(44)-C(46)-H(46A)	109.5
C(44)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(44)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
N(6)-C(47)-H(47A)	109.5
N(6)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
N(6)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
N(6)-C(48)-H(48A)	109.5
N(6)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
N(6)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
N(7)-C(49)-H(49A)	109.5
N(7)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
N(7)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
N(7)-C(50)-H(50A)	109.5
N(7)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
N(7)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(1)-N(1)-Ti(2)	151.0(3)
C(1)-N(1)-Ti(1)	114.7(2)
Ti(2)-N(1)-Ti(1)	92.67(13)
C(13)-N(2)-Ti(2)	147.7(3)
C(13)-N(2)-Ti(1)	119.0(2)
Ti(2)-N(2)-Ti(1)	92.80(13)
C(25)-N(3)-C(29)	116.5(3)
C(25)-N(3)-Ti(2)	118.4(3)
C(29)-N(3)-Ti(2)	124.5(3)
C(34)-N(4)-C(30)	116.4(4)
C(34)-N(4)-Ti(2)	123.8(3)
C(30)-N(4)-Ti(2)	119.8(3)
C(35)-N(5)-Ti(1)	174.9(3)
C(48)-N(6)-C(47)	109.6(3)
C(48)-N(6)-Ti(1)	129.9(3)
C(47)-N(6)-Ti(1)	120.5(3)
C(49)-N(7)-C(50)	110.1(3)
C(49)-N(7)-Ti(2)	125.4(3)
C(50)-N(7)-Ti(2)	124.1(3)
N(5)-Ti(1)-N(6)	105.81(14)
N(5)-Ti(1)-N(2)	119.25(14)
N(6)-Ti(1)-N(2)	114.65(13)
N(5)-Ti(1)-N(1)	123.79(14)
N(6)-Ti(1)-N(1)	111.39(13)
N(2)-Ti(1)-N(1)	80.77(12)
N(5)-Ti(1)-Ti(2)	140.70(11)
N(6)-Ti(1)-Ti(2)	113.47(10)
N(2)-Ti(1)-Ti(2)	41.14(8)
N(1)-Ti(1)-Ti(2)	40.75(9)
N(1)-Ti(2)-N(2)	91.29(13)
N(1)-Ti(2)-N(7)	115.58(14)

N(2)-Ti(2)-N(7)	107.12(14)
N(1)-Ti(2)-N(4)	134.41(13)
N(2)-Ti(2)-N(4)	91.67(13)
N(7)-Ti(2)-N(4)	106.83(13)
N(1)-Ti(2)-N(3)	92.04(13)
N(2)-Ti(2)-N(3)	166.18(13)
N(7)-Ti(2)-N(3)	83.45(13)
N(4)-Ti(2)-N(3)	76.47(11)
N(1)-Ti(2)-Ti(1)	46.58(10)
N(2)-Ti(2)-Ti(1)	46.06(10)
N(7)-Ti(2)-Ti(1)	112.39(11)
N(4)-Ti(2)-Ti(1)	128.57(8)
N(3)-Ti(2)-Ti(1)	138.61(9)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **15**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	27(2)	19(2)	24(2)	5(2)	8(2)	-2(2)
C(2)	29(2)	31(3)	21(2)	0(2)	4(2)	-5(2)
C(3)	25(2)	40(3)	32(2)	0(2)	-1(2)	-5(2)
C(4)	26(2)	47(3)	38(3)	6(2)	1(2)	6(2)
C(5)	34(2)	37(3)	40(3)	3(2)	11(2)	14(2)
C(6)	34(2)	22(3)	33(2)	4(2)	7(2)	-1(2)
C(7)	27(2)	37(3)	38(3)	-10(2)	2(2)	-6(2)
C(8)	45(3)	35(3)	47(3)	-3(2)	2(2)	0(2)
C(9)	79(4)	53(4)	47(3)	-20(3)	31(3)	-10(3)
C(10)	36(2)	27(3)	41(3)	-11(2)	8(2)	2(2)
C(11)	63(3)	56(4)	34(3)	-10(2)	8(2)	-2(3)
C(12)	56(3)	33(3)	56(3)	-9(2)	-1(2)	-1(3)
C(13)	34(2)	17(2)	32(2)	5(2)	12(2)	3(2)
C(14)	43(3)	20(3)	36(2)	-1(2)	14(2)	0(2)
C(15)	38(3)	45(3)	49(3)	-11(2)	19(2)	-2(3)
C(16)	43(3)	51(4)	66(3)	-7(3)	26(3)	10(3)
C(17)	29(2)	46(3)	57(3)	-2(3)	9(2)	-1(2)
C(18)	34(2)	29(3)	33(2)	3(2)	10(2)	1(2)
C(19)	36(2)	29(3)	34(2)	-4(2)	12(2)	0(2)
C(20)	72(3)	32(3)	45(3)	-11(2)	20(3)	-8(3)
C(21)	57(3)	44(3)	42(3)	-5(2)	4(2)	-2(3)
C(22)	33(2)	37(3)	36(2)	-2(2)	7(2)	3(2)
C(23)	40(3)	80(5)	52(3)	-6(3)	-2(2)	2(3)
C(24)	61(3)	34(3)	70(3)	-6(3)	26(3)	-14(3)
C(25)	35(2)	27(3)	34(2)	6(2)	9(2)	6(2)
C(26)	55(3)	27(3)	32(2)	7(2)	14(2)	-2(2)
C(27)	52(3)	50(4)	34(3)	-1(2)	20(2)	-21(3)
C(28)	39(3)	48(3)	33(3)	3(2)	11(2)	-9(2)
C(29)	41(3)	31(3)	25(2)	-2(2)	5(2)	-4(2)
C(30)	35(2)	28(3)	38(3)	-3(2)	6(2)	-4(2)
C(31)	36(3)	33(3)	50(3)	1(2)	2(2)	8(2)
C(32)	59(3)	22(3)	50(3)	3(2)	14(2)	9(3)
C(33)	48(3)	23(3)	45(3)	-8(2)	11(2)	-4(2)
C(34)	28(2)	33(3)	41(3)	0(2)	7(2)	1(2)
C(35)	39(2)	18(2)	21(2)	1(2)	5(2)	-5(2)
C(36)	39(2)	21(2)	23(2)	-1(2)	3(2)	-5(2)
C(37)	45(3)	32(3)	27(2)	4(2)	0(2)	-10(2)
C(38)	67(3)	34(3)	18(2)	-1(2)	7(2)	-14(3)
C(39)	57(3)	35(3)	27(2)	-4(2)	17(2)	-6(3)
C(40)	44(3)	25(3)	24(2)	1(2)	12(2)	-1(2)
C(41)	41(3)	34(3)	32(2)	11(2)	7(2)	2(2)
C(42)	40(3)	71(4)	49(3)	23(3)	3(2)	1(3)
C(43)	67(3)	54(4)	51(3)	-6(3)	21(3)	9(3)
C(44)	54(3)	32(3)	39(3)	9(2)	25(2)	8(3)
C(45)	41(3)	65(4)	64(3)	0(3)	4(3)	3(3)
C(46)	82(4)	66(4)	68(4)	15(3)	48(3)	34(3)
C(47)	42(3)	35(3)	32(2)	-10(2)	-4(2)	-6(2)
C(48)	60(3)	28(3)	47(3)	4(2)	9(2)	-8(3)
C(49)	46(3)	47(3)	40(3)	13(2)	-10(2)	-3(3)
C(50)	71(3)	41(3)	24(2)	-1(2)	7(2)	-4(3)
N(1)	28(2)	27(2)	22(2)	1(2)	1(1)	1(2)
N(2)	23(2)	18(2)	26(2)	-2(1)	4(1)	0(2)

