Experimental:

General Procedures. All operations were performed under a purified argon atmosphere using glovebox or vacuum line techniques. Toluene and hexane solvents were dried and purified by passing through activated alumina and Q5 columns. ^{1}H, $^{13}C\{^{1}H\}$, HMQC, COSY NMR experiments were performed on Bruker AC-200, AMX-300, and WH-400 or Varian 200 MHz spectrometers. Data are given in ppm relative to solvent signals for ^{1}H and ^{13}C spectra. Elemental analyses were performed by Ms. Roxanna Simank of this department; in some instances, low carbon values are found, which is a common phenomenon in organogroup 3 chemistry (see for example G. C. Bazan, W. P. Schaefer and J. E. Bercaw, *Organometallics*, 1993, ***12***, 2126-2130; J. Eppinger, M. Spiegler, W. Hieringer, W. A. Herrmann and R. Anwander, *J. Am. Chem. Soc.*, 2000, ***122***, 3080-3096; P. W. Roesky, *Inorg. Chem.*, 1998, ***37***, 4507-4511; D. M. Roitershtein, J. W. Ziller and W. J. Evans, *J. Am. Chem. Soc.*, 1998, ***120***, 11342-11346. [ArNC(CH_3)CHC(CH_3)NAr]ScCl_2(THF) was prepared by literature procedures. All other materials were obtained from Sigma-Aldrich and purified according to standard procedures.

Synthesis of [ArNC(CH_3)CHC(CH_3)NAr]ScCl_2. A 50 mL RB flask containing [ArNC(CH_3)CHC(CH_3)NAr]ScCl_2(THF) (1.50 g, 2.48 mmol) was heated at 130 ^{O}C under full dynamic vacuum for 18 hours. The resultant yellow powder was washed with toluene (2 x 15 mL) and evacuated to dryness. Yield: 1.29 g, 97.8%. ^{1}H NMR (CD_2Cl_2): δ 7.11 (s, 6H; C_6H_3), 4.90 (s, 1H; CH) 3.11 (sp, 4H; C*H*(CH_3)$_2$, $J_{H\text{-}H}$ = 6.9 Hz), 1.69 (s, 6H; NCCH_3), 1.21 (d, 12H; CH(C*H*$_3$)$_2$, $J_{H\text{-}H}$ = 6.6 Hz), 1.11 (d, 12H; CH(C*H*$_3$)$_2$, $J_{H\text{-}H}$ = 6.6 Hz). $^{13}C\{^{1}H\}$ NMR (CD_2Cl_2): δ 161.8 (N*C*CH$_3$), 143.2 (C_{ipso}), 141.5, 125.7, 123.5 (C_6H_3), 94.0 (CH), 28.8 (*C*H(CH_3)$_2$), 24.6

(NC*C*H$_3$), 23.5, 21.1 (CH(*C*H$_3$)$_2$). Anal. Calcd. for $C_{29}H_{41}N_2Cl_2Sc$: C, 65.29; H,˚7.75; N, 5.25. Found: C, 64.13, H,˚6.84; N, 5.03.

Synthesis of [ArNC(CH$_3$)CHC(CH$_3$)NAr]Sc(CH$_3$)$_2$. [ArNC(CH$_3$)CHC(CH$_3$)NAr]ScCl$_2$ (600 mg, 1.13 mmol) and 2.1 equivalents of MeLi (52 mg, 2.37 mmol) were added to a 50 mL RB flask attached to a swivel frit apparatus. Toluene (30 mL) was vacuum transferred onto the mixture and the resultant solution stirred for 4.5 hours. The reaction mixture was filtered and solvent removed *in vacuo* to afford 502 mg (90.6%) of [ArNC(CH$_3$)CHC(CH$_3$)NAr]Sc(CH$_3$)$_2$ as a yellow crystalline solid. ^{1}H NMR (C_7D_8): δ 7.11 (s, 6H; C_6H_3), 4.91 (s, 1H; CH) 3.32 (sp, 4H; C*H*(CH$_3$)$_2$, $J_{H\text{-}H}$ = 6.9 Hz), 1.57 (s, 6H; NCCH$_3$), 1.35 (d, 12H; CH(C*H*$_3$)$_2$, $J_{H\text{-}H}$ = 6.6 Hz), 1.14 (d, 12H; CH(C*H*$_3$)$_2$, $J_{H\text{-}H}$ = 6.6 Hz), -0.06 (Sc-CH$_3$). ^{13}C{^{1}H} NMR (C_6D_6): δ 167.9 (N*C*CH$_3$), 143.0 (C_{ipso}), 141.4, 127.0, 124.5 (C_6H_3), 96.0 (CH), 28.8 (*C*H(CH$_3$)$_2$), 28.6 (Sc-CH$_3$), 25.6, 24.3 (CH(*C*H$_3$)$_2$), 23.9 (NC*C*H$_3$). Anal. Calcd. for $C_{31}H_{47}N_2Sc$: C, 75.57; H,˚9.62; N, 5.69. Found: C, 75.00, H,˚9.20; N, 5.66 %.

Synthesis of {[ArNC(Me)CHC(Me)NAr]ScCH$_3$}$^+$[CH$_3$B(C$_6$F$_5$)$_3$]$^-$ and {[ArNC(Me)CHC(Me)NAr]ScC$_6$F$_5$}$^+$[CH$_3$B(C$_6$F$_5$)$_3$]$^-$

An NMR tube was charged with [ArNC(CH$_3$)CHC(CH$_3$)NAr]Sc(CH$_3$)$_2$ (10 mg, 0.020 mmol) and B(C_6F_5)$_3$ (23 mg, 0.020 mmol) to which cold (-35 ^{O}C) C_6D_5Br (0.5 mL) was added. Upon mixing, the tube was inserted in the NMR probe at —35^{O}C and slowly warmed to —23 ^{O}C. ^{1}H NMR (C_6D_5Br, 250K): δ 7.20–6.79 (ov m, 6H; C_6H_3), 5.19 (s, 1H; CH) 3.36 (br, 2H; C*H*(CH$_3$)$_2$), 2.14 (br, 2H; C*H*(CH$_3$)$_2$), 1.69 (br s, 3H; B-CH$_3$) 1.56 (s, 6H; NCCH$_3$), 1.16-0.74 (ov m, 24H; CH(C*H*$_3$)$_2$), 0.52 (s, 3H; Sc-CH$_3$). ^{11}B{^{1}H} NMR (C_6D_5Br, 250K): δ 16.8 (br s). ^{19}F NMR (C_6D_5Br, 250K): δ –134.3 (*ortho*-F), –159.4 (*para*-F), -163.6 (*meta*-F). The NMR tube was gradually warmed to RT generating {[ArNC(Me)CHC(Me)NAr]ScC$_6$F$_5$}$^+$[CH$_3$B(C_6F_5)$_3$]$^-$

from rapid C_6F_5 transfer and loss of free $MeB(C_6F_5)_2$. ^1H NMR (C_6D_5Br): δ 7.16–7.05 (ov m, 6H; C_6H_3), 5.69 (s, 1H; CH) 2.53 (br, 4H; $CH(CH_3)_2$), 1.75 (s, 6H; $NCCH_3$), 1.27 (br s, 3H; B-CH_3), 1.03-0.85 (ov m, 24H; $CH(CH_3)_2$). $^{11}B\{^1H\}$ NMR (C_6D_5Br): δ 15.2 (br s). ^{19}F NMR (C_6D_5Br, 250K): δ Isomer 1 (70%): -117.1, -123.0 (br s, 2F; Sc-C_6F_5, *ortho*-F), -133.2 (d, 6F; $^3J_{F-F}$ = 19 Hz, Me-$B(C_6F_5)_3$, *ortho*-F), –150.2 (t, 1F; $^3J_{F-F}$ = 21 Hz, Sc-C_6F_5, *para*-F), –159.3 (t, 3F; $^3J_{F-F}$ = 19 Hz, Me-$B(C_6F_5)_3$, *para*-F), -163.8 (t, 6F; $^3J_{F-F}$ = 19 Hz, Me-$B(C_6F_5)_3$, *meta*-F), -167.1 (br m, 2F; Sc-C_6F_5, *meta*-F). Isomer 2 (30%): -125.1 (br s, 2F; Sc-C_6F_5, *ortho*-F), -134.5 (d, 6F; $^3J_{F-F}$ = 19 Hz, Me-$B(C_6F_5)_3$, *ortho*-F), –150.9 (t, 1F; $^3J_{F-F}$ = 21 Hz, Sc-C_6F_5, *para*-F), –159.6 (t, 3F; $^3J_{F-F}$ = 19 Hz, Me-$B(C_6F_5)_3$, *para*-F), -164.7 (t, 6F; $^3J_{F-F}$ = 19 Hz, Me-$B(C_6F_5)_3$, *meta*-F), -167.1 (br m, 2F; Sc-C_6F_5, *meta*-F). The instability of these compounds made it impossible to acquire ^{13}C NMR spectra as further decomposition occurs over the timeframe required to collect the necessary data. Upon cooling the tube to —35°C and layering with 1 mL of hexanes, yellow crystals suitable for X-ray diffraction were obtained after 2 weeks.

Synthesis of $\{[ArNC(Me)CHC(Me)NAr]ScCH_3\}^+[B(C_6F_5)_4]^-$ (1a). A 25mL RB flask was charged with $[ArNC(CH_3)CHC(CH_3)NAr]Sc(CH_3)_2$ (35 mg, 0.072 mmol) and $[CPh_3][B(C_6F_5)_4]$ (66 mg, 0.072 mmol) to which bromobenzene (3 mL) was added. The solution was stirred for 5 minutes and then layered with hexanes (5 mL). The reaction mixture was cooled to —35°C for 24 hours, solvent decanted and yellow crystals washed with toluene (2 x 2mL) and dried under vacuum to yield 67 mg (71.7%) of $\{[ArNC(Me)CHC(Me)NAr]ScCH_3\}^+[B(C_6F_5)_4]^-$ as a fine yellow powder. ^1H NMR (C_6D_5Br): δ 7.24–7.02 (ov m, 6H; C_6H_3), 5.30 (s, 1H; CH) 2.35 (sp, 4H; $CH(CH_3)_2$, J_{H-H} = 6.6 Hz), 1.59 (s, 6H; $NCCH_3$), 1.14 (d, 12H; $CH(CH_3)_2$, J_{H-H} = 6.6 Hz), 0.88 (d, 12H; $CH(CH_3)_2$, J_{H-H} = 6.6 Hz), -0.10 (s, 3H; Sc-CH_3). $^{13}C\{^1H\}$ NMR (C_6D_5Br, 270K, C_6F_5 resonances not reported): δ 170.3 ($NCCH_3$), 141.1 (C_{ipso}), 139.8, 128.5, 127.7 (C_6H_3), 97.6

(CH), 45.3 (Sc-CH_3), 28.4 ($CH(CH_3)_2$), 24.0 ($NCCH_3$), 24.0, 23.7 ($CH(CH_3)_2$). ^{19}F NMR (C_6D_5Br): δ −132.9 (d, $^3J_{F-F}$ = 21 Hz, *ortho*-F), −163.0 (t, $^3J_{F-F}$ = 21 Hz, *para*-F), -166.9 (t, $^3J_{F-F}$ = 21 Hz, *meta*-F). $^{11}B\{^1H\}$ NMR (C_6D_5Br): δ −17.0. Anal. Calcd. for $C_{60}H_{49}N_2BF_{20}BrSc$: C, 54.86; H,˚3.76; N, 2.13. Found: C, 54.24, H,˚3.80; N, 1.98 %.

