Indenyl-, and Fluorenyl-Functionalised N-Heterocyclic Carbene Complexes of Titanium and Vanadium

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Supporting Information **Page**

Synthetic Methodology

3-(2,6-Diisopropyl-phenyl)-1-[2-(3*H*-inden-1-yl)-ethyl]-3*H*-imidazolium bromide, (IndH-NHC-H)Br. Bromoethylindene (20g, 90mmol) and 2,6-diisopropylphenylimidazole (21 g, 90 mmol) were dissolved in dioxane (100 ml) and heated to 110 °C for 1 week. The dioxan was removed in *vacuo* and the resulting viscous residue was dissolved in CH_2Cl_2 and precipitated with ether. The resulting viscous product was dried azeotropically with toluene.After removal of the toluene under reduced pressure the residue was washed with ether and dried under vacuum to give an off white powder. Yield: 25 g, 61%. MS ES^+ 371 $(M\text{-}Br^-)^+$.

^{1}H NMR (400 MHz, $CDCl_3$) 10.13 (1H, s, imidazolium-H); 8.01 (1H, s, Ar), 7.43-7.36 (3H, m, Ar); 7.23-7.11 (5H, m, Ar); 6.99 (1H, s, NC*H*); 6.48 (1H, s, NC*H*);5.10 (2H, t, *J* = 6.5 Hz, CH_2); 3.30 (2H, t, *J* = 6.5Hz, CH_2); 3.21 (2H, s, indenyl-CH_2); 2.02 (2H, sept, *J* = 7Hz, ^{i}pr-CH) 1.06 (6H, d, *J* = 7 Hz, ^{i}Pr-CH_3); 0.97 (6H, d, *J* = 7 Hz, ^{i}pr-CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) 144.3 (Ar, C), 143.1 (Ar, C), 137.8 (Ar, CH), 137.1 (Ar, C), 130.8 (Ar, CH), 127.2 (Ar, C), 125.4 (Ar, CH), 124.3 (Ar, CH) 124.2 (Ar, CH), 123.6 (Ar, CH), 123.0 (Ar, CH), 122.8 (Ar, CH), 118.0 (Ar, CH), 48.1 (CH_2), 37.1 (CH_2), 27.6 (CH) 27.6(CH_2), 23.2 (CH_3). MS, ES^+ 371 (M^+, 100%). Calculated (%) C, 68.44, H, 6.13 N, 5.32, found C, 68.45, H, 6.20 N, 5.23.

1-[2-(9*H*-Fluoren-9-yl)ethyl]-3-(2,6 diisopropylphenyl)-3*H*-imidazol-1-ium bromide, (FlH-NHC-H)Br. A glass ampoule fitted with a PTFE stopcock containing 9-(2-bromoethyl)-9*H*-fluorene (5.0 g, 18 mmol), 2,6-diisopropylphenylimidazole (4.2 g, 18 mmol) and dioxan (100 ml) was heated to 100 ℃ for 5 days. After removal of the

volatiles the residue was dissolved in the minimum amount of CH_2Cl_2 (ca 5 ml). This solution was then added slowly to ether (100 ml). The resulting solid was filtered, washed with diethyl ether (100 ml), and dried under vacuum. The solid was dried azeotropically with toluene. The product was isolated as above ginving an off-white solid. Yield: 4.6g, 50%. MS ES^+: 421 $(M\text{-}Br^-)^+$

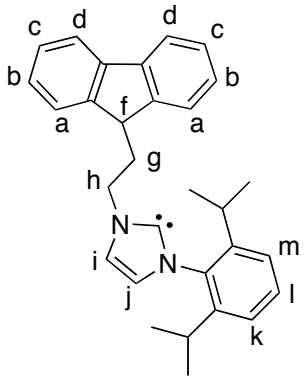
M.p.: 155 °C (ether). NMR (^1H, $CDCl_3$): 10.45 (1H, s, imid-*H*); 7.75 (2H, d, *J* = 7.5 Hz, Ar*H*) 7.63 (2H, d, *J* = 8.0 Hz, Ar*H*); 7.46 (1H, t, *J* = 8.5 Hz, Ar*H*); 7.37 (2H, t, *J* = 7.5 Hz, Ar*H*); 7.29 (2H, d, *J* = 7.5 Hz, Ar*H*); 7.23 (2H, d, *J* = 8.0 Hz, Ar*H*); 7.16 (1H, s, NC*H*); 6.90 (1H, s, NC*H*); 4.46 (2H, m, CH_2); 4.19 (1H, t, *J* = 5.0 Hz, Fluorenyl-*H*); 2.9 (2H, m, CH_2); 2.15 (2H, quin, *J* = 6.5 Hz, C*H*(CH_3)$_2$); 1.19 (6H, d, *J* = 6.5 Hz, CH(C*H*$_3$)$_2$); 1.19 (6H, d, *J* = 6.5 Hz, CH(C*H*$_3$)$_2$). NMR ($^{13}C\{^1H\}$, $CDCl_3$):145.2 (Ar), 145.1 (Ar), 141.0 (Ar), 138.1 (imid-*C*H), 131.8 (N*C*H), 130.1 (Ar), 127.7 (N*C*H), 127.5 (Ar) 124.8 (ArH), 124.5 (ArH), 123.6 (ArH), 123.2 (ArH), 120.1 (ArH), 47.6 (*C*H_2), 44.9 (Fluorenyl-*C*H) 33.9 (*C*H_2), 24.4 (*C*H_3) 24.2 (*C*H_3)15.2 (*C*HCH_3). Calculated (%) C, 71.85, H, 6.63, N, 5.59; Found C, 71.92, H, 6.57, N, 5.60.

General method for the first deprotonation of (IndH-NHC-H)Br and (FlH-NHC-H)Br. 1 eq. $KN(SiMe_3)_2$ (3 mmol) was dissolved in benzene (20 ml) and the resulting solution was added at room temperature to the imidazolium salt (3 mmol) to give a suspension. The mixture was stirred overnight. The precipitated potassium halide was removed by filtration through Celite giving rise to a solution of the crude neutral functionalized NHC. The crude products have been isolated as air sensitive powders.

However, this is not necessary for routine work and the solutions of the NHCs were used for the second deprotonation as described below.

^{1}H-NMR data for the crude neutral species are given below.

FluH-NHC:



^{1}H NMR (C_6D_6): 7.71 and 7.64 (2H each, d, J = 7 Hz, H_a and H_d) ; 7.35-7.21 (7 H, unresolved m, H_b, H_c H_k, H_l and H_m) 6.66 and 6.53(1H each, s, H_i and H_j); 4.11 (2H, t, J = 7 Hz, H_h); 4.05 (1H, t, J = 6 Hz, H_f), 2.45 (2H, quin, J = 7Hz, 2x C*H*(CH_3)$_2$); 2.36 (2H, m, H_g); 1.16 (6H, d, J = 7 Hz, CH(C*H*$_3$)$_2$); 1.07 (6H, d , J = 7 Hz, CH(C*H*$_3$)$_2$).

IndH-NHC: The ^{1}H-NMR (C_6D_6) spectrum of the crude product at room temperature shows broad peaks assignable to indenyl and DiPP aromatic protons (6.8 – 7.7 ppm), CH_2CH_2, indene and C*H*(CH_3)$_2$ protons (2.2 – 4.0 ppm) and CH(C*H*$_3$)$_2$ (0.8 – 1.2ppm). Even though the integration agrees with the proposed structure, the broadness of the spectrum inhibits further assignment.

Tautomerization of FlH-NHC and IndH-NHC

A solution of FlH-NHC obtained as described above dissolved in THF-d^8 was placed in a NMR tube equipped with Young's valve and heated to 60 °C. The ^{1}H NMR spectrum

was recorded periodically. After 8 h an equilibrium mixture was obtained comprising FlH-NHC and Fl-NHC-H (ca 1:1). The latter was identified by the appearance of a characteristic broad peak at 11.2 ppm which was assigned to the imidazolium proton. Simultaneously, the intensity of the fluorenyl proton at 2.6 ppm decreased to one half of its original intensity. All other signals due to the aromatic, backbone and CH_2CH_2 protons broadened. A similar behavior was observed with IndH-NHC where the corresponding signals are at 11.21 ppm (imidazolium appearing) and 2.2 indenyl proton decreasing in intensity. The final mixture contains ca 25% IndH-NHC and 75% Ind-NHC-H.

General Procedure for the Deprotonation of (FlH-NHC), and (IndH-NHC)

The filtrate of the crude (FlH-NHC) or (Ind-NHC) obtained as described above was added to 1 eq. KHMDS and the resulting solution allowed to stir overnight. The precipitated product is then isolated by filtration, washed with benzene (2 ml), then petrol (10 ml) and dried under vacuum to afford the product (70 - 80% yield).

(Fl-NHC)$^-$K$^+$. A solution of KHMDS (80 mg, 0.4 mmol) in benzene 10 ml was added to a suspension of the imidazolium salt (200 mg, 0.4 mmol) in benzene to form an orange solution. This solution became green by stirring overnight. It was filtered through Celite giving rise to the crude **(FlH-NHC)** as shown by ^{1}H-NMR spectroscopy (see above). A solution of KHMDS (80 mg, 0.4 mmol) in benzene was added to the solution of **(FlH-NHC)** to give a red reaction mixture which on stirring formed slowly a red precipitate. Stirring continued overnight, the precipitate was collected by filtration and washed with

benzene to give the product (90mg, 50% yield). NMR (^{1}H, THF-d^8): δ 0.81 [6H, d, *J* = 7 Hz, CH(C*H*$_3$)$_2$]; 1.10 [6H, d, J = 7 Hz, CH(C*H*$_3$)$_2$]; 2.33 (2H, sept, 7 Hz, C*H*(CH$_3$)$_2$); 3.67 (2H, m, Fl-C*H*$_2$CH$_2$); 4.52 (2H, m, NC*H*$_2$CH$_2$-Fl); 6.58 (2H, m, aromatic of DiPP); 6.97 (3H, m, overlapping 1H aromatic from DiPP and 2H aromatic from fluorene); 7.12 (2 H, d, *J* = 7 Hz, aromatic from fluorene); 7.26 (3H, m, overlapping 1H carbene backbone and 2H aromatic from fluorene); 7.51 (1H, s, carbene backbone); 8.02 (2H, d, *J* = 8 Hz, aromatic fluorene H). NMR, ^{13}C{^{1}H}, THF-d^8, δ, 206.9 (carbene C); 144.3 (aromatic); 136.2 (aromatic); 132.5 (aromatic); 126.2 (aromatic); 121.0 (aromatic); 120.5 (aromatic); 118.2 (aromatic); 117.5 (aromatic); 117.5 (aromatic); 116.7 (aromatic); 111.7 (aromatic); 106.5 (aromatic); 88.4 (fluorenyl C); 51.3 (Fl-CH$_2$*C*H$_2$N); 26.7 (Fl-*C*H$_2$CH$_2$-N); 25.6 (*C*H(CH$_3$)$_2$); 22.0 (CH(*C*H$_3$)$_2$); 21.10 (CH(*C*H$_3$)$_2$). Calculated(%): C, 78.56, H, 6.81, N, 6.11.Found: C, 78.41, H, 6.69, N, 5.97.

(Ind-NHC)$^-$K$^+$. This was prepared similarly from the solution of the crude **Ind-NHC** and KHMDS. Yield: ca 50% of red-purple air sensitive powder. ^{1}H NMR (pyridine-d5): 7.82 (1H, d, *J* = 8 Hz, indenyl); 7.72 (1H, d, *J* = 8 Hz, indenyl); 7.46-7.43 (1H, m, indenyl); 7.32-7.20 (4H, m, overlapping DiPP aromatic and 1H indenyl aromatic); 6.98 (2H, m, indenyl); 6.75 (1H, s, carbene backbone); 6.48 (1H, s, carbene backbone); 4.45 (2H, m, NC*H*$_2$CH$_2$-ind); 3.59 (2H, m, NCH$_2$C*H*$_2$-ind); 2.93 (2H, sept, *J* = 7 Hz, C*H*(CH$_3$)$_2$); 1.19 (6H, d, *J* = 7 Hz, CH(C*H*$_3$)$_2$); 1.14 (6H, d, *J* = 7 Hz, CH(C*H*$_3$)$_2$).
^{13}C{^{1}H} NMR (pyridine-d^5) 211.0 (C, carbene); 147.5 (Ar); 130.2 (Ar); 129.9 (ArH); 129.5 (Ar); 128.3 (Ar); 126.6 (Ar); 125.0 (Ar); 120.8 (ArH); 120.6 (ArH); 120.1 (ArH);

117.3 (ArH); 113.9 (ArH); 104.9 (Indenyl carbon); 93.4 (Bridge CH_2); 55.6 (Bridge CH_2); 32.6 (isopropyl CH); 29.32 (isopropyl CH_3).