N(3)	33(2)	24(2)	29(2)	4(2)	9(2)	4(2)
N(4)	23(2)	25(2)	29(2)	5(2)	6(1)	5(2)
N(5)	37(2)	19(2)	21(2)	6(1)	3(1)	-1(2)
N(6)	35(2)	22(2)	28(2)	0(2)	6(2)	-3(2)
N(7)	38(2)	28(2)	24(2)	7(2)	1(2)	2(2)
Ti(1)	31(1)	19(1)	20(1)	2(1)	4(1)	-1(1)
Ti(2)	28(1)	18(1)	22(1)	1(1)	4(1)	-1(1)

Data for compound 16

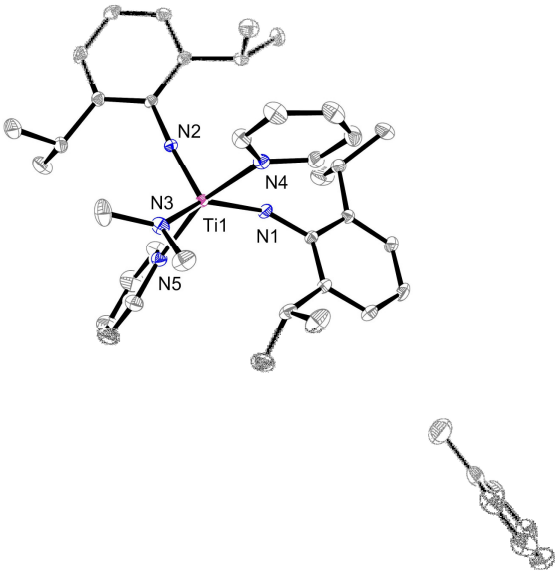


Table 1. Crystal data and structure refinement for **16**.

Identification code	cl1649
Empirical formula	C43 H59 N5 Ti
Formula weight	693.85
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C 1 c 1
Unit cell dimensions	a = 14.4789(10) A alpha = 90 deg. b = 15.7622(10) A beta = 110.076(2) deg. c = 18.8740(10) A gamma = 90 deg.
Volume	4045.7(4) A^3
Z, Calculated density	4, 1.139 Mg/m^3
Absorption coefficient	0.246 mm^-1
F(000)	1496
Crystal size	0.17 x 0.1 x 0.03 mm
Theta range for data collection	2.83 to 30.00 deg.
Limiting indices	-20<=h<=19, -22<=k<=22, -26<=l<=26
Reflections collected / unique	30095 / 11376 [R(int) = 0.0338]
Completeness to theta = 30.00	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.981 and 0.852
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11376 / 2 / 454
Goodness-of-fit on F^2	1.016
Final R indices [I>2sigma(I)]	R1 = 0.0407, wR2 = 0.0836
R indices (all data)	R1 = 0.0601, wR2 = 0.0907
Absolute structure parameter	0.114(14)
Largest diff. peak and hole	0.244 and -0.203 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **16**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	7596(1)	7828(1)	9110(1)	20(1)
C(2)	7885(1)	8643(1)	9448(1)	24(1)
C(3)	7686(2)	8851(1)	10100(1)	31(1)
C(5)	6875(2)	7540(1)	10077(1)	31(1)
C(6)	7054(1)	7288(1)	9427(1)	23(1)
C(7)	8436(2)	9273(1)	9134(1)	31(1)
C(08)	7193(2)	8309(1)	10419(1)	34(1)
C(8)	8003(2)	10167(1)	9049(1)	47(1)
C(9)	9516(2)	9296(2)	9631(2)	59(1)
C(10)	6666(2)	6436(1)	9080(1)	31(1)
C(11)	7168(2)	5697(1)	9583(1)	53(1)
C(12)	5547(2)	6384(2)	8853(1)	53(1)
C(13)	8756(1)	7580(1)	6699(1)	19(1)
C(14)	9440(1)	7121(1)	6465(1)	23(1)
C(15)	9974(1)	7541(1)	6081(1)	29(1)
C(16)	9856(2)	8400(1)	5925(1)	31(1)
C(17)	9193(1)	8850(1)	6164(1)	25(1)
C(18)	8648(1)	8469(1)	6551(1)	20(1)
C(19)	9596(1)	6173(1)	6614(1)	28(1)
C(20)	9324(2)	5678(1)	5870(1)	48(1)
C(21)	10647(2)	5971(1)	7115(1)	44(1)
C(22)	7904(1)	8977(1)	6778(1)	24(1)
C(23)	8296(2)	9845(1)	7116(1)	37(1)
C(24)	6952(2)	9078(1)	6108(1)	37(1)
C(25)	6996(2)	5296(1)	6470(1)	47(1)
C(26)	5897(2)	5474(2)	7152(1)	45(1)
N(4)	6067(1)	7518(1)	7068(1)	25(1)
C(28)	5477(2)	7324(1)	6363(1)	34(1)
C(29)	4587(2)	7707(1)	6011(1)	43(1)
C(30)	4263(2)	8318(1)	6393(1)	43(1)
C(31)	4860(2)	8541(1)	7106(1)	39(1)
C(32)	5751(1)	8128(1)	7423(1)	30(1)
N(5)	8676(1)	5914(1)	8297(1)	26(1)
C(34)	9583(2)	6223(1)	8642(1)	40(1)
C(35)	10361(2)	5737(2)	9076(1)	52(1)
C(36)	10206(2)	4889(2)	9176(1)	51(1)
C(37)	9283(2)	4567(1)	8830(1)	47(1)
C(38)	8542(2)	5087(1)	8398(1)	33(1)
C(39)	7354(2)	7255(2)	13229(1)	51(1)
C(40)	7882(2)	7499(2)	13961(2)	49(1)
C(41)	7522(2)	7369(2)	14537(1)	53(1)
C(42)	6621(2)	6991(2)	14393(2)	61(1)
C(43)	6082(2)	6751(2)	13664(2)	60(1)
C(44)	6435(2)	6880(2)	13091(1)	53(1)
C(45)	7733(3)	7402(2)	12595(2)	90(1)
N(1)	7816(1)	7575(1)	8485(1)	22(1)
N(2)	8185(1)	7186(1)	7056(1)	20(1)
N(3)	6778(1)	5794(1)	7039(1)	29(1)
Ti(1)	7502(1)	6783(1)	7574(1)	18(1)

Table 3. Bond lengths [A] and angles [deg] for **16**.

C(1)-N(1)	1.380(2)
C(1)-C(6)	1.423(2)
C(1)-C(2)	1.431(2)
C(2)-C(3)	1.395(2)
C(2)-C(7)	1.516(3)
C(3)-C(08)	1.377(3)
C(3)-H(3)	0.9500
C(5)-C(08)	1.377(3)
C(5)-C(6)	1.395(2)
C(5)-H(5)	0.9500
C(6)-C(10)	1.514(3)
C(7)-C(9)	1.523(3)
C(7)-C(8)	1.529(3)
C(7)-H(7)	1.0000
C(08)-H(08)	0.9500
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.521(3)
C(10)-C(12)	1.529(3)
C(10)-H(10)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-N(2)	1.380(2)
C(13)-C(14)	1.414(2)
C(13)-C(18)	1.427(2)
C(14)-C(15)	1.395(2)
C(14)-C(19)	1.524(3)
C(15)-C(16)	1.383(3)
C(15)-H(15)	0.9500
C(16)-C(17)	1.387(3)
C(16)-H(16)	0.9500
C(17)-C(18)	1.383(2)
C(17)-H(17)	0.9500
C(18)-C(22)	1.517(2)
C(19)-C(21)	1.524(3)
C(19)-C(20)	1.535(3)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(24)	1.526(3)
C(22)-C(23)	1.534(3)
C(22)-H(22)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-N(3)	1.450(3)
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-N(3)	1.453(3)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
N(4)-C(32)	1.340(2)
N(4)-C(28)	1.347(2)
N(4)-Ti(1)	2.2821(16)
C(28)-C(29)	1.372(3)
C(28)-H(28)	0.9500
C(29)-C(30)	1.378(3)

