Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting information for the manuscript: **Cationic Dialanes with Fluxional π-Bridged Cyclopentadienyl Ligands**

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S-1 Supporting experimental data

S-1.1 General experimental details and analytical methods

All manipulations of air and/or water sensitive compounds were performed under an inert argon atmosphere using standard Schlenk or glovebox techniques. All glassware used in reactions have been stored over-night in an oven at 180°C and were thoroughly flame-dried prior to usage. $AlCl_3$ (Sigma Ahldrich, sublimed), Cp*H (Sigma Aldrich), KHMDS (Sigma Aldrich, >95%), $SnCl_2$ and LAH (1.6 M in Et_2O, Sigma Ahldrich) were used as received. $GeCl_2$-Dioxane (Sigma-Ahldrich) was recrystallized from dioxane. $Li[Al(OR^F)_4]$ (with $R^F = C(CF_3)_3$),[1] $[Ph_3C][Al(OR^F)_4]$,[2] $[(AlCp^*)_4]$[3] ($Cp^* = C_5Me_5$), [GeCp][F{$Al(OR^F)_3$}$_2$][4] and [SnCp][F{$Al(OR^F)_3$}$_2$][4,5] were prepared using literature known procedures. *n*-Heptane (Sigma Ahldrich) and 1,2-difluorobenzene (fluorochem, 1,2-DFB) were refluxed over CaH_2, fractionally distilled, and stored over activated 3 Å molecular sieves. *n*-Pentane was collected from the solvent-purification system (SPS) and used as received.

NMR spectroscopy: NMR samples were prepared inside an inert atmosphere glovebox in NMR tubes equipped with a gas-tight J. Young valve. ^1H, ^{13}C, ^{19}F, ^{27}Al and ^{29}Si-NMR spectra were acquired either on a Bruker Biospin Avance II+ 400 MHz WB or a Bruker Avance III HD 300 MHz spectrometer. ^1H and ^{13}C NMR spectra are reported relative to TMS and were calibrated to residual solvent resonances.[4] Data analysis was performed using Bruker TOPSPIN 3.5 software. The broad resonance at δ = 70 ppm observed in ^{27}Al-NMR spectra corresponds to a background from Al-nuclei in the probe head. The graphical representations in the manuscript were created with OriginPro 2021.

IR and Raman spectroscopy: FTIR spectra were recorded inside a glovebox with a Bruker ALPHA equipped with QuickSnap Eco-ATR module and ZnSe crystal. The spectra were measured at RT in the range of 4000-550 cm^{-1} with 64 scans and a resolution of 2 cm^{-1}. The data were processed with the Bruker OPUS 7.5 software package and, if not stated otherwise, a baseline correction with 3 iterations was performed. FT Raman spectra were recorded with a VERTEX 70 with Bruker RAM II Modul (1064 nm exciting line of a Nd-YAG laser) and liquid nitrogen cooled Ge detector. The samples were flame-sealed in soda-lime glass Pasteur pipettes and were measured at RT in the range of 4000-80 cm^{-1} with up to 10,000 scans and a resolution of 4 cm^{-1}. The data were processed with the Bruker OPUS 7.5 software package and, if not stated otherwise, a baseline correction with 5 iterations was performed. All IR and Raman spectra were normalized to 1 and the intensities are reported as follows: ≥ 0.8 = very strong (vs), ≥ 0.6 = strong (s), ≥ 0.4 = medium (m), ≥ 0.2 = weak (w), < 0.2 = very weak (vw). The graphical representations were created with OriginPro 2021.

Single crystal X-ray analysis: Single crystal X-ray diffraction. Single crystal X-ray diffraction data were collected using either on a Bruker SMART APEXII QUAZAR detector with fixed-Chi D8 Goniometer, INCOATEC Mo microsource or Bruker D8 VENTURE with PHOTONIII detector, fixed-Chi D8 Goniometer and INCOATEC Mo/Cu microsource. Crystals were selected under perfluoropolyether oil, mounted on 0.1 to 0.3 mm diameter CryoLoops and quench-cooled using an Oxford Cryostream 800 open flow N2 cooling device.[6] Data were collected at 100 K using monochromated Mo Kα radiation (λ = 0.71073 Å). Data processing was done with SHELXS/XL and refined by least squares on weighted F2 values for all reflections, disordering of fragments was done with the help of the implemented DSR tool.[7] Graphical representations have been prepared using Olex2-1.2. Finalisation of gathered data was done using final cif tool.[8]