General method for the synthesis of silver carbene complexes. Imidazolium salt (1mmol), silver oxide (108 mg, 1 mmol) and 4Å molecular sieves in DCM (30 ml) were heated to reflux overnight under nitrogen in the dark. The resulting mixture was then filtered through Celite and the volatiles were removed under reduced pressure to give the desired product as a solid residue which was dried under vacuum in almost quantative yield.

Fl-NHC-Ag-Br

NMR (^{1}H, $CDCl_3$): 7.80 (2H, m, Ar); 7.61 (2H, m, Ar); 7.40 (5H, m, Ar); 7.22 (2H, d, *J* = 8 Hz, Ar); 6.76 (1H, m, carbene backbone); 6.70 (1H, m, carbene backbone); 3.82 (2H, m, N-C*H*$_2$CH$_2$-Fl); 2.82 (2H, m, N-CH$_2$C*H*$_2$-Fl); 2.25 (2H, septet, *J* = 7 Hz, C*H*(CH$_3$)$_2$); 1.21 (6H, d, *J* = 7 Hz, CH(C*H*$_3$)$_2$), 1.08 (6H, d, *J* = 7 Hz, CH(C*H*$_3$)$_2$)). NMR (^{13}C{^{1}H}, $CDCl_3$): 145.6 (C, Ar); 145.0 (C, Ar); 141.7 (C, Ar); 130.5 (CH, Ar) 127.8 (CH, Ar) 124.3 (CH, Ar); 124.2 (CH, Ar); 123.3 (CH, Ar) 120.9 (C, Ar); 120.2 (CH, Ar) 48.2 (Fl-CH$_2$*C*H$_2$N) 45.1 (*C*H, fluorene) 34.7 (Fl-*C*H$_2$CH$_2$-N); 28.2 *C*H(CH$_3$)$_2$), 24.5 CH(*C*H$_3$)$_2$), 24.34 CH(*C*H$_3$)$_2$). MS ES$^+$: 947 $[AgL_2]^+$. Calculated for $C_{30}H_{32}N_2AgBr$ (%): C, 59.23, H, 5.30, N, 4.60, Found: C, 59.36, H, 5.39, N, 4.50.

Ind-NHC-Ag-Br

^{1}H NMR ($CDCl_3$): 7.42-7.13 (7H, m, aromatic); 6.95 (1H, s, carbene backbone); 6.79 (1H, s, carbene backbone); 6.24 (1H, bs, indenyl H); 4.53 (2H, t, *J* = 7 Hz, bridge); 3.30

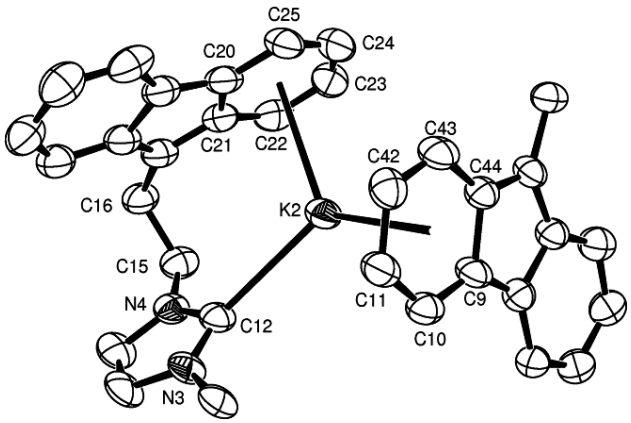
(2H, s, indenyl CH_2); 3.13 (2H, t, J = 7 Hz, bridge); 2.15 (2H, septet, J = 7Hz, isopropyl CH); 1.95 (6H, d, J = 7 Hz, isopropyl CH_3), 0.98 (6H, d, J = 7 Hz, isopropyl CH_3). $^{13}C\{^1H\}$ NMR ($CDCl_3$): 145.6 (C, Aromatic); 144.7 (c, aromatic); 144.2 (c, aromatic), 139.4 (c, aromatic); 131.5 (CH, aromatic); 130.5 (CH, aromatic); 126.4 (CH, aromatic); 125.2 (CH, aromatic); 124.2 (CH, aromatic); 51.1 (CH_2, bridge); 38.0 (CH_2, bridge); 29.9 (CH_2, indenyl); 28.2 (CH, isopropyl); 24.4 (CH_3, isopropyl). MS ES^+ (m/z): 847 $[AgL_2]^+$. Calculated for $C_{26}H_{30}N_2AgBr$ (%): C, 55.43, H, 5.42 N, 5.02. Found C, 55.90, H, 5.34, N, 4.95.

3-(2,6-Diisopropyl-phenyl)-1-[2-(fluorenyl-9-yl)-ethyl]-imidazol-2-ylidene dimethylamido- chloro-titanium (III), (Fl-NHC)(Cl)(NMe_2)Ti. In the glove box dichloro-bis(dimethylamido) titanium (40 mg, 0.2 mmol) and **(Fl-NHC)$^-$K$^+$** (100 mg ca 0.2mmol) were combined in a glass ampoule equipped with a Youngs' tap. Benzene (10ml) was added and the reaction mixture was stirred for 24h. After filtration yellow-brown crystals appeared within 48h. Yield: 32 mg, ca 25% based on Ti. Calculated (%) C, 70.27, H, 6.82 N, 7.68; Found C, 70.10, H, 6.75, N, 7.52.

3-(2,6-Diisopropyl-phenyl)-1-[2-(fluorenyl-9-yl)-ethyl]-imidazol-2-ylidene dimethylamido-bromo vanadium (III), (Ind-NHC)(Br)(NMe_2)V. Tetrakis(dimethylamido) vanadium (60 mg, 0.5 mmol) and **(IndH-NHC-H)Br** (0.5mmol) were dissolved in THF and combined at -78°C. After warming to room temperature and stirring overnight, the volatiles were removed under vacuum and the residue extracted into toluene. Filtration, concentration and crystallisation from

toluene/petrol at -30°C gave red-brown crystals. Yield: 95 mg, 0.18mmol, *ca*. 36%. Calculated (%) C, 61.77, H, 6.48 N, 7.72; Found C, 61.52, H, 6.32 N, 7.45.

Crystallographic Characterisation of $(Fl\text{-}NHC)^{-}K^{+}$



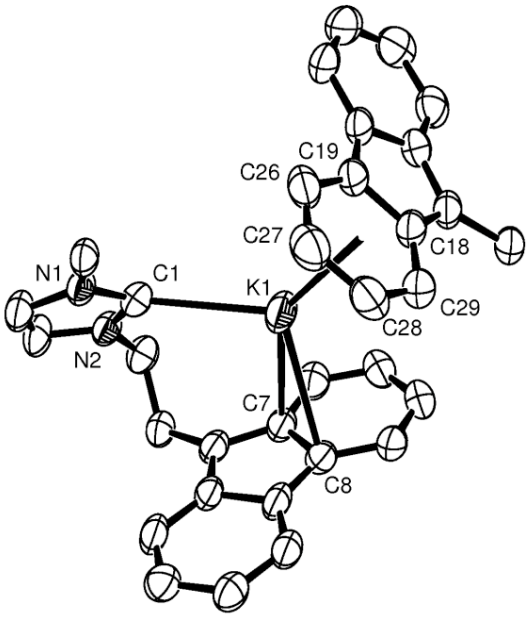


Table 1. Crystal data and structure refinement for (Fl-NHC)-K+

Identification code	$(Fl\text{-}NHC)^{-}K^{+}$	
Empirical formula	$C_{72}\,H_{74}\,K_2\,N_4$	
Formula weight	1073.55	
Temperature	120(2) K	
Wavelength	0.6868 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 20.531(7) Å	a= 90°.
	b = 13.027(4) Å	b= 92.220(5)°.
	c = 23.378(8) Å	g = 90°.
Volume	6248(4) $Å^3$	
Z	4	
Density (calculated)	1.141 Mg/m^3	
Absorption coefficient	0.195 mm^{-1}	
F(000)	2288	
Crystal size	0.20 x 0.01 x 0.01 mm^3	
Theta range for data collection	1.96 to 21.19°.	
Index ranges	-21<=h<=21, -13<=k<=13, -24<=l<=24	
Reflections collected	34299	
Independent reflections	7615 [R(int) = 0.1136]	
Completeness to theta = 21.19°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9980 and 0.6387	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7615 / 0 / 700	

Goodness-of-fit on F^2	0.922
Final R indices [I>2sigma(I)]	R1 = 0.0663, wR2 = 0.1520
R indices (all data)	R1 = 0.1220, wR2 = 0.1773
Extinction coefficient	0.0133(9)
Largest diff. peak and hole	0.362 and -0.297 e.$Å^{-3}$

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

	x	y	z	U(eq)
C(1)	5995(2)	531(4)	664(2)	42(1)
C(2)	6922(3)	1244(4)	334(2)	52(1)
C(3)	6421(3)	1655(4)	41(2)	54(1)
C(4)	5212(2)	1552(4)	61(2)	50(1)
C(5)	4985(2)	2483(4)	400(2)	46(1)
C(6)	4841(2)	2292(4)	1013(2)	44(1)
C(7)	4343(2)	1644(4)	1209(2)	45(1)
C(8)	4339(2)	1722(4)	1823(2)	46(1)
C(9)	4828(2)	2419(4)	2007(2)	46(1)
C(10)	5029(2)	2812(4)	2533(2)	47(1)
C(11)	5511(3)	3539(4)	2581(2)	51(1)
C(12)	3877(2)	5734(4)	2964(2)	46(1)
C(13)	3801(3)	6509(4)	3835(2)	57(2)
C(14)	3416(3)	7025(4)	3466(2)	60(2)
C(15)	3124(2)	6897(4)	2428(2)	53(1)
C(16)	3442(2)	7837(4)	2162(2)	53(1)
C(17)	4117(2)	7646(4)	1966(2)	47(1)
C(18)	4699(2)	8013(4)	2223(2)	47(1)
C(19)	5251(3)	7622(4)	1917(2)	49(1)
C(20)	4987(3)	6978(4)	1484(2)	50(1)
C(21)	4287(3)	7008(4)	1508(2)	49(1)
C(22)	3906(3)	6405(4)	1118(2)	58(2)

C(23)	4219(4)	5779(4)	735(2)	66(2)
C(24)	4897(4)	5743(5)	733(2)	68(2)
C(25)	5273(3)	6329(4)	1090(2)	58(2)
C(26)	5880(3)	7930(4)	2080(3)	59(2)
C(27)	5983(3)	8596(5)	2517(3)	66(2)
C(28)	5460(3)	8954(4)	2827(2)	61(2)
C(29)	4829(3)	8678(4)	2686(2)	55(1)
C(30)	4510(2)	4987(4)	3780(2)	47(1)
C(31)	4271(2)	4017(4)	3922(2)	49(1)
C(32)	3560(2)	3755(4)	3806(2)	57(2)
C(33)	3200(3)	3690(6)	4351(3)	98(2)
C(34)	3482(3)	2790(6)	3472(3)	124(3)
C(35)	4690(3)	3338(5)	4180(2)	64(2)
C(36)	5337(3)	3585(5)	4292(2)	70(2)
C(37)	5563(3)	4544(5)	4146(2)	63(2)
C(38)	5159(3)	5255(4)	3884(2)	51(1)
C(39)	5434(3)	6288(4)	3713(2)	57(2)
C(40)	5918(4)	6161(5)	3257(3)	109(3)
C(41)	5724(6)	6880(7)	4199(3)	181(5)
C(42)	5818(2)	3884(4)	2083(2)	51(1)
C(43)	5632(2)	3501(4)	1556(2)	52(1)
C(44)	5140(2)	2768(4)	1491(2)	44(1)
C(45)	3882(3)	1146(4)	2121(2)	56(2)
C(46)	3448(3)	516(4)	1831(3)	67(2)
C(47)	3462(3)	431(4)	1233(2)	63(2)
C(48)	3900(3)	977(4)	929(2)	54(1)
C(49)	7047(2)	-18(4)	1114(2)	42(1)

