Supporting Information for:
Cationic Aluminum Alkyl Complexes Incorporating Aminotroponimate Ligands

Andrey V. Korolev,[†] Eiji Ihara,[†] Ilia A. Guzei,[‡] Victor G. Young, Jr.,[§] and Richard F. Jordan^{†*}

[†]*Department of Chemistry, The University of Chicago, 5735 S. Ellis Ave., Chicago, Illinois 60637*

[‡]*Department of Chemistry, Iowa State University, Ames, Iowa 50011*

[§]*Department of Chemistry, University of Minnesota, Minneapolis, Minnesota 55455*

94 pages

Contents	Page
Additional Experimental Details and NMR Data for New Compounds (Part I) (see also Part II, pages S88-S94)	S3
I. X-ray Crystallographic Analysis of (ⁱ Pr ₂ -ATI)Al(C ₆ F ₅)(μ-H) ₂ B(C ₆ F ₅) ₂ (3)	S8
Molecular Structure and Atom Labeling Scheme for 3	S10
Unit Cell Diagram for 3	S11
Table 1. Crystal Data, Data Collection and Solution Refinement for 3	S12
Table 2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for 3	S13
Table 3. Bond Lengths (Å) and Angles (deg) for 3	S14
Table 4. Anisotropic Displacement Parameters for 3	S16
Table 5. Torsion Angles for 3	S17
Table 6. Hydrogen Coordinates and Isotropic Displacement Parameters for 3	S19
II. X-ray Crystallographic Analysis of [(ⁱ Pr ₂ -ATI)Al(Et)(ClPh)][B(C ₆ F ₅) ₄]·0.5PhCl (4c (ClPh)·0.5PhCl)	S20
Molecular Structure and Atom Labeling Scheme for 4c (ClPh)·0.5PhCl	S22
Unit Cell Diagram for 4c (ClPh)·0.5PhCl	S23
Table 1. Crystal Data, Data Collection and Solution Refinement for 4c (ClPh)·0.5PhCl	S24
Table 2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for 4c (ClPh)·0.5PhCl	S25
Table 3. Bond Lengths (Å) and Angles (deg) for 4c (ClPh)·0.5PhCl	S28
Table 4. Anisotropic Displacement Parameters for 4c (ClPh)·0.5PhCl	S34
Table 5. Hydrogen Coordinates and Isotropic Displacement Parameters for 4c (ClPh)·0.5PhCl	S37
Table 6. Torsion Angles for 4c (ClPh)·0.5PhCl	S38
III. X-ray Crystallographic Analysis of [(ⁱ Pr ₂ -ATI)Al(Et)(NCMe)][B(C ₆ F ₅) ₄] (8c)	S43
Molecular Structure and Atom Labeling Scheme for 8c	S45

Table 1. Crystal Data, Data Collection and Solution Refinement for 8c	S48
Table 2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for 8c	S49
Table 3. Bond Lengths (Å) and Angles (deg) for 8c	S51
Table 4. Anisotropic Displacement Parameters for 8c	S57
Table 5. Hydrogen Coordinates and Isotropic Displacement Parameters for 8c	S59
IV. X-ray Crystallographic Analysis of [AlEt(μ- ⁱ Pr ₂ -ATI)(μ-Et)AlEt ₂][B(C ₆ F ₅) ₄] (15)	S60
Molecular Structure and Atom Labeling Scheme for 15	S62
Unit Cell Diagram for 15	S65
Table 1. Crystal Data, Data Collection and Solution Refinement for 15	S66
Table 2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for 15	S67
Table 3. Bond Lengths (Å) and Angles (deg) for 15	S70
Table 4. Anisotropic Displacement Parameters for 15	S76
Table 5. Hydrogen Coordinates and Isotropic Displacement Parameters for 15	S79
Table 6. Torsion Angles for 15	S81
Additional Experimental Details and NMR Data for New Compounds (Part I)	S88

Additional Experimental Details and NMR Data for New Compounds (Part I)

NMR data for $(^i\text{Pr}_2\text{-ATI})\text{AlEt}_2$ (1c). ^1H NMR (CD_2Cl_2) δ 7.10 (m, 2H, H4&H6), 6.67 (d, $^3J_{\text{HH}} = 11.5$, 2H, H3&H7), 6.42 (t, $^3J_{\text{HH}} = 9$, 1H, H5), 3.96 (sept, $^3J_{\text{HH}} = 6.5$, 2H, Me_2CHN), 1.37 (d, $^3J_{\text{HH}} = 6.5$, 12H, Me_2CHN), 0.93 (t, $^3J_{\text{HH}} = 8$, 3H, AlCH_2CH_3), -0.04 (q, $^3J_{\text{HH}} = 8$, 2H, AlCH_2CH_3). ^1H NMR ($\text{C}_6\text{D}_5\text{CD}_3$) δ 6.76 (m, 2H, H4&H6), 6.34 (d, $^3J_{\text{HH}} = 11.5$, 2H, H3&H7), 6.20 (t, $^3J_{\text{HH}} = 9$, 1H, H5), 3.57 (sept, $^3J_{\text{HH}} = 6.5$, 2H, Me_2CHN), 1.26 (t, $^3J_{\text{HH}} = 8$, 3H, AlCH_2CH_3), 1.23 (d, $^3J_{\text{HH}} = 6.5$, 12H, Me_2CHN), 0.29 (q, $^3J_{\text{HH}} = 8$, 2H, AlCH_2CH_3). ^{13}C NMR ($\text{C}_6\text{D}_5\text{CD}_3$) δ 161.7 (s, C1&C2), 136.5 (d, $^1J_{\text{CH}} = 152$, C4&C6), 119.1 (d, $^1J_{\text{CH}} = 159$, C5), 113.5 (d, $^1J_{\text{CH}} = 152$, C3&C7), 47.5 (d, $^1J_{\text{CH}} = 133$, Me_2CHN), 22.2 (q, $^1J_{\text{CH}} = 126$, Me_2CHN), 9.8 (q, $^1J_{\text{CH}} = 123$, AlCH_2CH_3), 4.2 (t, $^1J_{\text{CH}} = 113$, AlCH_2CH_3).

NMR data for $[(^i\text{Pr}_2\text{-ATI})\text{AlH}]_2(\mu\text{-H})[\text{B}(\text{C}_6\text{F}_5)_4]$ (2a). ^1H NMR (C_6D_6 , liquid clathrate) δ 6.95 (t, $^3J_{\text{HH}} = 10.5$, 4H, H4&H6), 6.53 (t, $^3J_{\text{HH}} = 9.5$, 2H, H5), 6.52 (d, $^3J_{\text{HH}} = 11$, 4H, H3&H7), 4.54 (br, 3H, AlH), 3.28 (sept, $^3J_{\text{HH}} = 6$, 4H, Me_2CHN), 0.92 (d, $^3J_{\text{HH}} = 6$, 24H, Me_2CHN). ^1H NMR (CD_2Cl_2 , 0 °C) δ 7.52 (t, $^3J_{\text{HH}} = 10.5$, 4H, H4&H6), 7.13 (d, $^3J_{\text{HH}} = 11.5$, 4H, H3&H7), 7.03 (t, $^3J_{\text{HH}} = 9$, 2H, H5), 4.66 (br, 3H, AlH), 3.97 (sept, $^3J_{\text{HH}} = 6.5$, 4H, Me_2CHN), 1.30 (d, $^3J_{\text{HH}} = 6.5$, 24H, Me_2CHN). ^{13}C NMR (C_6D_6 , liquid clathrate) δ 158.7 (s, C1&C2), 138.5 (d, $^1J_{\text{CH}} = 157$, C4&C6), 137.1 126.1 (d, $^1J_{\text{CH}} = 162$, C5), 118.3 (d, $^1J_{\text{CH}} = 153$, C3&C7), 46.9 (d, $^1J_{\text{CH}} = 138$, Me_2CHN), 22.4 (q, $^1J_{\text{CH}} = 127$, Me_2CHN). ^{13}C , ^{11}B and ^{19}F NMR spectra confirmed that $\text{B}(\text{C}_6\text{F}_5)_4^-$ anion is free.

NMR data for $[(^i\text{Pr}_2\text{-ATI})\text{AlMe}]_2(\mu\text{-Me})[\text{B}(\text{C}_6\text{F}_5)_4]$ (2b). ^1H NMR (C_6D_6 , 50 °C, liquid clathrate) δ 6.94 (t, $^3J_{\text{HH}} = 10$, 4H, H4&H6), 6.50 (d, $^3J_{\text{HH}} = 12$, 4H, H3&H7), 6.47 (t, $^3J_{\text{HH}} = 9$, 2H, H5), 3.47 (sept, $^3J_{\text{HH}} = 6.5$, 4H, Me_2CHN), 0.97 (d, $^3J_{\text{HH}} = 6.5$, 24H, Me_2CHN), -0.11 (s, 9H, AlMe). ^{13}C NMR (C_6D_6 , 50 °C, liquid clathrate) δ 160.7 (s, C1&C2), 138.2 (d, $^1J_{\text{CH}} = 156$, C4&C6), 124.8 (d, $^1J_{\text{CH}} = 163$, C5), 117.0 (d, $^1J_{\text{CH}} = 153$, C3&C7), 46.0 (d, $^1J_{\text{CH}} = 136$, Me_2CHN), 22.6 (q, $^1J_{\text{CH}} = 126$, Me_2CHN), -2.7 (q, $^1J_{\text{CH}} = 120$, AlMe). ^{13}C , ^{11}B and ^{19}F NMR spectra confirmed that $\text{B}(\text{C}_6\text{F}_5)_4^-$ anion is free.

NMR data for [ⁱPr₂-ATI)AlEt][B(C₆F₅)₄] (4c). ¹H NMR (C₆D₆, liquid clathrate) δ 7.12 (t, ³J_{HH} = 11, 2H, H4&H6), 6.77 (t, ³J_{HH} = 9, 1H, H5), 6.77 (d, ³J_{HH} = 11.5, 2H, H3&H7), 3.33 (sept, ³J_{HH} = 6.5, 2H, Me₂CHN), 0.95 (t, ³J_{HH} = 8, 3H, AlCH₂CH₃), 0.89 (d, ³J_{HH} = 6.5, 12H, Me₂CHN), 0.22 (q, ³J_{HH} = 8, 2H, AlCH₂CH₃). ¹H NMR (C₆D₆, 50 °C, liquid clathrate) δ 7.15 (t, ³J_{HH} = 11, 2H, H4&H6), 6.82 (d, ³J_{HH} = 11, 2H, H3&H7), 6.79 (t, ³J_{HH} = 10, 1H, H5), 3.40 (sept, ³J_{HH} = 6.5, 2H, Me₂CHN), 0.96 (t, ³J_{HH} = 8, 3H, AlCH₂CH₃), 0.93 (d, ³J_{HH} = 6.5, 12H, Me₂CHN), 0.27 (q, ³J_{HH} = 8, 2H, AlCH₂CH₃). ¹H NMR (C₆D₅CD₃, liquid clathrate) δ 7.14 (t, ³J_{HH} = 10, 2H, H4&H6), 6.76 (d, ³J_{HH} = 12, 2H, H3&H7), 6.76 (t, ³J_{HH} = 9, 1H, H5), 3.32 (sept, ³J_{HH} = 6.5, 2H, Me₂CHN), 0.98 (t, ³J_{HH} = 8.5, 3H, AlCH₂CH₃), 0.92 (d, ³J_{HH} = 6.5, 12H, Me₂CHN), 0.23 (q, ³J_{HH} = 8.5, 2H, AlCH₂CH₃). ¹³C NMR (C₆D₆, liquid clathrate) δ 159.5 (s, C1&C2), 138.9 (d, ¹J_{CH} = 158, C4&C6), 129.5 (d, ¹J_{CH} = 163, C5), 120.7 (d, ¹J_{CH} = 154, C3&C7), 47.1 (d, ¹J_{CH} = 138, Me₂CHN), 22.6 (q, ¹J_{CH} = 127, Me₂CHN), 7.1 (q, ¹J_{CH} = 128, AlCH₂CH₃), 3.4 (t, ¹J_{CH} = 119, AlCH₂CH₃). ¹³C NMR (C₆D₆, 50 °C, liquid clathrate) δ 159.6 (s, C1&C2), 138.9 (d, ¹J_{CH} = 156, C4&C6), 129.5 (d, ¹J_{CH} = 161, C5), 120.8 (d, ¹J_{CH} = 154, C3&C7), 47.2 (d, ¹J_{CH} = 138, Me₂CHN), 22.7 (q, ¹J_{CH} = 127, Me₂CHN), 7.1 (q, ¹J_{CH} = 128, AlCH₂CH₃), 3.2 (t, ¹J_{CH} = 120, AlCH₂CH₃). ¹³C NMR (C₆D₅CD₃, liquid clathrate) δ 159.9 (s, C1&C2), 139.0 (d, ¹J_{CH} = 158, C4&C6), 129.2 (d, ¹J_{CH} = 163, C5), 120.8 (d, ¹J_{CH} = 154, C3&C7), 47.3 (d, ¹J_{CH} = 138, Me₂CHN), 22.5 (q, ¹J_{CH} = 127, Me₂CHN), 7.4 (q, ¹J_{CH} = 127, AlCH₂CH₃), 4.6 (t, ¹J_{CH} = 119, AlCH₂CH₃). ¹³C, ¹¹B and ¹⁹F NMR spectra confirmed that B(C₆F₅)₄⁻ anion is free.

