Electronic Supplementary Information for:

Monomeric Cp^{3t}Al(I): Synthesis, reactivity, and the concept of valence isomerism

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S1 Synthetic details and characterization of compounds

General remarks

All syntheses were carried out in an Argon-filled glovebox or with standard Schlenk techniques¹ unless otherwise stated. Cp^{3t}H, (Cp^{3t})₂Mg and (Cp*Al)₄ were prepared as described previously.²⁻⁴ All solvents were dried by distillation over appropriate drying agents⁵ and stored over molecular sieves. All solution NMR spectra were acquired on a Bruker Avance 400 NMR spectrometer (¹H: 400.1 MHz, ²⁷Al: 104 MHz, ¹³C: 101 MHz). ¹H NMR and ¹³C NMR spectra were referenced to external TMS via residual protons of the solvent (¹H) or the solvent itself (¹³C). ²⁷Al NMR spectra were referenced to external TMS via external Al(NO₃)₃. Elemental analyses were performed on an Elementar vario MICRO cube elemental analyzer. High-resolution mass spectrometry was obtained using a Thermo Scientific Exactive Plus spectrometer.



Synthesis of Cp^{3t}AlBr₂: $(Cp^{3t})_2Mg$ (5.00 g, 10.2 mmol) was dissolved in pentane (50 mL) and AlBr₃ (5.43 g, 20.3 mmol) was added. The colorless solution turned slightly yellowish and white solids precipitated immediately. After the reaction mixture was stirred for 30 minutes, the suspension was filtrered. The filtrate was

concentrated and stored at -30 °C overnight to obtain colorless crystals. These were isolated by filtration, washed with pentane (3 x 2 mL) and dried under reduced pressure to give **2** (4.92 g, 11.7 mmol, 58%).

¹H NMR (C_6D_6): δ 6.64 (s, 2 H, $C_5H_2(tBu)_3$), 1.41 (s, 18 H, *t*Bu), 1.24 (s, 9 H, *t*Bu) ppm. ¹³C{¹H} NMR (C_6D_6): δ 130.2 (Ar), 126.4 (Ar), 115.2 (Ar), 34.4 ($C(CH_3)_3$), 32.7 ($C(CH_3)_3$), 32.3 ($C(CH_3)_3$), 31.1 ($C(CH_3)_3$) ppm.

²⁷Al NMR (C_6D_6): δ –42 (s, br) ppm.

Anal. Found: C 47.55, H 6.93; Calcd. Data for C₁₇H₂₉AlBr₂: C 48.59, H 6.96.



Synthesis of Cp^{3t}Al \rightarrow Cp*AlBr₂: Cp^{3t}AlBr₂ (2.59 g, 6.16 mmol) was dissolved in toluene (20 mL) and (Cp*Al)₄ (1.00 g, 6.16 mmol) was added. The yellow suspension was sonicated over a period of two hours until (Cp*Al)₄ was consumed and the reaction mixture turned colorless. The mixture was filtered and

the solvent from the filtrate was removed under reduced pressure. The residue was treated with pentane (20 mL), filtrated and the residue was dried under reduced pressure to obtain analytically pure **3**. A second fraction of **3** can be crystallized after concentrating the filtrate and storage at -30 °C overnight to give an overall yield of 2.7 g (4.64 mmol, 75%).

¹H NMR (C₆D₆): δ 6.25 (s, 2 H, C₅*H*₂(*t*Bu)₃), 1.90 (s, 15 H, C₅Me₅), 1.38 (s, 18 H, *t*Bu), 1.24 (s, 9 H, *t*Bu) ppm.

¹³C{¹H} NMR (C₆D₆): δ 131.7 (Ar), 130.4 (Ar), 117.1 (Ar), 108.3 (Ar), 33.8(*C*(CH₃)₃), 33.8(*C*(*CH*₃)₃), 31.8(*C*(CH₃)₃), 31.8(*C*(CH₃)₃), 11.5 (C₅*Me*₅) ppm.

Note: No signal could be observed in the ²⁷Al NMR spectrum, probably due to its broadness.

LIFDI-MS (m/z) calculated for [C₂₇H₄₄Al₂Br₁ (C₂₇H₄₄Al₂Br₂ –Br] = 501.2252; found: 501.2236.



Synthesis of Cp^{3t}Al: 2 (1.00 g, 1.72 mmol) was dissolved in 20 ml pentane and cAAC^{Me} (0.490 g, 1.72 mmol) was added in portions. The reaction mixture turned yellow and slightly yellow solids precipitated immediately. After stirring for six hours, the suspension was filtered, and the solvent was removed from the filtrate

under reduced pressure to give **1** as a yellow oil (0.348 g, 1.33 mmol, 78%).

¹H NMR (C₆D₆): δ 5.94 (s, 2 H, C₅H₂(*t*Bu)₃), 1.37 (s, 18 H, *t*Bu), 1.20 (s, 9 H, *t*Bu) ppm.

¹³C{¹H} NMR (C₆D₆): δ 131.4 (Ar), 130.2 (Ar), 103.8 (Ar), 34.4 (C(*CH*₃)₃), 32.8 (*C*(*CH*₃)₃), 32.4 C(*CH*₃)₃), 30.9 (*C*(*CH*₃)₃) ppm.

²⁷AI NMR (C_6D_6): δ –161 (s) ppm.

LIFDI-MS (m/z) calculated for [C₁₇H₂₉AI₁] = 260.2079; found: 260.2071.



Generation of an equilibrium mixture of $Cp^{3t}AI \rightarrow Cp^{3t}AIBr_2$ (4) and $Cp^{3t}(Br)AI-AI(Br)Cp^{3t}$ (5), and their isolation: To a solution of $Cp^{3t}AI$ (30 mg, 0.12 mmol, 0.6 mL, 0.19 M in C_6D_6) $Cp^{3t}AIBr_2$ (48 mg, 0.12 mmol) was added. The solvent was

removed, and the residue was treated with 1 ml pentane, filtered and stored at room temperature overnight. Colorless crystals precipitated, which were isolated and dried under reduced pressure to give **4** (30 mg, 0.044 mmol, 36 %). Storing the mother liquor at -30 °C overnight afforded **5** (10 mg, 0.015 mmol, 12 %) as colorless crystals. Both species gave identical averaged NMR spectra for the equilibrium mixture of **4** and **5**. Recrystallization of solutions of both isolated **4** and **5** afforded again both species at the same conditions as described above. Equilibrium NMR parameters:

¹H NMR (C₆D₆): δ 6.39 (s, 2 H, C₅H₂(*t*Bu)₃), 1.43 (s, 18 H, *t*Bu), 1.29 (s, 9 H, *t*Bu) ppm.