Comments on elemental analysis and mass spectrometry: In our decade-long experience working with $[Al(OR^F)_4]^-$ (OR^F = $C(CF_3)_3$), the highly fluorinated anion yields erratic and not reproducible results from the elemental analyses. Hence, no elemental analysis is included. Moreover, the complexes are to labile to be transferred into the gas-phase in an ESI-MS. This was already discussed for our previously reported low-valent Al complex salts.[9]

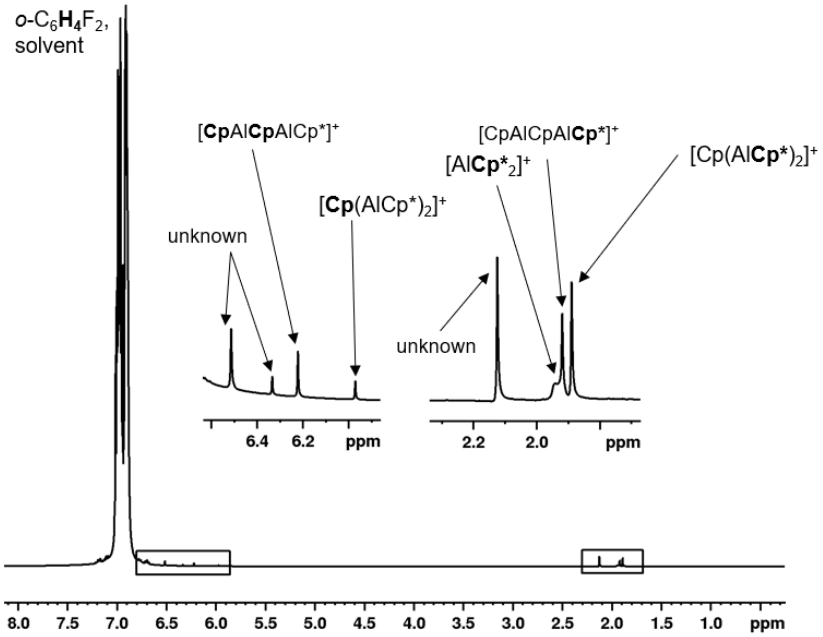
S-1.2 Experimental data for the reaction of [SnCp][F{Al(OR^F)$_3$}$_2$] with 0.25 [(AlCp*)$_4$]

[SnCp][F{Al(OR^F)$_3$}$_2$] (20 mg, 12 μmol) and [(AlCp*)$_4$] (2.0 mg, 12 μmol, 0.25 equiv.) were dissolved in 1,2-DFB (0.7 mL) at room temperature in a J. Young NMR tube. The formation of a metallic precipitate and brown solution was observed. NMR analysis revealed various new NMR signals in the ^{1}H NMR spectrum. Here, signals of [Cp(Al**Cp***)$_2$][F{Al(OR^F)$_3$}$_2$] **1A** could be assigned in retrospect (more cleanly prepared in next sections). Moreover, signals matching the [CpAlCpAl**Cp***]$^+$ cation, which was later obtained as its [Al(OR^F)$_4$]$^-$ salt in **4** (see page 12), are observed. Layering the solution gave colourless crystals of the asymmetric aluminocenoium cation [CpAlCp*][F{Al(OR^F)$_3$}$_2$] (S-Figure 65) along other colourless crystals, which could not be identified by scXRD.

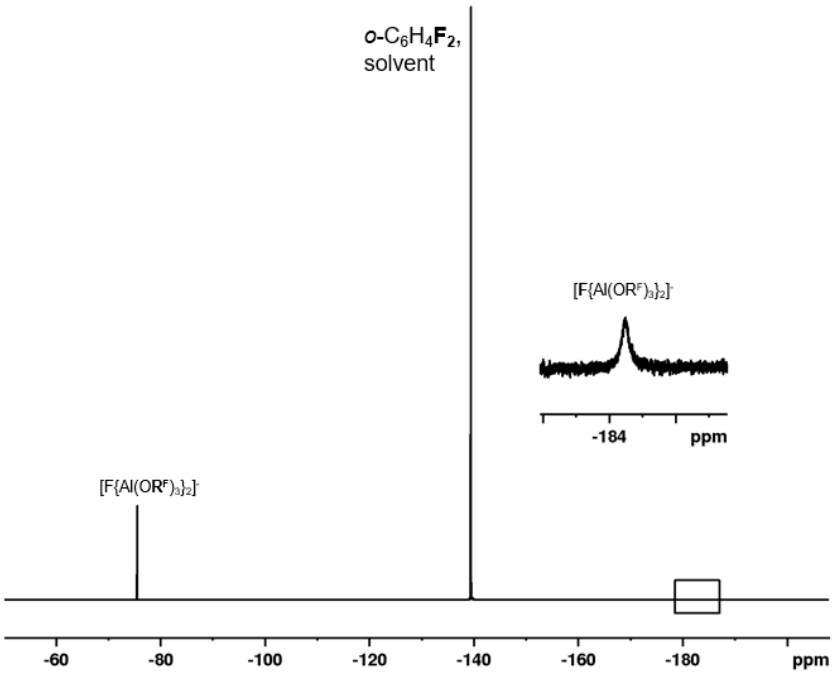
^{1}H NMR spectrum (400.17 MHz, 1,2-DFB, 298 K): δ = 1.89 (s, 30 H, [Cp(Al**Cp***)$_2$]$^+$), 1.92 (s, 15 H, [CpAlCpAl**Cp***]$^+$), 1.94 (s, 30 H, [AlCp*$_2$]$^+$), 2.13 (s, unknown compound), 5.97 (s, 5 H, [**Cp**(AlCp*)$_2$]$^+$), 6.22 (s, 10 H, [CpAlCpAl**Cp***]$^+$), 6.33 (s, unknown compound), 6.52 (s, unknown compound) ppm.