C(50)	7144(2)	387(4)	1665(2)	44(1)
C(51)	6860(2)	1406(4)	1827(2)	49(1)
C(52)	7358(3)	2259(4)	1786(2)	64(2)
C(53)	6587(3)	1385(4)	2427(2)	58(2)
C(54)	7527(2)	-180(4)	2049(2)	50(1)
C(55)	7803(2)	-1092(4)	1898(2)	51(1)
C(56)	7706(2)	-1468(4)	1355(2)	48(1)
C(57)	7322(2)	-939(4)	953(2)	44(1)
C(58)	7180(2)	-1387(4)	368(2)	49(1)
C(59)	6687(3)	-2246(4)	401(2)	62(2)
C(60)	7801(2)	-1772(5)	86(2)	67(2)
C(61)	3111(3)	3620(4)	1717(3)	58(2)
C(62)	2686(3)	4275(4)	1985(2)	53(1)
C(63)	2246(3)	4835(4)	1664(3)	59(2)
C(64)	2216(3)	4781(4)	1080(3)	63(2)
C(65)	2653(3)	4129(4)	814(2)	63(2)
C(66)	3097(3)	3565(4)	1134(3)	63(2)
C(67)	2787(5)	1111(4)	5362(2)	106(3)
C(68)	2146(4)	883(5)	5487(3)	112(3)
C(69)	2017(3)	127(5)	5887(4)	117(3)
C(70)	2528(5)	-402(4)	6160(2)	128(3)
C(71)	3168(4)	-175(5)	6035(3)	170(5)
C(72)	3298(3)	582(6)	5635(4)	147(4)
K(1)	5149(1)	-134(1)	1555(1)	60(1)
K(2)	4475(1)	4858(1)	1966(1)	49(1)
N(1)	6659(2)	549(3)	711(2)	42(1)
N(2)	5864(2)	1220(3)	246(2)	43(1)

N(3)	4081(2)	5733(3)	3524(2)	45(1)
N(4)	3469(2)	6551(3)	2941(2)	47(1)

Table 3. Bond lengths [Å] and angles [°] for (Fl-NHC)$^{-}$K^{+}.

C(1)-N(2)	1.347(6)
C(1)-N(1)	1.364(6)
C(1)-K(1)	2.896(5)
C(2)-C(3)	1.326(7)
C(2)-N(1)	1.387(6)
C(2)-H(2)	0.9500
C(3)-N(2)	1.378(6)
C(3)-H(3)	0.9500
C(4)-N(2)	1.456(6)
C(4)-C(5)	1.533(6)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.495(6)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(44)	1.399(6)
C(6)-C(7)	1.414(6)
C(6)-K(1)	3.454(5)
C(7)-C(48)	1.403(7)
C(7)-C(8)	1.442(6)
C(7)-K(1)	2.941(5)
C(8)-C(45)	1.407(7)
C(8)-C(9)	1.408(7)
C(8)-K(1)	3.014(5)
C(9)-C(10)	1.380(7)

C(9)-C(44)	1.460(6)
C(9)-K(2)	3.260(5)
C(10)-C(11)	1.371(7)
C(10)-K(2)	3.169(5)
C(10)-H(10)	0.9500
C(11)-C(42)	1.418(7)
C(11)-K(2)	3.051(5)
C(11)-H(11)	0.9500
C(12)-N(4)	1.355(6)
C(12)-N(3)	1.358(6)
C(12)-K(2)	2.911(5)
C(13)-C(14)	1.331(7)
C(13)-N(3)	1.383(6)
C(13)-H(13)	0.9500
C(14)-N(4)	1.382(6)
C(14)-H(14)	0.9500
C(15)-N(4)	1.441(6)
C(15)-C(16)	1.531(7)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.497(6)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.400(7)
C(17)-C(21)	1.411(7)
C(18)-C(29)	1.405(7)
C(18)-C(19)	1.455(7)

C(18)-K(1)#1	3.038(5)
C(19)-C(26)	1.390(7)
C(19)-C(20)	1.407(7)
C(19)-K(1)#1	3.049(5)
C(20)-C(25)	1.397(7)
C(20)-C(21)	1.440(7)
C(20)-K(2)	3.177(5)
C(21)-C(22)	1.416(7)
C(21)-K(2)	3.018(5)
C(22)-C(23)	1.388(7)
C(22)-K(2)	3.029(5)
C(22)-H(22)	0.9500
C(23)-C(24)	1.392(8)
C(23)-K(2)	3.142(5)
C(23)-H(23)	0.9500
C(24)-C(25)	1.351(8)
C(24)-K(2)	3.252(5)
C(24)-H(24)	0.9500
C(25)-K(2)	3.287(5)
C(25)-H(25)	0.9500
C(26)-C(27)	1.350(7)
C(26)-K(1)#1	3.159(5)
C(26)-H(26)	0.9500
C(27)-C(28)	1.399(8)
C(27)-K(1)#1	3.229(6)
C(27)-H(27)	0.9500
C(28)-C(29)	1.374(7)

C(28)-K(1)#1	3.244(6)
C(28)-H(28)	0.9500
C(29)-K(1)#1	3.154(5)
C(29)-H(29)	0.9500
C(30)-C(38)	1.389(7)
C(30)-C(31)	1.400(7)
C(30)-N(3)	1.428(6)
C(31)-C(35)	1.359(7)
C(31)-C(32)	1.514(7)
C(32)-C(34)	1.485(8)
C(32)-C(33)	1.500(7)
C(32)-H(32)	1.0000
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-C(36)	1.383(7)
C(35)-H(35)	0.9500
C(36)-C(37)	1.380(8)
C(36)-H(36)	0.9500
C(37)-C(38)	1.373(7)
C(37)-H(37)	0.9500
C(38)-C(39)	1.518(7)
C(39)-C(41)	1.479(8)
C(39)-C(40)	1.495(7)

C(39)-H(39A)	1.0000
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-C(43)	1.371(7)
C(42)-K(2)	3.038(5)
C(42)-H(42)	0.9500
C(43)-C(44)	1.395(7)
C(43)-K(2)	3.142(5)
C(43)-H(43)	0.9500
C(44)-K(2)	3.260(5)
C(45)-C(46)	1.371(7)
C(45)-K(1)	3.400(5)
C(45)-H(45)	0.9500
C(46)-C(47)	1.403(7)
C(46)-H(46)	0.9500
C(47)-C(48)	1.367(7)
C(47)-H(47)	0.9500
C(48)-K(1)	3.244(5)
C(48)-H(48)	0.9500
C(49)-C(57)	1.386(6)
C(49)-C(50)	1.399(7)
C(49)-N(1)	1.418(6)
C(50)-C(54)	1.384(7)

C(50)-C(51)	1.503(6)
C(51)-C(52)	1.515(7)
C(51)-C(53)	1.532(6)
C(51)-H(51)	1.0000
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800
C(54)-C(55)	1.368(7)
C(54)-H(54)	0.9500
C(55)-C(56)	1.369(7)
C(55)-H(55)	0.9500
C(56)-C(57)	1.387(6)
C(56)-H(56)	0.9500
C(57)-C(58)	1.505(7)
C(58)-C(59)	1.513(7)
C(58)-C(60)	1.544(6)
C(58)-H(58)	1.0000
C(59)-H(59A)	0.9800
C(59)-H(59B)	0.9800
C(59)-H(59C)	0.9800
C(60)-H(60A)	0.9800
C(60)-H(60B)	0.9800
C(60)-H(60C)	0.9800
C(61)-C(66)	1.363(7)

C(61)-C(62)	1.386(7)
C(61)-K(2)	3.265(5)
C(61)-H(61)	0.9500
C(62)-C(63)	1.363(7)
C(62)-H(62)	0.9500
C(63)-C(64)	1.368(7)
C(63)-H(63)	0.9500
C(64)-C(65)	1.398(7)
C(64)-H(64)	0.9500
C(65)-C(66)	1.371(7)
C(65)-H(65)	0.9500
C(66)-H(66)	0.9500
C(67)-C(68)	1.3900
C(67)-C(72)	1.3900
C(67)-H(67)	0.9500
C(68)-C(69)	1.3900
C(68)-H(68)	0.9500
C(69)-C(70)	1.3900
C(69)-H(69)	0.9500
C(70)-C(71)	1.3900
C(70)-H(70)	0.9500
C(71)-C(72)	1.3900
C(71)-H(71)	0.9500
C(72)-H(72)	0.9500
K(1)-C(18)#2	3.038(5)
K(1)-C(19)#2	3.049(5)
K(1)-C(29)#2	3.154(5)

K(1)-C(26)#2	3.159(5)
K(1)-C(27)#2	3.229(6)
K(1)-C(28)#2	3.244(6)

N(2)-C(1)-N(1)	102.6(4)
N(2)-C(1)-K(1)	127.7(3)
N(1)-C(1)-K(1)	125.1(3)
C(3)-C(2)-N(1)	106.1(4)
C(3)-C(2)-H(2)	126.9
N(1)-C(2)-H(2)	126.9
C(2)-C(3)-N(2)	107.0(5)
C(2)-C(3)-H(3)	126.5
N(2)-C(3)-H(3)	126.5
N(2)-C(4)-C(5)	112.1(4)
N(2)-C(4)-H(4A)	109.2
C(5)-C(4)-H(4A)	109.2
N(2)-C(4)-H(4B)	109.2
C(5)-C(4)-H(4B)	109.2
H(4A)-C(4)-H(4B)	107.9
C(6)-C(5)-C(4)	116.1(4)
C(6)-C(5)-H(5A)	108.3
C(4)-C(5)-H(5A)	108.3
C(6)-C(5)-H(5B)	108.3
C(4)-C(5)-H(5B)	108.3
H(5A)-C(5)-H(5B)	107.4
C(44)-C(6)-C(7)	107.9(4)
C(44)-C(6)-C(5)	126.5(4)

C(7)-C(6)-C(5)	125.5(5)
C(44)-C(6)-K(1)	92.5(3)
C(7)-C(6)-K(1)	57.3(3)
C(5)-C(6)-K(1)	117.6(3)
C(48)-C(7)-C(6)	133.1(5)
C(48)-C(7)-C(8)	118.7(5)
C(6)-C(7)-C(8)	108.2(4)
C(48)-C(7)-K(1)	89.3(3)
C(6)-C(7)-K(1)	98.8(3)
C(8)-C(7)-K(1)	78.8(3)
C(45)-C(8)-C(9)	132.4(5)
C(45)-C(8)-C(7)	119.1(5)
C(9)-C(8)-C(7)	108.5(4)
C(45)-C(8)-K(1)	93.4(3)
C(9)-C(8)-K(1)	100.9(3)
C(7)-C(8)-K(1)	73.2(3)
C(10)-C(9)-C(8)	134.1(4)
C(10)-C(9)-C(44)	119.6(5)
C(8)-C(9)-C(44)	106.2(4)
C(10)-C(9)-K(2)	73.9(3)
C(8)-C(9)-K(2)	117.7(3)
C(44)-C(9)-K(2)	77.1(3)
C(11)-C(10)-C(9)	121.4(5)
C(11)-C(10)-K(2)	72.5(3)
C(9)-C(10)-K(2)	81.3(3)
C(11)-C(10)-H(10)	119.3
C(9)-C(10)-H(10)	119.3

K(2)-C(10)-H(10)	117.4
C(10)-C(11)-C(42)	119.6(5)
C(10)-C(11)-K(2)	82.1(3)
C(42)-C(11)-K(2)	76.0(3)
C(10)-C(11)-H(11)	120.2
C(42)-C(11)-H(11)	120.2
K(2)-C(11)-H(11)	112.1
N(4)-C(12)-N(3)	101.8(4)
N(4)-C(12)-K(2)	123.7(3)
N(3)-C(12)-K(2)	130.5(3)
C(14)-C(13)-N(3)	106.0(5)
C(14)-C(13)-H(13)	127.0
N(3)-C(13)-H(13)	127.0
C(13)-C(14)-N(4)	106.6(5)
C(13)-C(14)-H(14)	126.7
N(4)-C(14)-H(14)	126.7
N(4)-C(15)-C(16)	112.6(4)
N(4)-C(15)-H(15A)	109.1
C(16)-C(15)-H(15A)	109.1
N(4)-C(15)-H(15B)	109.1
C(16)-C(15)-H(15B)	109.1
H(15A)-C(15)-H(15B)	107.8
C(17)-C(16)-C(15)	113.9(4)
C(17)-C(16)-H(16A)	108.8
C(15)-C(16)-H(16A)	108.8
C(17)-C(16)-H(16B)	108.8
C(15)-C(16)-H(16B)	108.8