¹³C{¹H} NMR (C₆D₆): δ 130.9 (Ar), 129.1 (Ar), 111.8 (Ar), 34.1 (C(CH₃)₃), 33.6 (C(CH₃)₃), 32.1 (C(CH₃)₃), 31.8 (C(CH₃)₃) ppm.

²⁷AI NMR (C_6D_6): δ –64 (s, br) ppm.

Anal. Found: C 61.53, H 8.65; Calcd. Data for C₃₄H₅₈Al₂Br₂: C 60.00, H 8.59.

Synthesis of Cp^{3t}Al→tBuAlCl₂: To a solution of Cp^{3t}Al (30 mg, 0.12 mmol,



0.6 mL, 0.19 M in C_6D_6) *t*BuAlCl₂ (17.9 mg, 0.12 mmol) was added. The solvent was removed, and the residue was treated with 1 ml pentane, filtered and stored at -30 °C overnight. Colorless crystals precipitated, which were isolated and dried under reduced pressure to give **6** (20 mg, 0.048 mmol, 40 %).

¹H NMR (C₆D₆): δ 6.13 (s, 2 H, C₅*H*₂(*t*Bu)₃), 1.30 (s, 9 H, *t*Bu), 1.22 (s, 18 H, *t*Bu), 1.09 (s, 9 H, *t*Bu) ppm.

¹³C{¹H} NMR (C₆D₆): δ 133.5 (Ar), 104.4. (Ar), 33.7 (C(*CH*₃)₃), 33.6 (*C*(*CH*₃)₃), 31.6 (*C*(*CH*₃)₃), 28.5 (*C*(*CH*₃)₃) ppm.

²⁷Al NMR (C₆D₆): δ 145.7 (Al(2), s, br) ppm. The signal for Al(1) was not observed.

Anal. Found: C 61.08, H 8.73; Calcd. Data for C₂₁H₃₈Al₂Cl₂: C 60.72, H 9.22.



Synthesis of Cp^{3t}Al \rightarrow AlBr₃: AlBr₃ (32.0 mg, 0.12 mmol) was dissolved in benzene (0.5 mL), and a solution of Cp^{3t}Al (30 mg, 0.12 mmol, 0.6 mL, 0.19 M in C₆D₆) was added. The solution was layered with pentane, which resulted in the precipitation of colorless crystals over a period of 12 h. The

crystals were isolated and dried under reduced pressure to give 7 (41 mg, 0.078 mmol, 65%).

¹H NMR (C₆D₆): δ 6.10 (s, 2 H, C₅H₂(*t*Bu)₃), 1.13 (s, 18 H, *t*Bu), 0.99 (s, 9 H, *t*Bu) ppm.

¹³C{¹H} NMR (C₆D₆): δ 135.0 (Ar), 134.3 (Ar), 104.5. (Ar), 33.8 (C(*CH*₃)₃), 33.6 (*C*(*CH*₃)₃), 31.8 (*C*(*CH*₃)₃), 31.5 (*C*(*CH*₃)₃) ppm.

²⁷Al NMR (C_6D_6): δ 95.0 (Al(2), s, br) ppm. The signal for Al(1) was not observed.

Anal. Found: C 39.59, H 5.34; Calcd. Data for C₁₇H₂₉Al₂Br₃: C 38.74, H 5.55.



Synthesis of $Cp^{3t}AI \rightarrow (Br)_2AI-AI(Br)(Cp^{3t})$: A solution of $AIBr_3$ (16.0 mg, 0.06 mmol) in benzene (0.5 mL) was added dropwise to a solution of $Cp^{3t}AI$ (30 mg, 0.12 mmol, 0.6 mL, 0.19 M in C_6D_6). All volatiles were removed in vacuo, and the residue washed with pentane (2 x 0.5 mL) and dried in vacuo. Hereby, **8** was isolated as a colorless solid (28 mg, 0.04

mmol, 67%). Single crystals were obtained by slowly evaporating the solvent from benzene solutions of **8**.

¹H-NMR (C₆D₆): δ 6.37 (s, 2 H, C₅H₂(*t*Bu)₃), 1.42 (s, 18 H, *t*Bu), 1.27 (s, 9 H, *t*Bu) ppm.

¹³C{¹H}-NMR (C₆D₆): δ 130.9 (Ar), 112.4.8 (Ar), 111.4. (Ar), 34.0 (C(CH₃)₃), 33.6 (C(CH₃)₃), 32.0 (C(CH₃)₃), 31.8(C(CH₃)₃) ppm.

 $^{27}\text{Al-NMR}$ (C₆D₆): δ -71.0 (Al(3), s, br) ppm. The signals for Al(1,2) were not observed.

Anal. Found: C 51.59., H 7.40; Calcd. Data for C₃₄H₅₈Al₂Br₂: C 51.86, H 7.42.



Synthesis of (Cp^{3t}AIO)₂: A solution of Cp^{3t}AI (30 mg, 0.12 mmol, 0.6 mL,

0.19 M in C_6D_6) was degassed and subjected to an atmosphere of N₂O. The solvent was removed, and the residue dissolved in small amounts of pentane (0.3 mL). Colorless crystals precipitated upon slow evaporation at -30 °C, which were isolated and dried under reduced pressure to give **9** (19 mg, 0.069 mmol, 57 %).

¹H NMR (C₆D₆): δ 6.49 (s, 2 H, C₅H₂(*t*Bu)₃), 1.61 (s, 18 H, *t*Bu), 1.39 (s, 9 H, *t*Bu) ppm.