NMR data for [ⁱPr₂-ATI)AlⁱBu][B(C₆F₅)₄] (4e). ¹H NMR (C₆D₆, 60 °C, liquid clathrate) δ 7.23 (m, ³J_{HH} = 10, 2H, H4&H6), 6.98 (d, ³J_{HH} = 11, 2H, H3&H7), 6.86 (t, ³J_{HH} = 9.5, 1H, H5), 3.59 (sept, ³J_{HH} = 6.5, 2H, Me₂CHN), 1.91 (nonet, ³J_{HH} = 6.5, 2H, AlCH₂CHMe₂), 1.06 (d, ³J_{HH} = 6.5, 12H, Me₂CHN), 0.93 (d, ³J_{HH} = 6.5, 6H, AlCH₂CHMe₂), 0.64 (d, ³J_{HH} = 7.5, 2H, AlCH₂CHMe₂). ¹³C NMR (C₆D₆, 50 °C, liquid clathrate) δ 159.6 (s, C1&C2), 139.1 (d, ¹J_{CH} = 157, C4&C6), 129.8 (d, ¹J_{CH} = 158, C5), 120.9 (d, ¹J_{CH} = 154, C3&C7), 47.3 (d, ¹J_{CH} = 138, Me₂CHN), 27.8 (q, ¹J_{CH} = 125, AlCH₂CHMe₂), 25.4 (d, ¹J_{CH} = 125, AlCH₂CHMe₂), 23.9 (t, ¹J_{CH} = 115, AlCH₂CHMe₂), 22.9 (q, ¹J_{CH} = 127, Me₂CHN). ¹³C, ¹¹B and ¹⁹F NMR spectra confirmed that B(C₆F₅)₄⁻ anion is free.

Reaction of $[(^i\text{Pr}_2\text{-ATI})\text{AlEt}][\text{B}(\text{C}_6\text{F}_5)_4]$ and $(^i\text{Pr}_2\text{-ATI})\text{AlEt}_2$ in 1:1 ratio in $\text{C}_6\text{D}_5\text{CD}_3$. A resealable NMR tube was charged with $[(^i\text{Pr}_2\text{-ATI})\text{AlEt}][\text{B}(\text{C}_6\text{F}_5)_4]$ (115 mg, 122 μmol) and $(^i\text{Pr}_2\text{-ATI})\text{AlEt}_2$ (35 mg, 120 μmol), and $\text{C}_6\text{D}_5\text{CD}_3$ (ca. 0.5 mL) was added by vacuum transfer at -78°C . The tube was warmed to room temperature and phase separation occurred producing a dark red, dense oil (clathrate) which composed ca. 90 % of the sample by volume and a pale yellow solution above it. NMR spectra of the clathrate were taken and contained only one set of $(^i\text{Pr}_2\text{-ATI})$ and Et resonances which appeared at the weighted average of $[(^i\text{Pr}_2\text{-ATI})\text{AlEt}][\text{B}(\text{C}_6\text{F}_5)_4]$ and $(^i\text{Pr}_2\text{-ATI})\text{AlEt}_2$. The sample was evaporated under vacuum and extracted with pentane (6 x 2 mL) leaving behind a yellow powder which was identified as $[(^i\text{Pr}_2\text{-ATI})\text{AlEt}][\text{B}(\text{C}_6\text{F}_5)_4]$ by NMR. The pentane washes were combined and evaporated under vacuum leaving a yellow solid which was identified as $(^i\text{Pr}_2\text{-ATI})\text{AlEt}_2$ by NMR. NMR data for 1:1 mixture: ^1H NMR ($\text{C}_6\text{D}_5\text{CD}_3$, liquid clathrate) δ 6.95 (br t, $^3J_{\text{HH}} = 10$, 4H, H4&H6), 6.55 (br d, $^3J_{\text{HH}} = 11$, 4H, H3&H7), 6.41 (br t, $^3J_{\text{HH}} = 8.5$, 2H, H5), 3.48 (br sept, $^3J_{\text{HH}} = 6.5$, 4H, Me_2CHN), 1.05 (br d, $^3J_{\text{HH}} = 5$, 24H, Me_2CHN), 0.96 (br t, $^3J_{\text{HH}} = 7$, 9H, AlCH_2CH_3), 0.16 (br q, $^3J_{\text{HH}} = 7$, 6H, AlCH_2CH_3). ^{13}C NMR ($\text{C}_6\text{D}_5\text{CD}_3$, liquid clathrate) δ 161.3 (s, C1&C2), 139.4 (d, $^1J_{\text{CH}} = 155$, C4&C6), 122.3 (d, $^1J_{\text{CH}} = 160$, C5), 117.3 (d, $^1J_{\text{CH}} = 153$, C3&C7), 47.6 (d, $^1J_{\text{CH}} = 137$, Me_2CHN), 22.3 (q, $^1J_{\text{CH}} = 126$, Me_2CHN), 8.0 (q, $^1J_{\text{CH}} = 126$, AlCH_2CH_3), 4.5 (t, $^1J_{\text{CH}} = 114$, AlCH_2CH_3). The same experiment was done in CD_2Cl_2 at -90°C . Signals were significantly broad, and only one set of signals was observed for $(^i\text{Pr}_2\text{-ATI})$ ligands and Et groups. ^1H NMR (CD_2Cl_2 , -90°C) δ 7.35 (br, 4H, H4&H6), 6.97 (br d, $^3J_{\text{HH}} = 11$, 4H, H3&H7), 6.77 (br, 2H, H5), 3.98 (br, 4H, Me_2CHN), 1.31 (br, 24H, Me_2CHN), 0.86 (br, 9H, AlCH_2CH_3), -0.15 (br, 6H, AlCH_2CH_3). $^{13}\text{C}\{\text{H}\}$ NMR (CD_2Cl_2 , -90°C) δ 160.4 (C1&C2), 137.8 (C4&C6), 122.0 (C5), 116.5 (C3&C7), 46.8 (Me_2CHN), 21.8 (Me_2CHN), 7.5 (AlCH_2CH_3), 4.4 (AlCH_2CH_3).

Reaction of $(^i\text{Pr}_2\text{-ATI})\text{AlEt}_2$ and $[\text{Ph}_3\text{C}][\text{B}(\text{C}_6\text{F}_5)_4]$ in 2:1 ratio in $\text{C}_6\text{D}_5\text{Cl}$. $(^i\text{Pr}_2\text{-ATI})\text{AlEt}_2$ (33 mg, 110 μmol) and $[\text{Ph}_3\text{C}][\text{B}(\text{C}_6\text{F}_5)_4]$ (52 mg, 56 μmol) were placed in an NMR tube. $\text{C}_6\text{D}_5\text{Cl}$ (ca. 0.5 mL) was added by vacuum transfer at -78°C . The tube was warmed to 23°C and a rapid reaction occurred affording a homogeneous solution after a few seconds. The NMR spectra contained only one set of $(^i\text{Pr}_2\text{-ATI})$ and Et resonances which appeared at the weighted

average of $[(^i\text{Pr}_2\text{-ATI})\text{AlEt}][\text{B}(\text{C}_6\text{F}_5)_4]$ and $(^i\text{Pr}_2\text{-ATI})\text{AlEt}_2$. ^1H NMR ($\text{C}_6\text{D}_5\text{Cl}$) δ 7.04 (t, $^3J_{\text{HH}} = 11$, 4H, H4&H6), 6.61 (d, $^3J_{\text{HH}} = 11$, 4H, H3&H7), 6.53 (t, $^3J_{\text{HH}} = 9$, 2H, H5), 3.61 (sept, $^3J_{\text{HH}} = 6.5$, 4H, Me_2CHN), 1.18 (d, $^3J_{\text{HH}} = 6.5$, 24H, Me_2CHN), 1.07 (t, $^3J_{\text{HH}} = 8$, 9H, AlCH_2CH_3), 0.24 (q, $^3J_{\text{HH}} = 8$, 6H, AlCH_2CH_3). The spectra did not change significantly down to -40°C . $^{13}\text{C}\{\text{H}\}$ NMR ($\text{C}_6\text{D}_5\text{Cl}$) δ 160.8 (C1&C2), 137.9 (C4&C6), 123.3 (C5), 116.6 (C3&C7), 47.4 (Me_2CHN), 22.5 (Me_2CHN), 8.9 (AlCH_2CH_3), 4.0 (AlCH_2CH_3). These spectra also contained resonances for Ph_3CH and ethylene. The same experiment was done in C_6D_6 at 60°C . ^1H NMR (C_6D_6 , 60°C , liquid clathrate) δ 6.96 (t, $^3J_{\text{HH}} = 10.5$, 4H, H4&H6), 6.59 (d, $^3J_{\text{HH}} = 11$, 4H, H3&H7), 6.43 (t, $^3J_{\text{HH}} = 9$, 2H, H5), 3.54 (sept, $^3J_{\text{HH}} = 6.5$, 4H, Me_2CHN), 1.08 (d, $^3J_{\text{HH}} = 6.5$, 24H, Me_2CHN), 1.00 (t, $^3J_{\text{HH}} = 8$, 9H, AlCH_2CH_3), 0.20 (q, $^3J_{\text{HH}} = 8$, 6H, AlCH_2CH_3). $^{13}\text{C}\{\text{H}\}$ NMR (C_6D_6 , 60°C , liquid clathrate) δ 161.2 (C1&C2), 138.7 (C4&C6), 122.5 (C5), 117.3 (C3&C7), 47.5 (Me_2CHN), 22.4 (Me_2CHN), 8.0 (AlCH_2CH_3), 4.2 (AlCH_2CH_3). These spectra also contained resonances for Ph_3CH and ethylene.

Reaction of $[(^i\text{Pr}_2\text{-ATI})\text{AlPr}][\text{B}(\text{C}_6\text{F}_5)_4]$ and $(^i\text{Pr}_2\text{-ATI})\text{AlPr}_2$ in 1:1 ratio in $\text{C}_6\text{D}_5\text{Cl}$. Resealable NMR tube was charged with $[(^i\text{Pr}_2\text{-ATI})\text{AlPr}][\text{B}(\text{C}_6\text{F}_5)_4]$ (75 mg, 79 μmol) and $(^i\text{Pr}_2\text{-ATI})\text{AlPr}_2$ (25 mg, 1.2 μmol), and $\text{C}_6\text{D}_5\text{Cl}$ (ca. 0.5 mL) was added by vacuum transfer at -78°C . A yellow solution formed when the tube was warmed to room temperature. NMR spectra were taken and contained only one set of $(^i\text{Pr}_2\text{-ATI})$ and Et resonances which appeared at the weighted average of $[(^i\text{Pr}_2\text{-ATI})\text{AlPr}][\text{B}(\text{C}_6\text{F}_5)_4]$ and $(^i\text{Pr}_2\text{-ATI})\text{AlPr}_2$. ^1H NMR ($\text{C}_6\text{D}_5\text{Cl}$) δ 7.03 (t, $^3J_{\text{HH}} = 10.5$, 2H, H4&H6), 6.59 (d, $^3J_{\text{HH}} = 11.5$, H3&H7), 6.53 (t, $^3J_{\text{HH}} = 9$, 1H, H5), 3.61 (sept, $^3J_{\text{HH}} = 6.5$, 2H, Me_2CHN), 1.46 (sext, $^3J_{\text{HH}} = 7.5$, 2H, $\text{AlCH}_2\text{CH}_2\text{CH}_3$), 1.19 (d, $^3J_{\text{HH}} = 6.5$, 12H, Me_2CHN), 1.02 (t, $^3J_{\text{HH}} = 7$, 3H, $\text{AlCH}_2\text{CH}_2\text{CH}_3$), 0.29 (t, $^3J_{\text{HH}} = 8$, 2H, $\text{AlCH}_2\text{CH}_2\text{CH}_3$). ^{13}C NMR ($\text{C}_6\text{D}_5\text{Cl}$) δ 160.8 (s, C1&C2), 137.9 (d, $^1J_{\text{CH}} = 155$, C4&C6), 123.3 (d, $^1J_{\text{CH}} = 162$, C5), 116.6 (d, $^1J_{\text{CH}} = 153$, C3&C7), 47.5 (d, $^1J_{\text{CH}} = 135$, Me_2CHN), 22.6 (q, $^1J_{\text{CH}} = 126$, Me_2CHN), 21.0 (q, $^1J_{\text{CH}} = 124$, $\text{AlCH}_2\text{CH}_2\text{CH}_3$), 19.4 (t, $^1J_{\text{CH}} = 125$, $\text{AlCH}_2\text{CH}_2\text{CH}_3$), 16.4 (t, $^1J_{\text{CH}} = 111$, $\text{AlCH}_2\text{CH}_2\text{CH}_3$). ^{13}C , ^{11}B and ^{19}F NMR spectra confirmed that $\text{B}(\text{C}_6\text{F}_5)_4^-$ anion is free.