C(29)-H(29)	0.9500
C(30)-C(31)	1.373(3)
C(30)-H(30)	0.9500
C(31)-C(32)	1.385(3)
C(31)-H(31)	0.9500
C(32)-H(32)	0.9500
N(5)-C(38)	1.340(2)
N(5)-C(34)	1.342(3)
N(5)-Ti(1)	2.2437(15)
C(34)-C(35)	1.376(3)
C(34)-H(34)	0.9500
C(35)-C(36)	1.378(4)
C(35)-H(35)	0.9500
C(36)-C(37)	1.368(4)
C(36)-H(36)	0.9500
C(37)-C(38)	1.375(3)
C(37)-H(37)	0.9500
C(38)-H(38)	0.9500
C(39)-C(40)	1.385(4)
C(39)-C(44)	1.396(4)
C(39)-C(45)	1.496(4)
C(40)-C(41)	1.373(4)
C(40)-H(40)	0.9500
C(41)-C(42)	1.374(4)
C(41)-H(41)	0.9500
C(42)-C(43)	1.381(4)
C(42)-H(42)	0.9500
C(43)-C(44)	1.360(4)
C(43)-H(43)	0.9500
C(44)-H(44)	0.9500
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
N(1)-Ti(1)	2.0450(13)
N(1)-H(1)	0.8800
N(2)-Ti(1)	1.7334(14)
N(3)-Ti(1)	1.9560(15)

N(1)-C(1)-C(6)	120.56(15)
N(1)-C(1)-C(2)	121.55(14)
C(6)-C(1)-C(2)	117.88(14)
C(3)-C(2)-C(1)	119.18(16)
C(3)-C(2)-C(7)	119.11(16)
C(1)-C(2)-C(7)	121.67(14)
C(08)-C(3)-C(2)	122.34(17)
C(08)-C(3)-H(3)	118.8
C(2)-C(3)-H(3)	118.8
C(08)-C(5)-C(6)	122.00(17)
C(08)-C(5)-H(5)	119.0
C(6)-C(5)-H(5)	119.0
C(5)-C(6)-C(1)	119.72(16)
C(5)-C(6)-C(10)	118.66(15)
C(1)-C(6)-C(10)	121.62(14)
C(2)-C(7)-C(9)	109.98(16)
C(2)-C(7)-C(8)	113.17(17)
C(9)-C(7)-C(8)	109.86(19)
C(2)-C(7)-H(7)	107.9
C(9)-C(7)-H(7)	107.9
C(8)-C(7)-H(7)	107.9
C(5)-C(08)-C(3)	118.74(16)
C(5)-C(08)-H(08)	120.6
C(3)-C(08)-H(08)	120.6
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(6)-C(10)-C(11)	112.46(16)
C(6)-C(10)-C(12)	111.62(18)
C(11)-C(10)-C(12)	111.46(19)

C(6)-C(10)-H(10)	107.0
C(11)-C(10)-H(10)	107.0
C(12)-C(10)-H(10)	107.0
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
N(2)-C(13)-C(14)	121.50(15)
N(2)-C(13)-C(18)	119.63(15)
C(14)-C(13)-C(18)	118.86(14)
C(15)-C(14)-C(13)	119.44(15)
C(15)-C(14)-C(19)	119.20(16)
C(13)-C(14)-C(19)	121.35(15)
C(16)-C(15)-C(14)	121.66(17)
C(16)-C(15)-H(15)	119.2
C(14)-C(15)-H(15)	119.2
C(15)-C(16)-C(17)	118.77(16)
C(15)-C(16)-H(16)	120.6
C(17)-C(16)-H(16)	120.6
C(18)-C(17)-C(16)	122.17(16)
C(18)-C(17)-H(17)	118.9
C(16)-C(17)-H(17)	118.9
C(17)-C(18)-C(13)	119.08(15)
C(17)-C(18)-C(22)	120.64(15)
C(13)-C(18)-C(22)	120.20(14)
C(14)-C(19)-C(21)	111.89(16)
C(14)-C(19)-C(20)	110.74(15)
C(21)-C(19)-C(20)	110.49(17)
C(14)-C(19)-H(19)	107.9
C(21)-C(19)-H(19)	107.9
C(20)-C(19)-H(19)	107.9
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(18)-C(22)-C(24)	110.33(14)
C(18)-C(22)-C(23)	113.03(15)
C(24)-C(22)-C(23)	110.57(16)
C(18)-C(22)-H(22)	107.6
C(24)-C(22)-H(22)	107.6
C(23)-C(22)-H(22)	107.6
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
N(3)-C(25)-H(25A)	109.5
N(3)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
N(3)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
N(3)-C(26)-H(26A)	109.5
N(3)-C(26)-H(26B)	109.5

H(26A)-C(26)-H(26B)	109.5
N(3)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(32)-N(4)-C(28)	116.62(16)
C(32)-N(4)-Ti(1)	124.94(12)
C(28)-N(4)-Ti(1)	118.43(13)
N(4)-C(28)-C(29)	123.4(2)
N(4)-C(28)-H(28)	118.3
C(29)-C(28)-H(28)	118.3
C(28)-C(29)-C(30)	119.08(19)
C(28)-C(29)-H(29)	120.5
C(30)-C(29)-H(29)	120.5
C(31)-C(30)-C(29)	118.6(2)
C(31)-C(30)-H(30)	120.7
C(29)-C(30)-H(30)	120.7
C(30)-C(31)-C(32)	118.9(2)
C(30)-C(31)-H(31)	120.5
C(32)-C(31)-H(31)	120.5
N(4)-C(32)-C(31)	123.28(18)
N(4)-C(32)-H(32)	118.4
C(31)-C(32)-H(32)	118.4
C(38)-N(5)-C(34)	116.71(17)
C(38)-N(5)-Ti(1)	124.32(13)
C(34)-N(5)-Ti(1)	118.95(13)
N(5)-C(34)-C(35)	123.5(2)
N(5)-C(34)-H(34)	118.3
C(35)-C(34)-H(34)	118.3
C(34)-C(35)-C(36)	118.9(2)
C(34)-C(35)-H(35)	120.5
C(36)-C(35)-H(35)	120.5
C(37)-C(36)-C(35)	118.2(2)
C(37)-C(36)-H(36)	120.9
C(35)-C(36)-H(36)	120.9
C(36)-C(37)-C(38)	119.8(2)
C(36)-C(37)-H(37)	120.1
C(38)-C(37)-H(37)	120.1
N(5)-C(38)-C(37)	122.9(2)
N(5)-C(38)-H(38)	118.6
C(37)-C(38)-H(38)	118.6
C(40)-C(39)-C(44)	117.8(2)
C(40)-C(39)-C(45)	121.8(3)
C(44)-C(39)-C(45)	120.4(3)
C(41)-C(40)-C(39)	121.3(2)
C(41)-C(40)-H(40)	119.3
C(39)-C(40)-H(40)	119.3
C(40)-C(41)-C(42)	120.0(2)
C(40)-C(41)-H(41)	120.0
C(42)-C(41)-H(41)	120.0
C(41)-C(42)-C(43)	119.3(3)
C(41)-C(42)-H(42)	120.3
C(43)-C(42)-H(42)	120.3
C(44)-C(43)-C(42)	120.8(3)
C(44)-C(43)-H(43)	119.6
C(42)-C(43)-H(43)	119.6
C(43)-C(44)-C(39)	120.6(2)
C(43)-C(44)-H(44)	119.7
C(39)-C(44)-H(44)	119.7
C(39)-C(45)-H(45A)	109.5
C(39)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(39)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(1)-N(1)-Ti(1)	147.60(12)
C(1)-N(1)-H(1)	106.2
Ti(1)-N(1)-H(1)	106.2
C(13)-N(2)-Ti(1)	173.62(12)
C(25)-N(3)-C(26)	110.25(16)
C(25)-N(3)-Ti(1)	126.87(13)
C(26)-N(3)-Ti(1)	122.85(13)
N(2)-Ti(1)-N(3)	107.98(7)
N(2)-Ti(1)-N(1)	104.27(6)
N(3)-Ti(1)-N(1)	147.75(6)
N(2)-Ti(1)-N(5)	96.16(6)
N(3)-Ti(1)-N(5)	89.27(6)
N(1)-Ti(1)-N(5)	87.62(6)