^{19}F NMR spectrum (376.54 MHz, 1,2-DFB, 298 K): δ = −184.48 (s, 1 F, [**F**{Al(OR^F)$_3$}$_2$]$^-$), –75.54 (s, 54 F, [F{Al(O**R^F**)$_3$}$_2$]$^-$) ppm.

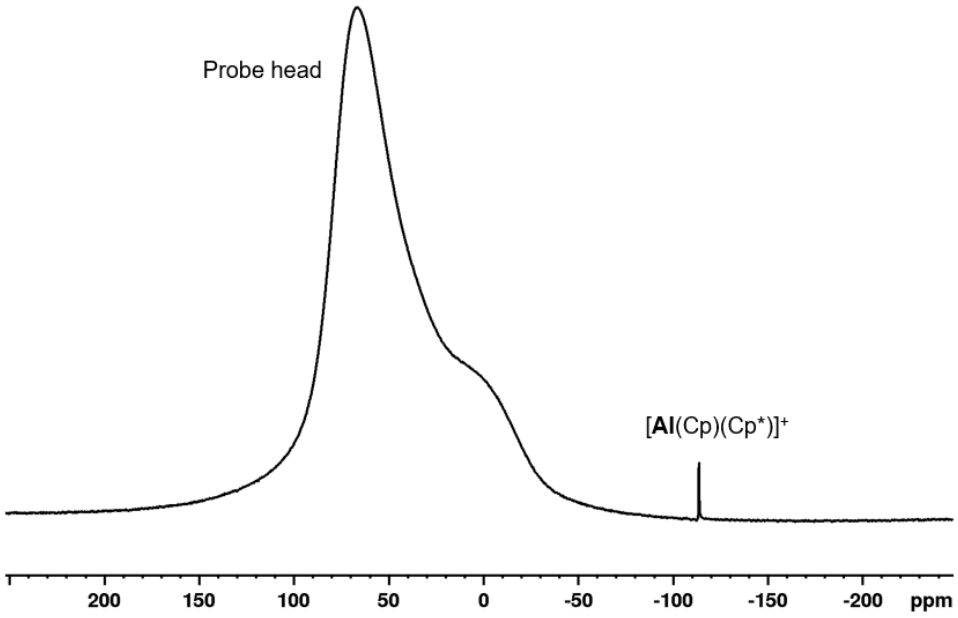
^{27}Al NMR spectrum (104.27 MHz, 1,2-DFB, 298 K): δ = –114.57 (s, [**Al**Cp*$_2$]$^+$), –113.83 (s, [**Al**(Cp)(Cp*)]$^+$), –37.03 (s, [Cp(Cp*)$_2$]$^+$) ppm.



S-Figure 1: ^{1}H NMR spectrum (400.17 MHz, 1,2-DFB, 300K) of the reaction between [SnCp][F{Al(OR^F)$_3$}$_2$] and 0.25 [(AlCp*)$_4$].



S-Figure 2: ^{19}F NMR spectrum (376.54 MHz, 1,2-DFB, 298 K) of the reaction between [SnCp][F{Al(OR^F)$_3$}$_2$] and 0.25 [(AlCp*)$_4$].



S-Figure 3: ^{27}Al NMR spectrum (104.27 MHz, 1,2-DFB, 298 K) of the reaction between [SnCp][F{Al(OR^F)$_3$}$_2$] and 0.25 [(AlCp*)$_4$].