Synthesis of {[ArNC(Me)CHC(Me)NAr]Sc(CH_3)(C_6H_6)}$^+$[B(C_6F_5)$_4$]$^-$ (1b). A 25mL RB flask was charged with [ArNC(CH_3)CHC(CH_3)NAr]Sc(CH_3)$_2$ (35 mg, 0.072 mmol) and [CPh_3][B(C_6F_5)$_4$] (66 mg, 0.072 mmol) to which bromobenzene (3 mL) was added. The solution was stirred for 5 minutes, benzene (2 mL) was added followed by an additional 5 minutes of stirring. The reaction mixture was layered with hexanes (5 mL), cooled to —35°C for 24 hours and solvent removed. The yellow crystals were washed with toluene (2 x 2mL) and dried under vacuum to give 54 mg (61.5%) of {[ArNC(Me)CHC(Me)NAr]Sc(CH_3)(C_6H_6)}$^+$[B(C_6F_5)$_4$]$^-$ as a fine yellow powder. ^1H NMR (C_6D_5Br, 270K): δ 7.22–7.10(ov m, 6H; C_6H_3), 6.85 (s, 6H; C_6H_6), 5.21 (s, 1H; CH) 2.46 (sp, 2H; C*H*(CH_3)$_2$, J_{H-H} = 6.8 Hz), 2.18 (sp, 2H; C*H*(CH_3)$_2$, J_{H-H} = 6.8 Hz), 1.55 (s, 6H; $NCCH_3$), 1.19 (d, 6H; CH(C*H*$_3$)$_2$, J_{H-H} = 6.8 Hz), 1.11 (d, 6H; CH(C*H*$_3$)$_2$, J_{H-H} = 6.8 Hz), 1.01 (d, 6H; CH(C*H*$_3$)$_2$, J_{H-H} = 6.8 Hz), 0.73 (d, 6H; CH(C*H*$_3$)$_2$, J_{H-H} = 6.8 Hz), -0.28 (s, 3H; Sc-CH_3). $^{13}C\{^1H\}$ NMR (C_6D_5Br, 270K, C_6F_5 resonances not reported): δ 169.7 (N*C*CH_3), 142.4 (C_{ipso}), 140.7, 139.8 (C_6H_3), 132.2 (C_6H_6), 129.9, 127.9, 124.7 (C_6H_3), 96.9 (CH), 41.5 (Sc-CH_3) 28.4, 27.5 (*C*H(CH_3)$_2$), 24.3, 23.9 (CH(*C*H_3)$_2$), 23.8 ($NCCH_3$), 23.7, 22.4 (CH(*C*H_3)$_2$). ^{19}F NMR (C_6D_5Br, 250K): δ −131.1 (d, $^3J_{F-F}$ = 21 Hz, *ortho*-F), −161.0 (t, $^3J_{F-F}$ = 21 Hz, *para*-F), −164.9 (t, $^3J_{F-F}$ = 21 Hz, *meta*-F). $^{11}B\{^1H\}$ NMR (C_6D_5Br, 250K): δ −17.0. Anal. Calcd. for $C_{60}H_{50}N_2BF_{20}Sc \cdot C_6H_5Br$: C, 56.96; H,˚3.98; N, 2.01. Found: C, 51.26, H,˚3.43; N, 1.85.

Synthesis of {[ArNC(Me)CHC(Me)NAr]Sc(CH_3)(C_7H_8)}$^+$[B(C_6F_5)$_4$]$^-$ (1c). A 25mL RB flask was charged with [ArNC(CH_3)CHC(CH_3)NAr]Sc(CH_3)$_2$ (35 mg, 0.072 mmol) and [CPh_3][B(C_6F_5)$_4$] (66 mg, 0.072 mmol) to which bromobenzene (3 mL) was added. The solution was stirred for 5 minutes, toluene (2 mL) was added followed by an additional 5 minutes of stirring. The reaction mixture was layered with hexanes (5 mL), cooled to —35°C for 24 hours and solvent removed. The yellow solid was washed with toluene (2 x 2mL) and dried under vacuum to give 87 mg (97.9%) of {[ArNC(Me)CHC(Me)NAr]Sc(CH_3)(C_7H_8)}$^+$[B(C_6F_5)$_4$]$^-$ as a bright yellow powder. ^{1}H NMR (C_6D_5Br, 260K): δ 7.22–7.10 (ov m, 6H; C_6H_3), 6.81 (d, 2H; *o*-C_7H_8, $J_{H\text{-}H}$ = 7.5 Hz), 6.66 (t, 1H; *p*-C_7H_8, $J_{H\text{-}H}$ = 7.5 Hz)), 6.39 (t, 2H; *m*-C_7H_8, $J_{H\text{-}H}$ = 7.5 Hz), 5.18 (s, 1H; CH), 2.44 (sp, 2H; C*H*(CH_3)$_2$, $J_{H\text{-}H}$ = 6.7 Hz), 2.19 (sp, 2H; C*H*(CH_3)$_2$, $J_{H\text{-}H}$ = 6.7 Hz), 1.86 (s, 3H; C*H*$_3$C$_6$H$_5$), 1.50 (s, 6H; NCC*H*$_3$), 1.16 (d, 6H; CH(C*H*$_3$)$_2$, $J_{H\text{-}H}$ = 6.7 Hz), 1.06 (d, 6H; CH(C*H*$_3$)$_2$, $J_{H\text{-}H}$ = 6.7 Hz), 1.01 (d, 6H; CH(C*H*$_3$)$_2$, $J_{H\text{-}H}$ = 6.7 Hz), 0.72 (d, 6H; CH(C*H*$_3$)$_2$, $J_{H\text{-}H}$ = 6.7 Hz), -0.29 (s, 3H; Sc-CH$_3$). ^{13}C{^{1}H} NMR (C_6D_5Br, 270K, C_6F_5 resonances not reported): δ 169.8 (N*C*CH$_3$), 142.3 (C_{ipso} of C_6H_3), 140.7, 139.9 (C_6H_3), 137.3 (C_{ipso} of $CH_3C_6H_5$), 133.2, 132.7 (CH_3*C*$_6$H$_5$), 128.3, 127.7 (C_6H_3), 126.0 (CH_3*C*$_6$H$_5$), 125.5 (C_6H_3), 97.6 (CH), 42.7 (Sc-CH$_3$), 28.8, 27.8 (*C*H(CH_3)$_2$), 24.7 (CH(*C*H$_3$)$_2$), 24.1 (NC*C*H$_3$), 24.1, 24.0, 22.6 (CH(*C*H$_3$)$_2$), 21.3 (C_6H_5*C*H$_3$). ^{19}F NMR (C_6D_5Br, 250K) : δ −131.2 (d, $^3J_{F\text{-}F}$ = 21 Hz, *ortho*-F), −161.0 (t, $^3J_{F\text{-}F}$ = 21 Hz, *para*-F), −164.9 (t, $^3J_{F\text{-}F}$ = 21 Hz, *meta*-F). ^{11}B NMR (C_6D_5Br, 250K) : δ −17.0. Anal. Calcd. for $C_{61}H_{52}N_2BF_{20}Sc \cdot C_6H_5Br$: C, 57.24; H, 4.09; N, 1.99. Found: C, 56.94, H, 3.87; N, 2.39.

Synthesis of {[ArNC(Me)CHC(Me)NAr]Sc(CH_3)(C_9H_{12})}$^+$[B(C_6F_5)$_4$]$^-$ (1d). A 25mL RB flask was charged with [ArNC(CH_3)CHC(CH_3)NAr]Sc(CH_3)$_2$ (45 mg, 0.091 mmol) and [CPh_3][B(C_6F_5)$_4$] (84 mg, 0.091 mmol) to which bromobenzene (5 mL) was added. The solution

was stirred for 5 minutes, mesitylene (1 mL) was added followed by an additional 5 minutes of stirring. The reaction mixture was layered with hexanes (5 mL), cooled to —35°C for 18 hours and solvent removed. The large yellow crystals were washed with toluene (3 x 2mL) and dried under vacuum to give 113mg $\{[ArNC(Me)CHC(Me)NAr]Sc(CH_3)(C_6H_6)\}^+[B(C_6F_5)_4]^-$ as a yellow powder in 97.4% yield. ^{1}H NMR (C_6D_5Br, 250K): δ 7.26–6.88 (ov m, 6H; C_6H_3), 6.59 (s, 3H; 1,3,5-CH_3-C_6H_3), 5.25 (s, 1H; CH) 2.37 (sp, 2H; C*H*$(CH_3)_2$, J_{H-H} = 6.6 Hz), 2.09 (sp, 2H; C*H*$(CH_3)_2$, J_{H-H} = 6.6 Hz), 1.43 (s, 6H; NCCH_3), 1.36 (s, 9H; 1,3,5-*CH*$_3$-C_6H_3) 1.17 (d, 6H; CH(C*H*$_3)_2$, J_{H-H} = 6.6 Hz), 1.08 (d, 6H; CH(C*H*$_3)_2$, J_{H-H} = 6.6 Hz), 0.95 (d, 6H; CH(C*H*$_3)_2$, J_{H-H} = 6.6 Hz), 0.74 (d, 6H; CH(C*H*$_3)_2$, J_{H-H} = 6.6 Hz), -0.14 (s, 3H; Sc-CH_3). ^{13}C{^{1}H} NMR (C_6D_5Br, 250K, C_6F_5 resonances not reported): δ 170.4 (N*C*CH_3), 141.7 (C_{ipso} of C_6H_3), 141.2, 140.8 (C_6H_3), 137.2 (C_{ipso} of 1,3,5-CH_3-C_6H_3), 130.0 (1,3,5-CH_3-*C*$_6H_3$), 127.0, 126.8, 124.9 (C_6H_3), 98.8 (CH), 43.5 (Sc-CH_3), 29.1, 28.3 (*C*H$(CH_3)_2$), 24.8 (NC*C*H_3), 24.6, 24.1, 23.5, 23.1 (CH(*C*H$_3)_2$), 21.4 (1,3,5-*C*H_3-C_6H_3). ^{19}F NMR (C_6D_5Br, 250K) : δ −131.2(d, $^3J_{F-F}$ = 21 Hz, *ortho*-F), −161.1 (t, $^3J_{F-F}$ = 21 Hz, *para*-F), −165.0 (t, $^3J_{F-F}$ = 21 Hz, *meta*-F). ^{11}B NMR (C_6D_5Br, 250K) : δ -16.6. Anal. Calcd. for $C_{63}H_{56}N_2BF_{20}Sc \cdot C_6H_5Br$: C, 57.80; H,˚4.29; N, 1.95. Found: C, 56.84, H,˚3.99; N, 2.03 %.

X-ray Crystallography. Suitable crystals were covered in Paratone oil, mounted on a glass fiber, and immediately placed in a cold stream on the diffractometer. 1a: Crystals were grown from a C_6D_5Br solution layered with hexanes at —35°C. Measurements were using a Nonius KappaCCD diffractometer with a graphite monochromated Mo-Kα radiation (λ = 0.71069) source at 173(2) K using the ω and φ scans to a maximum θ value of 25.07°. The sturcture was solved by direct methods and expanded using Fourier Techniques. The non-hydrogen atoms were refined anisotropically. A bromine atom of the solvent molecule was

disordered over three sites. Hydrogen atoms were included at geometrically idealized positions and were not refined. **1c:** Crystals were grown from a C_6H_5Br solution layered with hexanes at —35^{O}C. Measurements were using a Nonius KappaCCD diffractometer with a graphite monochromated Mo-Kα radiation (λ = 0.71069) source at 173(2) K using the ω and φ scans to a maximum θ value of 24.9 ^{O}. The sturcture was solved by direct methods and expanded using Fourier Techniques. The non-hydrogen atoms were refined anisotropically. A bromine atom of the solvent molecule was disordered. Hydrogen atoms were included at geometrically idealized positions and were not refined.

Kinetic Measurements: In a typical experiment, the compound of interest (0.0118 mmol) was dissolved in 0.5 mL C_6D_5Br cooled to —35°C and cold toluene (0.05 mL) added (2.14 x10^{-2} M). The NMR tube was kept at -35 °C until inserted into the NMR probe, at which time it was given 10 minutes to equilibrate to the specified temperature. The progress of reaction was monitored by integration of the backbone peak in the ^{1}H spectrum. The reaction was followed until 95% completion. Kinetic plots and rate data for various [toluene] are given below in Figure S1 and Table S1, respectively.

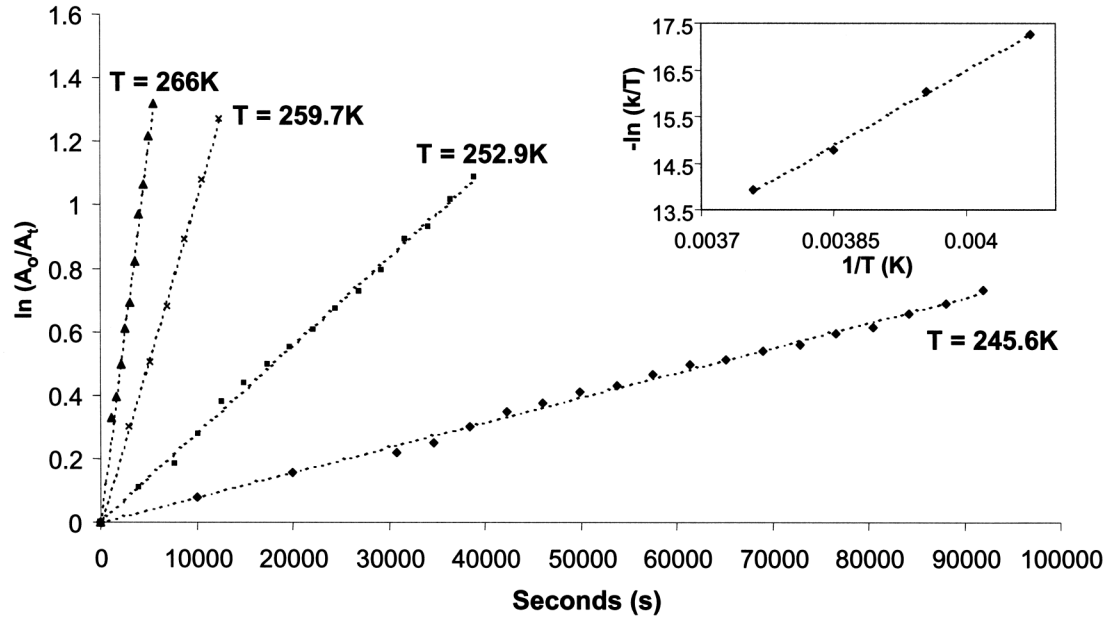

Figure S1. First order kinetic and Erying plots for the arene exchange reaction of **1d** to **1c**

Table S1: Rate Constants for Different [toluene] at 261K.