N(2)-Ti(1)-N(4)	101.03(6)
N(3)-Ti(1)-N(4)	86.47(6)
N(1)-Ti(1)-N(4)	87.12(6)
N(5)-Ti(1)-N(4)	162.78(5)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **16**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	18(1)	25(1)	16(1)	1(1)	5(1)	1(1)
C(2)	27(1)	24(1)	21(1)	-1(1)	9(1)	0(1)
C(3)	40(1)	29(1)	27(1)	-6(1)	16(1)	0(1)
C(5)	32(1)	38(1)	28(1)	0(1)	18(1)	-5(1)
C(6)	21(1)	30(1)	20(1)	0(1)	9(1)	-4(1)
C(7)	48(1)	22(1)	28(1)	-5(1)	18(1)	-6(1)
C(08)	40(1)	43(1)	25(1)	-4(1)	19(1)	3(1)
C(8)	65(2)	27(1)	53(1)	6(1)	24(1)	2(1)
C(9)	40(1)	61(2)	80(2)	21(1)	28(1)	-5(1)
C(10)	38(1)	33(1)	26(1)	-5(1)	17(1)	-14(1)
C(11)	83(2)	30(1)	47(1)	2(1)	24(1)	-8(1)
C(12)	42(1)	75(2)	47(1)	-15(1)	21(1)	-29(1)
C(13)	20(1)	22(1)	14(1)	-2(1)	6(1)	-4(1)
C(14)	24(1)	22(1)	23(1)	-3(1)	9(1)	-1(1)
C(15)	27(1)	31(1)	35(1)	-3(1)	19(1)	0(1)
C(16)	32(1)	35(1)	32(1)	5(1)	20(1)	-6(1)
C(17)	30(1)	21(1)	25(1)	2(1)	10(1)	-3(1)
C(18)	22(1)	22(1)	16(1)	-1(1)	6(1)	-2(1)
C(19)	31(1)	24(1)	33(1)	-1(1)	16(1)	1(1)
C(20)	74(2)	29(1)	45(1)	-8(1)	23(1)	-1(1)
C(21)	41(1)	33(1)	58(1)	9(1)	17(1)	6(1)
C(22)	29(1)	20(1)	27(1)	3(1)	14(1)	0(1)
C(23)	50(1)	25(1)	40(1)	-4(1)	22(1)	1(1)
C(24)	27(1)	41(1)	42(1)	8(1)	10(1)	3(1)
C(25)	39(1)	40(1)	59(1)	-24(1)	14(1)	-6(1)
C(26)	51(1)	43(1)	40(1)	-10(1)	15(1)	-26(1)
N(4)	24(1)	24(1)	26(1)	-1(1)	8(1)	-5(1)
C(28)	34(1)	34(1)	29(1)	-5(1)	3(1)	-3(1)
C(29)	33(1)	41(1)	40(1)	0(1)	-6(1)	-3(1)
C(30)	25(1)	41(1)	54(1)	7(1)	2(1)	5(1)
C(31)	35(1)	38(1)	46(1)	2(1)	16(1)	8(1)
C(32)	31(1)	32(1)	28(1)	1(1)	11(1)	1(1)
N(5)	27(1)	26(1)	23(1)	0(1)	7(1)	-1(1)
C(34)	35(1)	36(1)	42(1)	3(1)	2(1)	-5(1)
C(35)	35(1)	61(2)	48(1)	7(1)	-2(1)	1(1)
C(36)	48(2)	56(2)	40(1)	16(1)	5(1)	18(1)
C(37)	57(2)	33(1)	46(1)	12(1)	13(1)	7(1)
C(38)	36(1)	29(1)	32(1)	4(1)	8(1)	0(1)
C(39)	60(2)	42(1)	53(1)	10(1)	22(1)	21(1)
C(40)	39(1)	40(1)	61(2)	-4(1)	8(1)	1(1)
C(41)	55(2)	51(2)	45(1)	-7(1)	6(1)	2(1)
C(42)	64(2)	71(2)	51(1)	5(1)	22(1)	-4(2)
C(43)	54(2)	54(2)	61(2)	2(1)	5(1)	-12(1)
C(44)	58(2)	39(1)	48(1)	-2(1)	1(1)	4(1)
C(45)	97(3)	115(3)	74(2)	23(2)	48(2)	35(2)
N(1)	24(1)	24(1)	23(1)	-4(1)	12(1)	-9(1)
N(2)	24(1)	19(1)	20(1)	1(1)	10(1)	-1(1)
N(3)	28(1)	24(1)	29(1)	-3(1)	4(1)	-6(1)
Ti(1)	21(1)	17(1)	18(1)	-2(1)	8(1)	-4(1)

Data for compound 17

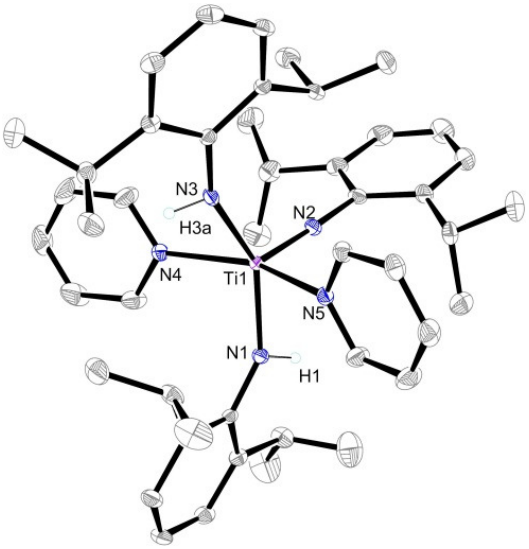


Table 1. Crystal data and structure refinement for **17**.