S-1.3 Experimental data for the preparartion of $[Cp(AlCp^*)_2][F\{Al(OR^F)_3\}_2]$ **1A**

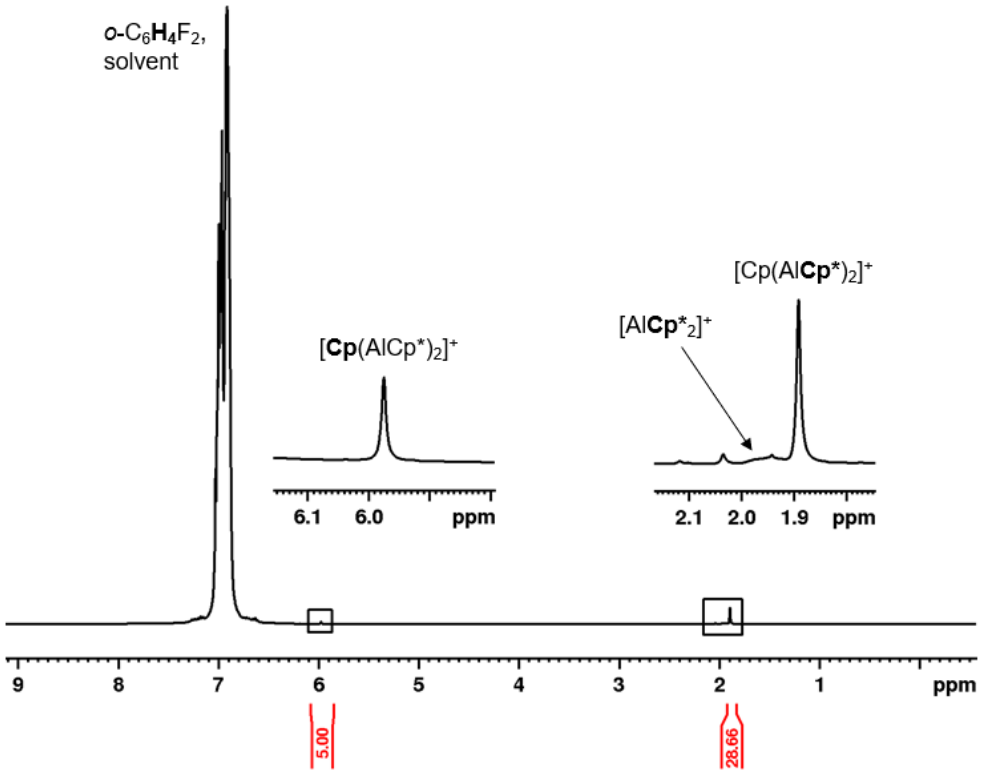
Procedure 1 via [GeCp]$^+$: $[GeCp][F\{Al(OR^F)_3\}_2]$ (20 mg, 12 μmol) and $[(AlCp^*)_4]$ (4.0 mg, 25 μmol, 0.5 equiv.) were dissolved in 1,2-DFB (1 mL) at room temperature. The formed metallic precipitate was filtered off and the colourless solution was layered with *n*-heptane at –30°C. The title compound was isolated as colourless crystals (8 mg, 4 μmol, 3 × 10^1 %).

^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 298 K): δ = 1.90 (s, 30 H, $[Cp(Al\mathbf{Cp^*})_2]^+$), 5.97 (s, 5 H, $[\mathbf{Cp}(AlCp^*)_2]^+$) ppm.

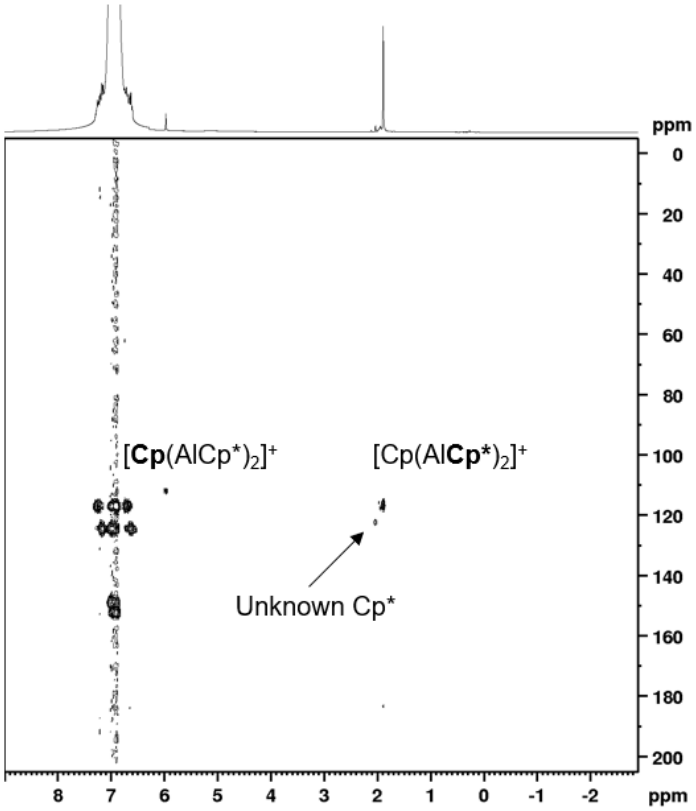
^{1}H, ^{13}C HMBC spectrum (300.18 MHz, 75.48 MHz, 1,2-DFB, 298 K): δ(^{13}C) = 112.1 ($[\mathbf{Cp}(AlCp^*)_2]^+$), 166.6 ($[Cp(Al\mathbf{Cp^*})_2]^+$) ppm.