Equivalents of Toluene	**[Toluene] (M)**	**Rate (s^{-1})**	**Temperature (K)**
8.1	0.17	4.467×10^{-4}	261
16.2	0.34	4.517×10^{-4}	261
24.3	0.51	4.490×10^{-4}	261
32.4	0.68	3.810×10^{-4}	261
81	1.71	3.481×10^{-4}	261
202.5	4.27	2.187×10^{-4}	261

Crystal data and structure refinement for $\{[ArNC(Me)CHC(Me)NAr]ScC_6F_5\}^+[CH_3B(C_6F_5)_3]^-$

Identification code	WP — 7 (Paul — 5)	
Empirical formula	$C_{54}H_{44}BF_{20}N_2Sc$ Æ 0.25 C_6H_{14}	
Formula weight	1178.22	
Temperature	170(2) K	
Wavelength	0.71073	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 12.2225(2)	α = 82.7740(6)¡.
	b = 13.9703(2)	β = 73.6650(6)¡.
	c = 16.9809(3)	γ = 73.6860(8)¡.
Volume	2667.00(7) ^{3}	
Z	2	
Density (calculated)	1.467 Mg/m^3	
Absorption coefficient	0.25 mm^{-1}	
F(000)	1201	
Crystal size	0.30 x 0.25 x 0.20 mm^3	
Theta range for data collection	2.7 to 24.0¡.	
Index ranges	-13<=h<=13, -15<=k<=15, -19<=l<=19	
Reflections collected	16150	
Independent reflections	8321 [R(int) = 0.023]	
Observed data [I>2sigma(I)]	6513	
Completeness to theta = 24.0¡	99.6 %	
Absorption correction	Multi-scan method	
Max. and min. transmission	0.952 and 0.929	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8321 / 0 / 716	
Goodness-of-fit on F^2	1.09	
Final R indices [I>2sigma(I)]	R1 = 0.074, wR2 = 0.233	
R indices (all data)	R1 = 0.090, wR2 = 0.252	
Extinction coefficient	0.013(3)	
Weighting scheme	$w = 1/[\sigma^2(Fo^2) + (0.1574P)^2 + 3.1431P]$	
	where $P = (Fo^2 + 2Fc^2)/3$	
$(\Delta/\theta)max$	0.008	
Largest diff. peak and hole	0.70 and -0.70 e. $^{-3}$	

{[ArNC(Me)CHC(Me)NAr]ScC$_6$F$_5$}$^+$[CH$_3$B(C$_6$F$_5$)$_3$]$^-$, ORTEP diagram.

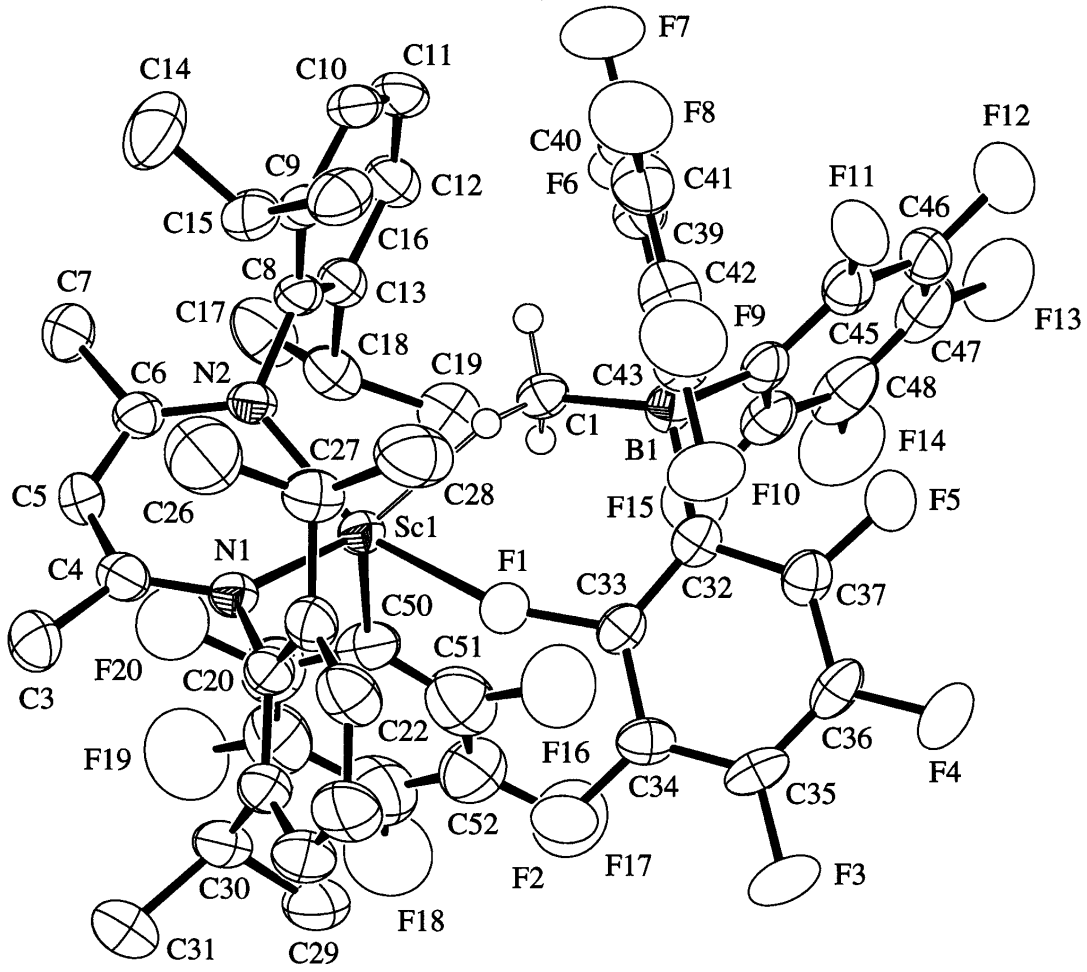

Table 1. Crystal data and structure refinement for $C_{66}H_{44}D_{10}BBr_2F_{20}N_2Sc$, **1a**.

Identification code	WP — 65 (Paul-9)
Empirical formula	$C_{66}H_{44}D_{10}BBr_2F_{20}N_2Sc$
Formula weight	1480.76
Temperature	173(2) K
Wavelength	0.71073
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 18.789(3)
	b = 14.249(3) β = 106.697(11)¡.
	c = 24.539(4)
Volume	6293(2) ^{3}
Z	4
Density (calculated)	1.562 Mg/m^3
Absorption coefficient	1.489 mm^{-1}
F(000)	2960
Crystal size	0.12 x 0.10 x 0.09 mm^3
Theta range for data collection	3.11 to 25.07¡.
Index ranges	-22<=h<=22, -16<=k<=16, -29<=l<=29
Reflections collected	21312
Independent reflections	11042 [R(int) = 0.0502]
Completeness to theta = 25.07¡	99.0 %
Absorption correction	Multi-scan method
Max. and min. transmission	0.8776 and 0.8415
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11042 / 0 / 848
Goodness-of-fit on F^2	1.014
Final R indices [I>2sigma(I)]	R1 = 0.0533, wR2 = 0.1289
R indices (all data)	R1 = 0.1072, wR2 = 0.1608
Largest diff. peak and hole	0.443 and -0.884 e. $^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (^{2}x 10^3) for $C_{66}H_{44}D_{10}BBr_2F_{20}N_2Sc$, **1a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
Sc(1)	4305(1)	6966(1)	1429(1)	30(1)
N(1)	5308(2)	6428(2)	1955(1)	32(1)
N(2)	4872(2)	8090(2)	1184(1)	31(1)
C(1)	4000(3)	6041(3)	701(2)	41(1)
C(3)	6545(3)	5815(3)	1983(2)	43(1)
C(4)	5901(2)	6472(3)	1756(2)	33(1)
C(5)	5963(2)	7116(3)	1337(2)	32(1)
C(6)	5526(2)	7886(3)	1094(2)	31(1)
C(7)	5835(3)	8516(3)	725(2)	42(1)
C(8)	5342(2)	5854(3)	2454(2)	35(1)
C(9)	5151(2)	4899(3)	2395(2)	40(1)
C(10)	5169(3)	4409(4)	2891(3)	54(1)
C(11)	5367(3)	4831(4)	3414(2)	59(2)
C(12)	5555(3)	5773(4)	3463(2)	51(1)
C(13)	5553(2)	6310(4)	2990(2)	41(1)
C(14)	5584(3)	7822(4)	3556(2)	61(2)
C(15)	5773(3)	7334(4)	3059(2)	44(1)
C(16)	6597(3)	7470(5)	3125(3)	66(2)
C(17)	4136(3)	4009(4)	1680(3)	67(2)
C(18)	4934(3)	4383(3)	1829(2)	48(1)
C(19)	5463(3)	3561(4)	1814(3)	61(2)
C(20)	4540(2)	8999(3)	1013(2)	32(1)
C(21)	4707(3)	9737(3)	1415(2)	38(1)
C(22)	4364(3)	10601(3)	1258(2)	46(1)
C(23)	3873(3)	10744(3)	723(2)	43(1)
C(24)	3720(3)	10022(3)	339(2)	43(1)
C(25)	4051(2)	9136(3)	465(2)	37(1)
C(26)	4122(3)	8700(4)	-517(2)	59(2)
C(27)	3887(3)	8382(3)	8(2)	44(1)
C(28)	3058(3)	8133(4)	-185(2)	57(1)

C(29)	6005(3)	10068(7)	2007(3)	112(3)
C(30)	5266(3)	9617(4)	1998(2)	52(1)
C(31)	5009(3)	10027(4)	2484(2)	56(1)
C(32)	2748(2)	6920(4)	1280(2)	41(1)
C(33)	2960(2)	7848(3)	1327(2)	38(1)
C(34)	3473(2)	8173(4)	1822(2)	41(1)
C(35)	3783(3)	7551(4)	2261(2)	46(1)
C(36)	3575(3)	6617(4)	2216(2)	44(1)
C(37)	3059(3)	6301(4)	1722(2)	45(1)
Br(1)	2027(1)	6479(1)	636(1)	62(1)
B(1)	1615(3)	3324(4)	-586(2)	31(1)
C(38)	1557(2)	2914(3)	34(2)	33(1)
C(39)	1940(3)	3232(3)	572(2)	38(1)
C(40)	1833(3)	2883(4)	1071(2)	45(1)
C(41)	1306(3)	2223(4)	1044(2)	46(1)
C(42)	889(3)	1885(3)	525(2)	42(1)
C(43)	1026(2)	2241(3)	43(2)	35(1)
C(44)	2348(2)	3991(3)	-521(2)	35(1)
C(45)	2376(2)	4843(3)	-791(2)	37(1)
C(46)	3030(3)	5279(3)	-798(2)	41(1)
C(47)	3703(2)	4888(4)	-529(2)	41(1)
C(48)	3712(2)	4052(4)	-247(2)	41(1)
C(49)	3057(2)	3629(3)	-254(2)	38(1)
C(50)	804(2)	3857(3)	-838(2)	30(1)
C(51)	652(2)	4676(3)	-586(2)	33(1)
C(52)	-17(3)	5142(3)	-744(2)	37(1)
C(53)	-594(2)	4780(3)	-1171(2)	37(1)
C(54)	-485(2)	3966(3)	-1423(2)	36(1)
C(55)	198(2)	3533(3)	-1264(2)	32(1)
C(56)	1760(2)	2507(3)	-1018(2)	33(1)
C(57)	1985(2)	1583(3)	-898(2)	35(1)
C(58)	2172(2)	984(3)	-1282(2)	43(1)
C(59)	2164(3)	1313(4)	-1808(2)	46(1)
C(60)	1946(3)	2210(4)	-1956(2)	44(1)
C(61)	1750(2)	2781(3)	-1573(2)	38(1)
F(1)	2449(2)	3930(2)	643(1)	49(1)