¹³C{¹H} NMR (C₆D₆): δ 127.9 (Ar), 125.9 (Ar), 108.4 (Ar), 34.2 (C(CH₃)₃), 33.4 (C(CH₃)₃), 32.2 (C(CH₃)₃), 31.9 (C(CH₃)₃) ppm.

Note: No signal could be observed in ²⁷Al NMR, probably due to its broadness.

Anal. Found: C 73.96, H 10.54; Calcd. Data for C₅₁H₈₇Al₃O₃: C 73.87, H 10.58.



Synthesis of (Cp^{3t}AINPh)₂: To a solution of Cp^{3t}AI (30 mg, 0.12 mmol, 0.6 mL, 0.19 M in C₆D₆) an excess of PhN₃ (40 mg, 0.34 mmol) was added, which was accompanied by the a color change of the solution to red. The solvent was removed, and the residue was washed with pentane (3 x 0.5 mL) to give colorless **10** (28 mg, 0.16 mmol, 66%). Colorless crystals precipitated out of

the reaction mixture in benzene, when stored overnight at room temperature. ¹H NMR (C_6D_6): δ 7.35 (t, ${}^2J_{H,H}$ = 7.5 Hz, 2H, *o*- C_6H_5N), 7.11 (d, ${}^2J_{H,H}$ = 7.5 Hz, 2H, *m*- C_6H_5N), 6.97 (t, ² $J_{H,H}$ = 7.5 Hz, 1H, *p*- C_6H_5N), 6.78 (s, 2 H, $C_5H_2(tBu)_3$), 1.57 (s, 9 H, *t*Bu), 1.18 (s, 18 H, *t*Bu) ppm. ¹³C{¹H} NMR (C_6D_6): δ 153.3 (Ar), 129.4 (Ar), 129.2 (Ar), 129.0 (Ar), 123.8 (Ar), 119.1 (Ar), 107.2. (Ar), 33.8 ($C(CH_3)_3$), 32.9 ($C(CH_3)_3$), 32.6 ($C(CH_3)_3$), 32.1 ($C(CH_3)_3$) ppm.

Note: Signals at δ 34.5, 22.7 and 14.3 ppm are due to remaining pentane. No signal could be observed in the ²⁷Al NMR spectrum, probably due to its broadness.

Anal. Found: C 80.21, H 9.93, N 4.32; Calcd. Data for C₄₆H₆₈Al₂N₂: C 78.59, H 9.75, N 3.98.

S2 NMR Spectra of all isolated species





Figure S2. ²⁷Al NMR (104 MHz, C₆D₆) spectrum of 1.







Figure S4. ¹H NMR (400 MHz, C₆D₆) spectrum of 2.



Figure S5. ^{27}Al NMR (104 MHz, $C_6D_6)$ spectrum of 2.



Figure S6. $^{13}C\{^{1}H\}$ NMR (101 MHz, $C_{6}D_{6})$ spectrum of 2.



Figure S7. ¹H NMR (400 MHz, C_6D_6) spectrum of 3.



Figure S8. ^{27}Al NMR (104 MHz, $C_6D_6)$ spectrum of 3.



Figure S9. $^{13}C\{^{1}H\}$ NMR (101 MHz, $C_{6}D_{6})$ spectrum of 3.



Figure S10. ¹H NMR (400 MHz, C₆D₆) spectrum of 4/5 at rt



Figure S11. ²⁷Al NMR (104 MHz, C₆D₆) spectrum of 4/5 at rt.



Figure S12. $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, $C_6D_6)$ spectrum of 4/5 at rt.





Figure S14. 27 Al NMR (104 MHz, C₆D₆) spectrum of 6.



Figure S15. $^{13}\text{C}\{^{1}\text{H}\}$ NMR (101 MHz, $C_6D_6)$ spectrum of 6.



Figure S16. ¹H NMR (400 MHz, C₆D₆) spectrum of 7.



Figure S17. $^{\rm 27}Al$ NMR (104 MHz, $C_6D_6)$ spectrum of 7.



Figure S18. ${}^{13}C{}^{1}H$ NMR (101 MHz, C_6D_6) spectrum of 7.



Figure S20. $^{\rm 27}Al$ NMR (104 MHz, $C_6D_6)$ spectrum of 8.



Figure S21. $^{13}C\{^{1}H\}$ NMR (101 MHz, $C_6D_6)$ spectrum of 8.



Figure S22. ¹H NMR (400 MHz, C₆D₆) spectrum of 9.



Figure S23. $^{\rm 27}Al$ NMR (104 MHz, $C_6D_6)$ spectrum of 9.



Figure S24. $^{13}\text{C}\{^{1}\text{H}\}$ NMR (101 MHz, $C_6D_6)$ spectrum of 9.



Figure S25. ¹H NMR (400 MHz, C_6D_6) spectrum of 10.



Figure S26. 27 Al NMR (104 MHz, C₆D₆) spectrum of 10.



Figure S27. $^{13}C\{^{1}H\}$ NMR (101 MHz, $C_{6}D_{6})$ spectrum of 10.



Figure S28. VT ¹H NMR (104 MHz, toluene-*d*₈) spectrum of 4/5 (rt to 100 °C).



Figure S29. VT ¹H NMR (104 MHz, toluene- d_8) spectrum of 4/5 (rt to -90 °C).



Figure S30. VT 27 Al NMR (104 MHz, toluene- d_8) spectrum of 4/5 (rt to 100 °C).



Figure S31. VT ²⁷AI NMR (104 MHz, toluene-*d*₈) spectrum of 4/5 (rt to -90 °C).



Figure S32. ¹H DOSY NMR (C₆D₆, 298 K) spectrum of 1.