Identification code	cl1671
Empirical formula	C46 H63 N5 Ti
Formula weight	733.91
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 9.6975(5) A alpha = 80.776(2) deg. b = 12.1115(6) A beta = 79.744(2) deg. c = 22.0445(10) A gamma = 73.268(2) deg.
Volume	2423.5(2) A^3
Z, Calculated density	2, 1.006 Mg/m^3
Absorption coefficient	0.208 mm^-1
F(000)	792
Crystal size	0.18 x 0.12 x 0.05 mm
Theta range for data collection	0.95 to 26.37 deg.
Limiting indices	-12<=h<=12, -15<=k<=15, -27<=l<=27
Reflections collected / unique	56608 / 9895 [R(int) = 0.0353]
Completeness to theta = 26.37	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.978 and 0.901
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9895 / 0 / 482
Goodness-of-fit on F^2	1.082
Final R indices [I>2sigma(I)]	R1 = 0.0591, wR2 = 0.1662
R indices (all data)	R1 = 0.0661, wR2 = 0.1721
Extinction coefficient	0.0111(14)
Largest diff. peak and hole	1.275 and -0.480 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **17**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	2842(2)	1723(2)	1769(1)	23(1)
C(2)	3139(2)	558(2)	2045(1)	28(1)
C(3)	4064(3)	-314(2)	1708(1)	37(1)
C(4)	4713(3)	-75(2)	1112(1)	39(1)
C(5)	4449(2)	1056(2)	845(1)	35(1)
C(6)	3531(2)	1968(2)	1155(1)	28(1)
C(7)	2467(3)	217(2)	2700(1)	38(1)
C(8)	1469(4)	-558(3)	2709(2)	63(1)
C(9)	3621(4)	-340(3)	3126(1)	71(1)
C(10)	3269(3)	3212(2)	844(1)	40(1)
C(11)	3427(7)	3325(4)	139(2)	99(2)
C(12)	4133(6)	3859(4)	1060(2)	87(1)
C(13)	-872(2)	5620(2)	2545(1)	28(1)
C(14)	-1994(2)	6179(2)	2176(1)	36(1)
C(15)	-2505(3)	7383(2)	2131(2)	51(1)
C(16)	-1958(4)	8032(2)	2440(2)	60(1)
C(17)	-858(3)	7497(2)	2792(1)	48(1)
C(18)	-275(3)	6294(2)	2845(1)	34(1)
C(19)	-2587(3)	5452(2)	1847(1)	44(1)
C(20)	-1544(4)	5069(3)	1265(1)	61(1)
C(21)	-4133(3)	6042(3)	1694(2)	70(1)
C(22)	1024(3)	5715(2)	3176(1)	37(1)
C(23)	2403(3)	5562(3)	2702(2)	51(1)
C(24)	1181(4)	6329(3)	3707(1)	55(1)
C(25)	-2005(2)	2304(2)	4063(1)	23(1)
C(26)	-2359(2)	1282(2)	4387(1)	27(1)
C(27)	-3125(2)	1318(2)	4984(1)	34(1)
C(28)	-3593(3)	2318(2)	5271(1)	37(1)
C(29)	-3333(2)	3322(2)	4942(1)	32(1)
C(30)	-2577(2)	3357(2)	4343(1)	26(1)
C(31)	-1879(3)	133(2)	4112(1)	34(1)
C(32)	-3107(3)	-468(3)	4191(1)	50(1)
C(33)	-548(3)	-661(2)	4384(1)	49(1)
C(34)	-2453(2)	4511(2)	3987(1)	32(1)
C(35)	-2346(3)	5391(2)	4392(1)	51(1)
C(36)	-3736(3)	5033(2)	3620(1)	44(1)
C(37)	-2477(3)	2244(3)	2398(2)	59(1)
C(38)	-3259(4)	1770(4)	2096(2)	80(1)
C(39)	-2648(4)	1305(3)	1570(2)	65(1)
C(40)	-1287(4)	1341(3)	1348(2)	72(1)
C(41)	-546(3)	1852(3)	1658(1)	52(1)
C(42)	1302(2)	2799(2)	4054(1)	30(1)
C(43)	2202(3)	2822(2)	4470(1)	39(1)
C(44)	3629(3)	2767(2)	4264(1)	46(1)
C(45)	4115(3)	2692(3)	3644(1)	53(1)
C(46)	3154(3)	2691(2)	3252(1)	39(1)
N(1)	1867(2)	2592(1)	2091(1)	23(1)
N(2)	-387(2)	4423(1)	2621(1)	24(1)
N(3)	-1111(2)	2281(2)	3491(1)	28(1)
N(4)	-1121(2)	2292(2)	2187(1)	29(1)
N(5)	1756(2)	2746(1)	3445(1)	24(1)
Ti(1)	162(1)	2933(1)	2773(1)	19(1)

Table 3. Bond lengths [A] and angles [deg] for **17**.

C(1)-N(1)	1.390(2)
C(1)-C(2)	1.414(3)
C(1)-C(6)	1.425(3)
C(2)-C(3)	1.393(3)
C(2)-C(7)	1.520(3)
C(3)-C(4)	1.376(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.373(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.392(3)
C(5)-H(5)	0.9500
C(6)-C(10)	1.523(3)
C(7)-C(9)	1.525(4)
C(7)-C(8)	1.527(4)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(12)	1.476(5)
C(10)-C(11)	1.522(4)
C(10)-H(10)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-N(2)	1.382(3)
C(13)-C(14)	1.420(3)
C(13)-C(18)	1.422(3)
C(14)-C(15)	1.392(3)
C(14)-C(19)	1.508(4)
C(15)-C(16)	1.380(5)
C(15)-H(15)	0.9500
C(16)-C(17)	1.376(4)
C(16)-H(16)	0.9500
C(17)-C(18)	1.396(3)
C(17)-H(17)	0.9500
C(18)-C(22)	1.506(3)
C(19)-C(20)	1.531(4)
C(19)-C(21)	1.536(4)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.528(4)
C(22)-C(24)	1.534(3)
C(22)-H(22)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-N(3)	1.397(2)
C(25)-C(26)	1.427(3)
C(25)-C(30)	1.429(3)
C(26)-C(27)	1.392(3)
C(26)-C(31)	1.523(3)
C(27)-C(28)	1.378(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.377(3)
C(28)-H(28)	0.9500
C(29)-C(30)	1.391(3)
C(29)-H(29)	0.9500
C(30)-C(34)	1.515(3)
C(31)-C(33)	1.524(4)
C(31)-C(32)	1.537(3)

C(31)-H(31)	1.0000
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-C(35)	1.531(3)
C(34)-C(36)	1.531(4)
C(34)-H(34)	1.0000
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-N(4)	1.329(3)
C(37)-C(38)	1.378(4)
C(37)-H(37)	0.9500
C(38)-C(39)	1.337(5)
C(38)-H(38)	0.9500
C(39)-C(40)	1.335(5)
C(39)-H(39)	0.9500
C(40)-C(41)	1.391(4)
C(40)-H(40)	0.9500
C(41)-N(4)	1.323(3)
C(41)-H(41)	0.9500
C(42)-N(5)	1.343(3)
C(42)-C(43)	1.382(3)
C(42)-H(42)	0.9500
C(43)-C(44)	1.364(4)
C(43)-H(43)	0.9500
C(44)-C(45)	1.373(4)
C(44)-H(44)	0.9500
C(45)-C(46)	1.379(3)
C(45)-H(45)	0.9500
C(46)-N(5)	1.332(3)
C(46)-H(46)	0.9500
N(1)-Ti(1)	2.0206(16)
N(1)-H(1)	0.8800
N(2)-Ti(1)	1.7230(17)
N(3)-Ti(1)	2.0293(17)
N(3)-H(3A)	0.8800
N(4)-Ti(1)	2.2953(17)
N(5)-Ti(1)	2.2669(17)