^{19}F NMR spectrum (282.45 MHz, 1,2-DFB, 298 K): δ = –184.45 (s, 1 F, $[\mathbf{F}\{Al(OR^F)_3\}_2]^-$), –75.54 (s, 54 F, $[F\{Al(O\mathbf{R^F})_3\}_2]^-$) ppm.

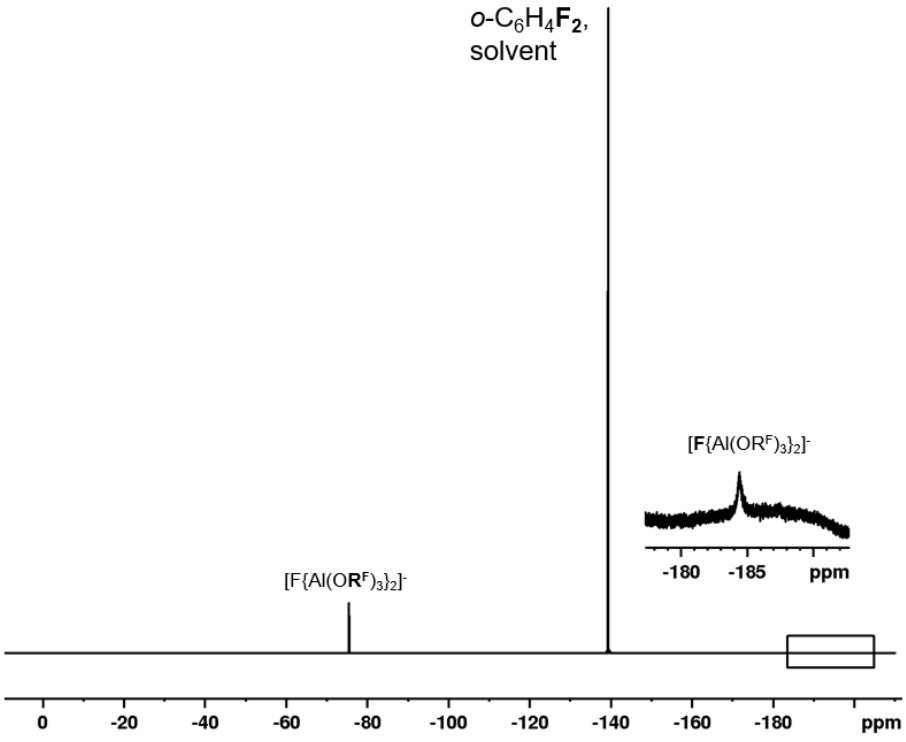
^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 298 K): δ = –114.54 (s, $[\mathbf{Al}Cp^*_2]^+$), –113.76 (s, $[\mathbf{Al}(Cp)(Cp^*)]^+$), –37.00 (s, $[Cp(Cp^*)_2]^+$) ppm.



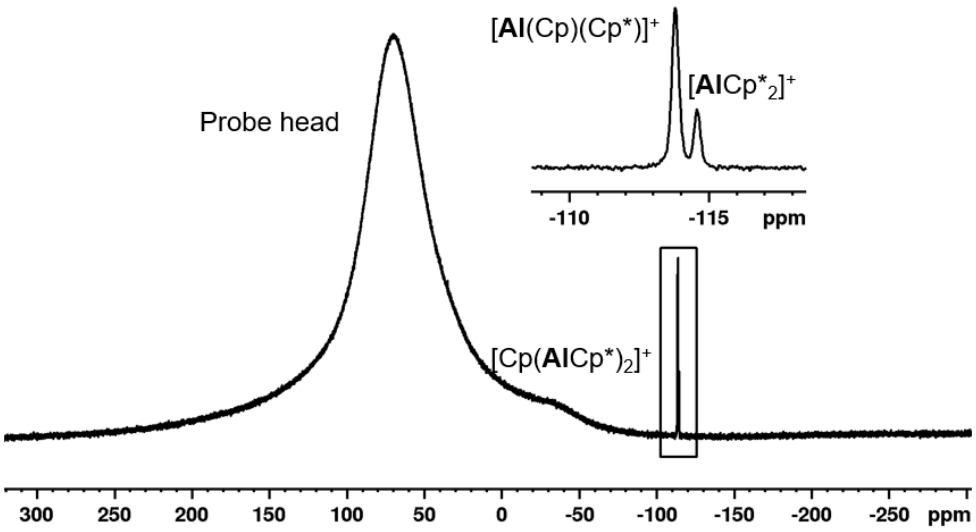
S-Figure 4: ^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 300K) of $[Cp(AlCp^*)_2][F\{Al(OR^F)_3\}_2]$ **1A.**