D = K·M_w^{α} D₍₁₎ =8.703 x e⁻¹⁰ m²/s $Mw = \sqrt[\alpha]{\frac{D}{K}}$

Depending on α and K, an average M_w of 253 g/mol is calculated. 6

S3 Crystal structure determinations

The crystal data of **2**, **3**, **4** and **6**, were collected on a Bruker D8 Quest diffractometer with a CMOS area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The crystal data of **5**, and **7-10** were collected on a Bruker X8-APEX II diffractometer with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The structures were solved using intrinsic phasing method (ShelXT, G. Sheldrick, *Acta Cryst.*, **2015**, *A71*, 3–8),⁷ refined with the ShelXL program (G. Sheldrick, *Acta Cryst.*, **2008**, *A64*, 112–122)⁸ and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factors calculations. All hydrogen atoms were assigned to idealised geometric positions. The structure of **4** was refined using TWIN keyword (matrix: Twin -1 0 0 0 1 0 0 0 -1). The BASF parameter was refined to 48%. The crystal of **5** was a pseudo-merohedral twin with domains rotated by 179.9 ° around real axis. The structure was refined using TWIN keyword (matrix: Twin 0.95 0.10 -0.05 0.975 -0.95 -0.03 0 0 -1 2). The BASF parameter was refined using TWIN keyword (matrix: twin -1 0 - 0.014 0 -1 0 0 0 1). The BASF parameter was refined using TWIN keyword (matrix: twin -1 0 - 0.014 0 -1 0 0 0 1). The BASF parameter was refined using TWIN keyword (matrix: twin -1 0 - 0.014 0 -1 0 0 0 1). The BASF parameter was refined to 7%.

Crystal data for **2**: $C_{17}H_{29}AlBr_2$, $M_r = 420.20$, colourless block, $0.675 \times 0.447 \times 0.289$ mm³, Monoclinic space group $P2_1/c$, a = 9.400(5) Å, b = 14.876(9) Å, c = 13.886(9) Å, $\beta = 105.24(4)^\circ$, V = 1873(2) Å³, Z = 4, $\rho_{calcd} = 1.490$ g·cm⁻³, $\mu = 4.365$ mm⁻¹, F(000) = 856, T = 100(2) K, $R_1 = 0.0725$, $wR^2 = 0.0841$, 3680 independent reflections [20≤52.042°] and 190 parameters.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-1878105. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif

Crystal data for **3**: $C_{27}H_{44}Al_2Br_2$, $M_r = 582.40$, colourless needle, $0.537 \times 0.133 \times 0.085 \text{ mm}^3$, Monoclinic space group $P2_1/c$, a = 8.824(3) Å, b = 29.234(6) Å, c = 12.125(3) Å, $\beta = 108.80(2)^\circ$, V = 2961.1(14) Å³, Z = 4, $\rho_{ca/cd} = 1.306 \text{ g} \cdot \text{cm}^{-3}$, $\mu = 2.809 \text{ mm}^{-1}$, F(000) = 1208, T = 100(2) K, $R_1 = 0.0711$, $wR^2 = 0.0700$, 5818 independent reflections $[20 \le 52.044^\circ]$ and 294 parameters.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-1878107. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif

Crystal data for **4**: $C_{34}H_{58}Al_2Br_2$, $M_r = 680.58$, colourless block, $0.216 \times 0.21 \times 0.143$ mm³, Monoclinic space group *Cc*, *a* = 19.582(6) Å, *b* = 8.479(2) Å, *c* = 21.301(8) Å, $\beta = 93.33(2)^\circ$, *V* = 3531(2) Å³, *Z* = 4, $\rho_{calcd} = 1.280 \text{ g} \cdot \text{cm}^{-3}$, $\mu = 2.366 \text{ mm}^{-1}$, *F*(000) = 1432, *T* = 100(2) K, *R*₁ = 0.0428, *wR*² = 0.1182, 6954 independent reflections [2 $\theta \le 52.042^\circ$] and 362 parameters.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-1878106. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif

Crystal data for **5**: : $C_{34}H_{58}Al_2Br_2$, $M_r = 680.58$, colourless block, $0.623 \times 0.544 \times 0.534$ mm³, Triclinic space group P $\overline{1}$, a = 10.367(2) Å, b = 12.452(3) Å, c = 15.704(3) Å, $\alpha = 69.094(5)^{\circ}$, $\beta = 88.918(6)^{\circ}$, $\gamma = 67.783(5)^{\circ}$, V = 1737.3(6) Å³, Z = 2, $\rho_{calcd} = 1.301$ g·cm⁻³, $\mu = 2.404$ mm⁻¹, F(000) = 716, T = 100(2) K, $R_1 = 0.0987$, $wR^2 = 0.2664$, 6846 independent reflections [2 $\theta \le 52.042^{\circ}$] and 362 parameters.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-1878104. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif

Crystal data for **6**: $C_{21}H_{38}Al_2Cl_2$, $M_r = 415.37$, colourless block, $0.303 \times 0.225 \times 0.166$ mm³, Monoclinic space group $P2_1$, a = 9.8915(4) Å, b = 21.5331(9) Å, c = 11.5146(5) Å, $\beta = 90.4570(10)^\circ$, V = 2452.47(18) Å³, Z = 4, $\rho_{calcd} = 1.125$ g·cm⁻³, $\mu = 0.339$ mm⁻¹, F(000) = 896, T = 100(2) K, $R_1 = 0.0437$, $wR^2 = 0.0778$, 9603 independent reflections [2 $\theta \le 52.042^\circ$] and 476 parameters.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-1878109. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif

Crystal data for **7**: $C_{17}H_{29}Al_2Br_3$, $M_r = 527.09$, colourless block, $0.297 \times 0.276 \times 0.232$ mm³, Triclinic space group $P \ \overline{1}$, a = 10.6448(18) Å, b = 10.6844(20) Å, c = 11.1041(12) Å, $\alpha = 63.541(5)^\circ$, $\beta = 81.455(7)^\circ$, $\gamma = 73.465(6)^\circ$, V = 1083.5(3) Å³, Z = 2, $\rho_{calcd} = 1.616$ g·cm⁻³, $\mu = 5.662$ mm⁻¹, F(000) = 524, T = 100(2) K, $R_1 = 0.0154$, $wR^2 = 0.0350$, 4275 independent reflections [2 $\theta \le 52.04^\circ$] and 208 parameters.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-1878108. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif

Crystal data for **8**: $C_{34}H_{58}AI_{3}Br_{3}$, $M_{r} = 787.47$, colourless plate, 0.256×0.234×0.213 mm³, Monoclinic space group $P2_{1}/c$, a = 10.1424(16) Å, b = 38.371(7) Å, c = 10.1825(19) Å, $\beta = 105.719(13)^{\circ}$, V = 3814.6(12) Å³, Z = 4, $\rho_{calcd} = 1.371$ g·cm⁻³, $\mu = 3.263$ mm⁻¹, F(000) = 1624, T = 100(2) K, $R_{1} = 0.0331$, $wR^{2} = 0.0517$, 7525 independent reflections [20≤52.04°] and 379 parameters.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-1879323. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif

Crystal data for **9**: $C_{51}H_{87}AI_3O_3$, $M_r = 829.14$, colourless plate, $0.36 \times 0.167 \times 0.084$ mm³, Monoclinic space group $P2_1/c$, a = 14.173(9) Å, b = 19.091(14) Å, c = 19.858(14) Å, $\beta = 109.37(2)^\circ$, V = 5069(6) Å³, Z = 4, $\rho_{calcd} = 1.086$ g·cm⁻³, $\mu = 0.112$ mm⁻¹, F(000) = 1824, T = 100(2) K, $R_1 = 0.1473$, $wR^2 = 0.1370$, 9985 independent reflections [2 $\theta \le 52.044^\circ$] and 541 parameters.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-1878111. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif

Crystal data for **10**: $C_{46}H_{68}Al_2N_2$, $M_r = 702.98$, colourless plate, $0.16 \times 0.138 \times 0.099 \text{ mm}^3$, Orthorhombic space group *Pbca*, a = 17.2467(17) Å, b = 13.0572(9) Å, c = 18.6141(16) Å, $V = 4191.8(6) \text{ Å}^3$, Z = 4, $\rho_{calcd} = 1.114 \text{ g} \cdot \text{cm}^{-3}$, $\mu = 0.102 \text{ mm}^{-1}$, F(000) = 1536, T = 100(2) K, $R_1 = 0.1067$, $wR^2 = 0.1138$, 4122 independent reflections [$2\theta \le 52.038^\circ$] and 235 parameters.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-1878110. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif

S4 Density functional theory (DFT) calculations

General remarks

Geometry optimizations of 4_{calc} and 5_{calc} were performed using the GAUSSIAN 16 program.⁹ The M06L hybrid functional and def2-SVP basis sets were used for all these computations.^{10,11}We ensured that the calculated geometries are minima on the potential energy surface by carrying out harmonic frequency calculations (zero negative eigenvalues of the Hessian). The transition state TS for the transformation of $\mathbf{4}_{calc}$ into $\mathbf{5}_{calc}$ was localized by optimization (opt=TS) of an initial structural guess, and its nature as transition state was also verified by harmonic frequency calculations (one negative eigenvalues of the Hessian).

Optimized structures



Cartesian coordinates for optimized structures

Br C C

HCCCHCC

Н Н



4_{calc}

Al	-1.63183200	0.18755100	0.13059300
AI	0.75687200	-0.80561800	-0.04552000
Br	0.14302600	-2.98688300	-0.67853300
Br	1.01761600	0.49143300	-1.98813500
С	-2.57590900	2.15107300	-0.24411600
С	-3.16466500	1.53880500	0.89500300
Н	-3.13929900	1.95672000	1.90016700
С	-3.79921900	0.30267700	0.53793000
С	-3.55144800	0.11012500	-0.88237600
С	-2.81991300	1.27019800	-1.32306700
Н	-2.44544900	1.41759600	-2.33361900
С	-1.82248600	3.46866900	-0.26090500
С	-0.62930000	3.38881900	0.69636300
Н	-0.07444100	4.33896500	0.71570900
Н	0.07931300	2.60362900	0.38096900

Н	-0.94317900	3.16837800	1.72869400
С	-1.31639900	3.77479700	-1.66753900
Н	-0.77780300	4.73294100	-1.67953400
Н	-2.14269100	3.85260300	-2.38953200
Н	-0.61988500	3.00137800	-2.02417300
С	-2,77627500	4,57771500	0.19514900
й	-2 26637000	5 55223800	0.18791900
 Ц	3 14534200	4 40577400	1 21682300
	-3.14334200	4.40377400	0.46650600
	-3.03132300	4.00022900	-0.40050000
C	-4.51998300	-0.54278500	1.59938300
C	-4.71638800	0.28749500	2.8/498/00
Н	-5.28439000	-0.29843800	3.61108200
Н	-5.27739600	1.21392700	2.68506200
Н	-3.76324400	0.55509100	3.35317800
С	-5.91953600	-0.94754300	1.12830400
Н	-6.45698600	-1.45531200	1.94229700
Н	-5.91302000	-1.63257600	0.27444100
н	-6.51114600	-0.06519100	0.84276400
C	-3 68728800	-1 76829400	2 00018400
ц	-4 23625100	-2 30185800	2 72170100
	-4.25025100	-2.39103000	2.12170100
	-2.73490900	-1.45105000	2.49470000
н	-3.40537300	-2.40778800	1.15505700
С	-3.95396200	-0.96922700	-1.89886700
С	-5.37484800	-0.66708300	-2.39324000
Н	-5.67241500	-1.39122800	-3.16627300
Н	-5.43178900	0.33655600	-2.83924100
Н	-6.12224100	-0.71193400	-1.59085200
С	-3.86289000	-2.39895600	-1.36435500
H	-4.09654400	-3,10646000	-2.17279100
H	-4 56221300	-2 61491900	-0 55001600
н	-2 84364100	-2 63517100	-1 01956300
C	2.04304100	-2.03317100	3 11023500
	-3.01119200	-0.91200000	-3.11023300
н	-3.24934600	-1.73424300	-3.79940900
н	-1.95451700	-1.02/11500	-2.81931100
Н	-3.10975500	0.01778200	-3.68564000
С	1.73504700	-0.27709400	1.76750300
С	2.28681600	0.97499800	1.37606300
Н	1.88926200	1.93367600	1.70752800
С	3.37001200	0.81495300	0.49648400
С	3.55511600	-0.60255100	0.30775100
Ċ	2,55757600	-1.25544200	1.07387700
Ĥ	2 52631000	-2 32390000	1 28111100
C	1 02308900	-0 55880000	3 00112600
C	2 00007500	-0.000000000	1 19156000
	2.09907500	-0.04040400	4.10100900
	1.05120000	-0.00410000	5.10050000
н	2.66670000	0.29018900	4.25614400
Н	2.81728300	-1.45214000	3.96464300
С	0.26328100	-1.88420000	3.04008500
Н	-0.22751200	-2.09326500	4.00276900
Н	0.92657800	-2.73353700	2.82157600
Н	-0.51992400	-1.88514400	2.26453400
С	0.05657100	0.56772500	3.45096000
Ĥ	-0 43832000	0 36488900	4 41337700
н	-0 73657800	0.68612200	2 69312600
Ц	0.56945500	1 53625400	3 54437100
	4 11503400	2.04911500	0.02602900
C	4.11503400	2.04611500	-0.03093600
C .	3.21531100	3.28876600	0.06236700
н	3.73135800	4.16029200	-0.36747800
Н	2.96270600	3.55231200	1.09921400
Н	2.27617900	3.14686800	-0.49493900
С	5.34671400	2.30422500	0.84465000
Н	5.88584300	3.20575000	0.51198600
Н	6.05673900	1.46757400	0.82888400
Н	5 05107000	2 45887400	1.89282600
C	4 53833700	1 96710800	-1 50566400
ы	4.00000100	2 02222100	-1.00000400
	4.5500000	1 70500000	2 46425000
н	3.67491900	1.78599000	-2.10135000