H(16A)-C(16)-H(16B)	107.7
C(18)-C(17)-C(21)	107.1(4)
C(18)-C(17)-C(16)	126.6(5)
C(21)-C(17)-C(16)	126.2(5)
C(17)-C(18)-C(29)	132.4(5)
C(17)-C(18)-C(19)	109.8(5)
C(29)-C(18)-C(19)	117.7(5)
C(17)-C(18)-K(1)#1	108.8(3)
C(29)-C(18)-K(1)#1	81.5(3)
C(19)-C(18)-K(1)#1	76.6(3)
C(26)-C(19)-C(20)	134.2(5)
C(26)-C(19)-C(18)	119.8(5)
C(20)-C(19)-C(18)	106.0(5)
C(26)-C(19)-K(1)#1	81.5(3)
C(20)-C(19)-K(1)#1	110.5(3)
C(18)-C(19)-K(1)#1	75.8(3)
C(25)-C(20)-C(19)	132.5(5)
C(25)-C(20)-C(21)	119.1(5)
C(19)-C(20)-C(21)	108.3(4)
C(25)-C(20)-K(2)	82.0(3)
C(19)-C(20)-K(2)	112.7(3)
C(21)-C(20)-K(2)	70.5(3)
C(17)-C(21)-C(22)	131.8(5)
C(17)-C(21)-C(20)	108.8(5)
C(22)-C(21)-C(20)	119.2(5)
C(17)-C(21)-K(2)	108.0(3)
C(22)-C(21)-K(2)	76.9(3)

C(20)-C(21)-K(2)	82.8(3)
C(23)-C(22)-C(21)	118.8(5)
C(23)-C(22)-K(2)	81.6(3)
C(21)-C(22)-K(2)	76.0(3)
C(23)-C(22)-H(22)	120.6
C(21)-C(22)-H(22)	120.6
K(2)-C(22)-H(22)	112.4
C(22)-C(23)-C(24)	120.7(6)
C(22)-C(23)-K(2)	72.5(3)
C(24)-C(23)-K(2)	81.9(3)
C(22)-C(23)-H(23)	119.6
C(24)-C(23)-H(23)	119.6
K(2)-C(23)-H(23)	116.5
C(25)-C(24)-C(23)	121.7(5)
C(25)-C(24)-K(2)	79.5(3)
C(23)-C(24)-K(2)	73.0(3)
C(25)-C(24)-H(24)	119.1
C(23)-C(24)-H(24)	119.1
K(2)-C(24)-H(24)	119.1
C(24)-C(25)-C(20)	120.3(5)
C(24)-C(25)-K(2)	76.6(3)
C(20)-C(25)-K(2)	73.1(3)
C(24)-C(25)-H(25)	119.8
C(20)-C(25)-H(25)	119.8
K(2)-C(25)-H(25)	121.6
C(27)-C(26)-C(19)	120.6(5)
C(27)-C(26)-K(1)#1	80.7(3)

C(19)-C(26)-K(1)#1	72.7(3)
C(27)-C(26)-H(26)	119.7
C(19)-C(26)-H(26)	119.7
K(1)#1-C(26)-H(26)	117.6
C(26)-C(27)-C(28)	120.4(5)
C(26)-C(27)-K(1)#1	74.9(3)
C(28)-C(27)-K(1)#1	78.1(3)
C(26)-C(27)-H(27)	119.8
C(28)-C(27)-H(27)	119.8
K(1)#1-C(27)-H(27)	118.0
C(29)-C(28)-C(27)	121.5(5)
C(29)-C(28)-K(1)#1	74.0(3)
C(27)-C(28)-K(1)#1	76.9(3)
C(29)-C(28)-H(28)	119.2
C(27)-C(28)-H(28)	119.2
K(1)#1-C(28)-H(28)	121.0
C(28)-C(29)-C(18)	119.8(5)
C(28)-C(29)-K(1)#1	81.3(3)
C(18)-C(29)-K(1)#1	72.3(3)
C(28)-C(29)-H(29)	120.1
C(18)-C(29)-H(29)	120.1
K(1)#1-C(29)-H(29)	117.0
C(38)-C(30)-C(31)	121.9(5)
C(38)-C(30)-N(3)	118.3(5)
C(31)-C(30)-N(3)	119.8(5)
C(35)-C(31)-C(30)	118.1(5)
C(35)-C(31)-C(32)	121.5(5)

C(30)-C(31)-C(32)	120.4(5)
C(34)-C(32)-C(33)	110.7(6)
C(34)-C(32)-C(31)	111.7(5)
C(33)-C(32)-C(31)	111.3(5)
C(34)-C(32)-H(32)	107.6
C(33)-C(32)-H(32)	107.6
C(31)-C(32)-H(32)	107.6
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(32)-C(34)-H(34A)	109.5
C(32)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(32)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(31)-C(35)-C(36)	121.4(5)
C(31)-C(35)-H(35)	119.3
C(36)-C(35)-H(35)	119.3
C(35)-C(36)-C(37)	119.6(6)
C(35)-C(36)-H(36)	120.2
C(37)-C(36)-H(36)	120.2
C(38)-C(37)-C(36)	121.2(5)
C(38)-C(37)-H(37)	119.4

C(36)-C(37)-H(37)	119.4
C(37)-C(38)-C(30)	117.9(5)
C(37)-C(38)-C(39)	119.4(5)
C(30)-C(38)-C(39)	122.7(5)
C(41)-C(39)-C(40)	110.2(6)
C(41)-C(39)-C(38)	113.8(5)
C(40)-C(39)-C(38)	110.7(5)
C(41)-C(39)-H(39A)	107.3
C(40)-C(39)-H(39A)	107.3
C(38)-C(39)-H(39A)	107.3
C(39)-C(40)-H(40A)	109.5
C(39)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(39)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(39)-C(41)-H(41A)	109.5
C(39)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(39)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(43)-C(42)-C(11)	120.4(5)
C(43)-C(42)-K(2)	81.5(3)
C(11)-C(42)-K(2)	77.1(3)
C(43)-C(42)-H(42)	119.8
C(11)-C(42)-H(42)	119.8

K(2)-C(42)-H(42)	112.0
C(42)-C(43)-C(44)	121.4(5)
C(42)-C(43)-K(2)	73.0(3)
C(44)-C(43)-K(2)	82.2(3)
C(42)-C(43)-H(43)	119.3
C(44)-C(43)-H(43)	119.3
K(2)-C(43)-H(43)	115.9
C(43)-C(44)-C(6)	133.2(4)
C(43)-C(44)-C(9)	117.6(5)
C(6)-C(44)-C(9)	109.2(4)
C(43)-C(44)-K(2)	72.7(3)
C(6)-C(44)-K(2)	117.7(3)
C(9)-C(44)-K(2)	77.1(3)
C(46)-C(45)-C(8)	120.5(5)
C(46)-C(45)-K(1)	90.3(3)
C(8)-C(45)-K(1)	62.2(3)
C(46)-C(45)-H(45)	119.8
C(8)-C(45)-H(45)	119.8
K(1)-C(45)-H(45)	117.6
C(45)-C(46)-C(47)	120.2(5)
C(45)-C(46)-H(46)	119.9
C(47)-C(46)-H(46)	119.9
C(48)-C(47)-C(46)	121.1(5)
C(48)-C(47)-H(47)	119.5
C(46)-C(47)-H(47)	119.5
C(47)-C(48)-C(7)	120.5(5)
C(47)-C(48)-K(1)	93.3(3)

C(7)-C(48)-K(1)	65.1(3)
C(47)-C(48)-H(48)	119.8
C(7)-C(48)-H(48)	119.8
K(1)-C(48)-H(48)	111.6
C(57)-C(49)-C(50)	122.1(5)
C(57)-C(49)-N(1)	119.6(4)
C(50)-C(49)-N(1)	118.3(4)
C(54)-C(50)-C(49)	116.9(4)
C(54)-C(50)-C(51)	121.7(5)
C(49)-C(50)-C(51)	121.4(5)
C(50)-C(51)-C(52)	111.3(4)
C(50)-C(51)-C(53)	111.9(4)
C(52)-C(51)-C(53)	110.0(4)
C(50)-C(51)-H(51)	107.8
C(52)-C(51)-H(51)	107.8
C(53)-C(51)-H(51)	107.8
C(51)-C(52)-H(52A)	109.5
C(51)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(51)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(51)-C(53)-H(53A)	109.5
C(51)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(51)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5

H(53B)-C(53)-H(53C)	109.5
C(55)-C(54)-C(50)	121.9(5)
C(55)-C(54)-H(54)	119.1
C(50)-C(54)-H(54)	119.1
C(54)-C(55)-C(56)	120.2(5)
C(54)-C(55)-H(55)	119.9
C(56)-C(55)-H(55)	119.9
C(55)-C(56)-C(57)	120.6(5)
C(55)-C(56)-H(56)	119.7
C(57)-C(56)-H(56)	119.7
C(49)-C(57)-C(56)	118.2(4)
C(49)-C(57)-C(58)	121.1(5)
C(56)-C(57)-C(58)	120.6(5)
C(57)-C(58)-C(59)	110.3(4)
C(57)-C(58)-C(60)	112.3(4)
C(59)-C(58)-C(60)	110.3(4)
C(57)-C(58)-H(58)	107.9
C(59)-C(58)-H(58)	107.9
C(60)-C(58)-H(58)	107.9
C(58)-C(59)-H(59A)	109.5
C(58)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	109.5
C(58)-C(59)-H(59C)	109.5
H(59A)-C(59)-H(59C)	109.5
H(59B)-C(59)-H(59C)	109.5
C(58)-C(60)-H(60A)	109.5
C(58)-C(60)-H(60B)	109.5

H(60A)-C(60)-H(60B)	109.5
C(58)-C(60)-H(60C)	109.5
H(60A)-C(60)-H(60C)	109.5
H(60B)-C(60)-H(60C)	109.5
C(66)-C(61)-C(62)	119.7(5)
C(66)-C(61)-K(2)	100.8(3)
C(62)-C(61)-K(2)	99.5(3)
C(66)-C(61)-H(61)	120.1
C(62)-C(61)-H(61)	120.1
K(2)-C(61)-H(61)	69.4
C(63)-C(62)-C(61)	119.7(5)
C(63)-C(62)-H(62)	120.1
C(61)-C(62)-H(62)	120.1
C(64)-C(63)-C(62)	121.7(5)
C(64)-C(63)-H(63)	119.2
C(62)-C(63)-H(63)	119.2
C(63)-C(64)-C(65)	118.1(6)
C(63)-C(64)-H(64)	121.0
C(65)-C(64)-H(64)	121.0
C(66)-C(65)-C(64)	120.5(5)
C(66)-C(65)-H(65)	119.7
C(64)-C(65)-H(65)	119.7
C(61)-C(66)-C(65)	120.3(5)
C(61)-C(66)-H(66)	119.9
C(65)-C(66)-H(66)	119.9
C(68)-C(67)-C(72)	120.0
C(68)-C(67)-H(67)	120.0

C(72)-C(67)-H(67)	120.0
C(67)-C(68)-C(69)	120.0
C(67)-C(68)-H(68)	120.0
C(69)-C(68)-H(68)	120.0
C(70)-C(69)-C(68)	120.0
C(70)-C(69)-H(69)	120.0
C(68)-C(69)-H(69)	120.0
C(69)-C(70)-C(71)	120.0
C(69)-C(70)-H(70)	120.0
C(71)-C(70)-H(70)	120.0
C(72)-C(71)-C(70)	120.0
C(72)-C(71)-H(71)	120.0
C(70)-C(71)-H(71)	120.0
C(71)-C(72)-C(67)	120.0
C(71)-C(72)-H(72)	120.0
C(67)-C(72)-H(72)	120.0
C(1)-K(1)-C(7)	85.02(14)
C(1)-K(1)-C(8)	105.13(14)
C(7)-K(1)-C(8)	27.98(13)
C(1)-K(1)-C(18)#2	144.09(14)
C(7)-K(1)-C(18)#2	126.05(14)
C(8)-K(1)-C(18)#2	110.45(14)
C(1)-K(1)-C(19)#2	116.72(13)
C(7)-K(1)-C(19)#2	149.74(15)
C(8)-K(1)-C(19)#2	138.08(14)
C(18)#2-K(1)-C(19)#2	27.66(12)
C(1)-K(1)-C(29)#2	154.09(15)