S-Figure 5: ^{1}H-^{13}C HMBC spectrum (300.18 MHz, 75.48 MHz, 1,2-DFB, 300K) of $[Cp(AlCp^*)_2][F\{Al(OR^F)_3\}_2]$ **1A**.



S-Figure 6: ^{19}F NMR spectrum (282.45 MHz, 1,2-DFB, 300K) of $[Cp(AlCp^*)_2][F\{Al(OR^F)_3\}_2]$ **1A**.



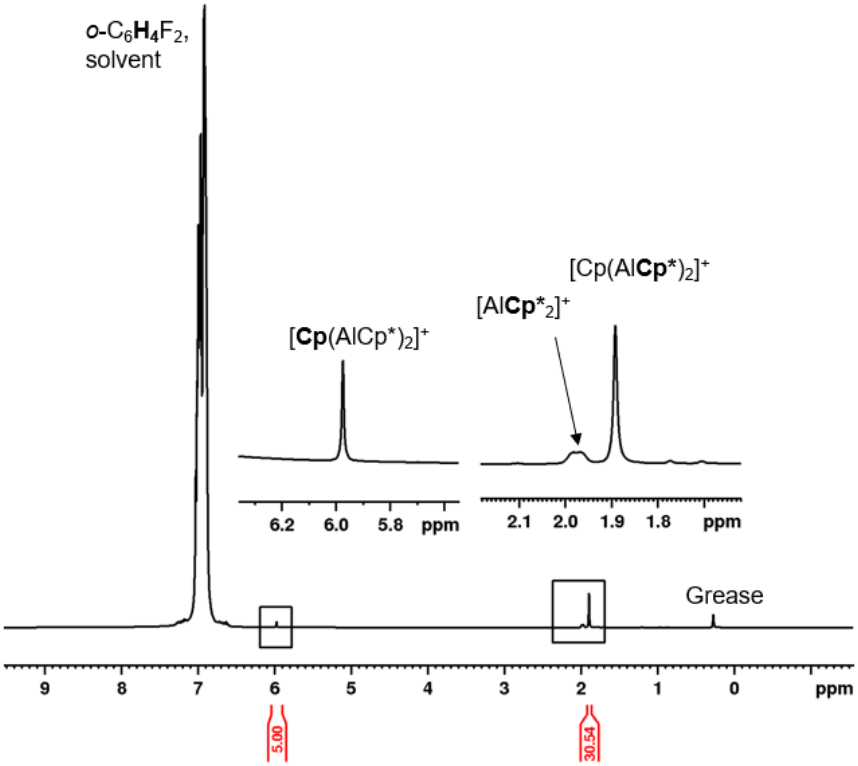
S-Figure 7: ^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 300K) of $[Cp(AlCp^*)_2][F\{Al(OR^F)_3\}_2]$ **1A**.

Procedure 2 via [SnCp]$^+$: [SnCp][F{Al(OR^F)$_3$}$_2$] (20 mg, 12 μmol) and [(AlCp*)$_4$] (3.9 mg, 24 μmol, 0.5 equiv.) were dissolved in 1,2-DFB (1 mL) at room temperature. The formed metallic precipitate was filtered off and the colourless solution was layered with *n*-heptane at –30°C. The title compound was isolated as colourless crystals (6 mg, 3 μmol, 3 × 10^1 % %).