Н	5.28371300	1.19184700	-1.70873900
С	4.53047700	-1.43450800	-0.53406000
С	5.98374600	-1.00998600	-0.29741700
Н	6.66630600	-1.69001300	-0.82920000
Н	6.23916700	-1.05664200	0.77190000
Н	6.21037600	0.00292600	-0.64553000
С	4.17651300	-1.38730000	-2.02675500
Н	4.90723600	-1.96768600	-2.61207500
Н	4.14464800	-0.37264900	-2.43743700
Н	3.18627700	-1.83500100	-2.20126600
С	4.45055300	-2.91251400	-0.12530500
Н	5.17910700	-3.49671400	-0.70622300
Н	3.46042100	-3.34692800	-0.32495100
Н	4.68327000	-3.06070200	0.93977900



5_{calc}

1.18799400	0.21237800	-0.50611600
-1.18852300	0.30519900	0.44178600
0.93228000	0.64957200	-2.84961900
-0.90395700	1.26510500	2.62911400
2.84923600	1.36552800	0.41267700
3.30663200	0.44575300	-0.56964300
3.71925600	0.72036700	-1.53820800
3.07564900	-0.90588100	-0.13253400
2.54786400	-0.80414100	1.22933100
2.41837600	0.57233600	1.51141600
1.96907700	0.97919800	2.41275600
3.01262200	2.87572000	0.38147300
4.49859600	3.18724700	0.59986500
4.67017400	4.27395100	0.62732600
5.12034400	2.77121500	-0.20636000
4.86004500	2.76649800	1.54930700
2.56918500	3.44552300	-0.96550600
2.76554000	4.52707100	-1.01113500
1.49110400	3.29698400	-1.13320900
3.09447400	2.97870200	-1.81188000
2.19155000	3.52206500	1.49438000
2.27701600	4.61756300	1.44949000
2.53091100	3.20919600	2.49258800
1.12444200	3.26277200	1.41769500
3.65044400	-2.07936100	-0.94341800
3.87358600	-1.66972700	-2.40543300
4.24101700	-2.53593400	-2.97406500
4.63133200	-0.88209900	-2.51158100
2.95181900	-1.31990700	-2.89032700
5.03280400	-2.43368100	-0.37455600
5.49133000	-3.24347700	-0.96264500
5.00401400	-2.75705300	0.67125000
5.70521400	-1.56473000	-0.42912700
2.74293800	-3.30938300	-0.97970400