F(2)	2240(2)	3218(2)	1579(1)	62(1)
F(3)	1187(2)	1878(2)	1528(1)	66(1)
F(4)	358(2)	1237(2)	494(1)	58(1)
F(5)	597(1)	1882(2)	-458(1)	41(1)
F(6)	1748(1)	5293(2)	-1084(1)	44(1)
F(7)	3010(2)	6101(2)	-1084(1)	55(1)
F(8)	4336(2)	5304(2)	-551(1)	58(1)
F(9)	4366(1)	3640(2)	26(1)	53(1)
F(10)	3108(1)	2783(2)	7(1)	43(1)
F(11)	1186(1)	5049(2)	-149(1)	43(1)
F(12)	-109(2)	5953(2)	-482(1)	49(1)
F(13)	-1257(2)	5228(2)	-1336(1)	56(1)
F(14)	-1055(1)	3585(2)	-1840(1)	53(1)
F(15)	242(1)	2727(2)	-1554(1)	38(1)
F(16)	2046(2)	1215(2)	-380(1)	46(1)
F(17)	2388(2)	101(2)	-1127(1)	60(1)
F(18)	2355(2)	738(2)	-2183(1)	65(1)
F(19)	1941(2)	2550(2)	-2472(1)	58(1)
F(20)	1547(2)	3661(2)	-1746(1)	43(1)
Br(2)	2790(1)	610(2)	2094(1)	89(1)
Br(2A)	2101(8)	-737(9)	2334(3)	163(7)
Br(2B)	2654(6)	38(13)	2330(5)	89(3)
C(62)	2117(3)	-100(5)	1512(3)	72(2)
C(63)	2094(3)	94(4)	967(4)	76(2)
C(64)	1585(4)	-411(5)	491(3)	79(2)
C(65)	1164(3)	-1043(5)	617(4)	82(2)
C(66)	1192(4)	-1256(5)	1186(4)	87(2)
C(67)	1668(4)	-776(6)	1633(4)	88(2)

Table 3. Bond lengths [ ] and angles [¡] for $C_{66}H_{44}D_{10}BBr_2F_{20}N_2Sc$, **1a**.

Sc(1)-N(1)	2.100(4)	C(21)-C(30)	1.523(7)
Sc(1)-N(2)	2.105(4)	C(22)-C(23)	1.386(7)
Sc(1)-C(1)	2.162(5)	C(23)-C(24)	1.370(7)
Sc(1)-C(35)	2.640(4)	C(24)-C(25)	1.402(6)
Sc(1)-C(34)	2.682(4)	C(25)-C(27)	1.519(6)
Sc(1)-C(36)	2.715(4)	C(26)-C(27)	1.544(7)
Sc(1)-C(33)	2.767(4)	C(27)-C(28)	1.535(7)
Sc(1)-C(37)	2.802(5)	C(29)-C(30)	1.525(9)
Sc(1)-C(32)	2.842(4)	C(30)-C(31)	1.524(7)
N(1)-C(4)	1.339(5)	C(32)-C(33)	1.376(6)
N(1)-C(8)	1.459(5)	C(32)-C(37)	1.389(7)
N(2)-C(6)	1.340(5)	C(32)-Br(1)	1.871(5)
N(2)-C(20)	1.447(5)	C(33)-C(34)	1.395(6)
C(3)-C(4)	1.503(6)	C(34)-C(35)	1.389(7)
C(4)-C(5)	1.409(6)	C(35)-C(36)	1.382(7)
C(5)-C(6)	1.397(6)	C(36)-C(37)	1.392(7)
C(6)-C(7)	1.506(6)	B(1)-C(44)	1.643(7)
C(8)-C(9)	1.405(6)	B(1)-C(56)	1.649(6)
C(8)-C(13)	1.417(6)	B(1)-C(50)	1.654(6)
C(9)-C(10)	1.394(7)	B(1)-C(38)	1.663(6)
C(9)-C(18)	1.520(7)	C(38)-C(39)	1.388(6)
C(10)-C(11)	1.369(8)	C(38)-C(43)	1.389(6)
C(11)-C(12)	1.384(8)	C(39)-F(1)	1.356(5)
C(12)-C(13)	1.389(6)	C(39)-C(40)	1.387(7)
C(13)-C(15)	1.513(7)	C(40)-F(2)	1.348(5)
C(14)-C(15)	1.532(6)	C(40)-C(41)	1.355(7)
C(15)-C(16)	1.522(7)	C(41)-F(3)	1.361(5)
C(17)-C(18)	1.533(7)	C(41)-C(42)	1.377(7)
C(18)-C(19)	1.543(7)	C(42)-F(4)	1.345(6)
C(20)-C(25)	1.407(6)	C(42)-C(43)	1.376(6)
C(20)-C(21)	1.413(6)	C(43)-F(5)	1.361(5)
C(21)-C(22)	1.392(7)	C(44)-C(45)	1.391(6)
		C(44)-C(49)	1.403(6)
		C(45)-F(6)	1.353(5)
		C(45)-C(46)	1.381(6)

C(46)-F(7)	1.360(5)	C(65)-C(66)	1.416(10)
C(46)-C(47)	1.366(7)	C(66)-C(67)	1.381(11)
C(47)-F(8)	1.344(5)		
C(47)-C(48)	1.376(7)	N(1)-Sc(1)-N(2)	90.79(14)
C(48)-F(9)	1.352(5)	N(1)-Sc(1)-C(1)	105.22(16)
C(48)-C(49)	1.367(6)	N(2)-Sc(1)-C(1)	105.23(16)
C(49)-F(10)	1.354(5)	N(1)-Sc(1)-C(35)	96.21(15)
C(50)-C(55)	1.385(6)	N(2)-Sc(1)-C(35)	108.18(15)
C(50)-C(51)	1.389(6)	C(1)-Sc(1)-C(35)	139.74(17)
C(51)-F(11)	1.348(5)	N(1)-Sc(1)-C(34)	121.82(14)
C(51)-C(52)	1.376(6)	N(2)-Sc(1)-C(34)	90.59(14)
C(52)-F(12)	1.358(5)	C(1)-Sc(1)-C(34)	130.15(16)
C(52)-C(53)	1.374(6)	C(35)-Sc(1)-C(34)	30.23(15)
C(53)-F(13)	1.354(5)	N(1)-Sc(1)-C(36)	92.57(14)
C(53)-C(54)	1.357(6)	N(2)-Sc(1)-C(36)	138.00(15)
C(54)-F(14)	1.362(5)	C(1)-Sc(1)-C(36)	114.12(17)
C(54)-C(55)	1.376(6)	C(35)-Sc(1)-C(36)	29.87(15)
C(55)-F(15)	1.365(5)	C(34)-Sc(1)-C(36)	52.90(15)
C(56)-C(57)	1.388(6)	N(1)-Sc(1)-C(33)	149.00(14)
C(56)-C(61)	1.411(6)	N(2)-Sc(1)-C(33)	98.80(14)
C(57)-F(16)	1.349(5)	C(1)-Sc(1)-C(33)	100.59(16)
C(57)-C(58)	1.391(6)	C(35)-Sc(1)-C(33)	52.79(15)
C(58)-F(17)	1.343(5)	C(34)-Sc(1)-C(33)	29.61(13)
C(58)-C(59)	1.368(7)	C(36)-Sc(1)-C(33)	60.89(14)
C(59)-F(18)	1.354(5)	N(1)-Sc(1)-C(37)	112.84(14)
C(59)-C(60)	1.360(7)	N(2)-Sc(1)-C(37)	149.23(14)
C(60)-F(19)	1.353(5)	C(1)-Sc(1)-C(37)	87.91(17)
C(60)-C(61)	1.369(6)	C(35)-Sc(1)-C(37)	52.13(16)
C(61)-F(20)	1.344(5)	C(34)-Sc(1)-C(37)	60.61(15)
Br(2)-C(62)	1.903(7)	C(36)-Sc(1)-C(37)	29.17(15)
Br(2A)-C(62)	2.221(12)	C(33)-Sc(1)-C(37)	50.89(14)
Br(2B)-C(62)	1.982(11)	N(1)-Sc(1)-C(32)	141.28(14)
C(62)-C(63)	1.354(9)	N(2)-Sc(1)-C(32)	124.61(14)
C(62)-C(67)	1.368(10)	C(1)-Sc(1)-C(32)	82.02(16)
C(63)-C(64)	1.468(10)	C(35)-Sc(1)-C(32)	60.67(14)
C(64)-C(65)	1.294(10)	C(34)-Sc(1)-C(32)	51.45(14)

C(36)-Sc(1)-C(32)	51.40(14)	C(21)-C(20)-N(2)	118.2(4)
C(33)-Sc(1)-C(32)	28.37(13)	C(22)-C(21)-C(20)	118.3(4)
C(37)-Sc(1)-C(32)	28.48(14)	C(22)-C(21)-C(30)	119.9(4)
C(4)-N(1)-C(8)	119.4(4)	C(20)-C(21)-C(30)	121.8(4)
C(4)-N(1)-Sc(1)	117.0(3)	C(23)-C(22)-C(21)	121.4(5)
C(8)-N(1)-Sc(1)	122.3(3)	C(24)-C(23)-C(22)	119.5(5)
C(6)-N(2)-C(20)	119.0(3)	C(23)-C(24)-C(25)	122.1(5)
C(6)-N(2)-Sc(1)	116.5(3)	C(24)-C(25)-C(20)	117.6(4)
C(20)-N(2)-Sc(1)	123.6(3)	C(24)-C(25)-C(27)	119.3(4)
N(1)-C(4)-C(5)	123.2(4)	C(20)-C(25)-C(27)	123.1(4)
N(1)-C(4)-C(3)	120.1(4)	C(25)-C(27)-C(28)	111.4(4)
C(5)-C(4)-C(3)	116.7(4)	C(25)-C(27)-C(26)	111.3(4)
C(6)-C(5)-C(4)	131.4(4)	C(28)-C(27)-C(26)	108.6(4)
N(2)-C(6)-C(5)	123.7(4)	C(31)-C(30)-C(29)	108.6(5)
N(2)-C(6)-C(7)	120.0(4)	C(31)-C(30)-C(21)	113.9(4)
C(5)-C(6)-C(7)	116.3(4)	C(29)-C(30)-C(21)	110.3(5)
C(9)-C(8)-C(13)	122.3(4)	C(33)-C(32)-C(37)	119.9(5)
C(9)-C(8)-N(1)	120.5(4)	C(33)-C(32)-Br(1)	121.0(4)
C(13)-C(8)-N(1)	117.1(4)	C(37)-C(32)-Br(1)	119.1(4)
C(10)-C(9)-C(8)	117.0(5)	C(33)-C(32)-Sc(1)	72.8(2)
C(10)-C(9)-C(18)	119.2(5)	C(37)-C(32)-Sc(1)	74.2(3)
C(8)-C(9)-C(18)	123.8(4)	Br(1)-C(32)-Sc(1)	125.8(2)
C(11)-C(10)-C(9)	122.0(5)	C(32)-C(33)-C(34)	120.2(5)
C(10)-C(11)-C(12)	120.0(5)	C(32)-C(33)-Sc(1)	78.8(3)
C(11)-C(12)-C(13)	121.5(5)	C(34)-C(33)-Sc(1)	71.8(2)
C(12)-C(13)-C(8)	117.1(5)	C(35)-C(34)-C(33)	119.7(5)
C(12)-C(13)-C(15)	120.2(5)	C(35)-C(34)-Sc(1)	73.2(3)
C(8)-C(13)-C(15)	122.7(4)	C(33)-C(34)-Sc(1)	78.6(3)
C(13)-C(15)-C(16)	111.8(4)	C(36)-C(35)-C(34)	120.4(5)
C(13)-C(15)-C(14)	114.1(4)	C(36)-C(35)-Sc(1)	78.1(3)
C(16)-C(15)-C(14)	108.6(4)	C(34)-C(35)-Sc(1)	76.5(3)
C(9)-C(18)-C(17)	112.0(5)	C(35)-C(36)-C(37)	119.5(5)
C(9)-C(18)-C(19)	112.6(4)	C(35)-C(36)-Sc(1)	72.1(3)
C(17)-C(18)-C(19)	108.8(4)	C(37)-C(36)-Sc(1)	78.9(3)
C(25)-C(20)-C(21)	121.1(4)	C(32)-C(37)-C(36)	120.4(5)
C(25)-C(20)-N(2)	120.7(4)	C(32)-C(37)-Sc(1)	77.4(3)