C(7)-K(1)-C(29)#2	118.95(14)
C(8)-K(1)-C(29)#2	94.85(14)
C(18)#2-K(1)-C(29)#2	26.14(13)
C(19)#2-K(1)-C(29)#2	46.46(13)
C(1)-K(1)-C(26)#2	103.23(14)
C(7)-K(1)-C(26)#2	171.63(14)
C(8)-K(1)-C(26)#2	144.79(15)
C(18)#2-K(1)-C(26)#2	46.77(13)
C(19)#2-K(1)-C(26)#2	25.80(13)
C(29)#2-K(1)-C(26)#2	52.68(14)
C(1)-K(1)-C(27)#2	109.68(15)
C(7)-K(1)-C(27)#2	150.75(16)
C(8)-K(1)-C(27)#2	123.22(16)
C(18)#2-K(1)-C(27)#2	53.04(14)
C(19)#2-K(1)-C(27)#2	44.45(15)
C(29)#2-K(1)-C(27)#2	44.53(14)
C(26)#2-K(1)-C(27)#2	24.37(13)
C(1)-K(1)-C(48)	91.61(14)
C(7)-K(1)-C(48)	25.62(13)
C(8)-K(1)-C(48)	45.85(14)
C(18)#2-K(1)-C(48)	109.61(14)
C(19)#2-K(1)-C(48)	126.74(15)
C(29)#2-K(1)-C(48)	114.24(14)
C(26)#2-K(1)-C(48)	152.50(15)
C(27)#2-K(1)-C(48)	158.67(15)
C(1)-K(1)-C(28)#2	131.77(15)
C(7)-K(1)-C(28)#2	129.02(14)

C(8)-K(1)-C(28)#2	101.15(14)
C(18)#2-K(1)-C(28)#2	44.85(14)
C(19)#2-K(1)-C(28)#2	52.06(14)
C(29)#2-K(1)-C(28)#2	24.74(13)
C(26)#2-K(1)-C(28)#2	43.73(15)
C(27)#2-K(1)-C(28)#2	24.96(14)
C(48)-K(1)-C(28)#2	134.56(15)
C(1)-K(1)-C(45)	128.51(13)
C(7)-K(1)-C(45)	44.83(12)
C(8)-K(1)-C(45)	24.39(12)
C(18)#2-K(1)-C(45)	86.41(13)
C(19)#2-K(1)-C(45)	114.06(13)
C(29)#2-K(1)-C(45)	74.16(13)
C(26)#2-K(1)-C(45)	126.81(14)
C(27)#2-K(1)-C(45)	111.91(15)
C(48)-K(1)-C(45)	49.74(14)
C(28)#2-K(1)-C(45)	87.09(14)
C(1)-K(1)-C(6)	64.48(12)
C(7)-K(1)-C(6)	23.86(12)
C(8)-K(1)-C(6)	41.21(12)
C(18)#2-K(1)-C(6)	149.38(12)
C(19)#2-K(1)-C(6)	171.49(14)
C(29)#2-K(1)-C(6)	135.65(13)
C(26)#2-K(1)-C(6)	161.91(14)
C(27)#2-K(1)-C(6)	143.97(15)
C(48)-K(1)-C(6)	45.25(13)
C(28)#2-K(1)-C(6)	134.26(13)

C(45)-K(1)-C(6)	64.03(11)
C(12)-K(2)-C(21)	82.47(14)
C(12)-K(2)-C(22)	95.72(15)
C(21)-K(2)-C(22)	27.08(13)
C(12)-K(2)-C(42)	120.02(15)
C(21)-K(2)-C(42)	121.53(15)
C(22)-K(2)-C(42)	131.55(15)
C(12)-K(2)-C(11)	98.65(14)
C(21)-K(2)-C(11)	140.11(15)
C(22)-K(2)-C(11)	158.07(15)
C(42)-K(2)-C(11)	26.92(13)
C(12)-K(2)-C(43)	144.34(15)
C(21)-K(2)-C(43)	120.12(14)
C(22)-K(2)-C(43)	116.90(15)
C(42)-K(2)-C(43)	25.57(12)
C(11)-K(2)-C(43)	45.98(13)
C(12)-K(2)-C(23)	121.58(16)
C(21)-K(2)-C(23)	46.08(14)
C(22)-K(2)-C(23)	25.91(14)
C(42)-K(2)-C(23)	111.19(17)
C(11)-K(2)-C(23)	137.35(16)
C(43)-K(2)-C(23)	92.13(16)
C(12)-K(2)-C(10)	98.62(14)
C(21)-K(2)-C(10)	165.48(15)
C(22)-K(2)-C(10)	163.06(15)
C(42)-K(2)-C(10)	45.63(13)
C(11)-K(2)-C(10)	25.38(12)

C(43)-K(2)-C(10)	52.45(13)
C(23)-K(2)-C(10)	138.48(15)
C(12)-K(2)-C(20)	95.69(14)
C(21)-K(2)-C(20)	26.72(13)
C(22)-K(2)-C(20)	46.71(15)
C(42)-K(2)-C(20)	94.82(14)
C(11)-K(2)-C(20)	115.02(14)
C(43)-K(2)-C(20)	96.71(13)
C(23)-K(2)-C(20)	52.37(15)
C(10)-K(2)-C(20)	139.59(14)
C(12)-K(2)-C(24)	134.96(15)
C(21)-K(2)-C(24)	52.51(14)
C(22)-K(2)-C(24)	45.08(15)
C(42)-K(2)-C(24)	87.52(16)
C(11)-K(2)-C(24)	114.39(16)
C(43)-K(2)-C(24)	72.46(15)
C(23)-K(2)-C(24)	25.07(14)
C(10)-K(2)-C(24)	124.42(14)
C(20)-K(2)-C(24)	43.51(15)
C(12)-K(2)-C(44)	142.67(13)
C(21)-K(2)-C(44)	134.74(13)
C(22)-K(2)-C(44)	119.30(14)
C(42)-K(2)-C(44)	44.87(13)
C(11)-K(2)-C(44)	52.88(13)
C(43)-K(2)-C(44)	25.08(12)
C(23)-K(2)-C(44)	93.71(15)
C(10)-K(2)-C(44)	44.87(12)

C(20)-K(2)-C(44)	117.19(13)
C(24)-K(2)-C(44)	82.25(14)
C(12)-K(2)-C(9)	117.27(13)
C(21)-K(2)-C(9)	160.11(13)
C(22)-K(2)-C(9)	138.39(15)
C(42)-K(2)-C(9)	52.43(13)
C(11)-K(2)-C(9)	44.51(14)
C(43)-K(2)-C(9)	44.81(12)
C(23)-K(2)-C(9)	115.36(14)
C(10)-K(2)-C(9)	24.74(12)
C(20)-K(2)-C(9)	141.44(12)
C(24)-K(2)-C(9)	107.78(14)
C(44)-K(2)-C(9)	25.88(11)
C(1)-N(1)-C(2)	111.9(4)
C(1)-N(1)-C(49)	125.2(4)
C(2)-N(1)-C(49)	122.8(4)
C(1)-N(2)-C(3)	112.4(4)
C(1)-N(2)-C(4)	124.8(4)
C(3)-N(2)-C(4)	122.6(4)
C(12)-N(3)-C(13)	112.9(4)
C(12)-N(3)-C(30)	124.5(4)
C(13)-N(3)-C(30)	122.5(4)
C(12)-N(4)-C(14)	112.7(4)
C(12)-N(4)-C(15)	124.2(4)
C(14)-N(4)-C(15)	123.1(4)

Symmetry transformations used to generate equivalent atoms:

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

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	40(3)	49(3)	37(3)	-2(3)	5(2)	3(2)
C(2)	43(3)	62(4)	52(3)	10(3)	19(3)	0(3)
C(3)	53(4)	68(4)	43(3)	11(3)	20(3)	-2(3)
C(4)	47(3)	63(4)	38(3)	2(3)	6(3)	4(3)
C(5)	43(3)	53(3)	43(3)	8(3)	10(2)	2(3)
C(6)	42(3)	49(3)	40(3)	-2(3)	12(2)	4(3)
C(7)	44(3)	46(3)	45(3)	5(3)	13(3)	6(3)
C(8)	48(3)	43(3)	49(3)	3(3)	14(3)	7(3)
C(9)	45(3)	55(3)	41(3)	3(3)	19(3)	6(3)
C(10)	46(3)	51(3)	47(3)	9(3)	16(3)	8(3)
C(11)	55(4)	58(4)	39(3)	1(3)	11(3)	2(3)
C(12)	41(3)	53(3)	45(3)	5(3)	17(2)	0(3)
C(13)	56(4)	69(4)	47(3)	-8(3)	25(3)	13(3)
C(14)	53(4)	67(4)	62(4)	-3(3)	30(3)	15(3)
C(15)	41(3)	58(4)	61(4)	11(3)	15(3)	6(3)
C(16)	48(3)	51(3)	61(3)	8(3)	20(3)	0(3)
C(17)	42(3)	49(3)	50(3)	12(3)	14(3)	0(3)
C(18)	47(3)	47(3)	48(3)	9(3)	15(3)	2(3)
C(19)	50(4)	45(3)	54(3)	12(3)	17(3)	1(3)
C(20)	52(4)	49(3)	50(3)	14(3)	21(3)	1(3)
C(21)	55(4)	48(3)	45(3)	10(3)	12(3)	-5(3)
C(22)	59(4)	62(4)	54(4)	18(3)	9(3)	0(3)

C(23)	99(6)	61(4)	39(3)	1(3)	7(3)	-9(4)
C(24)	95(5)	60(4)	51(4)	6(3)	30(4)	8(4)
C(25)	63(4)	61(4)	52(3)	6(3)	28(3)	3(3)
C(26)	43(4)	51(4)	82(4)	21(3)	15(3)	0(3)
C(27)	51(4)	60(4)	87(5)	9(4)	3(3)	-8(3)
C(28)	65(4)	53(4)	65(4)	4(3)	4(3)	-15(3)
C(29)	58(4)	51(3)	58(4)	6(3)	20(3)	-1(3)
C(30)	43(3)	64(4)	35(3)	-1(3)	13(2)	11(3)
C(31)	44(3)	63(4)	42(3)	8(3)	16(3)	-2(3)
C(32)	44(3)	75(4)	52(3)	10(3)	18(3)	-2(3)
C(33)	58(4)	162(7)	75(4)	-21(4)	39(3)	-13(4)
C(34)	55(4)	156(7)	164(8)	-92(7)	29(5)	-19(5)
C(35)	57(4)	75(4)	60(4)	23(3)	10(3)	-5(3)
C(36)	55(4)	90(5)	67(4)	27(4)	7(3)	9(4)
C(37)	48(4)	86(5)	55(3)	16(3)	17(3)	-9(3)
C(38)	46(4)	67(4)	43(3)	2(3)	10(3)	6(3)
C(39)	51(3)	63(4)	59(3)	-4(3)	14(3)	-3(3)
C(40)	134(6)	69(4)	132(6)	24(4)	101(5)	4(4)
C(41)	328(15)	129(7)	86(6)	-27(6)	9(7)	-119(9)
C(42)	45(3)	54(3)	55(4)	-5(3)	5(3)	1(3)
C(43)	42(3)	62(4)	54(4)	5(3)	22(3)	3(3)
C(44)	37(3)	46(3)	49(3)	3(3)	15(3)	6(3)
C(45)	67(4)	45(3)	57(3)	5(3)	29(3)	3(3)
C(46)	78(4)	53(4)	73(4)	1(3)	32(3)	-18(3)
C(47)	69(4)	53(4)	67(4)	1(3)	16(3)	-16(3)
C(48)	52(3)	59(4)	52(3)	5(3)	9(3)	1(3)
C(49)	39(3)	48(3)	41(3)	6(3)	13(2)	-2(3)