N(1)-C(1)-C(2)	119.90(17)
N(1)-C(1)-C(6)	121.72(18)
C(2)-C(1)-C(6)	118.36(18)
C(3)-C(2)-C(1)	119.49(19)
C(3)-C(2)-C(7)	118.49(19)
C(1)-C(2)-C(7)	122.01(18)
C(4)-C(3)-C(2)	121.9(2)
C(4)-C(3)-H(3)	119.0
C(2)-C(3)-H(3)	119.0
C(5)-C(4)-C(3)	118.9(2)
C(5)-C(4)-H(4)	120.5
C(3)-C(4)-H(4)	120.5
C(4)-C(5)-C(6)	122.0(2)
C(4)-C(5)-H(5)	119.0
C(6)-C(5)-H(5)	119.0
C(5)-C(6)-C(1)	119.3(2)
C(5)-C(6)-C(10)	120.51(19)
C(1)-C(6)-C(10)	120.24(19)
C(2)-C(7)-C(9)	111.7(2)
C(2)-C(7)-C(8)	112.0(2)
C(9)-C(7)-C(8)	111.3(3)
C(2)-C(7)-H(7)	107.2
C(9)-C(7)-H(7)	107.2
C(8)-C(7)-H(7)	107.2
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5

C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(12)-C(10)-C(11)	111.9(3)
C(12)-C(10)-C(6)	112.3(2)
C(11)-C(10)-C(6)	114.2(2)
C(12)-C(10)-H(10)	105.9
C(11)-C(10)-H(10)	105.9
C(6)-C(10)-H(10)	105.9
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
N(2)-C(13)-C(14)	119.9(2)
N(2)-C(13)-C(18)	120.29(19)
C(14)-C(13)-C(18)	119.81(19)
C(15)-C(14)-C(13)	118.5(2)
C(15)-C(14)-C(19)	122.4(2)
C(13)-C(14)-C(19)	119.1(2)
C(16)-C(15)-C(14)	121.5(3)
C(16)-C(15)-H(15)	119.3
C(14)-C(15)-H(15)	119.3
C(17)-C(16)-C(15)	120.2(2)
C(17)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
C(16)-C(17)-C(18)	121.1(3)
C(16)-C(17)-H(17)	119.4
C(18)-C(17)-H(17)	119.4
C(17)-C(18)-C(13)	118.8(2)
C(17)-C(18)-C(22)	121.3(2)
C(13)-C(18)-C(22)	119.78(19)
C(14)-C(19)-C(20)	110.7(2)
C(14)-C(19)-C(21)	113.7(2)
C(20)-C(19)-C(21)	111.1(2)
C(14)-C(19)-H(19)	107.0
C(20)-C(19)-H(19)	107.0
C(21)-C(19)-H(19)	107.0
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(18)-C(22)-C(23)	109.0(2)
C(18)-C(22)-C(24)	115.7(2)
C(23)-C(22)-C(24)	109.6(2)
C(18)-C(22)-H(22)	107.4
C(23)-C(22)-H(22)	107.4
C(24)-C(22)-H(22)	107.4
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5

N(3)-C(25)-C(26)	121.35(18)
N(3)-C(25)-C(30)	120.59(18)
C(26)-C(25)-C(30)	118.05(18)
C(27)-C(26)-C(25)	119.3(2)
C(27)-C(26)-C(31)	118.46(19)
C(25)-C(26)-C(31)	122.19(18)
C(28)-C(27)-C(26)	122.3(2)
C(28)-C(27)-H(27)	118.8
C(26)-C(27)-H(27)	118.8
C(29)-C(28)-C(27)	118.3(2)
C(29)-C(28)-H(28)	120.8
C(27)-C(28)-H(28)	120.8
C(28)-C(29)-C(30)	122.7(2)
C(28)-C(29)-H(29)	118.6
C(30)-C(29)-H(29)	118.6
C(29)-C(30)-C(25)	118.9(2)
C(29)-C(30)-C(34)	119.82(19)
C(25)-C(30)-C(34)	121.14(18)
C(26)-C(31)-C(33)	110.16(19)
C(26)-C(31)-C(32)	112.8(2)
C(33)-C(31)-C(32)	111.5(2)
C(26)-C(31)-H(31)	107.4
C(33)-C(31)-H(31)	107.4
C(32)-C(31)-H(31)	107.4
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-H(33A)	109.5
C(31)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(31)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(30)-C(34)-C(35)	114.2(2)
C(30)-C(34)-C(36)	109.75(18)
C(35)-C(34)-C(36)	110.0(2)
C(30)-C(34)-H(34)	107.5
C(35)-C(34)-H(34)	107.5
C(36)-C(34)-H(34)	107.5
C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
N(4)-C(37)-C(38)	123.4(3)
N(4)-C(37)-H(37)	118.3
C(38)-C(37)-H(37)	118.3
C(39)-C(38)-C(37)	120.1(3)
C(39)-C(38)-H(38)	120.0
C(37)-C(38)-H(38)	120.0
C(40)-C(39)-C(38)	117.7(3)
C(40)-C(39)-H(39)	121.1
C(38)-C(39)-H(39)	121.1
C(39)-C(40)-C(41)	120.4(3)
C(39)-C(40)-H(40)	119.8
C(41)-C(40)-H(40)	119.8
N(4)-C(41)-C(40)	122.6(3)
N(4)-C(41)-H(41)	118.7
C(40)-C(41)-H(41)	118.7
N(5)-C(42)-C(43)	123.2(2)
N(5)-C(42)-H(42)	118.4
C(43)-C(42)-H(42)	118.4
C(44)-C(43)-C(42)	119.4(2)
C(44)-C(43)-H(43)	120.3
C(42)-C(43)-H(43)	120.3
C(43)-C(44)-C(45)	118.1(2)
C(43)-C(44)-H(44)	121.0