C(36)-C(37)-Sc(1)	72.0(3)	C(46)-C(47)-C(48)	118.2(4)
C(44)-B(1)-C(56)	100.5(3)	F(9)-C(48)-C(49)	120.1(5)
C(44)-B(1)-C(50)	115.3(4)	F(9)-C(48)-C(47)	120.2(4)
C(56)-B(1)-C(50)	112.9(4)	C(49)-C(48)-C(47)	119.6(4)
C(44)-B(1)-C(38)	112.8(4)	F(10)-C(49)-C(48)	116.4(4)
C(56)-B(1)-C(38)	114.0(4)	F(10)-C(49)-C(44)	118.5(4)
C(50)-B(1)-C(38)	102.0(3)	C(48)-C(49)-C(44)	125.1(5)
C(39)-C(38)-C(43)	112.9(4)	C(55)-C(50)-C(51)	112.7(4)
C(39)-C(38)-B(1)	127.1(4)	C(55)-C(50)-B(1)	126.7(4)
C(43)-C(38)-B(1)	119.6(4)	C(51)-C(50)-B(1)	120.3(4)
F(1)-C(39)-C(40)	115.2(4)	F(11)-C(51)-C(52)	116.4(4)
F(1)-C(39)-C(38)	121.1(4)	F(11)-C(51)-C(50)	119.0(4)
C(40)-C(39)-C(38)	123.7(5)	C(52)-C(51)-C(50)	124.6(4)
F(2)-C(40)-C(41)	120.2(5)	F(12)-C(52)-C(53)	120.1(4)
F(2)-C(40)-C(39)	120.1(5)	F(12)-C(52)-C(51)	120.5(4)
C(41)-C(40)-C(39)	119.8(4)	C(53)-C(52)-C(51)	119.4(4)
C(40)-C(41)-F(3)	120.7(5)	F(13)-C(53)-C(54)	120.9(4)
C(40)-C(41)-C(42)	120.0(4)	F(13)-C(53)-C(52)	120.5(4)
F(3)-C(41)-C(42)	119.3(5)	C(54)-C(53)-C(52)	118.6(4)
F(4)-C(42)-C(41)	120.4(4)	C(53)-C(54)-F(14)	119.6(4)
F(4)-C(42)-C(43)	121.6(4)	C(53)-C(54)-C(55)	120.3(4)
C(41)-C(42)-C(43)	118.0(5)	F(14)-C(54)-C(55)	120.1(4)
F(5)-C(43)-C(42)	115.4(4)	F(15)-C(55)-C(54)	114.8(4)
F(5)-C(43)-C(38)	119.1(4)	F(15)-C(55)-C(50)	120.9(4)
C(42)-C(43)-C(38)	125.5(4)	C(54)-C(55)-C(50)	124.3(4)
C(45)-C(44)-C(49)	112.5(4)	C(57)-C(56)-C(61)	112.7(4)
C(45)-C(44)-B(1)	127.1(4)	C(57)-C(56)-B(1)	129.0(4)
C(49)-C(44)-B(1)	119.3(4)	C(61)-C(56)-B(1)	117.8(4)
F(6)-C(45)-C(46)	115.1(4)	F(16)-C(57)-C(56)	120.5(4)
F(6)-C(45)-C(44)	121.3(4)	F(16)-C(57)-C(58)	115.5(4)
C(46)-C(45)-C(44)	123.6(4)	C(56)-C(57)-C(58)	123.9(4)
F(7)-C(46)-C(47)	119.0(4)	F(17)-C(58)-C(59)	120.6(4)
F(7)-C(46)-C(45)	120.1(4)	F(17)-C(58)-C(57)	119.8(5)
C(47)-C(46)-C(45)	120.9(5)	C(59)-C(58)-C(57)	119.6(5)
F(8)-C(47)-C(46)	120.6(5)	F(18)-C(59)-C(60)	120.4(5)
F(8)-C(47)-C(48)	121.2(4)	F(18)-C(59)-C(58)	120.0(5)

C(60)-C(59)-C(58)	119.6(4)
F(19)-C(60)-C(59)	120.4(4)
F(19)-C(60)-C(61)	119.9(5)
C(59)-C(60)-C(61)	119.7(5)
F(20)-C(61)-C(60)	116.5(4)
F(20)-C(61)-C(56)	119.0(4)
C(60)-C(61)-C(56)	124.5(5)
C(63)-C(62)-C(67)	120.8(7)
C(63)-C(62)-Br(2)	117.3(6)
C(67)-C(62)-Br(2)	121.9(7)
C(63)-C(62)-Br(2B)	147.5(9)
C(67)-C(62)-Br(2B)	90.9(9)
C(63)-C(62)-Br(2A)	167.4(7)
C(62)-C(63)-C(64)	121.0(6)
C(65)-C(64)-C(63)	117.0(7)
C(64)-C(65)-C(66)	122.2(7)
C(67)-C(66)-C(65)	120.6(7)
C(62)-C(67)-C(66)	118.4(7)

Table 4. Anisotropic displacement parameters (^{2}x 10^3) for $C_{66}H_{44}D_{10}BBr_2F_{20}N_2Sc$, **1a**. The anisotropic displacement factor exponent takes the form:

$$-2\pi^2[\, h^2a^{*2}U^{11} + ... + 2\, h\, k\, a^*\, b^*\, U^{12}\,]$$

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Sc(1)	30(1)	31(1)	29(1)	1(1)	9(1)	1(1)
N(1)	31(2)	31(2)	32(2)	2(2)	9(2)	-1(2)
N(2)	35(2)	29(2)	27(2)	-2(2)	9(2)	2(2)
C(1)	41(3)	33(3)	47(3)	1(2)	10(2)	3(2)
C(3)	37(3)	46(3)	49(3)	5(2)	16(2)	6(2)
C(4)	34(2)	29(3)	36(2)	-1(2)	7(2)	1(2)
C(5)	34(2)	35(3)	31(2)	-4(2)	14(2)	0(2)
C(6)	36(2)	33(3)	25(2)	0(2)	9(2)	1(2)
C(7)	38(3)	46(3)	48(3)	12(2)	22(2)	6(2)
C(8)	28(2)	41(3)	34(2)	9(2)	7(2)	2(2)
C(9)	34(3)	38(3)	47(3)	14(2)	10(2)	6(2)
C(10)	43(3)	44(3)	76(4)	25(3)	20(3)	4(2)
C(11)	52(3)	71(4)	56(4)	30(3)	22(3)	13(3)
C(12)	44(3)	73(4)	38(3)	14(3)	14(2)	9(3)
C(13)	32(2)	51(3)	39(3)	8(2)	11(2)	0(2)
C(14)	63(4)	77(4)	48(3)	-15(3)	27(3)	-16(3)
C(15)	43(3)	52(3)	35(3)	-7(2)	8(2)	-8(2)
C(16)	54(3)	85(5)	67(4)	-22(3)	30(3)	-24(3)
C(17)	51(3)	40(3)	98(5)	1(3)	0(3)	-4(3)
C(18)	48(3)	32(3)	58(3)	4(2)	7(3)	-5(2)
C(19)	65(4)	40(3)	73(4)	2(3)	14(3)	7(3)
C(20)	34(2)	31(3)	34(2)	3(2)	14(2)	0(2)
C(21)	39(3)	38(3)	39(3)	-3(2)	15(2)	4(2)
C(22)	51(3)	38(3)	49(3)	-5(2)	15(3)	6(2)
C(23)	45(3)	32(3)	56(3)	6(2)	20(3)	10(2)
C(24)	40(3)	49(3)	41(3)	10(2)	12(2)	4(2)
C(25)	39(3)	34(3)	38(3)	4(2)	11(2)	2(2)
C(26)	71(4)	65(4)	45(3)	-6(3)	20(3)	-1(3)
C(27)	52(3)	38(3)	34(3)	2(2)	1(2)	7(2)

C(28)	62(4)	59(4)	49(3)	-3(3)	16(3)	-17(3)
C(29)	44(4)	236(10)	54(4)	-39(5)	9(3)	14(5)
C(30)	65(4)	46(3)	39(3)	-10(2)	6(3)	15(3)
C(31)	60(3)	61(4)	46(3)	-17(3)	16(3)	-11(3)
C(32)	34(3)	48(3)	43(3)	-10(2)	17(2)	-6(2)
C(33)	31(2)	42(3)	43(3)	-6(2)	14(2)	2(2)
C(34)	33(3)	42(3)	52(3)	-9(2)	20(2)	1(2)
C(35)	41(3)	65(4)	39(3)	-12(3)	20(2)	-2(3)
C(36)	41(3)	57(3)	38(3)	7(2)	19(2)	5(2)
C(37)	44(3)	40(3)	57(3)	3(3)	22(3)	-3(2)
Br(1)	49(1)	68(1)	65(1)	-16(1)	9(1)	-16(1)
B(1)	31(3)	32(3)	30(3)	-2(2)	8(2)	4(2)
C(38)	32(2)	32(3)	34(2)	-2(2)	8(2)	8(2)
C(39)	36(3)	40(3)	37(3)	-5(2)	7(2)	11(2)
C(40)	43(3)	60(3)	27(3)	-6(2)	4(2)	18(3)
C(41)	48(3)	57(3)	34(3)	10(2)	16(2)	19(3)
C(42)	40(3)	45(3)	43(3)	7(2)	17(2)	8(2)
C(43)	35(2)	40(3)	29(2)	2(2)	7(2)	7(2)
C(44)	32(2)	33(3)	37(2)	-6(2)	7(2)	2(2)
C(45)	33(3)	38(3)	42(3)	-7(2)	12(2)	1(2)
C(46)	43(3)	33(3)	50(3)	-3(2)	18(2)	-5(2)
C(47)	31(3)	50(3)	44(3)	-16(2)	12(2)	-12(2)
C(48)	29(3)	47(3)	43(3)	-15(2)	6(2)	1(2)
C(49)	36(3)	37(3)	41(3)	-10(2)	11(2)	-2(2)
C(50)	30(2)	31(3)	29(2)	-1(2)	6(2)	3(2)
C(51)	30(2)	36(3)	32(2)	0(2)	10(2)	-2(2)
C(52)	44(3)	29(3)	43(3)	0(2)	22(2)	8(2)
C(53)	32(2)	40(3)	42(3)	11(2)	12(2)	12(2)
C(54)	31(3)	41(3)	32(2)	7(2)	4(2)	0(2)
C(55)	39(3)	27(2)	30(2)	1(2)	11(2)	2(2)
C(56)	23(2)	37(3)	39(3)	-5(2)	9(2)	-1(2)
C(57)	28(2)	35(3)	40(3)	-5(2)	6(2)	1(2)
C(58)	29(2)	31(3)	59(3)	-13(2)	0(2)	6(2)
C(59)	29(2)	59(4)	47(3)	-25(3)	7(2)	2(2)
C(60)	34(3)	56(4)	42(3)	-12(2)	12(2)	-10(2)
C(61)	32(2)	39(3)	42(3)	-4(2)	11(2)	1(2)

F(1)	48(2)	50(2)	41(2)	-12(1)	3(1)	1(1)
F(2)	66(2)	82(2)	30(2)	-9(1)	1(1)	23(2)
F(3)	76(2)	92(2)	37(2)	20(2)	27(2)	28(2)
F(4)	53(2)	69(2)	57(2)	19(2)	26(2)	1(2)
F(5)	42(2)	43(2)	38(1)	0(1)	12(1)	-6(1)
F(6)	37(2)	37(2)	58(2)	10(1)	13(1)	5(1)
F(7)	52(2)	44(2)	74(2)	5(2)	24(2)	-8(1)
F(8)	37(2)	69(2)	71(2)	-12(2)	21(2)	-17(1)
F(9)	29(2)	63(2)	62(2)	-10(2)	4(1)	2(1)
F(10)	37(2)	36(2)	51(2)	2(1)	6(1)	8(1)
F(11)	41(2)	41(2)	44(2)	-15(1)	8(1)	0(1)
F(12)	56(2)	38(2)	56(2)	-3(1)	23(2)	14(1)
F(13)	41(2)	60(2)	62(2)	6(2)	8(1)	21(1)
F(14)	37(2)	60(2)	51(2)	-4(1)	-4(1)	0(1)
F(15)	37(1)	36(2)	38(1)	-9(1)	4(1)	1(1)
F(16)	51(2)	37(2)	48(2)	5(1)	11(1)	9(1)
F(17)	55(2)	39(2)	77(2)	-14(2)	4(2)	13(1)
F(18)	52(2)	78(2)	64(2)	-41(2)	15(2)	8(2)
F(19)	59(2)	79(2)	42(2)	-16(2)	24(2)	-14(2)
F(20)	52(2)	41(2)	38(1)	3(1)	15(1)	1(1)
Br(2)	53(1)	107(2)	97(1)	-51(1)	4(1)	20(1)
Br(2A)	230(13)	194(13)	81(5)	37(6)	73(7)	135(11)
Br(2B)	79(5)	110(7)	77(5)	-35(5)	19(4)	40(5)
C(62)	49(4)	74(5)	91(5)	-22(4)	17(4)	23(3)
C(63)	52(4)	48(4)	135(7)	-7(4)	40(4)	4(3)
C(64)	92(5)	62(5)	95(5)	23(4)	46(5)	35(4)
C(65)	40(4)	73(5)	120(7)	-26(5)	1(4)	7(3)
C(66)	50(4)	74(5)	145(8)	11(5)	42(5)	3(4)
C(67)	73(5)	98(6)	103(6)	8(5)	43(5)	30(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (^{2}x 10^3) for $C_{66}H_{44}D_{10}BBr_2F_{20}N_2Sc$, **1a**.