Н	3.20240600	-4.09754900	-1.59429100
н	1 77145500	-3 06948300	-1 43713100
	2 5 4 6 5 2 7 0 0	2 7400000	0.00007000
П	2.54652700	-3.74800200	0.00367000
С	2.14172200	-1.86242900	2.26717500
С	3.23214100	-2.91486100	2.49640600
Ĥ	2 94923100	-3 55827800	3 34264500
	4 10127600	-0.00027000	2 75420400
п	4.19127600	-2.44198200	2.75428100
Н	3.40281100	-3.57755800	1.64204500
С	1.92100900	-1.19327200	3.63062600
н	1 67684300	-1 95985200	4 38004800
	1.07004000	0.47704700	2.00004000
н	1.08869600	-0.47781700	3.61865700
Н	2.82305400	-0.66820500	3.97687100
С	0.82069900	-2.53719500	1.88410300
Ĥ	0 57137600	-3 34476400	2 59041400
н Ц	0.07107000	0.04470400	0.07160000
п	0.62653500	-2.90370000	0.07 100000
Н	-0.00116700	-1.80365500	1.93289300
С	-2.84908500	1.35770500	-0.56593400
C	-2 44003400	0 42245300	-1 55980900
Ŭ	2.0124600	0.70110000	2 51522400
	-2.00124600	0.70116000	-2.51555400
C	-2.60735800	-0.90351700	-1.10652200
С	-3.09207500	-0.82044300	0.27210700
С	-3 30698100	0 58245300	0 52795400
ы	3 69521900	0.00000000	1 46167200
	-3.06321600	0.99090000	1.40107200
C	-2.87244300	2.87000400	-0.71354800
С	-3.45388400	3.51666200	0.54109400
н	-3.44097700	4.61295900	0.45003700
н	-2.87506800	3 25216600	1 / 3003000
11	-2.07 500000	3.23210000	1.4030000
н	-4.49824300	3.21150900	0.70829700
С	-1.44964800	3.39138800	-0.94131100
Н	-1.44663200	4.47702500	-1.12224400
н	-0 96939600	2 90658800	-1 80607400
11	-0.303335000	2.30030000	-1.00007400
	-0.01744600	3.20017900	-0.05525600
С	-3.74246300	3.22649700	-1.92330800
Н	-3.80616000	4.31781800	-2.04796400
н	-4 76621000	2 84176000	-1 80730600
 	2 2220000	2.0117.0000	2 95517600
	-3.33360000	2.01004900	-2.00017000
С	-2.30309500	-2.09878900	-2.01873900
С	-2.06966000	-1.61213200	-3.45490300
н	-1 89868800	-2 47717100	-4 11147700
н	1 10001200	0.06123300	-3 54160400
	-1.19091200	-0.90125500	-5.54100400
н	-2.94233000	-1.06905300	-3.84576400
С	-3.48962500	-3.06672200	-2.10437200
Н	-3.28409100	-3.83662200	-2.86263900
н	-4 40368300	-2 53015300	-2 41576500
11	-4.4000000	2.55315500	-2.41070000
п	-3.71199700	-3.59379000	-1.17184900
С	-1.02953500	-2.82498500	-1.57673400
Н	-0.83299400	-3.70094500	-2.21451600
н	-1 06356200	-3 16827100	-0 53487600
н Ц	0.16276600	2 15005200	1 67950700
	-0.10370000	-2.15095500	-1.0/009/00
C	-3.66408900	-1.85986100	1.25262800
С	-3.68993100	-1.29049100	2.67775100
н	-2 69007300	-0 99459800	3 02632000
 ப	4 07105600	2 05440100	3 37031000
		-2.00+40100	0.37031900
н	-4.34991300	-0.41916400	2.78071400
С	-2.86613900	-3.16144000	1.34191700
Н	-1.82753000	-2.97487800	1.64932200
н	_2 83854300	-3 73650600	0 41150700
11	-2.00004000	-0.7000000	0.40004000
н	-3.31364000	-3.81000800	2.10361300
С	-5.11808600	-2.15033800	0.85301400
Н	-5.20858200	-2.57481100	-0.15394100
н	-5 71759300	-1 22846800	0.87405800
 ப	5.7 17 00000	2 26040200	1 5501/600
11	-0.070703000	-2.00040200	1.00014000