Reaction of (*i*Pr₂-ATI)Al^{*i*}Bu₂ and [Ph₃C][B(C₆F₅)₄] in 2:1 ratio in C₆D₅Cl.

(*i*Pr₂-ATI)Al^{*i*}Bu₂ (33 mg, 96 μmol) and [Ph₃C][B(C₆F₅)₄] (43 mg, 47 μmol) were placed in an NMR tube. C₆D₅Cl (ca. 0.5 mL) was added by vacuum transfer at -78 °C. The tube was warmed to 23 °C and a rapid reaction occurred affording a homogeneous solution after a few seconds. NMR spectra were taken and contained only one set of (*i*Pr₂-ATI) and ^{*i*}Bu resonances which appeared at the weighted average of [(*i*Pr₂-ATI)Al^{*i*}Bu]⁺ and (*i*Pr₂-ATI)Al^{*i*}Bu₂. ¹H NMR (C₆D₅Cl) δ 7.03 (m, 4H, H4&H6), 6.59 (d, ³J_{HH} = 11, 4H, H3&H7), 6.51 (t, ³J_{HH} = 9, 2H, H5), 3.63 (sept, ³J_{HH} = 6.5, 4H, Me₂CHN), 1.91 (nonet, ³J_{HH} = 6.5, 3H, AlCH₂CHMe₂), 1.24 (d, ³J_{HH} = 6.5, 24H, Me₂CHN), 0.98 (d, ³J_{HH} = 6.5, 18H, AlCH₂CHMe₂), 0.35 (d, ³J_{HH} = 6.5, 6H, AlCH₂CHMe₂). This spectrum also contained resonances for Ph₃CH and isobutylene.

[(*i*Pr₂-ATI)Al(Et)(THF)][B(C₆F₅)₄] was synthesized quantitatively using the procedure for **8c** described in Experimental Section with 1 equiv of THF. The product was observed by NMR only. ¹H NMR (CD₂Cl₂) δ 7.56 (m, 2H, H4&H6), 7.22 (d, ³J_{HH} = 12, 2H, H3&H7), 7.06 (t, ³J_{HH} = 9, 1H, H5), 4.12 (m, 6H, CH₂CH₂O and Me₂CHN), 2.16 (m, 4H, CH₂CH₂O), 1.39 (d, ³J_{HH} = 6.5, 12H, Me₂CHN), 1.14 (t, ³J_{HH} = 8, 3H, AlCH₂CH₃), 0.46 (q, ³J_{HH} = 8, 2H, AlCH₂CH₃). ¹³C{H} NMR (CD₂Cl₂) δ 161.1 (C1&C2), 139.1 (C4&C6), 126.7 (C5), 118.7 (C3&C7), 74.1 (CH₂CH₂O), 47.4 (Me₂CHN), 25.8 (CH₂CH₂O), 23.0 (Me₂CHN), 8.2 (AlCH₂CH₃), the AlCH₂CH₃ resonance was not observed.

[(*i*Pr₂-ATI)Al(Et)(NCPh)][B(C₆F₅)₄] was synthesized quantitatively using the procedure for **8c** described in Experimental Section with 1 equiv of PhCN. The product was observed by NMR only. ¹H NMR (CD₂Cl₂) δ 7.71 (m, 3H, Ph), 7.54 (m, 4H, Ph and H4&H6), 7.18 (d, ³J_{HH} = 11.5, 2H, H3&H7), 7.02 (t, ³J_{HH} = 9, 1H, H5), 4.13 (sept, ³J_{HH} = 6.5, 2H, Me₂CHN), 1.47 (d, ³J_{HH} = 6.5, 12H, Me₂CHN), 1.21 (t, ³J_{HH} = 8, 3H, AlCH₂CH₃), 0.51 (q, ³J_{HH} = 8, 2H, AlCH₂CH₃). ¹³C{H} NMR (CD₂Cl₂) δ 161.4 (C1&C2), 139.0 (C4&C6), 134.6 (Ph), 133.1 (Ph), 130.0 (Ph), 126.1 (C5), 120.4 (PhCN), 118.7 (C3&C7), 110.9 (C_{ipso}), 47.6 (Me₂CHN), 23.3 (Me₂CHN), 8.3 (AlCH₂CH₃), the AlCH₂CH₃ resonance was not observed.

I. X-ray Crystallographic Analysis of $(\text{Pr}_2\text{-ATI})\text{Al}(\text{C}_6\text{F}_5)(\mu\text{-H})_2\text{B}(\text{C}_6\text{F}_5)_2$ (3)

DATA COLLECTION

A crystal of the compound was attached to a glass fiber and mounted on the Siemens SMART system for a data collection at 173(2) K. An initial set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames are oriented such that orthogonal wedges of reciprocal space were surveyed. This produces orientation matrices determined from 95 reflections. Final cell constants are calculated from a set of 4883 strong reflections from the actual data collection. Please refer to Table 1 for additional crystal and refinement information.

The data collection technique used for this specimen is generally known as a hemisphere collection. Here a randomly oriented region of reciprocal space is surveyed to the extent of 1.3 hemispheres to a resolution of 0.84 Å. Three major swaths of frames are collected with 0.30° steps in ω . In the event the lattice is triclinic some additional sets of frames are collected to better model the absorption correction.

STRUCTURE SOLUTION AND REFINEMENT

The space group $\bar{P}1$ was determined based on systematic absences and intensity statistics.¹ A successful direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Several full-matrix least squares / difference Fourier cycles were performed which located the remainder of the non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters unless stated otherwise. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters, except for the bridging hydrides which were refined as isotropic atoms.

The unexpected decomposition product was found.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, 160 Kolthoff Hall, Chemistry Department, The University of Minnesota. All calculations were performed using SGI INDY R4400-SC or Pentium computers using the SHELXTL V5.0 suite of programs. All publications arising from this report MUST either 1) include Victor G. Young, Jr. as a coauthor or 2) acknowledge both Victor G. Young, Jr. and the X-Ray Crystallographic Laboratory.

1. SHELXTL-Plus V5.0, Siemens Industrial Automation, Inc., Madison, WI.

$$\begin{aligned}
 R_{\text{int}} &= \sum |F_o^2 - \langle F_o^2 \rangle| / \sum |F_o^2| \\
 R1 &= \sum ||F_o| - |F_c|| / \sum |F_o| \\
 wR2 &= [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}, \\
 \text{where } w &= q/\sigma^2(F_o^2) + (a \cdot P)^2 + b \cdot P \\
 \text{Goof} = S &= [\sum [w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}
 \end{aligned}$$

Table 1. Crystal data, data collection, and solution and refinement for 3

Crystal Data

Empirical formula	$C_{31}H_{21}AlBF_{15}N_2$
Crystal Habit, color	Block, Yellow
Crystal size	0.40 x 0.32 x 0.28 mm
Crystal system	Triclinic
Space group	$P\bar{1}$
	$a = 10.0419(3) \text{ \AA}$ $\alpha = 105.921(1)^\circ$
	$b = 10.0407(3) \text{ \AA}$ $\beta = 96.061(1)^\circ$
	$c = 15.9755(4) \text{ \AA}$ $\gamma = 95.456(1)^\circ$
Volume	$1527.31(8) \text{ \AA}^3$
Z	2
Formula weight	744.29
Density (calculated)	1.618 Mg/m^3
Absorption coefficient	0.186 mm^{-1}
F(000)	748

Data Collection

Diffractionmeter	Siemens SMART Platform CCD
Wavelength	$0.71073 \text{ \AA}$
Temperature	$173(2) \text{ K}$
θ range for data collection	1.34 to 25.00°
Index ranges	$-11 \leq h \leq 11$, $-11 \leq k \leq 11$, $0 \leq l \leq 18$
Reflections collected	8426
Independent reflections	5101 ($R_{\text{int}} = 0.0220$)

Solution and Refinement

System used	SHELXTL-V5.0
Solution	Direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2(F_o^2) + (AP)^2 + (BP)]^{-1}$, where $P = (F_o^2 + 2F_c^2)/3$, $A = 0.0363$, and $B = 0.8363$
Absorption correction	SADABS (Sheldrick, 1996)
Max. and min. transmission	1.000 and 0.790
Extinction coefficient	$0.0048(8)$
Data / restraints / parameters	5100 / 0 / 464
R indices ($I > 2\sigma(I)$) = 3884)	$R1 = 0.0446$, $wR2 = 0.0951$
R indices (all data)	$R1 = 0.0687$, $wR2 = 0.1091$
Goodness-of-fit on F^2	0.997
Largest diff. peak and hole	0.283 and $-0.249 \text{ e\AA}^{-3}$

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

	x	y	z	U(eq)	SOF
Al(1)	1284(1)	3814(1)	2576(1)	24(1)	1
N(1)	1817(2)	4742(2)	3768(1)	26(1)	1
N(2)	232(2)	5243(2)	2565(1)	25(1)	1
C(1)	1583(2)	6086(3)	3958(2)	25(1)	1
C(2)	2180(3)	7095(3)	4745(2)	34(1)	1
C(3)	2184(3)	8533(3)	5040(2)	38(1)	1
C(4)	1516(3)	9404(3)	4663(2)	40(1)	1
C(5)	621(3)	8997(3)	3896(2)	39(1)	1
C(6)	223(3)	7690(3)	3307(2)	33(1)	1
C(7)	649(2)	6376(3)	3261(2)	24(1)	1
C(8)	2570(3)	4211(3)	4436(2)	31(1)	1
C(9)	3068(3)	2835(3)	4005(2)	43(1)	1
C(10)	1668(3)	4027(3)	5115(2)	40(1)	1
C(11)	-839(3)	5296(3)	1856(2)	29(1)	1
C(12)	-855(3)	4100(3)	1027(2)	39(1)	1
C(13)	-2215(3)	5255(3)	2184(2)	42(1)	1
C(14)	372(3)	1872(3)	2162(2)	28(1)	1
C(15)	673(3)	854(3)	1458(2)	31(1)	1
F(15)	1734(2)	1133(2)	1046(1)	46(1)	1
C(16)	-53(3)	-460(3)	1130(2)	38(1)	1
F(16)	291(2)	-1409(2)	439(1)	58(1)	1
C(17)	-1141(3)	-786(3)	1528(2)	40(1)	1
F(17)	-1865(2)	-2064(2)	1218(1)	56(1)	1
C(18)	-1483(3)	175(3)	2240(2)	38(1)	1
F(18)	-2541(2)	-165(2)	2623(1)	61(1)	1
C(19)	-729(3)	1470(3)	2533(2)	34(1)	1
F(19)	-1107(2)	2408(2)	3232(1)	51(1)	1
B(1)	3104(3)	4224(3)	1896(2)	27(1)	1
C(20)	4016(2)	3399(3)	1213(2)	25(1)	1
C(21)	4004(3)	3576(3)	384(2)	26(1)	1
F(21)	3208(2)	4466(2)	150(1)	34(1)	1
C(22)	4757(3)	2887(3)	-235(2)	30(1)	1
F(22)	4693(2)	3100(2)	-1032(1)	43(1)	1
C(23)	5581(3)	1974(3)	-23(2)	34(1)	1
F(23)	6321(2)	1289(2)	-614(1)	52(1)	1
C(24)	5625(3)	1762(3)	790(2)	34(1)	1
F(24)	6435(2)	863(2)	1000(1)	54(1)	1
C(25)	4857(3)	2461(3)	1389(2)	29(1)	1
F(25)	4950(2)	2205(2)	2181(1)	47(1)	1
C(26)	3568(2)	5880(3)	2342(2)	25(1)	1
C(27)	4611(3)	6366(3)	3034(2)	29(1)	1
F(27)	5261(2)	5431(2)	3340(1)	37(1)	1
C(28)	5044(3)	7757(3)	3441(2)	35(1)	1
F(28)	6079(2)	8168(2)	4106(1)	54(1)	1
C(29)	4378(3)	8753(3)	3181(2)	33(1)	1
F(29)	4766(2)	10117(2)	3587(1)	50(1)	1
C(30)	3326(3)	8333(3)	2506(2)	29(1)	1
F(30)	2664(2)	9297(2)	2260(1)	41(1)	1
C(31)	2956(2)	6926(3)	2095(2)	26(1)	1
F(31)	1923(2)	6582(2)	1427(1)	36(1)	1