C(45)-C(44)-H(44)	121.0
C(44)-C(45)-C(46)	119.5(2)
C(44)-C(45)-H(45)	120.3
C(46)-C(45)-H(45)	120.3
N(5)-C(46)-C(45)	123.3(2)
N(5)-C(46)-H(46)	118.3
C(45)-C(46)-H(46)	118.3
C(1)-N(1)-Ti(1)	144.60(14)
C(1)-N(1)-H(1)	107.7
Ti(1)-N(1)-H(1)	107.7
C(13)-N(2)-Ti(1)	175.80(15)
C(25)-N(3)-Ti(1)	154.45(14)
C(25)-N(3)-H(3A)	102.8
Ti(1)-N(3)-H(3A)	102.8
C(41)-N(4)-C(37)	115.7(2)
C(41)-N(4)-Ti(1)	123.51(16)
C(37)-N(4)-Ti(1)	120.50(16)
C(46)-N(5)-C(42)	116.46(18)
C(46)-N(5)-Ti(1)	122.10(14)
C(42)-N(5)-Ti(1)	121.13(14)
N(2)-Ti(1)-N(1)	99.41(7)
N(2)-Ti(1)-N(3)	113.50(7)
N(1)-Ti(1)-N(3)	147.04(7)
N(2)-Ti(1)-N(5)	100.04(7)
N(1)-Ti(1)-N(5)	88.65(6)
N(3)-Ti(1)-N(5)	87.38(7)
N(2)-Ti(1)-N(4)	104.20(7)
N(1)-Ti(1)-N(4)	87.41(7)
N(3)-Ti(1)-N(4)	83.04(7)
N(5)-Ti(1)-N(4)	155.76(6)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for **17**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	17(1)	28(1)	24(1)	-6(1)	-4(1)	-6(1)
C(2)	26(1)	26(1)	29(1)	-4(1)	-2(1)	-4(1)
C(3)	34(1)	27(1)	44(1)	-8(1)	0(1)	0(1)
C(4)	31(1)	38(1)	43(1)	-19(1)	3(1)	-1(1)
C(5)	29(1)	49(1)	26(1)	-12(1)	2(1)	-11(1)
C(6)	25(1)	37(1)	23(1)	-5(1)	-3(1)	-9(1)
C(7)	50(1)	22(1)	33(1)	-1(1)	6(1)	-4(1)
C(8)	78(2)	39(2)	67(2)	-11(1)	29(2)	-29(2)
C(9)	92(3)	62(2)	39(2)	9(1)	-13(2)	5(2)
C(10)	49(1)	38(1)	28(1)	0(1)	2(1)	-10(1)
C(11)	164(5)	83(3)	51(2)	17(2)	-30(3)	-42(3)
C(12)	115(4)	66(2)	87(3)	3(2)	-18(2)	-42(2)
C(13)	26(1)	22(1)	31(1)	-2(1)	1(1)	-2(1)
C(14)	29(1)	32(1)	41(1)	3(1)	-4(1)	-2(1)
C(15)	35(1)	34(1)	71(2)	10(1)	-9(1)	5(1)
C(16)	58(2)	20(1)	94(2)	-2(1)	-9(2)	-1(1)
C(17)	49(2)	23(1)	72(2)	-9(1)	-4(1)	-8(1)
C(18)	36(1)	22(1)	42(1)	-4(1)	1(1)	-9(1)
C(19)	36(1)	44(1)	48(1)	4(1)	-18(1)	-5(1)
C(20)	63(2)	70(2)	46(2)	-10(1)	-20(1)	-2(2)
C(21)	43(2)	72(2)	95(3)	-4(2)	-33(2)	-7(2)
C(22)	45(1)	26(1)	44(1)	-6(1)	-9(1)	-16(1)
C(23)	40(1)	52(2)	64(2)	-9(1)	-10(1)	-12(1)
C(24)	73(2)	46(2)	59(2)	-13(1)	-16(2)	-28(2)
C(25)	20(1)	29(1)	23(1)	-6(1)	-2(1)	-8(1)
C(26)	26(1)	30(1)	26(1)	-2(1)	-5(1)	-7(1)
C(27)	33(1)	39(1)	29(1)	3(1)	-1(1)	-11(1)
C(28)	33(1)	51(1)	21(1)	-4(1)	1(1)	-6(1)
C(29)	27(1)	40(1)	26(1)	-12(1)	-1(1)	-4(1)
C(30)	20(1)	33(1)	27(1)	-10(1)	-1(1)	-8(1)
C(31)	42(1)	30(1)	31(1)	-2(1)	-1(1)	-15(1)
C(32)	56(2)	46(2)	58(2)	-4(1)	-12(1)	-27(1)
C(33)	46(2)	38(1)	61(2)	-14(1)	-6(1)	-2(1)
C(34)	31(1)	30(1)	35(1)	-15(1)	8(1)	-8(1)
C(35)	61(2)	45(2)	54(2)	-27(1)	12(1)	-24(1)

C(36)	43(1)	37(1)	45(1)	-2(1)	1(1)	-4(1)
C(37)	33(1)	99(3)	57(2)	-36(2)	4(1)	-30(2)
C(38)	48(2)	130(4)	87(3)	-38(2)	-10(2)	-50(2)
C(39)	64(2)	61(2)	90(2)	-27(2)	-45(2)	-16(2)
C(40)	50(2)	101(3)	76(2)	-63(2)	-26(2)	3(2)
C(41)	31(1)	86(2)	44(1)	-39(1)	-5(1)	-8(1)
C(42)	33(1)	32(1)	28(1)	-5(1)	-5(1)	-10(1)
C(43)	51(2)	38(1)	32(1)	-6(1)	-14(1)	-13(1)
C(44)	47(2)	50(2)	49(2)	-11(1)	-24(1)	-11(1)
C(45)	30(1)	78(2)	57(2)	-20(2)	-10(1)	-15(1)
C(46)	29(1)	54(2)	35(1)	-11(1)	-4(1)	-10(1)
N(1)	23(1)	21(1)	24(1)	-3(1)	0(1)	-6(1)
N(2)	23(1)	24(1)	24(1)	-6(1)	-3(1)	-4(1)
N(3)	34(1)	24(1)	27(1)	-11(1)	7(1)	-13(1)
N(4)	25(1)	31(1)	32(1)	-11(1)	-4(1)	-7(1)
N(5)	25(1)	21(1)	28(1)	-4(1)	-7(1)	-5(1)
Ti(1)	19(1)	18(1)	20(1)	-5(1)	-1(1)	-5(1)

Data for compound [V(N-*o*-$Cl_2C_6H_3$)$_2$(NH *o*-$Cl_2C_6H_3$)$_2$(NMe_2)$_2$]

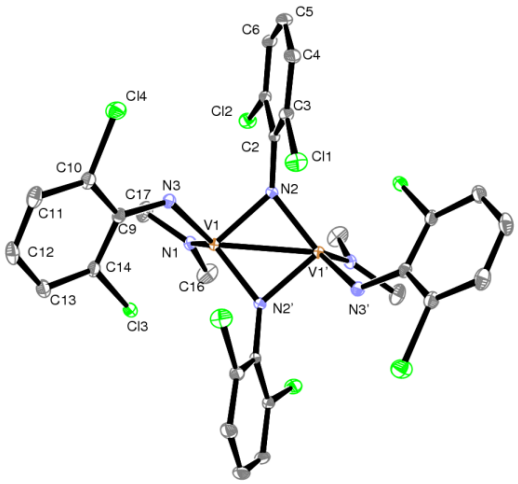


Table 1. Crystal data and structure refinement for cl786-1.

Identification code	cl786-1
Empirical formula	C28 H28 Cl8 N6 V2
Formula weight	834.04
Temperature	180(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, F d d 2
Unit cell dimensions	a = 23.961(5) A alpha = 90 deg. b = 32.093(6) A beta = 90 deg. c = 8.9451(18) A gamma = 90 deg.
Volume	6879(2) A^3
Z, Calculated density	16, 1.611 Mg/m^3
Absorption coefficient	1.196 mm^-1
F(000)	3360
Crystal size	0.25 x 0.236 x 0.099 mm
Theta range for data collection	3.06 to 32.17 deg.
Limiting indices	-34<=h<=35, -47<=k<=34, -13<=l<=13
Reflections collected / unique	17470 / 5691 [R(int) = 0.0404]
Completeness to theta = 25.00	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8912 and 0.7926
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5691 / 1 / 201
Goodness-of-fit on F^2	0.884
Final R indices [I>2sigma(I)]	R1 = 0.0347, wR2 = 0.0789
R indices (all data)	R1 = 0.0549, wR2 = 0.0833
Absolute structure parameter	-0.02(2)
Largest diff. peak and hole	0.373 and -0.512 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for cl786-1.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(2)	11947(1)	2400(1)	12685(2)	22(1)
C(2)	11405(1)	2322(1)	12214(3)	24(1)
C(3)	11276(1)	2200(1)	10741(3)	31(1)
C(4)	10738(1)	2099(1)	10299(4)	40(1)
C(5)	10307(1)	2129(1)	11314(5)	44(1)
C(6)	10404(1)	2270(1)	12730(4)	38(1)
C(7)	10947(1)	2362(1)	13170(3)	29(1)
N(3)	11954(1)	3154(1)	11314(3)	27(1)
C(9)	12056(1)	3507(1)	10512(3)	27(1)
C(10)	11721(1)	3658(1)	9350(3)	34(1)
C(11)	11844(2)	4018(1)	8561(4)	42(1)
C(12)	12327(2)	4236(1)	8911(4)	44(1)
C(13)	12674(1)	4102(1)	10026(4)	36(1)
C(14)	12531(1)	3748(1)	10809(3)	30(1)
Cl(4)	11115(1)	3382(1)	8887(1)	49(1)
C(16)	12610(2)	3042(1)	16104(4)	55(1)
C(17)	11892(2)	3457(1)	14940(4)	51(1)
N(1)	12297(1)	3116(1)	14757(3)	29(1)
Cl(1)	11807(1)	2164(1)	9434(1)	45(1)
Cl(2)	11071(1)	2544(1)	14977(1)	40(1)
Cl(3)	12951(1)	3570(1)	12254(1)	35(1)
V(1)	12390(1)	2891(1)	12877(1)	21(1)

Table 3. Bond lengths [A] and angles [deg] for cl786-1.