Atom	x	y	z	U(eq)
H(1A)	3731	5498	787	61
H(1B)	4450	5828	612	61
H(1C)	3681	6379	373	61
H(3A)	6441	5404	2271	64
H(3B)	6996	6180	2154	64
H(3C)	6616	5433	1670	64
H(5)	6375	7007	1193	39
H(7A)	5488	9034	582	63
H(7B)	5903	8156	404	63
H(7C)	6315	8770	949	63
H(10)	5040	3763	2864	65
H(11)	5375	4477	3743	70
H(12)	5689	6058	3828	62
H(14A)	5054	7742	3518	91
H(14B)	5700	8492	3552	91
H(14C)	5878	7544	3915	91
H(15)	5493	7665	2702	53
H(16A)	6718	8140	3166	99
H(16B)	6715	7223	2788	99
H(16C)	6889	7133	3464	99
H(17A)	4018	3681	1314	101
H(17B)	3791	4534	1654	101
H(17C)	4089	3572	1976	101
H(18)	4962	4840	1527	57
H(19A)	5301	3253	1442	91
H(19B)	5454	3107	2112	91
H(19C)	5969	3801	1878	91
H(22)	4468	11103	1524	55
H(23)	3645	11339	624	52
H(24)	3378	10124	-25	52
H(26A)	4013	8200	-803	89

H(26B)	4656	8835	-402	89
H(26C)	3846	9267	-678	89
H(27)	4175	7806	168	52
H(28A)	2970	7643	-478	85
H(28B)	2768	8693	-343	85
H(28C)	2906	7904	141	85
H(29A)	6183	9799	1703	168
H(29B)	6370	9947	2376	168
H(29C)	5938	10746	1950	168
H(30)	5352	8930	2070	62
H(31A)	4538	9736	2487	83
H(31B)	4940	10706	2430	83
H(31C)	5385	9902	2846	83
D(33)	2757	8268	1021	45
D(34)	3608	8817	1858	49
D(35)	4140	7768	2595	55
D(36)	3782	6195	2519	53
D(37)	2920	5658	1686	54
D(63)	2411	565	891	91
D(64)	1567	-280	107	95
D(65)	823	-1375	317	99
D(66)	881	-1734	1262	104
D(67)	1684	-912	2015	105

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

Identification code	**1c**	
Empirical formula	C67 H57 B Br F20 N2 Sc	
Formula weight	1405.83	
Temperature	173(2) K	
Wavelength	0.71073	
Crystal system	Monoclinic	
Space group	$P2_i/n$	
Unit cell dimensions	a = 18.9115(4)	α= 90¡.
	b = 14.0831(3)	β= 107.0566(9)¡.
	c = 24.6274(6)	γ = 90¡.
Volume	6270.6(2) ^{3}	
Z	4	
Density (calculated)	1.489 Mg/m^3	
Absorption coefficient	0.857 mm^{-1}	
F(000)	2856	
Crystal size	0.20 x 0.20 x 0.18 mm^3	
Theta range for data collection	1.61 to 24.88¡.	
Index ranges	-22<=h<=22, -16<=k<=15, -29<=l<=28	
Reflections collected	18966	
Independent reflections	10673 [R(int) = 0.0404]	
Completeness to theta = 24.88¡	97.9 %	
Absorption correction	None	
Max. and min. transmission	0.8609 and 0.8472	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10673 / 0 / 835	
Goodness-of-fit on F^2	1.015	
Final R indices [I>2sigma(I)]	R1 = 0.0558, wR2 = 0.1303	
R indices (all data)	R1 = 0.1042, wR2 = 0.1559	
Largest diff. peak and hole	0.526 and -0.580 e. $^{-3}$	

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

	x	y	z	U(eq)
Sc(1)	-4296(1)	-3079(1)	3570(1)	33(1)
N(1)	-5300(2)	-3613(2)	3045(1)	35(1)
N(2)	-4858(2)	-1935(2)	3812(1)	33(1)
C(1)	-4003(2)	-4016(3)	4310(2)	39(1)
C(3)	-6544(2)	-4214(3)	3005(2)	44(1)
C(4)	-5897(2)	-3560(2)	3238(2)	35(1)
C(5)	-5954(2)	-2913(2)	3656(2)	36(1)
C(6)	-5513(2)	-2131(2)	3898(1)	33(1)
C(7)	-5818(2)	-1492(3)	4264(2)	45(1)
C(8)	-5346(2)	-4190(3)	2547(2)	40(1)
C(9)	-5160(2)	-5169(3)	2609(2)	45(1)
C(10)	-5176(2)	-5675(3)	2116(2)	58(1)
C(11)	-5364(3)	-5238(4)	1594(2)	64(1)
C(12)	-5548(2)	-4289(4)	1544(2)	57(1)
C(13)	-5549(2)	-3741(3)	2013(2)	43(1)
C(14)	-5565(3)	-2207(4)	1447(2)	67(1)
C(15)	-5761(2)	-2703(3)	1945(2)	48(1)
C(16)	-6585(3)	-2565(4)	1877(2)	75(2)
C(17)	-4156(3)	-6090(4)	3322(2)	76(2)
C(18)	-4955(2)	-5691(3)	3173(2)	53(1)
C(19)	-5487(3)	-6509(3)	3180(2)	65(1)
C(20)	-4529(2)	-1007(3)	3986(2)	34(1)
C(21)	-4693(2)	-268(3)	3586(2)	41(1)
C(22)	-4360(2)	610(3)	3742(2)	49(1)
C(23)	-3874(2)	742(3)	4275(2)	52(1)
C(24)	-3716(2)	23(3)	4664(2)	45(1)
C(25)	-4036(2)	-874(3)	4533(2)	39(1)
C(26)	-4109(3)	-1321(4)	5513(2)	66(1)
C(27)	-3868(2)	-1637(3)	4990(2)	49(1)
C(28)	-3051(3)	-1891(3)	5183(2)	63(1)

C(29)	-5997(3)	72(6)	2985(2)	111(3)
C(30)	-5255(3)	-384(3)	3004(2)	58(1)
C(31)	-5003(3)	14(4)	2516(2)	64(1)
C(32)	-2770(2)	-3167(3)	3734(2)	49(1)
C(33)	-2975(2)	-2216(3)	3674(2)	46(1)
C(34)	-3478(2)	-1885(3)	3174(2)	46(1)
C(35)	-3785(2)	-2508(3)	2734(2)	53(1)
C(36)	-3582(3)	-3455(4)	2790(2)	56(1)
C(37)	-3085(2)	-3783(3)	3284(2)	54(1)
C(38)	-2173(3)	-3529(4)	4254(2)	76(2)
F(1)	-623(1)	1905(2)	5448(1)	45(1)
F(2)	-399(1)	1249(2)	4497(1)	63(1)
F(3)	-1235(2)	1882(2)	3468(1)	74(1)
F(4)	-2291(2)	3224(2)	3413(1)	68(1)
F(5)	-2491(1)	3951(2)	4345(1)	54(1)
F(6)	-2059(1)	1219(2)	5375(1)	50(1)
F(7)	-2400(1)	101(2)	6126(1)	63(1)
F(8)	-2372(1)	761(2)	7173(1)	70(1)
F(9)	-1955(1)	2591(2)	7457(1)	60(1)
F(10)	-1559(1)	3711(2)	6731(1)	48(1)
F(11)	-3134(1)	2795(2)	4989(1)	46(1)
F(12)	-4386(1)	3640(2)	4992(1)	58(1)
F(13)	-4356(1)	5308(2)	5572(1)	64(1)
F(14)	-3032(1)	6131(2)	6094(1)	61(1)
F(15)	-1775(1)	5346(2)	6068(1)	49(1)
F(16)	-1240(1)	5103(2)	5120(1)	51(1)
F(17)	49(1)	6025(2)	5437(1)	60(1)
F(18)	1210(1)	5301(2)	6284(1)	70(1)
F(19)	1026(1)	3660(2)	6806(1)	61(1)
F(20)	-262(1)	2781(2)	6534(1)	45(1)
B(1)	-1640(2)	3354(3)	5568(2)	35(1)
C(39)	-1586(2)	2933(3)	4956(2)	36(1)
C(40)	-1056(2)	2256(3)	4950(2)	39(1)
C(41)	-928(2)	1901(3)	4465(2)	46(1)
C(42)	-1353(3)	2225(3)	3945(2)	51(1)
C(43)	-1879(2)	2887(3)	3921(2)	49(1)

C(44)	-1978(2)	3247(3)	4417(2)	43(1)
C(45)	-1772(2)	2536(3)	6013(2)	35(1)
C(46)	-1999(2)	1598(3)	5895(2)	39(1)
C(47)	-2185(2)	1004(3)	6277(2)	44(1)
C(48)	-2176(2)	1328(3)	6799(2)	48(1)
C(49)	-1962(2)	2245(3)	6944(2)	45(1)
C(50)	-1761(2)	2814(3)	6560(2)	39(1)
C(51)	-2381(2)	4027(3)	5515(2)	37(1)
C(52)	-3081(2)	3648(3)	5253(2)	39(1)
C(53)	-3732(2)	4062(3)	5256(2)	45(1)
C(54)	-3724(2)	4897(3)	5542(2)	48(1)
C(55)	-3054(2)	5310(3)	5805(2)	45(1)
C(56)	-2407(2)	4882(3)	5783(2)	42(1)
C(57)	-838(2)	3912(2)	5820(2)	34(1)
C(58)	-698(2)	4732(3)	5559(2)	39(1)
C(59)	-29(2)	5208(3)	5706(2)	44(1)
C(60)	548(2)	4849(3)	6129(2)	46(1)
C(61)	451(2)	4029(3)	6392(2)	43(1)
C(62)	-227(2)	3585(3)	6238(2)	36(1)
Br(1)	-2216(1)	5550(1)	2103(1)	107(1)
Br(1A)	-3006(6)	4135(8)	2272(3)	162(4)
Br(1B)	-2399(5)	4917(6)	2319(3)	114(2)
C(63)	-2889(2)	4850(3)	1510(2)	91(2)
C(64)	-3359(3)	4158(4)	1611(2)	97(2)
C(65)	-3838(2)	3675(3)	1159(3)	102(2)
C(66)	-3847(2)	3884(3)	605(2)	96(2)
C(67)	-3377(3)	4577(3)	504(2)	102(2)
C(68)	-2898(2)	5060(2)	956(3)	86(2)

Table 3. Bond lengths [ ] and angles [¡] for **1c.**

Sc(1)-N(1)	2.098(3)	C(21)-C(30)	1.522(6)
Sc(1)-N(2)	2.109(3)	C(22)-C(23)	1.376(6)
Sc(1)-C(1)	2.186(4)	C(23)-C(24)	1.367(6)
Sc(1)-C(35)	2.643(4)	C(24)-C(25)	1.397(5)
Sc(1)-C(34)	2.655(4)	C(25)-C(27)	1.520(5)
Sc(1)-C(36)	2.704(4)	C(26)-C(27)	1.553(6)
Sc(1)-C(33)	2.722(4)	C(27)-C(28)	1.519(6)
Sc(1)-C(37)	2.769(4)	C(29)-C(30)	1.532(8)
Sc(1)-C(32)	2.796(4)	C(30)-C(31)	1.524(6)
N(1)-C(4)	1.349(4)	C(32)-C(33)	1.389(6)
N(1)-C(8)	1.452(5)	C(32)-C(37)	1.395(6)
N(2)-C(6)	1.345(4)	C(32)-C(38)	1.526(6)
N(2)-C(20)	1.456(4)	C(33)-C(34)	1.397(6)
C(3)-C(4)	1.504(5)	C(34)-C(35)	1.383(6)
C(4)-C(5)	1.402(5)	C(35)-C(36)	1.384(6)
C(5)-C(6)	1.404(5)	C(36)-C(37)	1.381(6)
C(6)-C(7)	1.504(5)	F(1)-C(40)	1.353(4)
C(8)-C(13)	1.407(5)	F(2)-C(41)	1.343(5)
C(8)-C(9)	1.420(5)	F(3)-C(42)	1.347(4)
C(9)-C(10)	1.401(6)	F(4)-C(43)	1.351(5)
C(9)-C(18)	1.516(6)	F(5)-C(44)	1.362(5)
C(10)-C(11)	1.373(7)	F(6)-C(46)	1.360(4)
C(11)-C(12)	1.378(7)	F(7)-C(47)	1.353(4)
C(12)-C(13)	1.390(6)	F(8)-C(48)	1.351(4)
C(13)-C(15)	1.512(6)	F(9)-C(49)	1.351(4)
C(14)-C(15)	1.548(6)	F(10)-C(50)	1.352(4)
C(15)-C(16)	1.529(6)	F(11)-C(52)	1.355(4)
C(17)-C(18)	1.552(6)	F(12)-C(53)	1.353(4)
C(18)-C(19)	1.534(6)	F(13)-C(54)	1.349(4)
C(20)-C(21)	1.403(5)	F(14)-C(55)	1.353(4)
C(20)-C(25)	1.409(5)	F(15)-C(56)	1.363(4)
C(21)-C(22)	1.391(5)	F(16)-C(58)	1.358(4)
		F(17)-C(59)	1.357(4)
		F(18)-C(60)	1.356(4)
		F(19)-C(61)	1.357(4)