Table 3. Bond lengths [Å] and angles [°] for 3

Al(1)-N(2)	1.864(2)	Al(1)-N(1)	1.870(2)
Al(1)-C(14)	1.976(3)	Al(1)-B(1)	2.283(3)
Al(1)-H(14A)	1.82(2)	Al(1)-H(14B)	1.93(2)
N(1)-C(1)	1.349(3)	N(1)-C(8)	1.488(3)
N(2)-C(7)	1.350(3)	N(2)-C(11)	1.492(3)
C(1)-C(2)	1.411(4)	C(1)-C(7)	1.488(4)
C(2)-C(3)	1.390(4)	C(2)-H(2A)	0.95
C(3)-C(4)	1.377(4)	C(3)-H(3A)	0.95
C(4)-C(5)	1.377(4)	C(4)-H(4A)	0.95
C(5)-C(6)	1.383(4)	C(5)-H(5A)	0.95
C(6)-C(7)	1.411(4)	C(6)-H(6A)	0.95
C(8)-C(10)	1.522(4)	C(8)-C(9)	1.522(4)
C(8)-H(8A)	1.00	C(9)-H(9A)	0.98
C(9)-H(9B)	0.98	C(9)-H(9C)	0.98
C(10)-H(10A)	0.98	C(10)-H(10B)	0.98
C(10)-H(10C)	0.98	C(11)-C(12)	1.522(4)
C(11)-C(13)	1.529(4)	C(11)-H(11A)	1.00
C(12)-H(12A)	0.98	C(12)-H(12B)	0.98
C(12)-H(12C)	0.98	C(13)-H(13A)	0.98
C(13)-H(13B)	0.98	C(13)-H(13C)	0.98
C(14)-C(15)	1.378(4)	C(14)-C(19)	1.386(4)
C(15)-F(15)	1.357(3)	C(15)-C(16)	1.380(4)
C(16)-F(16)	1.345(3)	C(16)-C(17)	1.377(4)
C(17)-F(17)	1.348(3)	C(17)-C(18)	1.374(4)
C(18)-F(18)	1.343(3)	C(18)-C(19)	1.374(4)
C(19)-F(19)	1.363(3)	B(1)-C(20)	1.605(4)
B(1)-C(26)	1.620(4)	B(1)-H(14A)	1.18(2)
B(1)-H(14B)	1.17(2)	C(20)-C(21)	1.382(4)
C(20)-C(25)	1.388(4)	C(21)-F(21)	1.354(3)
C(21)-C(22)	1.382(4)	C(22)-F(22)	1.344(3)
C(22)-C(23)	1.376(4)	C(23)-F(23)	1.344(3)
C(23)-C(24)	1.370(4)	C(24)-F(24)	1.355(3)
C(24)-C(25)	1.377(4)	C(25)-F(25)	1.353(3)
C(26)-C(27)	1.386(4)	C(26)-C(31)	1.391(4)
C(27)-F(27)	1.359(3)	C(27)-C(28)	1.374(4)
C(28)-F(28)	1.350(3)	C(28)-C(29)	1.385(4)
C(29)-F(29)	1.344(3)	C(29)-C(30)	1.371(4)
C(30)-F(30)	1.346(3)	C(30)-C(31)	1.380(4)
C(31)-F(31)	1.353(3)		
N(2)-Al(1)-N(1)	86.28(9)	N(2)-Al(1)-C(14)	117.72(10)
N(1)-Al(1)-C(14)	122.35(11)	N(2)-Al(1)-B(1)	106.66(10)
N(1)-Al(1)-B(1)	105.40(11)	C(14)-Al(1)-B(1)	114.44(11)
N(2)-Al(1)-H(14A)	131.8(8)	N(1)-Al(1)-H(14A)	88.2(8)
C(14)-Al(1)-H(14A)	105.4(8)	B(1)-Al(1)-H(14A)	30.8(8)
N(2)-Al(1)-H(14B)	89.3(7)	N(1)-Al(1)-H(14B)	130.8(8)
C(14)-Al(1)-H(14B)	102.9(7)	B(1)-Al(1)-H(14B)	31.0(7)
H(14A)-Al(1)-H(14B)	59.8(11)	C(1)-N(1)-C(8)	120.9(2)
C(1)-N(1)-Al(1)	111.1(2)	C(8)-N(1)-Al(1)	127.5(2)
C(7)-N(2)-C(11)	120.5(2)	C(7)-N(2)-Al(1)	111.4(2)
C(11)-N(2)-Al(1)	127.7(2)	N(1)-C(1)-C(2)	122.2(2)
N(1)-C(1)-C(7)	113.2(2)	C(2)-C(1)-C(7)	124.5(2)
C(3)-C(2)-C(1)	132.1(3)	C(3)-C(2)-H(2A)	113.9(2)
C(1)-C(2)-H(2A)	113.9(2)	C(4)-C(3)-C(2)	129.9(3)
C(4)-C(3)-H(3A)	115.1(2)	C(2)-C(3)-H(3A)	115.1(2)
C(3)-C(4)-C(5)	126.0(3)	C(3)-C(4)-H(4A)	117.0(2)
C(5)-C(4)-H(4A)	117.0(2)	C(4)-C(5)-C(6)	130.4(3)
C(4)-C(5)-H(5A)	114.8(2)	C(6)-C(5)-H(5A)	114.8(2)
C(5)-C(6)-C(7)	132.0(3)	C(5)-C(6)-H(6A)	114.0(2)

C(7)-C(6)-H(6A)	114.0(2)	N(2)-C(7)-C(6)	122.3(2)
N(2)-C(7)-C(1)	113.2(2)	C(6)-C(7)-C(1)	124.4(2)
N(1)-C(8)-C(10)	109.8(2)	N(1)-C(8)-C(9)	110.8(2)
C(10)-C(8)-C(9)	110.3(2)	N(1)-C(8)-H(8A)	108.62(14)
C(10)-C(8)-H(8A)	108.6(2)	C(9)-C(8)-H(8A)	108.6(2)
C(8)-C(9)-H(9A)	109.5(2)	C(8)-C(9)-H(9B)	109.5(2)
H(9A)-C(9)-H(9B)	109.5	C(8)-C(9)-H(9C)	109.5(2)
H(9A)-C(9)-H(9C)	109.5	H(9B)-C(9)-H(9C)	109.5
C(8)-C(10)-H(10A)	109.5(2)	C(8)-C(10)-H(10B)	109.5(2)
H(10A)-C(10)-H(10B)	109.5	C(8)-C(10)-H(10C)	109.5(2)
H(10A)-C(10)-H(10C)	109.5	H(10B)-C(10)-H(10C)	109.5
N(2)-C(11)-C(12)	111.3(2)	N(2)-C(11)-C(13)	109.7(2)
C(12)-C(11)-C(13)	110.5(2)	N(2)-C(11)-H(11A)	108.44(13)
C(12)-C(11)-H(11A)	108.4(2)	C(13)-C(11)-H(11A)	108.4(2)
C(11)-C(12)-H(12A)	109.5(2)	C(11)-C(12)-H(12B)	109.47(14)
H(12A)-C(12)-H(12B)	109.5	C(11)-C(12)-H(12C)	109.5(2)
H(12A)-C(12)-H(12C)	109.5	H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5(2)	C(11)-C(13)-H(13B)	109.5(2)
H(13A)-C(13)-H(13B)	109.5	C(11)-C(13)-H(13C)	109.5(2)
H(13A)-C(13)-H(13C)	109.5	H(13B)-C(13)-H(13C)	109.5
C(15)-C(14)-C(19)	114.5(2)	C(15)-C(14)-Al(1)	124.7(2)
C(19)-C(14)-Al(1)	120.5(2)	F(15)-C(15)-C(14)	119.5(2)
F(15)-C(15)-C(16)	116.6(2)	C(14)-C(15)-C(16)	123.9(3)
F(16)-C(16)-C(17)	120.4(3)	F(16)-C(16)-C(15)	121.1(3)
C(17)-C(16)-C(15)	118.5(3)	F(17)-C(17)-C(18)	120.0(3)
F(17)-C(17)-C(16)	119.5(3)	C(18)-C(17)-C(16)	120.5(3)
F(18)-C(18)-C(17)	119.7(3)	F(18)-C(18)-C(19)	122.0(3)
C(17)-C(18)-C(19)	118.4(3)	F(19)-C(19)-C(18)	117.0(2)
F(19)-C(19)-C(14)	118.8(2)	C(18)-C(19)-C(14)	124.2(3)
C(20)-B(1)-C(26)	117.3(2)	C(20)-B(1)-Al(1)	140.3(2)
C(26)-B(1)-Al(1)	102.3(2)	C(20)-B(1)-H(14A)	108.2(12)
C(26)-B(1)-H(14A)	108.0(12)	Al(1)-B(1)-H(14A)	52.6(12)
C(20)-B(1)-H(14B)	108.9(12)	C(26)-B(1)-H(14B)	108.2(12)
Al(1)-B(1)-H(14B)	57.6(12)	H(14A)-B(1)-H(14B)	106(2)
C(21)-C(20)-C(25)	114.8(2)	C(21)-C(20)-B(1)	121.2(2)
C(25)-C(20)-B(1)	124.0(2)	F(21)-C(21)-C(22)	117.1(2)
F(21)-C(21)-C(20)	119.0(2)	C(22)-C(21)-C(20)	123.9(2)
F(22)-C(22)-C(23)	120.1(2)	F(22)-C(22)-C(21)	121.0(2)
C(23)-C(22)-C(21)	118.9(3)	F(23)-C(23)-C(24)	120.5(3)
F(23)-C(23)-C(22)	120.2(3)	C(24)-C(23)-C(22)	119.3(2)
F(24)-C(24)-C(23)	119.5(2)	F(24)-C(24)-C(25)	120.3(3)
C(23)-C(24)-C(25)	120.2(3)	F(25)-C(25)-C(24)	117.2(2)
F(25)-C(25)-C(20)	119.9(2)	C(24)-C(25)-C(20)	122.9(3)
C(27)-C(26)-C(31)	114.3(2)	C(27)-C(26)-B(1)	121.3(2)
C(31)-C(26)-B(1)	124.4(2)	F(27)-C(27)-C(28)	116.9(2)
F(27)-C(27)-C(26)	119.2(2)	C(28)-C(27)-C(26)	124.0(2)
F(28)-C(28)-C(27)	121.3(2)	F(28)-C(28)-C(29)	119.5(2)
C(27)-C(28)-C(29)	119.2(2)	F(29)-C(29)-C(30)	120.7(2)
F(29)-C(29)-C(28)	119.9(2)	C(30)-C(29)-C(28)	119.4(2)
F(30)-C(30)-C(29)	119.5(2)	F(30)-C(30)-C(31)	121.0(2)
C(29)-C(30)-C(31)	119.5(2)	F(31)-C(31)-C(30)	116.5(2)
F(31)-C(31)-C(26)	119.8(2)	C(30)-C(31)-C(26)	123.6(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for 3
anisotropic displacement factor exponent takes the form: $-2\pi^2 [$
($h a$)² $U_{11} + \dots + 2 h k a b U_{12}$]