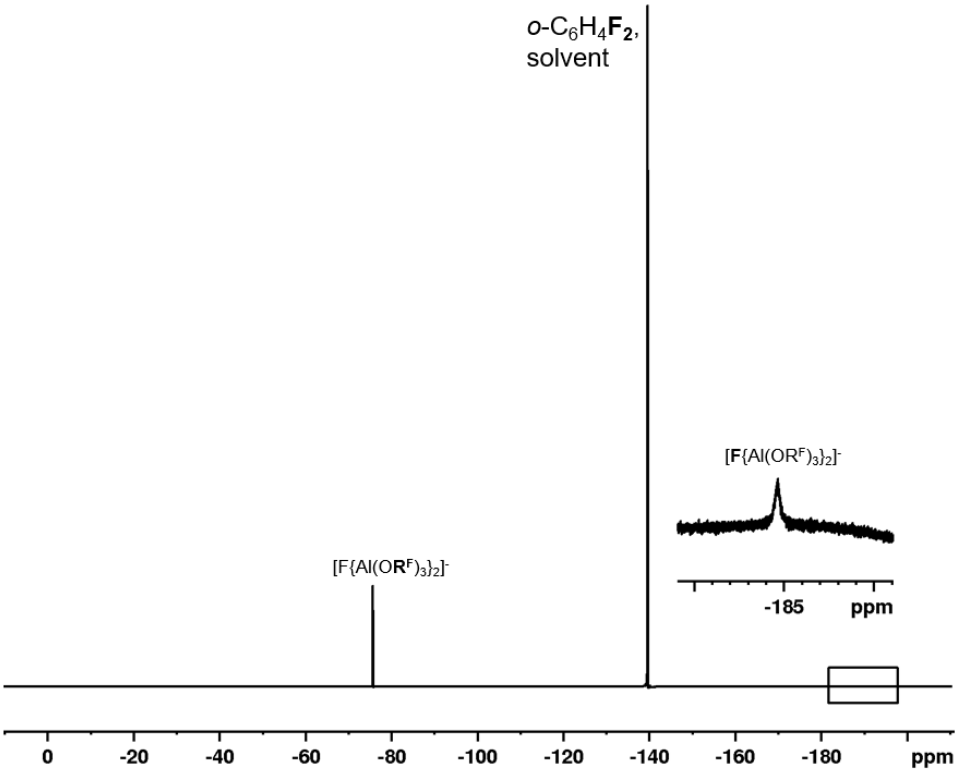
^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 298 K): δ = 1.89 (s, 30 H, [Cp(Al**Cp***)$_2$]$^+$), 5.97 (s, 5 H, [**Cp**(AlCp*)$_2$]$^+$) ppm.

^{19}F NMR spectrum (282.45 MHz, 1,2-DFB, 298 K): δ = –184.45 (s, 1 F, [**F**{Al(OR^F)$_3$}$_2$]$^-$), –75.54 (s, 54 F, [F{Al(O**R^F**)$_3$}$_2$]$^-$) ppm.

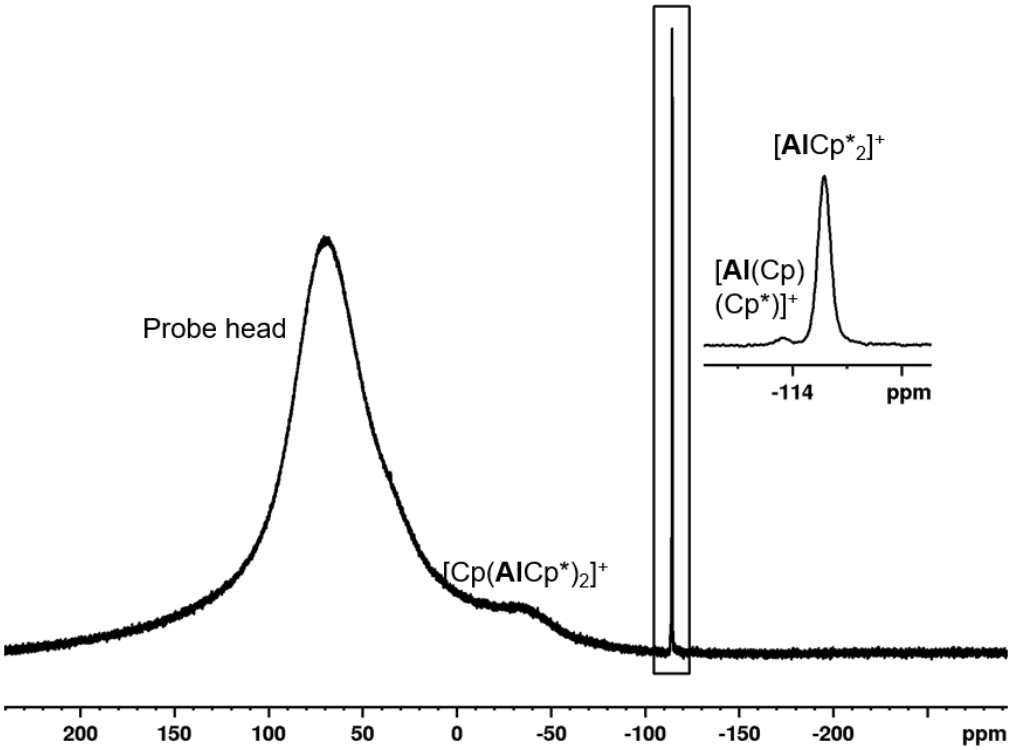
^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 298 K): δ = –114.57 (s, [**Al**Cp*$_2$]$^+$), –113.80 (s, [**Al**(Cp)(Cp*)]$^+$), –37.03 (s, [Cp(Cp*)$_2$]$^+$) ppm.