F(20)-C(62)	1.358(4)	C(63)-C(68)	1.3900
B(1)-C(39)	1.651(5)	C(64)-C(65)	1.3900
B(1)-C(45)	1.657(5)	C(65)-C(66)	1.3900
B(1)-C(57)	1.658(5)	C(66)-C(67)	1.3900
B(1)-C(51)	1.664(6)	C(67)-C(68)	1.3900
C(39)-C(40)	1.387(5)		
C(39)-C(44)	1.388(5)	N(1)-Sc(1)-N(2)	90.48(11)
C(40)-C(41)	1.378(5)	N(1)-Sc(1)-C(1)	105.03(13)
C(41)-C(42)	1.376(6)	N(2)-Sc(1)-C(1)	104.54(13)
C(42)-C(43)	1.352(6)	N(1)-Sc(1)-C(35)	95.79(13)
C(43)-C(44)	1.386(6)	N(2)-Sc(1)-C(35)	108.51(13)
C(45)-C(46)	1.393(5)	C(1)-Sc(1)-C(35)	140.51(15)
C(45)-C(50)	1.398(5)	N(1)-Sc(1)-C(34)	121.37(12)
C(46)-C(47)	1.381(5)	N(2)-Sc(1)-C(34)	90.93(12)
C(47)-C(48)	1.359(6)	C(1)-Sc(1)-C(34)	130.94(14)
C(48)-C(49)	1.370(6)	C(35)-Sc(1)-C(34)	30.27(13)
C(49)-C(50)	1.374(5)	N(1)-Sc(1)-C(36)	92.43(13)
C(51)-C(56)	1.380(5)	N(2)-Sc(1)-C(36)	138.42(14)
C(51)-C(52)	1.399(5)	C(1)-Sc(1)-C(36)	114.60(15)
C(52)-C(53)	1.365(6)	C(35)-Sc(1)-C(36)	29.96(14)
C(53)-C(54)	1.368(6)	C(34)-Sc(1)-C(36)	52.95(14)
C(54)-C(55)	1.373(6)	N(1)-Sc(1)-C(33)	149.09(12)
C(55)-C(56)	1.379(6)	N(2)-Sc(1)-C(33)	99.05(12)
C(57)-C(62)	1.382(5)	C(1)-Sc(1)-C(33)	100.91(14)
C(57)-C(58)	1.385(5)	C(35)-Sc(1)-C(33)	53.30(13)
C(58)-C(59)	1.383(5)	C(34)-Sc(1)-C(33)	30.08(12)
C(59)-C(60)	1.366(6)	C(36)-Sc(1)-C(33)	61.21(13)
C(60)-C(61)	1.362(6)	N(1)-Sc(1)-C(37)	112.42(13)
C(61)-C(62)	1.376(5)	N(2)-Sc(1)-C(37)	150.21(12)
Br(1)-Br(1B)	1.142(9)	C(1)-Sc(1)-C(37)	88.22(14)
Br(1)-C(63)	1.907(4)	C(35)-Sc(1)-C(37)	52.60(14)
Br(1)-Br(1A)	2.598(12)	C(34)-Sc(1)-C(37)	61.27(13)
Br(1A)-Br(1B)	1.571(13)	C(36)-Sc(1)-C(37)	29.20(13)
Br(1A)-C(63)	2.198(10)	C(33)-Sc(1)-C(37)	51.59(13)
Br(1B)-C(63)	1.937(9)	N(1)-Sc(1)-C(32)	141.45(12)
C(63)-C(64)	1.3900	N(2)-Sc(1)-C(32)	125.23(12)

C(1)-Sc(1)-C(32)	81.59(14)	C(19)-C(18)-C(17)	108.7(4)
C(35)-Sc(1)-C(32)	61.89(13)	C(21)-C(20)-C(25)	121.4(3)
C(34)-Sc(1)-C(32)	52.68(12)	C(21)-C(20)-N(2)	118.2(3)
C(36)-Sc(1)-C(32)	52.06(13)	C(25)-C(20)-N(2)	120.4(3)
C(33)-Sc(1)-C(32)	29.11(12)	C(22)-C(21)-C(20)	118.5(4)
C(37)-Sc(1)-C(32)	29.03(13)	C(22)-C(21)-C(30)	119.4(4)
C(4)-N(1)-C(8)	118.6(3)	C(20)-C(21)-C(30)	122.1(3)
C(4)-N(1)-Sc(1)	117.6(2)	C(23)-C(22)-C(21)	120.4(4)
C(8)-N(1)-Sc(1)	122.7(2)	C(24)-C(23)-C(22)	121.1(4)
C(6)-N(2)-C(20)	118.2(3)	C(23)-C(24)-C(25)	121.1(4)
C(6)-N(2)-Sc(1)	116.8(2)	C(24)-C(25)-C(20)	117.5(4)
C(20)-N(2)-Sc(1)	124.1(2)	C(24)-C(25)-C(27)	119.0(3)
N(1)-C(4)-C(5)	123.1(3)	C(20)-C(25)-C(27)	123.4(3)
N(1)-C(4)-C(3)	120.2(3)	C(25)-C(27)-C(28)	111.8(4)
C(5)-C(4)-C(3)	116.7(3)	C(25)-C(27)-C(26)	111.3(4)
C(4)-C(5)-C(6)	131.1(3)	C(28)-C(27)-C(26)	109.1(3)
N(2)-C(6)-C(5)	123.6(3)	C(21)-C(30)-C(31)	114.2(4)
N(2)-C(6)-C(7)	120.4(3)	C(21)-C(30)-C(29)	111.4(4)
C(5)-C(6)-C(7)	116.1(3)	C(31)-C(30)-C(29)	108.5(4)
C(13)-C(8)-C(9)	121.9(4)	C(33)-C(32)-C(37)	118.3(4)
C(13)-C(8)-N(1)	118.1(3)	C(33)-C(32)-C(38)	121.7(4)
C(9)-C(8)-N(1)	120.0(3)	C(37)-C(32)-C(38)	119.8(4)
C(10)-C(9)-C(8)	117.3(4)	C(33)-C(32)-Sc(1)	72.5(2)
C(10)-C(9)-C(18)	118.8(4)	C(37)-C(32)-Sc(1)	74.4(2)
C(8)-C(9)-C(18)	124.0(4)	C(38)-C(32)-Sc(1)	128.0(3)
C(11)-C(10)-C(9)	121.2(4)	C(32)-C(33)-C(34)	120.8(4)
C(10)-C(11)-C(12)	120.5(4)	C(32)-C(33)-Sc(1)	78.4(2)
C(11)-C(12)-C(13)	121.7(4)	C(34)-C(33)-Sc(1)	72.3(2)
C(12)-C(13)-C(8)	117.5(4)	C(35)-C(34)-C(33)	120.0(4)
C(12)-C(13)-C(15)	120.6(4)	C(35)-C(34)-Sc(1)	74.4(2)
C(8)-C(13)-C(15)	121.9(3)	C(33)-C(34)-Sc(1)	77.6(2)
C(13)-C(15)-C(16)	111.3(4)	C(34)-C(35)-C(36)	119.5(4)
C(13)-C(15)-C(14)	114.0(3)	C(34)-C(35)-Sc(1)	75.4(2)
C(16)-C(15)-C(14)	109.2(4)	C(36)-C(35)-Sc(1)	77.5(2)
C(9)-C(18)-C(19)	112.5(4)	C(37)-C(36)-C(35)	120.5(4)
C(9)-C(18)-C(17)	111.3(4)	C(37)-C(36)-Sc(1)	78.0(2)

C(35)-C(36)-Sc(1)	72.6(2)	C(48)-C(47)-C(46)	120.4(4)
C(36)-C(37)-C(32)	120.9(4)	F(8)-C(48)-C(47)	121.1(4)
C(36)-C(37)-Sc(1)	72.8(2)	F(8)-C(48)-C(49)	120.0(4)
C(32)-C(37)-Sc(1)	76.6(2)	C(47)-C(48)-C(49)	118.9(4)
C(39)-B(1)-C(45)	114.6(3)	F(9)-C(49)-C(48)	120.3(4)
C(39)-B(1)-C(57)	102.5(3)	F(9)-C(49)-C(50)	120.4(4)
C(45)-B(1)-C(57)	112.3(3)	C(48)-C(49)-C(50)	119.4(4)
C(39)-B(1)-C(51)	114.2(3)	F(10)-C(50)-C(49)	116.1(3)
C(45)-B(1)-C(51)	99.3(3)	F(10)-C(50)-C(45)	119.0(3)
C(57)-B(1)-C(51)	114.5(3)	C(49)-C(50)-C(45)	124.9(4)
C(40)-C(39)-C(44)	113.2(3)	C(56)-C(51)-C(52)	113.1(3)
C(40)-C(39)-B(1)	119.7(3)	C(56)-C(51)-B(1)	127.4(3)
C(44)-C(39)-B(1)	126.8(3)	C(52)-C(51)-B(1)	118.7(3)
F(1)-C(40)-C(41)	116.1(3)	F(11)-C(52)-C(53)	116.3(3)
F(1)-C(40)-C(39)	119.2(3)	F(11)-C(52)-C(51)	119.1(3)
C(41)-C(40)-C(39)	124.7(4)	C(53)-C(52)-C(51)	124.6(4)
F(2)-C(41)-C(42)	120.1(4)	F(12)-C(53)-C(52)	120.5(4)
F(2)-C(41)-C(40)	121.0(4)	F(12)-C(53)-C(54)	119.7(4)
C(42)-C(41)-C(40)	118.9(4)	C(52)-C(53)-C(54)	119.8(4)
F(3)-C(42)-C(43)	121.1(4)	F(13)-C(54)-C(53)	121.4(4)
F(3)-C(42)-C(41)	119.5(4)	F(13)-C(54)-C(55)	120.1(4)
C(43)-C(42)-C(41)	119.4(4)	C(53)-C(54)-C(55)	118.5(4)
C(42)-C(43)-F(4)	120.0(4)	F(14)-C(55)-C(54)	119.5(4)
C(42)-C(43)-C(44)	120.0(4)	F(14)-C(55)-C(56)	120.3(4)
F(4)-C(43)-C(44)	119.9(4)	C(54)-C(55)-C(56)	120.2(4)
F(5)-C(44)-C(43)	115.2(4)	F(15)-C(56)-C(51)	121.1(3)
F(5)-C(44)-C(39)	121.2(4)	F(15)-C(56)-C(55)	115.0(3)
C(43)-C(44)-C(39)	123.7(4)	C(51)-C(56)-C(55)	123.8(4)
C(46)-C(45)-C(50)	112.4(3)	C(62)-C(57)-C(58)	113.1(3)
C(46)-C(45)-B(1)	128.2(3)	C(62)-C(57)-B(1)	126.4(3)
C(50)-C(45)-B(1)	118.7(3)	C(58)-C(57)-B(1)	120.0(3)
F(6)-C(46)-C(47)	115.8(3)	F(16)-C(58)-C(59)	116.2(3)
F(6)-C(46)-C(45)	120.2(3)	F(16)-C(58)-C(57)	119.2(3)
C(47)-C(46)-C(45)	123.9(4)	C(59)-C(58)-C(57)	124.6(4)
F(7)-C(47)-C(48)	119.8(4)	F(17)-C(59)-C(60)	120.6(4)
F(7)-C(47)-C(46)	119.8(4)	F(17)-C(59)-C(58)	120.3(4)