	U11	U22	U33	U23	U13	U12
Al (1)	25 (1)	22 (1)	26 (1)	6 (1)	3 (1)	3 (1)
N (1)	26 (1)	26 (1)	27 (1)	8 (1)	5 (1)	6 (1)
N (2)	25 (1)	25 (1)	24 (1)	7 (1)	3 (1)	4 (1)
C (1)	22 (1)	26 (1)	26 (1)	5 (1)	9 (1)	3 (1)
C (2)	33 (2)	34 (2)	32 (2)	7 (1)	1 (1)	3 (1)
C (3)	37 (2)	32 (2)	36 (2)	-1 (1)	2 (1)	-1 (1)
C (4)	45 (2)	24 (2)	44 (2)	0 (1)	8 (2)	4 (1)
C (5)	46 (2)	28 (2)	43 (2)	8 (1)	9 (2)	12 (1)
C (6)	36 (2)	29 (2)	33 (2)	8 (1)	4 (1)	9 (1)
C (7)	22 (1)	25 (1)	25 (1)	6 (1)	8 (1)	5 (1)
C (8)	32 (2)	37 (2)	25 (1)	12 (1)	2 (1)	11 (1)
C (9)	55 (2)	45 (2)	34 (2)	17 (1)	5 (1)	25 (2)
C (10)	42 (2)	52 (2)	35 (2)	22 (2)	8 (1)	15 (2)
C (11)	29 (2)	30 (2)	29 (2)	10 (1)	1 (1)	8 (1)
C (12)	39 (2)	38 (2)	32 (2)	3 (1)	-8 (1)	10 (1)
C (13)	28 (2)	56 (2)	43 (2)	16 (2)	3 (1)	9 (1)
C (14)	29 (2)	26 (1)	29 (2)	11 (1)	-4 (1)	4 (1)
C (15)	28 (2)	30 (2)	36 (2)	9 (1)	2 (1)	5 (1)
F (15)	43 (1)	36 (1)	53 (1)	-2 (1)	15 (1)	5 (1)
C (16)	41 (2)	26 (2)	41 (2)	2 (1)	-9 (1)	10 (1)
F (16)	61 (1)	34 (1)	63 (1)	-11 (1)	1 (1)	9 (1)
C (17)	37 (2)	26 (2)	52 (2)	17 (1)	-15 (1)	-6 (1)
F (17)	55 (1)	29 (1)	74 (1)	14 (1)	-23 (1)	-13 (1)
C (18)	36 (2)	41 (2)	39 (2)	20 (1)	-2 (1)	-6 (1)
F (18)	56 (1)	62 (1)	64 (1)	26 (1)	8 (1)	-22 (1)
C (19)	37 (2)	32 (2)	32 (2)	12 (1)	1 (1)	0 (1)
F (19)	55 (1)	49 (1)	43 (1)	2 (1)	21 (1)	-7 (1)
B (1)	26 (2)	28 (2)	27 (2)	8 (1)	3 (1)	3 (1)
C (20)	23 (1)	24 (1)	27 (1)	6 (1)	2 (1)	0 (1)
C (21)	23 (1)	23 (1)	33 (2)	9 (1)	3 (1)	4 (1)
F (21)	39 (1)	34 (1)	34 (1)	13 (1)	6 (1)	11 (1)
C (22)	29 (2)	34 (2)	28 (2)	8 (1)	7 (1)	-3 (1)
F (22)	46 (1)	52 (1)	32 (1)	13 (1)	16 (1)	7 (1)
C (23)	26 (2)	34 (2)	37 (2)	0 (1)	12 (1)	6 (1)
F (23)	49 (1)	56 (1)	53 (1)	8 (1)	24 (1)	22 (1)
C (24)	28 (2)	31 (2)	44 (2)	9 (1)	2 (1)	14 (1)
F (24)	52 (1)	56 (1)	59 (1)	15 (1)	9 (1)	33 (1)
C (25)	29 (2)	32 (2)	27 (1)	9 (1)	3 (1)	7 (1)
F (25)	56 (1)	56 (1)	37 (1)	21 (1)	9 (1)	28 (1)
C (26)	24 (1)	29 (1)	23 (1)	9 (1)	7 (1)	4 (1)
C (27)	28 (2)	31 (2)	30 (2)	11 (1)	4 (1)	8 (1)
F (27)	35 (1)	34 (1)	44 (1)	16 (1)	-5 (1)	7 (1)
C (28)	30 (2)	37 (2)	32 (2)	7 (1)	-4 (1)	-1 (1)
F (28)	52 (1)	41 (1)	57 (1)	11 (1)	-24 (1)	-4 (1)
C (29)	38 (2)	21 (1)	38 (2)	4 (1)	5 (1)	1 (1)
F (29)	56 (1)	26 (1)	58 (1)	3 (1)	-6 (1)	2 (1)
C (30)	29 (2)	28 (2)	36 (2)	14 (1)	9 (1)	11 (1)
F (30)	44 (1)	31 (1)	52 (1)	16 (1)	5 (1)	14 (1)
C (31)	22 (1)	33 (2)	25 (1)	11 (1)	5 (1)	4 (1)
F (31)	34 (1)	36 (1)	36 (1)	12 (1)	-5 (1)	3 (1)

Table 5. Torsion angles [$^{\circ}$] for 3

N(2)-Al(1)-N(1)-C(1)	-19.3(2)	C(14)-Al(1)-N(1)-C(1)	-140.0(2)
B(1)-Al(1)-N(1)-C(1)	86.9(2)	N(2)-Al(1)-N(1)-C(8)	168.5(2)
C(14)-Al(1)-N(1)-C(8)	47.8(2)	B(1)-Al(1)-N(1)-C(8)	-85.2(2)
N(1)-Al(1)-N(2)-C(7)	18.8(2)	C(14)-Al(1)-N(2)-C(7)	143.6(2)
B(1)-Al(1)-N(2)-C(7)	-86.2(2)	N(1)-Al(1)-N(2)-C(11)	-168.5(2)
C(14)-Al(1)-N(2)-C(11)	-43.6(2)	B(1)-Al(1)-N(2)-C(11)	86.6(2)
C(8)-N(1)-C(1)-C(2)	8.5(4)	Al(1)-N(1)-C(1)-C(2)	-164.2(2)
C(8)-N(1)-C(1)-C(7)	-171.5(2)	Al(1)-N(1)-C(1)-C(7)	15.8(3)
N(1)-C(1)-C(2)-C(3)	173.4(3)	C(7)-C(1)-C(2)-C(3)	-6.5(5)
C(1)-C(2)-C(3)-C(4)	4.8(5)	C(2)-C(3)-C(4)-C(5)	3.0(5)
C(3)-C(4)-C(5)-C(6)	-3.5(5)	C(4)-C(5)-C(6)-C(7)	-4.5(6)
C(11)-N(2)-C(7)-C(6)	-7.5(4)	Al(1)-N(2)-C(7)-C(6)	165.9(2)
C(11)-N(2)-C(7)-C(1)	172.4(2)	Al(1)-N(2)-C(7)-C(1)	-14.3(3)
C(5)-C(6)-C(7)-N(2)	-172.1(3)	C(5)-C(6)-C(7)-C(1)	8.0(5)
N(1)-C(1)-C(7)-N(2)	-1.1(3)	C(2)-C(1)-C(7)-N(2)	178.9(2)
N(1)-C(1)-C(7)-C(6)	178.8(2)	C(2)-C(1)-C(7)-C(6)	-1.2(4)
C(1)-N(1)-C(8)-C(10)	74.9(3)	Al(1)-N(1)-C(8)-C(10)	-113.6(2)
C(1)-N(1)-C(8)-C(9)	-163.0(2)	Al(1)-N(1)-C(8)-C(9)	8.5(3)
C(7)-N(2)-C(11)-C(12)	162.9(2)	Al(1)-N(2)-C(11)-C(12)	-9.3(3)
C(7)-N(2)-C(11)-C(13)	-74.5(3)	Al(1)-N(2)-C(11)-C(13)	113.3(2)
N(2)-Al(1)-C(14)-C(15)	119.3(2)	N(1)-Al(1)-C(14)-C(15)	-136.4(2)
B(1)-Al(1)-C(14)-C(15)	-7.1(3)	N(2)-Al(1)-C(14)-C(19)	-55.0(2)
N(1)-Al(1)-C(14)-C(19)	49.2(3)	B(1)-Al(1)-C(14)-C(19)	178.5(2)
C(19)-C(14)-C(15)-F(15)	-179.8(2)	Al(1)-C(14)-C(15)-F(15)	5.5(4)
C(19)-C(14)-C(15)-C(16)	0.7(4)	Al(1)-C(14)-C(15)-C(16)	-174.0(2)
F(15)-C(15)-C(16)-F(16)	0.4(4)	C(14)-C(15)-C(16)-F(16)	179.9(3)
F(15)-C(15)-C(16)-C(17)	-179.8(2)	C(14)-C(15)-C(16)-C(17)	-0.3(4)
F(16)-C(16)-C(17)-F(17)	-0.2(4)	C(15)-C(16)-C(17)-F(17)	180.0(2)
F(16)-C(16)-C(17)-C(18)	179.2(3)	C(15)-C(16)-C(17)-C(18)	-0.6(4)
F(17)-C(17)-C(18)-F(18)	-0.1(4)	C(16)-C(17)-C(18)-F(18)	-179.5(3)
F(17)-C(17)-C(18)-C(19)	-179.5(2)	C(16)-C(17)-C(18)-C(19)	1.1(4)
F(18)-C(18)-C(19)-F(19)	-0.4(4)	C(17)-C(18)-C(19)-F(19)	178.9(2)
F(18)-C(18)-C(19)-C(14)	179.9(3)	C(17)-C(18)-C(19)-C(14)	-0.8(4)
C(15)-C(14)-C(19)-F(19)	-179.8(2)	Al(1)-C(14)-C(19)-F(19)	-4.9(3)
C(15)-C(14)-C(19)-C(18)	-0.1(4)	Al(1)-C(14)-C(19)-C(18)	174.8(2)
N(2)-Al(1)-B(1)-C(20)	-138.9(3)	N(1)-Al(1)-B(1)-C(20)	130.4(3)
C(14)-Al(1)-B(1)-C(20)	-6.9(3)	N(2)-Al(1)-B(1)-C(26)	45.6(2)
N(1)-Al(1)-B(1)-C(26)	-45.1(2)	C(14)-Al(1)-B(1)-C(26)	177.6(2)
C(26)-B(1)-C(20)-C(21)	-72.5(3)	Al(1)-B(1)-C(20)-C(21)	112.4(3)
C(26)-B(1)-C(20)-C(25)	108.0(3)	Al(1)-B(1)-C(20)-C(25)	-67.1(4)
C(25)-C(20)-C(21)-F(21)	179.6(2)	B(1)-C(20)-C(21)-F(21)	0.1(4)
C(25)-C(20)-C(21)-C(22)	0.1(4)	B(1)-C(20)-C(21)-C(22)	-179.4(2)
F(21)-C(21)-C(22)-F(22)	0.0(4)	C(20)-C(21)-C(22)-F(22)	179.6(2)
F(21)-C(21)-C(22)-C(23)	179.9(2)	C(20)-C(21)-C(22)-C(23)	-0.5(4)
F(22)-C(22)-C(23)-F(23)	-0.2(4)	C(21)-C(22)-C(23)-F(23)	179.9(2)
F(22)-C(22)-C(23)-C(24)	-179.5(2)	C(21)-C(22)-C(23)-C(24)	0.6(4)
F(23)-C(23)-C(24)-F(24)	0.7(4)	C(22)-C(23)-C(24)-F(24)	180.0(2)
F(23)-C(23)-C(24)-C(25)	-179.6(2)	C(22)-C(23)-C(24)-C(25)	-0.3(4)
F(24)-C(24)-C(25)-F(25)	-0.1(4)	C(23)-C(24)-C(25)-F(25)	-179.9(2)
F(24)-C(24)-C(25)-C(20)	179.6(2)	C(23)-C(24)-C(25)-C(20)	-0.1(4)
C(21)-C(20)-C(25)-F(25)	180.0(2)	B(1)-C(20)-C(25)-F(25)	-0.5(4)
C(21)-C(20)-C(25)-C(24)	0.2(4)	B(1)-C(20)-C(25)-C(24)	179.7(3)
C(20)-B(1)-C(26)-C(27)	-78.8(3)	Al(1)-B(1)-C(26)-C(27)	98.0(2)
C(20)-B(1)-C(26)-C(31)	103.1(3)	Al(1)-B(1)-C(26)-C(31)	-80.1(3)
C(31)-C(26)-C(27)-F(27)	178.6(2)	B(1)-C(26)-C(27)-F(27)	0.3(4)
C(31)-C(26)-C(27)-C(28)	-1.3(4)	B(1)-C(26)-C(27)-C(28)	-179.6(3)
F(27)-C(27)-C(28)-F(28)	0.9(4)	C(26)-C(27)-C(28)-F(28)	-179.1(2)
F(27)-C(27)-C(28)-C(29)	-177.2(2)	C(26)-C(27)-C(28)-C(29)	2.8(4)
F(28)-C(28)-C(29)-F(29)	0.2(4)	C(27)-C(28)-C(29)-F(29)	178.3(2)