N(2)-C(2)	1.390(3)
N(2)-V(1)#1	1.849(2)
N(2)-V(1)	1.905(2)
C(2)-C(7)	1.397(4)
C(2)-C(3)	1.408(4)
C(3)-C(4)	1.386(4)
C(3)-Cl(1)	1.732(3)
C(4)-C(5)	1.379(5)
C(4)-H(4)	0.9500
C(5)-C(6)	1.366(5)
C(5)-H(5)	0.9500
C(6)-C(7)	1.390(4)
C(6)-H(6)	0.9500
C(7)-Cl(2)	1.744(3)
N(3)-C(9)	1.363(3)
N(3)-V(1)	1.940(2)
N(3)-H(3A)	0.9200
N(3)-H(3B)	0.9200
C(9)-C(10)	1.398(4)
C(9)-C(14)	1.402(4)
C(10)-C(11)	1.385(4)
C(10)-Cl(4)	1.750(3)
C(11)-C(12)	1.390(5)
C(11)-H(11)	0.9500
C(12)-C(13)	1.368(5)
C(12)-H(12)	0.9500
C(13)-C(14)	1.376(4)
C(13)-H(13)	0.9500
C(14)-Cl(3)	1.735(3)
C(16)-N(1)	1.439(4)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-N(1)	1.472(4)
C(17)-H(17A)	0.9800

C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
N(1)-V(1)	1.844(2)
Cl(3)-V(1)	2.6192(9)
V(1)-N(2)#1	1.849(2)
V(1)-V(1)#1	2.5617(10)
C(2)-N(2)-V(1)#1	137.69(17)
C(2)-N(2)-V(1)	134.24(17)
V(1)#1-N(2)-V(1)	86.04(9)
N(2)-C(2)-C(7)	122.2(3)
N(2)-C(2)-C(3)	122.6(2)
C(7)-C(2)-C(3)	115.2(2)
C(4)-C(3)-C(2)	122.4(3)
C(4)-C(3)-Cl(1)	118.3(2)
C(2)-C(3)-Cl(1)	119.3(2)
C(5)-C(4)-C(3)	119.5(3)
C(5)-C(4)-H(4)	120.3
C(3)-C(4)-H(4)	120.3
C(6)-C(5)-C(4)	120.4(3)
C(6)-C(5)-H(5)	119.8
C(4)-C(5)-H(5)	119.8
C(5)-C(6)-C(7)	119.5(3)
C(5)-C(6)-H(6)	120.2
C(7)-C(6)-H(6)	120.2
C(6)-C(7)-C(2)	122.8(3)
C(6)-C(7)-Cl(2)	119.6(2)
C(2)-C(7)-Cl(2)	117.6(2)
C(9)-N(3)-V(1)	130.21(19)
C(9)-N(3)-H(3A)	104.7
V(1)-N(3)-H(3A)	104.7
C(9)-N(3)-H(3B)	104.7
V(1)-N(3)-H(3B)	104.7
H(3A)-N(3)-H(3B)	105.7
N(3)-C(9)-C(10)	125.2(3)
N(3)-C(9)-C(14)	120.3(3)
C(10)-C(9)-C(14)	114.5(3)
C(11)-C(10)-C(9)	123.1(3)
C(11)-C(10)-Cl(4)	118.5(2)
C(9)-C(10)-Cl(4)	118.4(2)
C(10)-C(11)-C(12)	118.8(3)
C(10)-C(11)-H(11)	120.6
C(12)-C(11)-H(11)	120.6
C(13)-C(12)-C(11)	120.8(3)
C(13)-C(12)-H(12)	119.6
C(11)-C(12)-H(12)	119.6
C(12)-C(13)-C(14)	118.7(3)
C(12)-C(13)-H(13)	120.6
C(14)-C(13)-H(13)	120.6
C(13)-C(14)-C(9)	124.1(3)
C(13)-C(14)-Cl(3)	120.5(2)
C(9)-C(14)-Cl(3)	115.4(2)
N(1)-C(16)-H(16A)	109.5
N(1)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
N(1)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
N(1)-C(17)-H(17A)	109.5
N(1)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
N(1)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-N(1)-C(17)	111.9(3)
C(16)-N(1)-V(1)	129.5(2)
C(17)-N(1)-V(1)	118.2(2)
C(14)-Cl(3)-V(1)	97.84(10)
N(1)-V(1)-N(2)#1	112.70(10)
N(1)-V(1)-N(2)	109.75(10)
N(2)#1-V(1)-N(2)	93.01(9)
N(1)-V(1)-N(3)	114.90(10)
N(2)#1-V(1)-N(3)	128.05(10)
N(2)-V(1)-N(3)	89.73(9)
N(1)-V(1)-V(1)#1	114.10(7)
N(2)#1-V(1)-V(1)#1	47.91(6)
N(2)-V(1)-V(1)#1	46.06(6)

N(3)-V(1)-V(1)#1	122.52(7)
N(1)-V(1)-Cl(3)	85.98(8)
N(2)#1-V(1)-Cl(3)	87.76(7)
N(2)-V(1)-Cl(3)	162.42(7)
N(3)-V(1)-Cl(3)	76.12(7)
V(1)#1-V(1)-Cl(3)	135.17(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x+5/2,-y+1/2,z

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for cl786-1.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(2)	20(1)	20(1)	24(1)	1(1)	0(1)	-1(1)
C(2)	21(1)	16(1)	35(2)	2(1)	0(1)	0(1)
C(3)	26(1)	29(1)	40(2)	2(1)	-7(1)	1(1)
C(4)	36(2)	35(2)	48(2)	4(2)	-21(2)	-5(1)
C(5)	24(2)	37(2)	73(2)	10(2)	-16(2)	-3(1)
C(6)	20(1)	33(2)	60(2)	13(2)	4(2)	1(1)
C(7)	24(1)	22(1)	41(2)	4(1)	3(1)	1(1)
N(3)	25(1)	26(1)	29(1)	3(1)	-1(1)	1(1)
C(9)	28(1)	25(1)	27(1)	2(1)	6(1)	5(1)
C(10)	38(2)	30(2)	33(2)	4(1)	3(1)	6(1)
C(11)	57(2)	35(2)	35(2)	8(1)	0(2)	10(2)
C(12)	66(2)	26(2)	42(2)	8(1)	10(2)	2(2)
C(13)	42(2)	25(2)	40(2)	2(1)	10(2)	-1(1)
C(14)	32(2)	23(1)	35(2)	4(1)	5(1)	4(1)
Cl(4)	42(1)	57(1)	49(1)	16(1)	-15(1)	-3(1)
C(16)	58(2)	74(3)	32(2)	-12(2)	-8(2)	14(2)
C(17)	65(2)	42(2)	47(2)	-15(2)	7(2)	16(2)
N(1)	31(1)	24(1)	32(1)	-3(1)	0(1)	-2(1)
Cl(1)	45(1)	62(1)	29(1)	-8(1)	-2(1)	0(1)
Cl(2)	33(1)	46(1)	42(1)	-3(1)	13(1)	0(1)
Cl(3)	31(1)	28(1)	47(1)	6(1)	-5(1)	-5(1)
V(1)	19(1)	20(1)	22(1)	0(1)	0(1)	0(1)