C(50)	36(3)	47(3)	51(3)	4(3)	9(2)	1(3)
C(51)	51(3)	52(3)	46(3)	2(3)	7(3)	5(3)
C(52)	68(4)	56(4)	69(4)	2(3)	25(3)	-2(3)
C(53)	60(4)	60(4)	57(3)	-3(3)	30(3)	-1(3)
C(54)	48(3)	55(4)	47(3)	-7(3)	6(3)	0(3)
C(55)	45(3)	55(4)	53(4)	2(3)	9(3)	4(3)
C(56)	38(3)	50(3)	55(4)	-3(3)	12(3)	4(3)
C(57)	37(3)	55(3)	42(3)	3(3)	11(2)	-4(3)
C(58)	48(3)	52(3)	48(3)	-3(3)	15(3)	4(3)
C(59)	57(4)	79(4)	50(3)	-5(3)	16(3)	-16(3)
C(60)	55(4)	94(4)	55(3)	-22(3)	30(3)	-5(3)
C(61)	42(3)	51(3)	81(4)	-1(3)	10(3)	1(3)
C(62)	43(3)	55(3)	63(3)	0(3)	18(3)	-7(3)
C(63)	52(4)	52(4)	73(4)	-10(3)	25(3)	7(3)
C(64)	58(4)	57(4)	74(4)	1(3)	15(3)	4(3)
C(65)	69(4)	65(4)	58(4)	-6(3)	21(3)	-3(3)
C(66)	61(4)	59(4)	72(4)	-11(3)	31(3)	1(3)
C(67)	154(8)	68(5)	100(6)	-2(4)	62(6)	-4(6)
C(68)	125(8)	66(6)	143(8)	-19(5)	-33(6)	15(5)
C(69)	96(7)	65(5)	193(10)	-39(6)	59(7)	2(5)
C(70)	166(9)	138(8)	83(6)	-8(5)	28(6)	-13(9)
C(71)	168(12)	133(9)	201(11)	33(8)	-94(9)	-61(8)
C(72)	78(7)	92(7)	272(14)	-26(8)	26(8)	-17(5)
K(1)	57(1)	64(1)	62(1)	16(1)	28(1)	11(1)
K(2)	50(1)	54(1)	44(1)	4(1)	18(1)	4(1)
N(1)	40(3)	47(3)	39(2)	5(2)	13(2)	2(2)
N(2)	41(3)	50(3)	39(2)	2(2)	12(2)	5(2)

N(3)	37(2)	60(3)	39(3)	0(2)	16(2)	8(2)
N(4)	39(3)	50(3)	52(3)	6(2)	19(2)	4(2)

Crystallographic Characterisation of (Fl-NHC)Ti(NMe_2)Cl

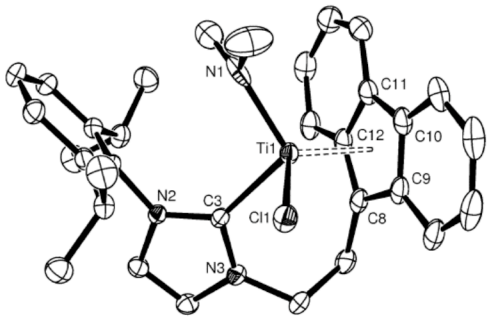


Table 1. Crystal data and structure refinement for (Fl-NHC)Ti(NMe_2)Cl.

Identification code	**(Fl-NHC)Ti(NMe_2)Cl**	
Empirical formula	C32 H37 Cl N3 Ti	
Formula weight	547.00	
Temperature	120(2) K	
Wavelength	0.71073 ≈	
Crystal system	Triclinic	
Space group	p-1	
Unit cell dimensions	a = 8.3495(6) ≈	α= 73.535(9)∞.
	b = 10.7139(13) ≈	β= 86.508(7)∞.
	c = 16.8282(19) ≈	γ = 71.966(7)∞.
Volume	1372.1(2) $≈^3$	
Z	2	
Density (calculated)	1.324 Mg/m^3	
Absorption coefficient	0.436 mm^{-1}	
F(000)	578	
Crystal size	0.10 x 0.10 x 0.05 mm^3	
Theta range for data collection	3.25 to 27.62∞.	
Index ranges	-10<=h<=10, -13<=k<=13, -21<=l<=21	
Reflections collected	22627	

Independent reflections	6276 [R(int) = 0.0411]
Completeness to theta = 27.62∞	98.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9786 and 0.9577
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6276 / 0 / 340
Goodness-of-fit on F^2	1.088
Final R indices [I>2sigma(I)]	R1 = 0.0484, wR2 = 0.1081
R indices (all data)	R1 = 0.0629, wR2 = 0.1140
Largest diff. peak and hole	0.679 and -0.548 e.≈$^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($\approx^2$x 10^3) for (Fl-NHC)Ti(NMe_2)Cl. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2111(3)	1132(3)	6234(2)	39(1)
C(2)	-337(4)	1329(4)	7037(2)	59(1)
C(3)	4775(3)	357(2)	8210(1)	18(1)
C(4)	7163(3)	-1470(2)	8494(1)	22(1)
C(5)	7256(3)	-665(2)	8960(1)	22(1)
C(6)	5410(3)	1512(2)	9204(1)	26(1)
C(7)	5181(3)	2906(2)	8587(2)	29(1)
C(8)	3652(3)	3389(2)	8029(1)	24(1)
C(9)	1948(3)	3915(2)	8249(1)	26(1)
C(10)	863(3)	4315(2)	7530(1)	26(1)
C(11)	1925(3)	4157(2)	6836(1)	25(1)
C(12)	3634(3)	3600(2)	7148(1)	23(1)
C(13)	4949(3)	3338(2)	6585(2)	30(1)
C(14)	4555(4)	3699(2)	5756(2)	35(1)
C(15)	2878(4)	4286(3)	5453(2)	37(1)
C(16)	1566(3)	4502(2)	5975(2)	33(1)
C(17)	-906(3)	4770(2)	7598(2)	33(1)
C(18)	-1561(3)	4861(2)	8353(2)	40(1)
C(19)	-503(4)	4500(2)	9057(2)	40(1)
C(20)	1206(3)	4028(2)	9019(2)	32(1)
C(21)	5170(3)	-1497(2)	7488(1)	19(1)
C(22)	3985(3)	-2199(2)	7759(1)	20(1)
C(23)	3172(3)	-2240(2)	8596(1)	22(1)
C(24)	1366(3)	-2276(3)	8598(2)	34(1)
C(25)	4219(3)	-3454(2)	9271(1)	30(1)
C(26)	3648(3)	-2925(2)	7254(1)	26(1)
C(27)	4453(3)	-2949(2)	6514(1)	29(1)
C(28)	5617(3)	-2247(2)	6262(1)	27(1)
C(29)	6014(3)	-1509(2)	6744(1)	22(1)
C(30)	7343(3)	-790(2)	6457(1)	25(1)
C(31)	6894(3)	248(3)	5610(2)	36(1)

C(32)	9078(3)	-1830(3)	6445(2)	37(1)
Cl(1)	1011(1)	941(1)	9045(1)	26(1)
N(1)	1393(2)	1280(2)	6954(1)	27(1)
N(2)	5656(2)	-845(2)	8036(1)	17(1)
N(3)	5800(2)	426(2)	8788(1)	21(1)
Ti(1)	2264(1)	1873(1)	7809(1)	19(1)

Table 3. Bond lengths [≈] and angles [∞] for (Fl-NHC)Ti(NMe_2)Cl.

C(1)-N(1)	1.347(3)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-N(1)	1.428(3)
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800
C(3)-N(3)	1.365(3)
C(3)-N(2)	1.372(3)
C(3)-Ti(1)	2.221(2)
C(4)-C(5)	1.340(3)
C(4)-N(2)	1.389(3)
C(4)-H(4)	0.9500
C(5)-N(3)	1.378(3)
C(5)-H(5)	0.9500
C(6)-N(3)	1.467(3)
C(6)-C(7)	1.521(3)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.497(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.427(3)
C(8)-C(12)	1.436(3)
C(8)-Ti(1)	2.382(2)
C(9)-C(20)	1.422(3)
C(9)-C(10)	1.438(3)
C(9)-Ti(1)	2.437(2)
C(10)-C(17)	1.413(3)
C(10)-C(11)	1.439(3)
C(10)-Ti(1)	2.431(2)
C(11)-C(16)	1.416(3)
C(11)-C(12)	1.433(3)

C(11)-Ti(1)	2.471(2)
C(12)-C(13)	1.419(3)
C(12)-Ti(1)	2.442(2)
C(13)-C(14)	1.369(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.406(4)
C(14)-H(14)	0.9500
C(15)-C(16)	1.366(4)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(17)-C(18)	1.369(4)
C(17)-H(17)	0.9500
C(18)-C(19)	1.410(4)
C(18)-H(18)	0.9500
C(19)-C(20)	1.362(4)
C(19)-H(19)	0.9500
C(20)-H(20)	0.9500
C(21)-C(29)	1.400(3)
C(21)-C(22)	1.402(3)
C(21)-N(2)	1.447(2)
C(22)-C(26)	1.395(3)
C(22)-C(23)	1.521(3)
C(23)-C(24)	1.520(3)
C(23)-C(25)	1.525(3)
C(23)-H(23)	1.0000
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-C(27)	1.381(3)
C(26)-H(26)	0.9500
C(27)-C(28)	1.383(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.396(3)

C(28)-H(28)	0.9500
C(29)-C(30)	1.520(3)
C(30)-C(31)	1.524(3)
C(30)-C(32)	1.533(3)
C(30)-H(30)	1.0000
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
Cl(1)-Ti(1)	2.3703(7)
N(1)-Ti(1)	1.984(2)

N(1)-C(1)-H(1A)	109.5
N(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
N(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
N(1)-C(2)-H(2A)	109.5
N(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
N(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
N(3)-C(3)-N(2)	102.54(17)
N(3)-C(3)-Ti(1)	123.49(14)
N(2)-C(3)-Ti(1)	133.85(14)
C(5)-C(4)-N(2)	107.08(18)
C(5)-C(4)-H(4)	126.5
N(2)-C(4)-H(4)	126.5
C(4)-C(5)-N(3)	106.32(18)
C(4)-C(5)-H(5)	126.8
N(3)-C(5)-H(5)	126.8
N(3)-C(6)-C(7)	111.55(18)

N(3)-C(6)-H(6A)	109.3
C(7)-C(6)-H(6A)	109.3
N(3)-C(6)-H(6B)	109.3
C(7)-C(6)-H(6B)	109.3
H(6A)-C(6)-H(6B)	108.0
C(8)-C(7)-C(6)	113.62(18)
C(8)-C(7)-H(7A)	108.8
C(6)-C(7)-H(7A)	108.8
C(8)-C(7)-H(7B)	108.8
C(6)-C(7)-H(7B)	108.8
H(7A)-C(7)-H(7B)	107.7
C(9)-C(8)-C(12)	106.67(19)
C(9)-C(8)-C(7)	126.3(2)
C(12)-C(8)-C(7)	126.4(2)
C(9)-C(8)-Ti(1)	74.89(12)
C(12)-C(8)-Ti(1)	74.97(12)
C(7)-C(8)-Ti(1)	122.51(14)
C(20)-C(9)-C(8)	132.1(2)
C(20)-C(9)-C(10)	118.6(2)
C(8)-C(9)-C(10)	109.13(19)
C(20)-C(9)-Ti(1)	120.08(15)
C(8)-C(9)-Ti(1)	70.69(12)
C(10)-C(9)-Ti(1)	72.61(12)
C(17)-C(10)-C(9)	120.3(2)
C(17)-C(10)-C(11)	132.3(2)
C(9)-C(10)-C(11)	107.3(2)
C(17)-C(10)-Ti(1)	118.34(15)
C(9)-C(10)-Ti(1)	73.04(12)
C(11)-C(10)-Ti(1)	74.44(12)
C(16)-C(11)-C(12)	120.3(2)
C(16)-C(11)-C(10)	132.3(2)
C(12)-C(11)-C(10)	107.3(2)
C(16)-C(11)-Ti(1)	124.50(16)
C(12)-C(11)-Ti(1)	71.93(12)
C(10)-C(11)-Ti(1)	71.42(12)
C(13)-C(12)-C(11)	118.9(2)