F(28)-C(28)-C(29)-C(30)	-180.0(2)	C(27)-C(28)-C(29)-C(30)	-1.9(4)
F(29)-C(29)-C(30)-F(30)	-1.1(4)	C(28)-C(29)-C(30)-F(30)	179.0(2)
F(29)-C(29)-C(30)-C(31)	179.5(2)	C(28)-C(29)-C(30)-C(31)	-0.4(4)
F(30)-C(30)-C(31)-F(31)	1.5(4)	C(29)-C(30)-C(31)-F(31)	-179.1(2)
F(30)-C(30)-C(31)-C(26)	-177.5(2)	C(29)-C(30)-C(31)-C(26)	1.9(4)
C(27)-C(26)-C(31)-F(31)	-180.0(2)	B(1)-C(26)-C(31)-F(31)	-1.7(4)
C(27)-C(26)-C(31)-C(30)	-1.1(4)	B(1)-C(26)-C(31)-C(30)	177.2(2)

Symmetry transformations used to generate equivalent atoms:

Table 6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 3

	x	y	z	U(eq)	SOF
H(2A)	2672(3)	6720(3)	5149(2)	40	1
H(3A)	2733(3)	8983(3)	5586(2)	45	1
H(4A)	1687(3)	10375(3)	4959(2)	47	1
H(5A)	212(3)	9733(3)	3749(2)	47	1
H(6A)	-466(3)	7674(3)	2847(2)	39	1
H(8A)	3369(3)	4914(3)	4741(2)	37	1
H(9A)	3696(15)	2981(5)	3599(10)	64	1
H(9B)	2298(4)	2149(7)	3679(11)	64	1
H(9C)	3532(18)	2488(11)	4458(2)	64	1
H(10A)	2183(6)	3727(20)	5571(7)	60	1
H(10B)	894(11)	3319(15)	4828(3)	60	1
H(10C)	1346(16)	4917(6)	5382(9)	60	1
H(11A)	-645(3)	6197(3)	1712(2)	35	1
H(12A)	26(7)	4153(12)	819(7)	58	1
H(12B)	-1557(13)	4170(12)	572(4)	58	1
H(12C)	-1045(19)	3208(3)	1157(3)	58	1
H(13A)	-2914(4)	5306(21)	1721(5)	63	1
H(13B)	-2198(7)	6050(12)	2705(8)	63	1
H(13C)	-2415(9)	4382(10)	2336(12)	63	1
H(14A)	3061(24)	3688(25)	2464(16)	26(7)	1
H(14B)	1988(25)	4071(25)	1547(16)	26(7)	1

II. X-ray Crystallographic Analysis of $[(^i\text{Pr}_2\text{-ATI})\text{Al}(\text{Et})(\text{ClPh})][\text{B}(\text{C}_6\text{F}_5)_4]\cdot 0.5\text{PhCl}$ (**4c**(ClPh)-0.5PhCl)

Crystallographic Experimental Section

Data Collection

A yellow crystal with approximate dimensions $0.4 \times 0.4 \times 0.4 \text{ mm}^3$ was selected under oil under ambient conditions and attached to the tip of a glass capillary. The crystal was mounted in a stream of cold nitrogen at 173(2) K and centered in the X-ray beam by using a video camera.

The crystal evaluation and data collection were performed on a Bruker CCD-1000 diffractometer with Mo K_α ($\lambda = 0.71073 \text{ \AA}$) radiation and the diffractometer to crystal distance of 5.08 cm.

The initial cell constants were obtained from three series of ω scans at different starting angles. Each series consisted of 20 frames collected at intervals of 0.3° in a 6° range about ω with the exposure time of 10 seconds per frame. A total of 77 reflections was obtained. The reflections were successfully indexed by an automated indexing routine built in the SMART program. The final cell constants were calculated from a set of 3342 strong reflections from the actual data collection.

The data were collected by using the hemisphere data collection routine. The reciprocal space was surveyed to the extent of a full sphere to a resolution of $0.80 \text{ \AA}$. A total of 20812 data were harvested by collecting two sets of frames with 0.4° scans in ω with an exposure time 10 sec per frame. These highly redundant datasets were corrected for Lorentz and polarization effects. The absorption correction was based on fitting a function to the empirical transmission surface as sampled by multiple equivalent measurements. [1]

Structure Solution and Refinement

The systematic absences in the diffraction data were uniquely consistent for the space group $P2_1/c$ that yielded chemically reasonable and computationally stable results of refinement [2]. A successful solution by the direct methods provided most non-hydrogen atoms from the E -map. The remaining non-hydrogen atoms were located in an alternating series of least-squares cycles and difference Fourier maps. All non-hydrogen

atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were included in the structure factor calculation at idealized positions and were allowed to ride on the neighboring atoms with relative isotropic displacement coefficients.

There were one and a half solvate molecules of chlorobenzene present in the asymmetric unit. One full molecule was refined anisotropically while the other was severely disordered over a crystallographic inversion center in such a way that only one half of it was symmetry independent. A significant amount of time was invested in identifying and refining the disordered molecule. Bond length restraints were applied to model that molecule but the resulting isotropic displacement coefficients suggested the molecules were mobile. In addition, the refinement was computationally unstable. Option SQUEEZE of program PLATON [3] was used to correct the diffraction data for diffuse scattering effects and to identify the solvate molecule. PLATON calculated the upper limit of volume that can be occupied by the solvent to be 429.0 Å³, or 9.2% of the unit cell volume. The program calculated 120 electrons in the unit cell for the diffuse species. This corresponds to one half molecule of chlorobenzene molecule in the asymmetric unit. Please note that all derived results in the following tables are based on known contents. No data are given for the diffusely scattering species.

The final least-squares refinement of 637 parameters against 7243 data resulted in residuals R (based on F^2 for $I \geq 2\sigma$) and wR (based on F^2 for all data) of 0.0879 and 0.1855, respectively. The final difference Fourier map was featureless.

The ORTEP diagrams were drawn with 30% probability ellipsoids.

References

- [1] Blessing, R.H. *Acta Cryst.* **1995**, *A51*, 33-38.
- [2] All software and sources of the scattering factors are contained in the SHELXTL (version 5.1) program library (G. Sheldrick, Bruker Analytical X-Ray Systems, Madison, WI).
- [3] Spek, A.L. *Acta Cryst.*, **1990**, *A46*, C-34.

Table 1. Crystal data and structure refinement for **4c(ClPh)·0.5PhCl**

Identification code	jor37
Empirical formula	C ₄₈ H _{31.50} Al B Cl _{1.50} F ₂₀ N ₂
Formula weight	1107.22
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁ /c
Unit cell dimensions	a = 14.2338(9) Å α = 90° b = 20.0259(13) Å β = 98.450(1)° c = 16.5459(11) Å γ = 90°
Volume	4665.1(5) Å ³
Z	4
Density (calculated)	1.576 Mg/m ³
Absorption coefficient	0.248 mm ⁻¹
F(000)	2228
Crystal size	0.40 x 0.40 x 0.40 mm ³
Theta range for data collection	1.45 to 24.00°
Index ranges	-16 ≤ h ≤ 16, 0 ≤ k ≤ 22, 0 ≤ l ≤ 18
Reflections collected	20812
Independent reflections	7243 [R(int) = 0.0877]
Completeness to theta = 24.00°	99.1 %
Absorption correction	Empirical with SADABS
Max. and min. transmission	0.9073 and 0.9073
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	7243 / 0 / 637
Goodness-of-fit on F ²	1.017
Final R indices [I > 2σ(I)]	R1 = 0.0879, wR2 = 0.1855
R indices (all data)	R1 = 0.1631, wR2 = 0.2041
Largest diff. peak and hole	0.650 and -0.668 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4c(ClPh)**·0.5PhCl
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Al	2171(2)	7069(1)	8138(1)	35(1)
N(1)	2621(4)	6345(2)	7642(3)	32(1)
N(2)	1268(3)	7166(2)	7220(3)	30(1)
B	3406(5)	3143(4)	8817(4)	24(2)
Cl	1169(2)	6473(1)	9065(1)	83(1)
F(1)	5243(2)	2298(2)	8927(2)	42(1)
F(2)	6783(2)	2649(2)	8321(2)	48(1)
F(3)	6927(3)	3869(2)	7637(3)	54(1)
F(4)	5427(3)	4728(2)	7515(2)	52(1)
F(5)	3840(2)	4367(2)	8058(2)	35(1)
F(6)	2054(2)	1940(2)	8716(2)	38(1)
F(7)	2151(3)	959(2)	9767(3)	56(1)
F(8)	3516(3)	927(2)	11107(2)	54(1)
F(9)	4776(3)	1958(2)	11368(2)	51(1)
F(10)	4715(2)	2955(2)	10304(2)	37(1)
F(11)	1933(2)	4041(2)	7775(2)	39(1)
F(12)	1079(3)	3779(2)	6303(2)	54(1)
F(13)	1355(3)	2595(2)	5557(2)	63(1)
F(14)	2658(3)	1717(2)	6325(2)	60(1)
F(15)	3578(3)	1987(2)	7804(2)	42(1)
F(16)	4411(3)	4311(2)	9779(2)	36(1)
F(17)	3623(3)	5166(2)	10679(2)	53(1)
F(18)	1735(3)	5116(2)	10761(3)	60(1)
F(19)	655(3)	4141(2)	9937(2)	52(1)
F(20)	1446(2)	3244(2)	9057(2)	35(1)
C(1)	2841(5)	7685(4)	8903(4)	56(2)
C(2)	2552(7)	7755(5)	9749(5)	89(3)
C(3)	3490(5)	5951(4)	7953(5)	55(2)
C(4)	3584(6)	5930(5)	8871(6)	91(4)
C(5)	4347(5)	6271(4)	7681(6)	68(3)
C(6)	2113(5)	6208(3)	6917(4)	33(2)

C(7)	2369(6)	5709(4)	6383(5)	60(3)
C(8)	1918(8)	5449(4)	5666(6)	82(3)
C(9)	1044(9)	5591(6)	5250(6)	85(3)
C(10)	439(7)	6085(6)	5422(5)	77(3)
C(11)	574(5)	6547(4)	6044(5)	51(2)
C(12)	1293(4)	6645(3)	6699(4)	30(2)
C(13)	593(5)	7715(4)	7064(6)	58(2)
C(14)	590(6)	8123(4)	7825(8)	104(4)
C(15)	824(5)	8144(4)	6356(6)	78(3)
C(16)	4459(4)	3327(3)	8549(4)	24(2)
C(17)	5245(5)	2915(3)	8580(4)	29(2)
C(18)	6057(5)	3088(3)	8284(4)	29(2)
C(19)	6128(5)	3698(4)	7937(4)	31(2)
C(20)	5380(5)	4130(3)	7856(4)	31(2)
C(21)	4567(5)	3924(3)	8159(4)	28(2)
C(22)	3420(4)	2494(3)	9424(4)	22(2)
C(23)	2777(4)	1972(3)	9352(4)	29(2)
C(24)	2820(5)	1449(4)	9891(4)	35(2)
C(25)	3485(5)	1429(3)	10574(4)	35(2)
C(26)	4126(5)	1952(4)	10694(4)	36(2)
C(27)	4065(4)	2458(3)	10131(4)	31(2)
C(28)	2781(4)	3017(3)	7894(4)	23(2)
C(29)	2131(4)	3443(3)	7465(4)	29(2)
C(30)	1694(5)	3312(4)	6682(4)	36(2)
C(31)	1831(5)	2736(4)	6301(4)	38(2)
C(32)	2475(5)	2287(4)	6700(4)	39(2)
C(33)	2934(5)	2449(3)	7460(4)	32(2)
C(34)	2974(4)	3732(3)	9335(3)	18(1)
C(35)	3470(4)	4236(3)	9779(4)	23(2)
C(36)	3075(6)	4696(3)	10266(4)	37(2)
C(37)	2117(6)	4660(3)	10308(4)	37(2)
C(38)	1586(5)	4174(4)	9897(4)	31(2)
C(39)	2029(5)	3738(3)	9433(4)	23(2)
C(40)	388(5)	5985(4)	8367(4)	41(2)
C(41)	726(6)	5399(4)	8105(6)	70(3)
C(42)	130(6)	5032(4)	7571(7)	89(4)