тs

Al 1.1005600 0.00109100 0.08139400 Br -0.30782800 -2.37174700 -0.62686800 Br 1.05154600 0.63341600 -2.37062500 C -2.43823000 2.07407400 -0.05056700 C -2.88797900 1.31035500 1.04479900 H -2.62259900 1.62322200 2.08567900 C -3.38201500 0.2094800 -0.61168700 C -3.322780400 0.00226700 -0.83969400 C -2.62035200 1.26046900 -1.19189800 H -2.33210400 1.5377600 -2.20357400 C -1.84441900 3.46975400 -0.00467600 C -0.76941100 3.5637000 1.08092000 H -0.0505600 2.84963700 0.38969400 C -1.22872200 3.83360700 -1.8349400 H -0.7644300 3.12682200 -1.64456900 C -2.97573200 4.45232900 0.32195900 H -3.43579900 4	AI	-1 27101800	0 08435700	0 05793700
Br -0.30782800 -2.37174700 -0.62668800 Br 1.05154600 0.63341600 -2.37062500 C -2.43823000 2.07407400 -0.05067200 C -2.88797900 1.31035500 1.04479900 H -2.82259900 1.62322200 2.08567900 C -3.38201500 0.02026700 -0.3369400 C -2.62035200 1.26046900 -1.19189800 H -2.33210400 1.53777600 -2.20357400 C -1.84441900 3.46975400 -0.00467600 C -1.84441900 3.46975400 -0.00467600 C -0.76941100 3.5637000 1.8080300 H -0.35403200 4.57493300 1.10807100 H -1.17648600 3.35637600 2.08129600 H -1.38092600 3.84370400 -2.15586900 H -0.43643100 3.12682200 -1.34456900 C -2.95951300 5.44457800 0.32915200 H -3.3756200 <th< td=""><td>AI</td><td>1 19054600</td><td>-0.09109100</td><td>-0.08139400</td></th<>	AI	1 19054600	-0.09109100	-0.08139400
Br 1.05154600 0.63341600 -2.37062500 C -2.43823000 2.07407400 -0.05067200 C -2.88797900 1.31035500 1.04479900 C -3.38201500 0.022904800 0.61168700 C -3.322780400 0.00226700 -0.33965400 C -3.22780400 1.53777600 -2.20357400 C -3.22780400 1.53777600 -2.20357400 C -3.32210400 1.53777600 -2.20357400 C -0.33403200 4.57409300 1.0807100 H -0.33403200 4.57409300 1.0807100 H -0.76941100 3.5637000 2.89692400 H -0.78448300 4.83866600 -1.3349400 H -0.78448300 4.83866600 -1.35349400 H -0.78448300 3.48376400 -2.15586900 C -2.97573200 4.45232900 0.3219500 H -3.377099400 4.41484800 0.43652200 C -3.31581600	Br	-0 30782800	-2 37174700	-0.62686800
C -2.43823000 2.07407400 -0.05067200 C -2.88797900 1.31035500 1.04479900 H -2.82259900 1.6232200 2.08567900 C -3.322780400 0.00226700 -0.83969400 C -3.22780400 1.53777600 -2.20357400 C -2.62035200 1.26046900 -1.19189800 H -2.33210400 1.53777600 -2.20357400 C -1.84441900 3.46975400 -0.00467600 C -0.76941100 3.56370000 1.08033000 H -0.3303200 4.57409300 1.08033000 H -0.05005600 2.84963700 0.88692400 H -1.17648600 3.35637600 2.08129600 C -1.22872200 3.83360700 -1.35349400 H -0.78448300 4.83866600 -1.131347700 H -0.78448300 4.83866600 -1.35349400 C -2.97573200 4.45232900 0.32195900 C -2.95951300 5.48457800 0.35915200 H -3.43579900 4.23056500 1.29621400 H -3.43579900 4.23056500 1.29621400 H -3.43579900 4.23056500 1.29621400 H -3.43579900 4.23056500 3.02814900 C -3.91561400 -0.9292100 3.02814900 H -3.343579900 4.23056500 1.29621400 H -3.343579900 4.23056500 1.29621400 H -3.343579900 4.23056500 1.29621400 H -3.377099400 -0.445232000 3.02814900 H -3.3750900 -2.5144600 3.32530700 C -4.03824400 -0.94291400 1.60200600 C -3.31750900 -2.32393300 1.10656500 3.73719200 H -4.44101100 0.56385400 3.15816000 C -5.53507300 -1.04921900 1.28747300 H -4.34101100 0.56385400 3.15816000 C -3.37750900 -2.32393300 1.61798700 H -3.32081400 -2.99515800 2.29989200 C -3.37655600 -0.88519900 -1.97663600 C -3.37750900 -2.3239300 1.61798700 H -3.32081400 -2.80755100 0.63929000 C -3.37655600 -0.88519900 -1.97863600 C -3.376055600 -0.88519900 -1.97863600 C -3.36055600 -0.88519900 -1.97863600 C -3.36055600 -0.88519900 -1.97863600 C -3.164520300 -0.251242000 -2.37758100 H -2.9491600 -2.85784400 -2.57727100 H -4.67633400 -2.85584400 -1.65543200 C -3.94317900 -2.85584400 -1.65543200 C -2.81969800 -0.816400 -3.31972500 H -2.9491600 -2.85584400 -1.65543200 C -2.81969800 -0.80136400 -3.1972500 H -2.29491600 -2.85584400 -1.65543200 C -2.81969800 -0.80136400 -3.19731500 C -2.81969800 -0.80136400 -3.1972500 H -2.2974000 -1.94843100 -2.93284000 C -2.81969800 -0.87739900 -2.37382400 C -2.44176800 0.95526200	Br	1 05154600	0.63341600	-2 37062500
C -2.88797900 1.31035500 1.04479900 H -2.82259900 1.62322200 2.08567900 C -3.38201500 0.02026700 -0.83969400 C -2.62035200 1.26046900 -1.19189800 H -2.33210400 1.53777600 -2.20357400 C -2.33403200 4.57409300 1.08033000 H -0.34030200 4.57409300 1.0807100 H -0.34030200 4.57409300 1.0807100 H -0.34030200 3.8360700 -8.89692400 C -1.7548600 3.84370400 -2.15586900 H -0.76941100 3.12682200 -1.31347700 H -0.43643100 3.12682200 -1.5456900 C -2.97573200 4.45232900 0.32195900 H -3.43579900 4.23056500 1.29621400 H -3.43579900 4.23056500 1.29621400 H -3.43579900 -3.24358400 -0.32195900 C -3.91561400 -0.	C	-2 43823000	2 07407400	-0.05067200
H -2.82259900 1.62322200 2.08567900 C -3.38201500 0.022904800 0.61168700 C -3.22780400 0.00226700 -0.83969400 C -2.62035200 1.26046900 -1.19189800 H -2.33210400 1.53777600 -2.20357400 C -1.84441900 3.46975400 -0.00467600 C -0.76941100 3.5637000 1.08033000 H -0.33403200 4.57409300 1.10807100 H -0.34643100 3.3636700 2.08129600 C -1.2872200 3.83360700 -1.31347700 H -0.78448300 4.83866600 -1.31347700 H -0.43643100 3.12682200 -1.64456900 C -2.97573200 4.45232900 0.32195900 H -2.59591300 5.48457800 0.35915200 H -3.3759900 4.23056500 1.29621400 C -4.03824400 -0.94291400 1.6020600 C -4.03824400 -0.	C	-2 88797900	1 31035500	1 04479900
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С	2.33541000	-1.29217700	1.38776800	
Ĥ	2.04097300	-2.32175100	1.57332100	
С	1.06523100	-0.22071900	3.40082000	
C	2.02454200	-0.31282600	4.59480200	
Н	1.46670600	-0.35697300	5.54302900	
Н	2.69352400	0.55899300	4.63889200	
Н	2.65508500	-1.21150300	4.53294400	
С	0.15126300	-1.44465400	3.39370900	
Н	-0.50801900	-1.45043700	4.27486400	
Н	0.71911600	-2.38592600	3.40632800	
Н	-0.48177700	-1.46552200	2.49170800	
С	0.21900200	1.04298600	3.53852900	
Н	-0.37769700	1.01256400	4.46297400	
Н	-0.47415000	1.15272100	2.68987600	
Н	0.83592600	1.95292600	3.58027700	
С	4.11665000	1.65704500	-0.29590700	
С	3.34576300	2.98577200	-0.34590900	
Н	3.94530000	3.74293900	-0.87124800	
Н	3.12944300	3.39621400	0.64987000	
Н	2.39530800	2.88105800	-0.89155600	
С	5.34927000	1.85059000	0.60297400	
Н	5.99111100	2.65376600	0.20953700	
Н	5.95867500	0.93807900	0.66611100	
Н	5.05911200	2.12352000	1.62813300	
С	4.59158600	1.37867700	-1.72089900	
Н	5.19331600	2.23240700	-2.06582000	
Н	3.75333300	1.26697400	-2.42038200	
Н	5.23213800	0.49422200	-1.80200200	
С	3.93760600	-1.92172400	-0.54386900	
C	5.44277200	-1.78323300	-0.28343300	
н	5.99272800	-2.58946000	-0.79205000	
н	5.66379700	-1.85822600	0.79215500	
Н	5.86055900	-0.83352800	-0.63752600	
C	3.62190100	-1.84930700	-2.04012900	
н	4.23497700	-2.58109600	-2.58776500	
H	3.80099600	-0.86523800	-2.48285000	
Н	2.56648900	-2.09/8/300	-2.22/55100	
	3.54508600	-3.33448200	-0.09256300	
	4.07767100	-4.0/41/400	-0.70710800	
	2.400/0000	-3.32390900 2 52017500	-U.Z 1039900	
П	3.01337700	-3.32017500	0.90004000	

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