C(13)-C(12)-C(8)	131.9(2)
C(11)-C(12)-C(8)	109.18(19)
C(13)-C(12)-Ti(1)	120.72(14)
C(11)-C(12)-Ti(1)	74.16(12)
C(8)-C(12)-Ti(1)	70.43(11)
C(14)-C(13)-C(12)	119.1(2)
C(14)-C(13)-H(13)	120.5
C(12)-C(13)-H(13)	120.5
C(13)-C(14)-C(15)	121.6(2)
C(13)-C(14)-H(14)	119.2
C(15)-C(14)-H(14)	119.2
C(16)-C(15)-C(14)	121.4(2)
C(16)-C(15)-H(15)	119.3
C(14)-C(15)-H(15)	119.3
C(15)-C(16)-C(11)	118.7(2)
C(15)-C(16)-H(16)	120.7
C(11)-C(16)-H(16)	120.7
C(18)-C(17)-C(10)	118.9(3)
C(18)-C(17)-H(17)	120.6
C(10)-C(17)-H(17)	120.6
C(17)-C(18)-C(19)	121.1(2)
C(17)-C(18)-H(18)	119.4
C(19)-C(18)-H(18)	119.4
C(20)-C(19)-C(18)	121.7(2)
C(20)-C(19)-H(19)	119.2
C(18)-C(19)-H(19)	119.2
C(19)-C(20)-C(9)	119.3(2)
C(19)-C(20)-H(20)	120.3
C(9)-C(20)-H(20)	120.3
C(29)-C(21)-C(22)	122.68(19)
C(29)-C(21)-N(2)	118.66(18)
C(22)-C(21)-N(2)	118.39(18)
C(26)-C(22)-C(21)	117.5(2)
C(26)-C(22)-C(23)	121.05(19)
C(21)-C(22)-C(23)	121.39(18)
C(24)-C(23)-C(22)	113.22(19)

C(24)-C(23)-C(25)	109.83(19)
C(22)-C(23)-C(25)	110.71(17)
C(24)-C(23)-H(23)	107.6
C(22)-C(23)-H(23)	107.6
C(25)-C(23)-H(23)	107.6
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(23)-C(25)-H(25A)	109.5
C(23)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(27)-C(26)-C(22)	121.2(2)
C(27)-C(26)-H(26)	119.4
C(22)-C(26)-H(26)	119.4
C(26)-C(27)-C(28)	120.1(2)
C(26)-C(27)-H(27)	120.0
C(28)-C(27)-H(27)	120.0
C(27)-C(28)-C(29)	121.3(2)
C(27)-C(28)-H(28)	119.3
C(29)-C(28)-H(28)	119.3
C(28)-C(29)-C(21)	117.3(2)
C(28)-C(29)-C(30)	119.65(19)
C(21)-C(29)-C(30)	123.09(18)
C(29)-C(30)-C(31)	112.13(19)
C(29)-C(30)-C(32)	110.76(18)
C(31)-C(30)-C(32)	110.18(19)
C(29)-C(30)-H(30)	107.9
C(31)-C(30)-H(30)	107.9
C(32)-C(30)-H(30)	107.9
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
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(1)-N(1)-C(2)	117.0(2)
C(1)-N(1)-Ti(1)	127.08(17)
C(2)-N(1)-Ti(1)	114.24(18)
C(3)-N(2)-C(4)	111.39(16)
C(3)-N(2)-C(21)	128.44(17)
C(4)-N(2)-C(21)	120.13(16)
C(3)-N(3)-C(5)	112.67(17)
C(3)-N(3)-C(6)	124.79(18)
C(5)-N(3)-C(6)	122.52(18)
N(1)-Ti(1)-C(3)	105.58(7)
N(1)-Ti(1)-Cl(1)	103.97(6)
C(3)-Ti(1)-Cl(1)	92.36(5)
N(1)-Ti(1)-C(8)	144.47(8)
C(3)-Ti(1)-C(8)	81.88(7)
Cl(1)-Ti(1)-C(8)	110.46(6)
N(1)-Ti(1)-C(10)	106.29(8)
C(3)-Ti(1)-C(10)	139.81(8)
Cl(1)-Ti(1)-C(10)	102.98(6)
C(8)-Ti(1)-C(10)	58.00(8)
N(1)-Ti(1)-C(9)	140.64(8)
C(3)-Ti(1)-C(9)	110.48(8)
Cl(1)-Ti(1)-C(9)	89.97(6)
C(8)-Ti(1)-C(9)	34.42(8)
C(10)-Ti(1)-C(9)	34.36(8)
N(1)-Ti(1)-C(12)	109.93(8)

C(3)-Ti(1)-C(12)	89.59(7)
Cl(1)-Ti(1)-C(12)	144.14(5)
C(8)-Ti(1)-C(12)	34.60(7)
C(10)-Ti(1)-C(12)	56.70(7)
C(9)-Ti(1)-C(12)	56.15(7)
N(1)-Ti(1)-C(11)	91.07(7)
C(3)-Ti(1)-C(11)	122.41(8)
Cl(1)-Ti(1)-C(11)	136.99(6)
C(8)-Ti(1)-C(11)	57.57(8)
C(10)-Ti(1)-C(11)	34.14(7)
C(9)-Ti(1)-C(11)	56.36(7)
C(12)-Ti(1)-C(11)	33.91(7)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\approx^2$x 10^3)for (Fl-NHC)Ti(NMe_2)Cl. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	38(2)	34(1)	39(2)	-7(1)	-4(1)	-5(1)
C(2)	41(2)	100(3)	45(2)	-24(2)	0(1)	-31(2)
C(3)	21(1)	18(1)	16(1)	-6(1)	2(1)	-8(1)
C(4)	18(1)	21(1)	24(1)	-7(1)	-2(1)	-4(1)
C(5)	18(1)	26(1)	23(1)	-7(1)	-2(1)	-7(1)
C(6)	32(1)	25(1)	25(1)	-13(1)	-2(1)	-9(1)
C(7)	37(1)	22(1)	33(1)	-12(1)	-1(1)	-14(1)
C(8)	31(1)	16(1)	27(1)	-9(1)	4(1)	-9(1)
C(9)	36(1)	16(1)	28(1)	-8(1)	7(1)	-9(1)
C(10)	32(1)	15(1)	30(1)	-5(1)	6(1)	-6(1)
C(11)	29(1)	17(1)	27(1)	-5(1)	3(1)	-5(1)
C(12)	29(1)	15(1)	27(1)	-6(1)	6(1)	-8(1)
C(13)	32(1)	22(1)	37(1)	-11(1)	11(1)	-11(1)
C(14)	48(2)	26(1)	32(1)	-9(1)	19(1)	-14(1)
C(15)	57(2)	29(1)	23(1)	-4(1)	4(1)	-13(1)
C(16)	41(1)	23(1)	29(1)	-3(1)	-2(1)	-7(1)
C(17)	30(1)	18(1)	49(2)	-8(1)	5(1)	-4(1)
C(18)	35(1)	23(1)	62(2)	-17(1)	21(1)	-8(1)
C(19)	54(2)	26(1)	45(2)	-20(1)	29(1)	-17(1)
C(20)	50(2)	21(1)	31(1)	-12(1)	12(1)	-14(1)
C(21)	21(1)	15(1)	21(1)	-7(1)	-3(1)	-3(1)
C(22)	19(1)	16(1)	25(1)	-6(1)	-3(1)	-3(1)
C(23)	22(1)	18(1)	26(1)	-7(1)	2(1)	-6(1)
C(24)	22(1)	36(1)	44(1)	-10(1)	5(1)	-13(1)
C(25)	29(1)	31(1)	26(1)	-7(1)	2(1)	-6(1)
C(26)	26(1)	22(1)	33(1)	-9(1)	-4(1)	-9(1)
C(27)	37(1)	22(1)	31(1)	-13(1)	-6(1)	-8(1)
C(28)	33(1)	24(1)	23(1)	-10(1)	-2(1)	-4(1)
C(29)	24(1)	19(1)	21(1)	-6(1)	0(1)	-4(1)
C(30)	30(1)	25(1)	23(1)	-9(1)	7(1)	-10(1)
C(31)	43(2)	30(1)	30(1)	-4(1)	5(1)	-11(1)

C(32)	31(1)	35(1)	42(1)	-8(1)	7(1)	-11(1)
Cl(1)	33(1)	23(1)	25(1)	-7(1)	7(1)	-11(1)
N(1)	16(1)	15(1)	39(1)	7(1)	0(1)	-2(1)
N(2)	18(1)	16(1)	18(1)	-6(1)	0(1)	-6(1)
N(3)	23(1)	20(1)	21(1)	-7(1)	0(1)	-8(1)
Ti(1)	20(1)	15(1)	21(1)	-6(1)	0(1)	-5(1)

Crystallographic Characterisation of (Ind-NHC)V(NMe_2)Br

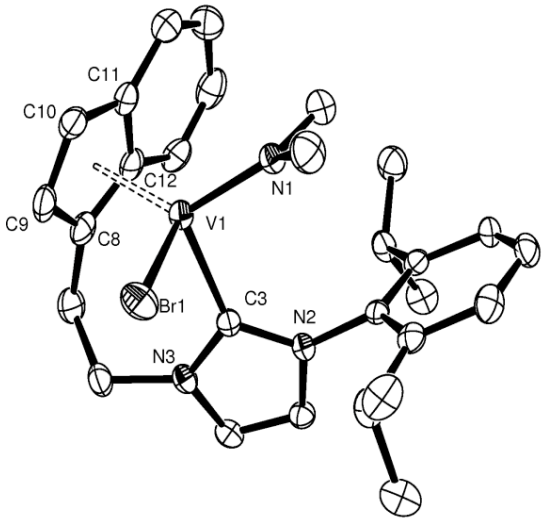


Table 1. Crystal data and structure refinement for (Ind-NHC)V(NMe_2)Br.

Identification code	**(Ind-NHC)V(NMe_2)Br**	
Empirical formula	C28 H35 Br N3 V	
Formula weight	544.44	
Temperature	120(2) K	
Wavelength	0.71073 ≈	
Crystal system	Triclinic	
Space group	p-1	
Unit cell dimensions	a = 8.208(4) ≈	α= 100.63(8)∞.
	b = 9.877(6) ≈	β= 97.83(4)∞.
	c = 17.305(10) ≈	γ = 105.38(5)∞.
Volume	1303.8(13) ≈^{3}	
Z	2	
Density (calculated)	1.387 Mg/m^3	
Absorption coefficient	1.933 mm^{-1}	
F(000)	564	
Crystal size	0.10 x 0.05 x 0.01 mm^3	
Theta range for data collection	3.64 to 27.42∞.	

Index ranges	-10<=h<=10, -12<=k<=12, -22<=l<=22
Reflections collected	18939
Independent reflections	5819 [R(int) = 0.0700]
Completeness to theta = 27.42∞	97.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9809 and 0.8302
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5819 / 0 / 304
Goodness-of-fit on F^2	1.019
Final R indices [I>2sigma(I)]	R1 = 0.0534, wR2 = 0.0875
R indices (all data)	R1 = 0.0977, wR2 = 0.0988
Largest diff. peak and hole	0.378 and -0.528 e.≈$^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($\approx^2$x 10^3) for (Ind-NHC)V(NMe_2)Br. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Br(1)	-3079(1)	6321(1)	950(1)	32(1)
V(1)	-678(1)	7123(1)	2191(1)	21(1)
N(3)	1421(3)	5424(3)	1200(2)	22(1)
N(2)	379(3)	4117(3)	1992(2)	19(1)
N(1)	-2074(3)	6427(3)	2897(2)	25(1)
C(12)	2187(4)	8829(4)	2784(2)	26(1)
C(8)	1896(4)	8637(4)	1920(2)	27(1)
C(9)	520(4)	9165(4)	1706(2)	31(1)
C(11)	927(4)	9451(4)	3077(2)	27(1)
C(10)	-160(4)	9603(4)	2394(2)	28(1)
C(13)	3433(4)	8565(4)	3343(2)	32(1)
C(14)	3451(5)	8936(4)	4145(2)	40(1)
C(15)	2230(5)	9585(4)	4443(2)	40(1)
C(16)	980(5)	9814(4)	3923(2)	36(1)
C(7)	2926(5)	8032(4)	1355(2)	34(1)
C(6)	1887(4)	6595(4)	773(2)	28(1)
C(3)	429(4)	5406(4)	1771(2)	19(1)
C(4)	1342(4)	3389(4)	1564(2)	22(1)
C(5)	1996(4)	4209(4)	1072(2)	23(1)
C(18)	236(4)	3588(4)	3331(2)	22(1)
C(17)	-602(4)	3475(3)	2544(2)	20(1)
C(25)	-2341(4)	2635(4)	2236(2)	23(1)
C(24)	-3250(4)	1980(4)	2770(2)	29(1)
C(23)	-2463(4)	2116(4)	3558(2)	29(1)
C(22)	-737(4)	2896(4)	3834(2)	26(1)
C(26)	-3134(4)	2366(4)	1348(2)	28(1)
C(27)	-2860(4)	987(4)	867(2)	36(1)
C(28)	-5056(4)	2244(4)	1198(2)	37(1)
C(19)	2168(4)	4373(4)	3626(2)	26(1)
C(20)	3168(4)	3252(4)	3606(2)	35(1)
C(1)	-3939(4)	5814(4)	2785(2)	37(1)

C(21)	2604(5)	5337(4)	4481(2)	38(1)
C(2)	-1307(5)	6511(4)	3723(2)	36(1)

Table 3. Bond lengths [≈] and angles [∞] for (Ind-NHC)V(NMe_2)Br.