C(43)	-759(7)	5221(5)	7291(6)	67(3)
C(44)	-1092(6)	5820(5)	7553(6)	67(3)
C(45)	-495(6)	6201(4)	8099(6)	61(3)

Table 3. Bond lengths [Å] and angles [°] for **4c(ClPh)-0.5PhCl**

Al-N(1)	1.827(6)
Al-N(2)	1.850(5)
Al-C(1)	1.919(7)
Al-Cl	2.540(3)
N(1)-C(6)	1.335(8)
N(1)-C(3)	1.494(8)
N(2)-C(12)	1.357(8)
N(2)-C(13)	1.458(8)
B-C(34)	1.632(9)
B-C(22)	1.641(9)
B-C(16)	1.665(10)
B-C(28)	1.670(9)
Cl-C(40)	1.774(7)
F(1)-C(17)	1.364(7)
F(2)-C(18)	1.352(6)
F(3)-C(19)	1.351(7)
F(4)-C(20)	1.330(7)
F(5)-C(21)	1.355(6)
F(6)-C(23)	1.360(6)
F(7)-C(24)	1.362(7)
F(8)-C(25)	1.333(7)
F(9)-C(26)	1.339(7)
F(10)-C(27)	1.360(7)
F(11)-C(29)	1.348(7)
F(12)-C(30)	1.370(7)
F(13)-C(31)	1.345(7)
F(14)-C(32)	1.343(7)
F(15)-C(33)	1.368(7)
F(16)-C(35)	1.348(7)
F(17)-C(36)	1.342(7)
F(18)-C(37)	1.345(7)
F(19)-C(38)	1.337(7)
F(20)-C(39)	1.380(6)
C(1)-C(2)	1.522(10)

C(3)-C(5)	1.505(10)
C(3)-C(4)	1.507(12)
C(6)-C(7)	1.417(10)
C(6)-C(12)	1.461(9)
C(7)-C(8)	1.366(11)
C(8)-C(9)	1.360(12)
C(9)-C(10)	1.370(13)
C(10)-C(11)	1.376(12)
C(11)-C(12)	1.391(9)
C(13)-C(14)	1.501(12)
C(13)-C(15)	1.527(11)
C(16)-C(21)	1.378(8)
C(16)-C(17)	1.385(8)
C(17)-C(18)	1.364(9)
C(18)-C(19)	1.359(9)
C(19)-C(20)	1.363(9)
C(20)-C(21)	1.390(9)
C(22)-C(27)	1.378(8)
C(22)-C(23)	1.384(8)
C(23)-C(24)	1.371(9)
C(24)-C(25)	1.363(9)
C(25)-C(26)	1.385(9)
C(26)-C(27)	1.371(9)
C(28)-C(29)	1.376(8)
C(28)-C(33)	1.380(8)
C(29)-C(30)	1.378(9)
C(30)-C(31)	1.342(9)
C(31)-C(32)	1.381(9)
C(32)-C(33)	1.367(9)
C(34)-C(39)	1.378(8)
C(34)-C(35)	1.380(8)
C(35)-C(36)	1.396(9)
C(36)-C(37)	1.378(9)
C(37)-C(38)	1.354(9)
C(38)-C(39)	1.374(9)
C(40)-C(45)	1.341(10)

C(40)-C(41)	1.364(10)
C(41)-C(42)	1.349(11)
C(42)-C(43)	1.337(11)
C(43)-C(44)	1.381(11)
C(44)-C(45)	1.377(11)

N(1)-Al-N(2)	87.8(2)
N(1)-Al-C(1)	129.3(3)
N(2)-Al-C(1)	133.8(3)
N(1)-Al-Cl	99.43(19)
N(2)-Al-Cl	99.30(19)
C(1)-Al-Cl	99.9(2)
C(6)-N(1)-C(3)	120.9(6)
C(6)-N(1)-Al	112.8(4)
C(3)-N(1)-Al	126.3(5)
C(12)-N(2)-C(13)	123.0(6)
C(12)-N(2)-Al	111.1(4)
C(13)-N(2)-Al	125.8(5)
C(34)-B-C(22)	102.9(5)
C(34)-B-C(16)	113.8(5)
C(22)-B-C(16)	114.1(5)
C(34)-B-C(28)	113.4(5)
C(22)-B-C(28)	113.4(5)
C(16)-B-C(28)	99.7(5)
C(40)-Cl-Al	102.7(2)
C(2)-C(1)-Al	119.4(6)
N(1)-C(3)-C(5)	109.8(6)
N(1)-C(3)-C(4)	108.0(7)
C(5)-C(3)-C(4)	111.0(7)
N(1)-C(6)-C(7)	123.4(6)
N(1)-C(6)-C(12)	114.0(6)
C(7)-C(6)-C(12)	122.5(6)
C(8)-C(7)-C(6)	132.8(8)
C(9)-C(8)-C(7)	129.6(9)
C(8)-C(9)-C(10)	127.1(9)
C(9)-C(10)-C(11)	128.1(9)

C(10)-C(11)-C(12)	133.2(8)
N(2)-C(12)-C(11)	121.3(6)
N(2)-C(12)-C(6)	113.4(5)
C(11)-C(12)-C(6)	125.3(7)
N(2)-C(13)-C(14)	110.2(7)
N(2)-C(13)-C(15)	110.4(7)
C(14)-C(13)-C(15)	111.4(8)
C(21)-C(16)-C(17)	112.8(6)
C(21)-C(16)-B	118.9(6)
C(17)-C(16)-B	127.8(6)
F(1)-C(17)-C(18)	115.8(6)
F(1)-C(17)-C(16)	120.2(6)
C(18)-C(17)-C(16)	123.9(6)
F(2)-C(18)-C(19)	120.0(6)
F(2)-C(18)-C(17)	120.1(6)
C(19)-C(18)-C(17)	119.9(6)
F(3)-C(19)-C(18)	120.1(7)
F(3)-C(19)-C(20)	119.4(6)
C(18)-C(19)-C(20)	120.4(6)
F(4)-C(20)-C(19)	121.7(6)
F(4)-C(20)-C(21)	121.1(6)
C(19)-C(20)-C(21)	117.1(6)
F(5)-C(21)-C(16)	119.3(6)
F(5)-C(21)-C(20)	115.0(6)
C(16)-C(21)-C(20)	125.6(6)
C(27)-C(22)-C(23)	112.6(6)
C(27)-C(22)-B	120.5(5)
C(23)-C(22)-B	126.7(5)
F(6)-C(23)-C(24)	115.1(6)
F(6)-C(23)-C(22)	121.2(6)
C(24)-C(23)-C(22)	123.7(6)
F(7)-C(24)-C(25)	119.2(7)
F(7)-C(24)-C(23)	119.2(6)
C(25)-C(24)-C(23)	121.5(6)
F(8)-C(25)-C(24)	121.5(7)
F(8)-C(25)-C(26)	121.2(6)

C(24)-C(25)-C(26)	117.3(6)
F(9)-C(26)-C(27)	121.8(6)
F(9)-C(26)-C(25)	119.1(6)
C(27)-C(26)-C(25)	119.2(6)
F(10)-C(27)-C(26)	115.2(6)
F(10)-C(27)-C(22)	119.2(6)
C(26)-C(27)-C(22)	125.7(6)
C(29)-C(28)-C(33)	112.8(6)
C(29)-C(28)-B	127.3(6)
C(33)-C(28)-B	119.8(6)
F(11)-C(29)-C(28)	121.1(5)
F(11)-C(29)-C(30)	115.9(6)
C(28)-C(29)-C(30)	122.9(7)
C(31)-C(30)-F(12)	119.9(6)
C(31)-C(30)-C(29)	122.0(7)
F(12)-C(30)-C(29)	118.1(6)
C(30)-C(31)-F(13)	121.5(7)
C(30)-C(31)-C(32)	117.8(6)
F(13)-C(31)-C(32)	120.7(7)
F(14)-C(32)-C(33)	121.8(7)
F(14)-C(32)-C(31)	119.5(6)
C(33)-C(32)-C(31)	118.6(7)
C(32)-C(33)-F(15)	115.0(6)
C(32)-C(33)-C(28)	125.7(7)
F(15)-C(33)-C(28)	119.3(6)
C(39)-C(34)-C(35)	111.3(6)
C(39)-C(34)-B	121.2(5)
C(35)-C(34)-B	127.2(5)
F(16)-C(35)-C(34)	120.9(6)
F(16)-C(35)-C(36)	114.2(6)
C(34)-C(35)-C(36)	124.9(6)
F(17)-C(36)-C(37)	121.1(6)
F(17)-C(36)-C(35)	120.3(7)
C(37)-C(36)-C(35)	118.7(6)
F(18)-C(37)-C(38)	121.8(7)
F(18)-C(37)-C(36)	118.5(7)

C(38)-C(37)-C(36)	119.8(6)
F(19)-C(38)-C(37)	119.6(7)
F(19)-C(38)-C(39)	122.4(6)
C(37)-C(38)-C(39)	117.9(6)
C(38)-C(39)-C(34)	127.4(6)
C(38)-C(39)-F(20)	114.3(6)
C(34)-C(39)-F(20)	118.2(5)
C(45)-C(40)-C(41)	122.0(7)
C(45)-C(40)-Cl	120.3(7)
C(41)-C(40)-Cl	117.7(6)
C(42)-C(41)-C(40)	117.4(8)
C(43)-C(42)-C(41)	123.0(8)
C(42)-C(43)-C(44)	119.2(8)
C(45)-C(44)-C(43)	118.7(8)
C(40)-C(45)-C(44)	119.7(8)

Symmetry transformations used to generate equivalent atoms:

Table4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 4c(ClPh)-0.5PhCl. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Al	43(1)	38(1)	25(1)	-2(1)	2(1)	-7(1)
N(1)	26(3)	31(3)	35(4)	5(3)	-11(3)	-3(3)
N(2)	25(3)	23(3)	43(4)	12(3)	10(3)	14(3)
B	9(4)	33(5)	28(4)	-1(4)	-4(3)	9(3)
Cl	103(2)	112(2)	36(1)	-13(1)	24(1)	-56(2)
F(1)	33(2)	36(2)	57(3)	6(2)	7(2)	9(2)
F(2)	31(2)	55(3)	60(3)	-1(2)	12(2)	14(2)
F(3)	47(3)	60(3)	61(3)	-6(2)	26(2)	-12(2)
F(4)	67(3)	42(3)	54(3)	7(2)	33(2)	-4(2)
F(5)	39(2)	30(2)	37(2)	10(2)	9(2)	9(2)
F(6)	41(2)	35(2)	34(2)	-2(2)	-5(2)	-12(2)
F(7)	61(3)	49(3)	60(3)	12(2)	15(2)	-19(2)
F(8)	66(3)	52(3)	47(3)	25(2)	16(2)	8(2)
F(9)	53(3)	68(3)	30(2)	15(2)	-3(2)	8(2)
F(10)	33(2)	38(2)	34(2)	2(2)	-14(2)	-7(2)
F(11)	45(3)	40(2)	29(2)	0(2)	-6(2)	17(2)
F(12)	47(3)	93(3)	21(2)	19(2)	-5(2)	6(2)
F(13)	68(3)	105(4)	13(2)	-13(2)	-4(2)	-31(3)
F(14)	84(3)	58(3)	41(3)	-30(2)	22(2)	-28(2)
F(15)	51(3)	32(2)	43(3)	-16(2)	10(2)	4(2)
F(16)	35(2)	40(2)	31(2)	-12(2)	-2(2)	-11(2)
F(17)	75(3)	44(3)	38(3)	-24(2)	7(2)	-19(2)
F(18)	81(3)	56(3)	50(3)	-23(2)	33(2)	12(2)
F(19)	39(3)	76(3)	44(3)	-10(2)	20(2)	7(2)
F(20)	25(2)	50(3)	31(2)	-7(2)	4(2)	-3(2)
C(1)	66(6)	59(5)	43(5)	-18(4)	14(4)	-30(4)
C(2)	103(8)	123(9)	43(6)	-26(6)	17(5)	-28(7)
C(3)	53(6)	27(4)	78(7)	17(4)	-20(5)	6(4)
C(4)	68(7)	88(7)	98(8)	51(6)	-48(6)	-27(5)
C(5)	24(5)	63(6)	112(8)	15(5)	-4(5)	14(4)
C(6)	44(5)	15(4)	38(5)	3(3)	2(4)	-1(3)