C(60)-C(59)-C(58)	119.0(4)
F(18)-C(60)-C(59)	120.4(4)
F(18)-C(60)-C(61)	120.4(4)
C(59)-C(60)-C(61)	119.2(4)
F(19)-C(61)-C(60)	119.4(4)
F(19)-C(61)-C(62)	120.6(4)
C(60)-C(61)-C(62)	120.0(4)
F(20)-C(62)-C(61)	114.8(3)
F(20)-C(62)-C(57)	121.1(3)
C(61)-C(62)-C(57)	124.1(3)
Br(1B)-Br(1)-C(63)	74.2(4)
Br(1B)-Br(1)-Br(1A)	19.8(5)
C(63)-Br(1)-Br(1A)	55.9(3)
Br(1B)-Br(1A)-C(63)	59.1(4)
Br(1B)-Br(1A)-Br(1)	14.3(3)
C(63)-Br(1A)-Br(1)	45.9(2)
Br(1)-Br(1B)-Br(1A)	145.9(7)
Br(1)-Br(1B)-C(63)	71.3(4)
Br(1A)-Br(1B)-C(63)	76.8(5)
C(64)-C(63)-C(68)	120.0
C(64)-C(63)-Br(1)	123.0(4)
C(68)-C(63)-Br(1)	117.0(4)
C(64)-C(63)-Br(1B)	89.3(5)
C(68)-C(63)-Br(1B)	149.6(5)
Br(1)-C(63)-Br(1B)	34.6(3)
C(64)-C(63)-Br(1A)	45.2(4)
C(68)-C(63)-Br(1A)	163.6(4)
Br(1)-C(63)-Br(1A)	78.2(4)
Br(1B)-C(63)-Br(1A)	44.1(4)
C(65)-C(64)-C(63)	120.0
C(64)-C(65)-C(66)	120.0
C(67)-C(66)-C(65)	120.0
C(68)-C(67)-C(66)	120.0
C(67)-C(68)-C(63)	120.0

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (^{2}x 10 ^{3}) for **1c**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Sc(1)	33(1)	36(1)	32(1)	-1(1)	10(1)	-1(1)
N(1)	36(2)	34(2)	33(2)	-3(1)	8(1)	1(1)
N(2)	38(2)	32(2)	29(2)	-1(1)	10(1)	-5(1)
C(1)	43(2)	40(2)	33(2)	1(2)	8(2)	0(2)
C(3)	38(2)	42(2)	52(2)	-7(2)	13(2)	-6(2)
C(4)	36(2)	33(2)	33(2)	4(2)	7(2)	1(2)
C(5)	37(2)	37(2)	35(2)	2(2)	16(2)	-3(2)
C(6)	36(2)	35(2)	29(2)	3(2)	9(2)	2(2)
C(7)	46(2)	46(2)	47(2)	-6(2)	22(2)	-4(2)
C(8)	32(2)	45(2)	43(2)	-11(2)	11(2)	-3(2)
C(9)	35(2)	42(2)	55(3)	-15(2)	8(2)	-5(2)
C(10)	50(3)	54(3)	71(3)	-23(3)	20(2)	-4(2)
C(11)	58(3)	77(4)	64(3)	-33(3)	26(3)	-9(3)
C(12)	49(3)	77(3)	44(3)	-10(2)	15(2)	-2(2)
C(13)	34(2)	59(3)	34(2)	-7(2)	10(2)	-1(2)
C(14)	69(3)	84(4)	55(3)	16(3)	27(3)	11(3)
C(15)	45(2)	64(3)	32(2)	4(2)	10(2)	7(2)
C(16)	58(3)	95(4)	76(3)	25(3)	28(3)	23(3)
C(17)	54(3)	58(3)	100(4)	-1(3)	-1(3)	4(2)
C(18)	49(3)	39(2)	65(3)	-6(2)	5(2)	3(2)
C(19)	65(3)	46(3)	78(3)	-1(2)	13(3)	-6(2)
C(20)	35(2)	35(2)	36(2)	-6(2)	15(2)	-3(2)
C(21)	45(2)	38(2)	41(2)	2(2)	15(2)	-4(2)
C(22)	58(3)	40(2)	54(3)	5(2)	22(2)	-4(2)
C(23)	56(3)	38(2)	64(3)	-11(2)	23(2)	-15(2)
C(24)	47(2)	43(2)	45(2)	-10(2)	12(2)	-7(2)
C(25)	41(2)	38(2)	41(2)	-6(2)	15(2)	-4(2)
C(26)	74(3)	80(3)	45(3)	3(2)	19(2)	-6(3)
C(27)	53(3)	46(2)	39(2)	-2(2)	1(2)	-7(2)
C(28)	69(3)	69(3)	48(3)	5(2)	13(2)	10(3)

C(29)	45(3)	218(8)	66(4)	45(4)	8(3)	-11(4)
C(30)	76(3)	45(2)	48(3)	12(2)	9(2)	-15(2)
C(31)	68(3)	77(3)	49(3)	14(2)	19(2)	12(3)
C(32)	34(2)	57(3)	54(3)	7(2)	13(2)	2(2)
C(33)	38(2)	53(3)	50(2)	-2(2)	17(2)	-10(2)
C(34)	38(2)	50(2)	56(3)	9(2)	22(2)	-1(2)
C(35)	45(3)	76(3)	43(2)	7(2)	19(2)	-7(2)
C(36)	53(3)	75(3)	50(3)	-19(2)	30(2)	-13(2)
C(37)	53(3)	47(2)	72(3)	-6(2)	36(3)	1(2)
C(38)	64(3)	70(3)	96(4)	18(3)	28(3)	12(3)
F(1)	44(1)	49(1)	40(1)	-3(1)	11(1)	5(1)
F(2)	61(2)	73(2)	62(2)	-20(1)	30(1)	-2(1)
F(3)	86(2)	101(2)	44(1)	-23(1)	34(1)	-30(2)
F(4)	73(2)	91(2)	32(1)	9(1)	3(1)	-21(2)
F(5)	53(2)	59(2)	43(1)	14(1)	4(1)	-3(1)
F(6)	52(1)	41(1)	53(1)	-5(1)	11(1)	-12(1)
F(7)	56(2)	44(1)	79(2)	16(1)	6(1)	-14(1)
F(8)	55(2)	83(2)	71(2)	44(2)	19(1)	-5(1)
F(9)	62(2)	83(2)	43(1)	15(1)	25(1)	11(1)
F(10)	58(2)	47(1)	42(1)	-4(1)	18(1)	-2(1)
F(11)	40(1)	43(1)	51(1)	-1(1)	7(1)	-9(1)
F(12)	35(1)	68(2)	65(2)	9(1)	4(1)	-3(1)
F(13)	47(2)	71(2)	74(2)	10(1)	21(1)	18(1)
F(14)	64(2)	47(1)	75(2)	-2(1)	28(1)	7(1)
F(15)	44(1)	42(1)	61(2)	-7(1)	16(1)	-6(1)
F(16)	54(2)	48(1)	50(1)	11(1)	15(1)	-7(1)
F(17)	73(2)	51(1)	63(2)	1(1)	33(1)	-22(1)
F(18)	51(2)	78(2)	77(2)	-8(2)	15(1)	-33(1)
F(19)	41(1)	72(2)	60(2)	0(1)	-2(1)	-7(1)
F(20)	41(1)	44(1)	45(1)	5(1)	7(1)	-4(1)
B(1)	35(2)	38(2)	31(2)	0(2)	8(2)	-4(2)
C(39)	37(2)	37(2)	35(2)	-2(2)	10(2)	-13(2)
C(40)	40(2)	44(2)	32(2)	0(2)	8(2)	-10(2)
C(41)	44(2)	50(2)	50(3)	-13(2)	22(2)	-9(2)
C(42)	62(3)	62(3)	36(2)	-12(2)	24(2)	-24(2)
C(43)	52(3)	63(3)	31(2)	3(2)	8(2)	-24(2)

C(44)	43(2)	43(2)	41(2)	6(2)	10(2)	-11(2)
C(45)	26(2)	39(2)	39(2)	4(2)	9(2)	-1(2)
C(46)	32(2)	42(2)	41(2)	5(2)	6(2)	-1(2)
C(47)	29(2)	37(2)	61(3)	12(2)	5(2)	-10(2)
C(48)	33(2)	60(3)	49(3)	26(2)	10(2)	1(2)
C(49)	34(2)	63(3)	38(2)	10(2)	12(2)	8(2)
C(50)	32(2)	42(2)	41(2)	5(2)	10(2)	0(2)
C(51)	37(2)	34(2)	39(2)	6(2)	12(2)	-5(2)
C(52)	42(2)	37(2)	39(2)	9(2)	12(2)	-1(2)
C(53)	36(2)	49(2)	48(2)	16(2)	8(2)	-2(2)
C(54)	37(2)	49(3)	59(3)	19(2)	17(2)	12(2)
C(55)	55(3)	33(2)	50(2)	4(2)	20(2)	6(2)
C(56)	38(2)	41(2)	46(2)	8(2)	11(2)	-2(2)
C(57)	37(2)	33(2)	34(2)	-7(2)	14(2)	-7(2)
C(58)	42(2)	40(2)	35(2)	1(2)	12(2)	0(2)
C(59)	56(3)	36(2)	47(2)	-6(2)	29(2)	-15(2)
C(60)	38(2)	53(3)	50(3)	-10(2)	16(2)	-15(2)
C(61)	38(2)	54(3)	36(2)	-6(2)	7(2)	-3(2)
C(62)	37(2)	35(2)	36(2)	-5(2)	12(2)	-5(2)
Br(1)	63(1)	124(1)	121(1)	-62(1)	9(1)	24(1)
Br(1A)	192(8)	204(9)	109(5)	30(5)	72(6)	108(8)
Br(1B)	133(6)	113(5)	112(5)	-27(4)	61(4)	36(5)
C(63)	53(4)	95(5)	122(6)	-26(4)	23(4)	28(3)
C(64)	76(4)	114(5)	114(6)	18(5)	49(4)	36(4)
C(65)	65(4)	96(5)	157(7)	2(5)	50(5)	1(4)
C(66)	34(3)	86(4)	155(7)	-40(5)	6(3)	9(3)
C(67)	132(6)	78(4)	114(5)	42(4)	66(5)	60(4)
C(68)	65(4)	63(3)	134(6)	-12(4)	35(4)	8(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (^{2}x 10 ^{3}) for **1c.**

	x	y	z	U(eq)
H(1A)	-3535	-3805	4576	59
H(1B)	-3948	-4667	4188	59
H(1C)	-4393	-3995	4498	59
H(3A)	-6442	-4633	2719	66
H(3B)	-6988	-3838	2830	66
H(3C)	-6622	-4598	3314	66
H(5)	-6361	-3023	3800	43
H(7A)	-5469	-974	4412	67
H(7B)	-5892	-1858	4582	67
H(7C)	-6293	-1229	4038	67
H(10)	-5055	-6331	2143	69
H(11)	-5367	-5594	1266	77
H(12)	-5678	-4002	1179	68
H(14A)	-5711	-1538	1432	101
H(14B)	-5829	-2518	1089	101
H(14C)	-5031	-2251	1505	101
H(15)	-5480	-2372	2302	57
H(16A)	-6704	-1887	1841	112
H(16B)	-6700	-2821	2212	112
H(16C)	-6877	-2900	1537	112
H(17A)	-4040	-6427	3686	113
H(17B)	-3806	-5565	3351	113
H(17C)	-4116	-6530	3024	113
H(18)	-4977	-5228	3475	64
H(19A)	-5330	-6826	3550	97
H(19B)	-5481	-6967	2881	97
H(19C)	-5988	-6259	3113	97
H(22)	-4468	1122	3480	59
H(23)	-3644	1343	4373	62
H(24)	-3382	134	5031	54

H(26A)	-3997	-1827	5799	99
H(26B)	-4642	-1193	5395	99
H(26C)	-3840	-744	5676	99
H(27)	-4154	-2220	4827	58
H(28A)	-2965	-2390	5472	94
H(28B)	-2761	-1328	5343	94
H(28C)	-2902	-2120	4857	94
H(29A)	-6166	-175	3298	167
H(29B)	-6364	-79	2622	167
H(29C)	-5937	762	3022	167
H(30)	-5343	-1080	2935	70
H(31A)	-5388	-95	2156	96
H(31B)	-4546	-306	2505	96
H(31C)	-4911	697	2571	96
H(33)	-2770	-1786	3976	55
H(34)	-3610	-1232	3137	56
H(35)	-4133	-2287	2395	64
H(36)	-3786	-3883	2486	67
H(37)	-2956	-4436	3319	65
H(38A)	-2109	-4214	4218	113
H(38B)	-2320	-3401	4597	113
H(38C)	-1705	-3204	4282	113
H(64)	-3353	4014	1989	116
H(65)	-4159	3202	1228	123
H(66)	-4174	3554	296	116
H(67)	-3384	4720	126	122
H(68)	-2577	5533	887	103