Br(1)-V(1)	2.552(2)
V(1)-N(1)	1.885(3)
V(1)-C(3)	2.185(3)
V(1)-C(10)	2.323(4)
V(1)-C(9)	2.353(4)
V(1)-C(8)	2.403(4)
V(1)-C(11)	2.432(4)
V(1)-C(12)	2.454(4)
N(3)-C(3)	1.363(4)
N(3)-C(5)	1.394(4)
N(3)-C(6)	1.479(4)
N(2)-C(3)	1.388(4)
N(2)-C(4)	1.398(4)
N(2)-C(17)	1.456(4)
N(1)-C(2)	1.460(4)
N(1)-C(1)	1.460(4)
C(12)-C(13)	1.420(5)
C(12)-C(11)	1.439(5)
C(12)-C(8)	1.449(5)
C(8)-C(9)	1.398(5)
C(8)-C(7)	1.518(5)
C(9)-C(10)	1.426(5)
C(9)-H(9)	0.9500
C(11)-C(16)	1.434(5)
C(11)-C(10)	1.436(5)
C(10)-H(10)	0.9500
C(13)-C(14)	1.366(5)
C(13)-H(13)	0.9500
C(14)-C(15)	1.428(5)
C(14)-H(14)	0.9500
C(15)-C(16)	1.364(5)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(7)-C(6)	1.534(5)

C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(4)-C(5)	1.349(5)
C(4)-H(4)	0.9500
C(5)-H(5)	0.9500
C(18)-C(22)	1.407(5)
C(18)-C(17)	1.411(5)
C(18)-C(19)	1.535(5)
C(17)-C(25)	1.418(5)
C(25)-C(24)	1.408(5)
C(25)-C(26)	1.531(5)
C(24)-C(23)	1.392(5)
C(24)-H(24)	0.9500
C(23)-C(22)	1.389(5)
C(23)-H(23)	0.9500
C(22)-H(22)	0.9500
C(26)-C(28)	1.532(4)
C(26)-C(27)	1.547(5)
C(26)-H(26)	1.0000
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(19)-C(20)	1.542(5)
C(19)-C(21)	1.542(5)
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(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800

C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(2)-H(2A)	0.9800
C(2)-H(2B)	0.9800
C(2)-H(2C)	0.9800

N(1)-V(1)-C(3)	105.33(13)
N(1)-V(1)-C(10)	109.26(14)
C(3)-V(1)-C(10)	141.75(13)
N(1)-V(1)-C(9)	144.30(13)
C(3)-V(1)-C(9)	109.93(13)
C(10)-V(1)-C(9)	35.50(12)
N(1)-V(1)-C(8)	152.14(13)
C(3)-V(1)-C(8)	83.05(13)
C(10)-V(1)-C(8)	58.72(13)
C(9)-V(1)-C(8)	34.18(12)
N(1)-V(1)-C(11)	97.30(13)
C(3)-V(1)-C(11)	125.05(12)
C(10)-V(1)-C(11)	35.07(12)
C(9)-V(1)-C(11)	57.49(13)
C(8)-V(1)-C(11)	57.82(13)
N(1)-V(1)-C(12)	117.56(13)
C(3)-V(1)-C(12)	91.73(13)
C(10)-V(1)-C(12)	57.95(13)
C(9)-V(1)-C(12)	56.78(13)
C(8)-V(1)-C(12)	34.69(12)
C(11)-V(1)-C(12)	34.25(12)
N(1)-V(1)-Br(1)	96.24(10)
C(3)-V(1)-Br(1)	92.96(11)
C(10)-V(1)-Br(1)	98.95(12)
C(9)-V(1)-Br(1)	87.46(11)
C(8)-V(1)-Br(1)	110.02(11)
C(11)-V(1)-Br(1)	133.81(10)
C(12)-V(1)-Br(1)	143.19(10)
C(3)-N(3)-C(5)	111.9(3)

C(3)-N(3)-C(6)	125.0(3)
C(5)-N(3)-C(6)	123.1(3)
C(3)-N(2)-C(4)	110.8(3)
C(3)-N(2)-C(17)	128.0(3)
C(4)-N(2)-C(17)	121.1(3)
C(2)-N(1)-C(1)	108.6(3)
C(2)-N(1)-V(1)	120.3(2)
C(1)-N(1)-V(1)	131.0(2)
C(13)-C(12)-C(11)	118.8(3)
C(13)-C(12)-C(8)	133.1(3)
C(11)-C(12)-C(8)	108.1(3)
C(13)-C(12)-V(1)	124.2(2)
C(11)-C(12)-V(1)	72.0(2)
C(8)-C(12)-V(1)	70.7(2)
C(9)-C(8)-C(12)	106.9(3)
C(9)-C(8)-C(7)	126.2(3)
C(12)-C(8)-C(7)	126.8(3)
C(9)-C(8)-V(1)	71.0(2)
C(12)-C(8)-V(1)	74.6(2)
C(7)-C(8)-V(1)	121.4(2)
C(8)-C(9)-C(10)	110.3(3)
C(8)-C(9)-V(1)	74.9(2)
C(10)-C(9)-V(1)	71.1(2)
C(8)-C(9)-H(9)	124.8
C(10)-C(9)-H(9)	124.8
V(1)-C(9)-H(9)	120.8
C(16)-C(11)-C(10)	133.2(3)
C(16)-C(11)-C(12)	119.4(3)
C(10)-C(11)-C(12)	107.4(3)
C(16)-C(11)-V(1)	124.6(3)
C(10)-C(11)-V(1)	68.3(2)
C(12)-C(11)-V(1)	73.7(2)
C(9)-C(10)-C(11)	107.1(3)
C(9)-C(10)-V(1)	73.4(2)
C(11)-C(10)-V(1)	76.6(2)
C(9)-C(10)-H(10)	126.4

C(11)-C(10)-H(10)	126.4
V(1)-C(10)-H(10)	115.8
C(14)-C(13)-C(12)	120.0(3)
C(14)-C(13)-H(13)	120.0
C(12)-C(13)-H(13)	120.0
C(13)-C(14)-C(15)	121.5(4)
C(13)-C(14)-H(14)	119.2
C(15)-C(14)-H(14)	119.2
C(16)-C(15)-C(14)	120.1(4)
C(16)-C(15)-H(15)	119.9
C(14)-C(15)-H(15)	119.9
C(15)-C(16)-C(11)	120.0(3)
C(15)-C(16)-H(16)	120.0
C(11)-C(16)-H(16)	120.0
C(8)-C(7)-C(6)	113.6(3)
C(8)-C(7)-H(7A)	108.9
C(6)-C(7)-H(7A)	108.9
C(8)-C(7)-H(7B)	108.9
C(6)-C(7)-H(7B)	108.9
H(7A)-C(7)-H(7B)	107.7
N(3)-C(6)-C(7)	111.4(3)
N(3)-C(6)-H(6A)	109.3
C(7)-C(6)-H(6A)	109.3
N(3)-C(6)-H(6B)	109.3
C(7)-C(6)-H(6B)	109.3
H(6A)-C(6)-H(6B)	108.0
N(3)-C(3)-N(2)	103.5(3)
N(3)-C(3)-V(1)	124.5(2)
N(2)-C(3)-V(1)	132.0(2)
C(5)-C(4)-N(2)	106.9(3)
C(5)-C(4)-H(4)	126.5
N(2)-C(4)-H(4)	126.5
C(4)-C(5)-N(3)	106.9(3)
C(4)-C(5)-H(5)	126.6
N(3)-C(5)-H(5)	126.6
C(22)-C(18)-C(17)	117.9(3)

C(22)-C(18)-C(19)	120.4(3)
C(17)-C(18)-C(19)	121.7(3)
C(18)-C(17)-C(25)	122.3(3)
C(18)-C(17)-N(2)	119.6(3)
C(25)-C(17)-N(2)	117.8(3)
C(24)-C(25)-C(17)	116.9(3)
C(24)-C(25)-C(26)	122.0(3)
C(17)-C(25)-C(26)	120.9(3)
C(23)-C(24)-C(25)	121.5(3)
C(23)-C(24)-H(24)	119.2
C(25)-C(24)-H(24)	119.2
C(22)-C(23)-C(24)	120.3(3)
C(22)-C(23)-H(23)	119.8
C(24)-C(23)-H(23)	119.8
C(23)-C(22)-C(18)	120.9(3)
C(23)-C(22)-H(22)	119.6
C(18)-C(22)-H(22)	119.6
C(25)-C(26)-C(28)	113.3(3)
C(25)-C(26)-C(27)	110.3(3)
C(28)-C(26)-C(27)	109.5(3)
C(25)-C(26)-H(26)	107.9
C(28)-C(26)-H(26)	107.9
C(27)-C(26)-H(26)	107.9
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(18)-C(19)-C(20)	109.3(3)

C(18)-C(19)-C(21)	113.5(3)
C(20)-C(19)-C(21)	108.9(3)
C(18)-C(19)-H(19)	108.4
C(20)-C(19)-H(19)	108.4
C(21)-C(19)-H(19)	108.4
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
N(1)-C(1)-H(1A)	109.5
N(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
N(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	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(1)-C(2)-H(2A)	109.5
N(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
N(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\approx^2$x 10^3)for (Ind-NHC)V(NMe_2)Br. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Br(1)	29(1)	42(1)	25(1)	8(1)	3(1)	10(1)
V(1)	24(1)	20(1)	22(1)	8(1)	7(1)	6(1)
N(3)	19(1)	26(2)	21(2)	8(1)	6(1)	5(1)
N(2)	19(1)	21(2)	19(2)	7(1)	5(1)	5(1)
N(1)	29(2)	23(2)	26(2)	9(1)	13(1)	8(1)
C(12)	26(2)	15(2)	32(2)	7(2)	3(2)	-1(2)
C(8)	26(2)	17(2)	37(2)	9(2)	9(2)	0(2)
C(9)	37(2)	19(2)	34(2)	13(2)	5(2)	2(2)
C(11)	31(2)	17(2)	33(2)	9(2)	7(2)	4(2)
C(10)	32(2)	21(2)	32(2)	8(2)	6(2)	10(2)
C(13)	28(2)	21(2)	42(2)	5(2)	1(2)	3(2)
C(14)	38(2)	28(2)	46(3)	11(2)	-10(2)	3(2)
C(15)	50(2)	35(3)	26(2)	3(2)	0(2)	5(2)
C(16)	46(2)	25(2)	35(2)	6(2)	9(2)	8(2)
C(7)	34(2)	30(2)	38(2)	14(2)	15(2)	3(2)
C(6)	33(2)	31(2)	27(2)	15(2)	13(2)	11(2)
C(3)	18(2)	19(2)	18(2)	5(2)	1(1)	2(1)
C(4)	22(2)	21(2)	24(2)	6(2)	6(1)	7(2)
C(5)	17(2)	30(2)	22(2)	6(2)	5(1)	8(2)
C(18)	25(2)	17(2)	25(2)	5(2)	8(2)	7(2)
C(17)	23(2)	16(2)	23(2)	5(2)	11(1)	7(2)
C(25)	24(2)	21(2)	28(2)	8(2)	6(2)	12(2)
C(24)	19(2)	28(2)	42(2)	13(2)	11(2)	6(2)
C(23)	32(2)	28(2)	37(2)	16(2)	22(2)	13(2)
C(22)	34(2)	22(2)	25(2)	12(2)	11(2)	9(2)
C(26)	17(2)	32(2)	33(2)	12(2)	1(2)	2(2)
C(27)	27(2)	47(3)	32(2)	5(2)	5(2)	13(2)
C(28)	28(2)	32(2)	48(3)	9(2)	-2(2)	8(2)
C(19)	25(2)	29(2)	22(2)	10(2)	2(1)	2(2)
C(20)	25(2)	41(3)	36(2)	11(2)	2(2)	8(2)
C(1)	30(2)	38(3)	46(3)	14(2)	16(2)	7(2)

C(21)	43(2)	36(3)	30(2)	11(2)	0(2)	6(2)
C(2)	50(2)	33(2)	30(2)	13(2)	14(2)	15(2)