C(7)	65(6)	40(5)	68(6)	-25(5)	-10(5)	3(4)
C(8)	105(9)	49(6)	91(8)	-41(6)	10(7)	-22(6)
C(9)	97(9)	105(9)	50(7)	-23(6)	-3(7)	-50(7)
C(10)	78(8)	115(9)	33(6)	6(6)	-9(5)	-29(7)
C(11)	49(5)	60(6)	36(5)	23(4)	-18(4)	-2(4)
C(12)	27(4)	39(5)	24(4)	10(4)	4(3)	-3(3)
C(13)	32(5)	42(5)	100(8)	4(5)	10(5)	7(4)
C(14)	64(7)	52(6)	205(14)	-20(8)	51(8)	16(5)
C(15)	27(5)	69(6)	137(9)	56(6)	8(5)	6(4)
C(16)	29(4)	26(4)	13(3)	-1(3)	-10(3)	2(3)
C(17)	24(4)	27(4)	31(4)	-6(3)	-11(3)	0(3)
C(18)	17(4)	31(4)	38(4)	-8(4)	2(3)	11(3)
C(19)	30(5)	44(5)	21(4)	-11(4)	18(3)	-16(4)
C(20)	40(5)	28(4)	25(4)	-10(3)	8(4)	-7(4)
C(21)	32(5)	23(4)	25(4)	-4(3)	-9(3)	12(3)
C(22)	20(4)	26(4)	20(4)	-9(3)	1(3)	-2(3)
C(23)	24(4)	32(4)	27(4)	4(3)	-6(3)	1(3)
C(24)	24(4)	41(5)	42(5)	-10(4)	13(4)	-8(4)
C(25)	41(5)	32(5)	36(5)	17(4)	18(4)	12(4)
C(26)	36(5)	48(5)	20(4)	9(4)	-5(3)	9(4)
C(27)	20(4)	40(5)	30(4)	-8(4)	-1(3)	2(3)
C(28)	19(4)	31(4)	20(4)	-4(3)	5(3)	-12(3)
C(29)	32(4)	39(5)	15(4)	2(3)	1(3)	0(4)
C(30)	27(4)	63(5)	18(4)	0(4)	8(3)	0(4)
C(31)	32(5)	68(6)	14(4)	-11(4)	6(3)	-18(4)
C(32)	39(5)	51(5)	29(4)	-27(4)	17(4)	-20(4)
C(33)	32(4)	35(4)	29(4)	1(4)	6(3)	-6(4)
C(34)	11(4)	27(4)	14(3)	5(3)	-3(3)	6(3)
C(35)	23(4)	20(4)	23(4)	3(3)	-11(3)	-1(3)
C(36)	64(6)	22(4)	24(4)	-10(3)	4(4)	-7(4)
C(37)	50(6)	39(5)	26(4)	-3(4)	18(4)	8(4)
C(38)	27(5)	47(5)	20(4)	14(4)	1(3)	5(4)
C(39)	30(4)	24(4)	13(3)	1(3)	-5(3)	-1(3)
C(40)	46(5)	45(5)	31(4)	4(4)	5(4)	-21(4)
C(41)	53(6)	25(5)	124(9)	9(5)	-16(6)	3(4)
C(42)	44(6)	39(6)	181(12)	-34(7)	7(7)	-4(5)

C(43)	55(7)	59(6)	85(7)	-13(5)	3(5)	-13(5)
C(44)	37(5)	69(7)	92(8)	21(6)	6(5)	1(5)
C(45)	45(6)	42(5)	97(7)	-8(5)	17(5)	12(5)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for $4\text{c}(\text{ClPh}) \cdot 0.5\text{PhCl}$

	x	y	z	U(eq)
H(1A)	3521	7559	8978	67
H(1B)	2791	8132	8646	67
H(2A)	1889	7901	9697	133
H(2B)	2961	8086	10065	133
H(2C)	2621	7323	10030	133
H(3)	3419	5486	7732	67
H(4A)	3587	6386	9086	136
H(4B)	4179	5706	9093	136
H(4C)	3048	5683	9034	136
H(5A)	4264	6287	7082	102
H(5B)	4915	6010	7884	102
H(5C)	4420	6726	7899	102
H(7)	2975	5518	6558	72
H(8)	2267	5121	5421	98
H(9)	830	5317	4791	102
H(10)	-148	6114	5066	92
H(11)	73	6863	6022	61
H(13)	-56	7521	6906	70
H(14A)	510	7827	8282	156
H(14B)	65	8444	7741	156
H(14C)	1193	8364	7949	156
H(15A)	1478	8309	6481	117
H(15B)	385	8523	6277	117
H(15C)	758	7875	5856	117
H(41)	1356	5254	8291	84
H(42)	353	4621	7385	107
H(43)	-1157	4948	6917	80
H(44)	-1720	5965	7360	80
H(45)	-707	6616	8284	73

Table 6. Torsion angles [°] for **4c**(ClPh)·0.5PhCl

N(2)-Al-N(1)-C(6)	-2.4(5)
C(1)-Al-N(1)-C(6)	-152.1(5)
Cl-Al-N(1)-C(6)	96.7(5)
N(2)-Al-N(1)-C(3)	174.0(6)
C(1)-Al-N(1)-C(3)	24.2(7)
Cl-Al-N(1)-C(3)	-87.0(6)
N(1)-Al-N(2)-C(12)	7.1(4)
C(1)-Al-N(2)-C(12)	154.4(5)
Cl-Al-N(2)-C(12)	-92.1(4)
N(1)-Al-N(2)-C(13)	-174.3(6)
C(1)-Al-N(2)-C(13)	-27.0(7)
Cl-Al-N(2)-C(13)	86.5(5)
N(1)-Al-Cl-C(40)	-56.0(3)
N(2)-Al-Cl-C(40)	33.3(4)
C(1)-Al-Cl-C(40)	171.1(4)
N(1)-Al-C(1)-C(2)	-119.8(7)
N(2)-Al-C(1)-C(2)	104.4(7)
Cl-Al-C(1)-C(2)	-8.8(8)
C(6)-N(1)-C(3)-C(5)	90.0(8)
Al-N(1)-C(3)-C(5)	-86.1(8)
C(6)-N(1)-C(3)-C(4)	-148.9(6)
Al-N(1)-C(3)-C(4)	35.0(8)
C(3)-N(1)-C(6)-C(7)	-2.4(10)
Al-N(1)-C(6)-C(7)	174.2(6)
C(3)-N(1)-C(6)-C(12)	-179.2(6)
Al-N(1)-C(6)-C(12)	-2.6(7)
N(1)-C(6)-C(7)-C(8)	172.8(9)
C(12)-C(6)-C(7)-C(8)	-10.7(14)
C(6)-C(7)-C(8)-C(9)	-1.8(18)
C(7)-C(8)-C(9)-C(10)	6.9(19)
C(8)-C(9)-C(10)-C(11)	0.1(18)
C(9)-C(10)-C(11)-C(12)	-4.1(17)
C(13)-N(2)-C(12)-C(11)	-10.5(10)
Al-N(2)-C(12)-C(11)	168.2(5)

C(13)-N(2)-C(12)-C(6)	171.3(6)
Al-N(2)-C(12)-C(6)	-10.0(7)
C(10)-C(11)-C(12)-N(2)	177.4(8)
C(10)-C(11)-C(12)-C(6)	-4.6(13)
N(1)-C(6)-C(12)-N(2)	8.5(8)
C(7)-C(6)-C(12)-N(2)	-168.3(6)
N(1)-C(6)-C(12)-C(11)	-169.6(6)
C(7)-C(6)-C(12)-C(11)	13.5(11)
C(12)-N(2)-C(13)-C(14)	166.9(7)
Al-N(2)-C(13)-C(14)	-11.5(9)
C(12)-N(2)-C(13)-C(15)	-69.7(9)
Al-N(2)-C(13)-C(15)	111.9(7)
C(34)-B-C(16)-C(21)	-51.4(7)
C(22)-B-C(16)-C(21)	-169.0(5)
C(28)-B-C(16)-C(21)	69.7(6)
C(34)-B-C(16)-C(17)	137.0(6)
C(22)-B-C(16)-C(17)	19.3(9)
C(28)-B-C(16)-C(17)	-101.9(7)
C(21)-C(16)-C(17)-F(1)	-178.2(5)
B-C(16)-C(17)-F(1)	-6.2(9)
C(21)-C(16)-C(17)-C(18)	2.2(9)
B-C(16)-C(17)-C(18)	174.3(6)
F(1)-C(17)-C(18)-F(2)	2.1(8)
C(16)-C(17)-C(18)-F(2)	-178.4(5)
F(1)-C(17)-C(18)-C(19)	-179.1(5)
C(16)-C(17)-C(18)-C(19)	0.5(10)
F(2)-C(18)-C(19)-F(3)	-0.6(9)
C(17)-C(18)-C(19)-F(3)	-179.5(5)
F(2)-C(18)-C(19)-C(20)	176.4(6)
C(17)-C(18)-C(19)-C(20)	-2.5(10)
F(3)-C(19)-C(20)-F(4)	-2.5(9)
C(18)-C(19)-C(20)-F(4)	-179.5(6)
F(3)-C(19)-C(20)-C(21)	178.6(5)
C(18)-C(19)-C(20)-C(21)	1.5(9)
C(17)-C(16)-C(21)-F(5)	177.8(5)
B-C(16)-C(21)-F(5)	4.9(8)

C(17)-C(16)-C(21)-C(20)	-3.2(9)
B-C(16)-C(21)-C(20)	-176.1(6)
F(4)-C(20)-C(21)-F(5)	1.6(8)
C(19)-C(20)-C(21)-F(5)	-179.4(5)
F(4)-C(20)-C(21)-C(16)	-177.5(6)
C(19)-C(20)-C(21)-C(16)	1.5(9)
C(34)-B-C(22)-C(27)	-71.7(7)
C(16)-B-C(22)-C(27)	52.1(8)
C(28)-B-C(22)-C(27)	165.4(6)
C(34)-B-C(22)-C(23)	102.1(7)
C(16)-B-C(22)-C(23)	-134.2(6)
C(28)-B-C(22)-C(23)	-20.9(9)
C(27)-C(22)-C(23)-F(6)	176.6(6)
B-C(22)-C(23)-F(6)	2.4(10)
C(27)-C(22)-C(23)-C(24)	-4.6(9)
B-C(22)-C(23)-C(24)	-178.8(6)
F(6)-C(23)-C(24)-F(7)	-1.2(9)
C(22)-C(23)-C(24)-F(7)	179.9(6)
F(6)-C(23)-C(24)-C(25)	-177.4(6)
C(22)-C(23)-C(24)-C(25)	3.7(11)
F(7)-C(24)-C(25)-F(8)	2.5(10)
C(23)-C(24)-C(25)-F(8)	178.7(6)
F(7)-C(24)-C(25)-C(26)	-177.3(6)
C(23)-C(24)-C(25)-C(26)	-1.1(10)
F(8)-C(25)-C(26)-F(9)	-1.4(10)
C(24)-C(25)-C(26)-F(9)	178.4(6)
F(8)-C(25)-C(26)-C(27)	-179.8(6)
C(24)-C(25)-C(26)-C(27)	0.0(10)
F(9)-C(26)-C(27)-F(10)	0.7(9)
C(25)-C(26)-C(27)-F(10)	179.1(6)
F(9)-C(26)-C(27)-C(22)	-179.8(6)
C(25)-C(26)-C(27)-C(22)	-1.4(11)
C(23)-C(22)-C(27)-F(10)	-176.9(5)
B-C(22)-C(27)-F(10)	-2.4(9)
C(23)-C(22)-C(27)-C(26)	3.5(10)
B-C(22)-C(27)-C(26)	178.1(6)