S-Figure 8: ^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 300K) of [Cp(AlCp*)$_2$][F{Al(OR^F)$_3$}$_2$] **1A.**



S-Figure 9: ^{19}F NMR spectrum (282.45 MHz, 1,2-DFB, 300K) of $[Cp(AlCp^*)_2][F\{Al(OR^F)_3\}_2]$ **1A**.



S-Figure 10: ^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 300K) of $[Cp(AlCp^*)_2][F\{Al(OR^F)_3\}_2]$ **1A**.

S-1.4 Experimental data for the preparation of $[AlCp_2][Al(OR^F)_4]$ **3**

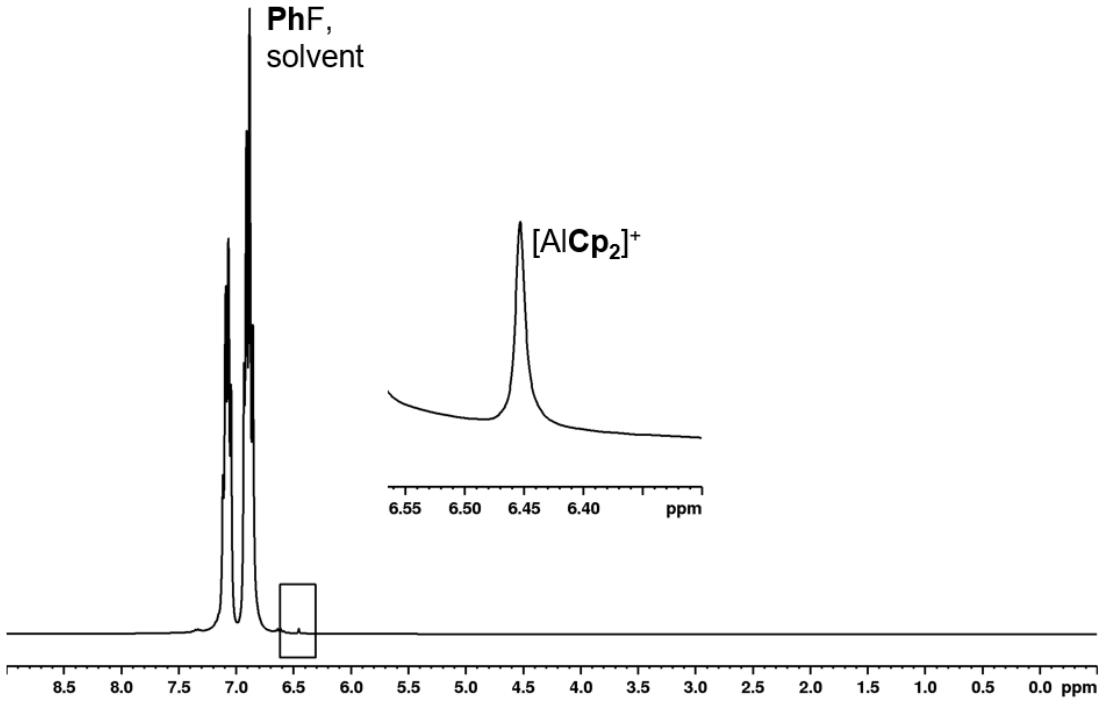
Procedure: Synthesis of $AlCp_3$ was adapted from a previously reported procedure.[10]

$MgCl_2$ (550 mg, 3.24 mmol) and $AlCl_3$ (288 mg, 2.16 mmol, 0.67 equiv.) were suspended in 10 mL toluene and stirred for 24 h at 50°C. The obtained colourless was filtrated of from precipitated $MgCl_2$ onto a solution of $Ph_3C[Al(OR^F)_4]$ (1.21 g, 1.00 mmol, 0.31 equiv) in toluene (10 mL). The reaction mixture was stirred for 3h at room temperature. Then, the colourless solution was filtered off from the formed beige precipitate, which was dried thoroughly. The title compound was isolated as beige powder (1.00 g, 889 μmol, 89 %).

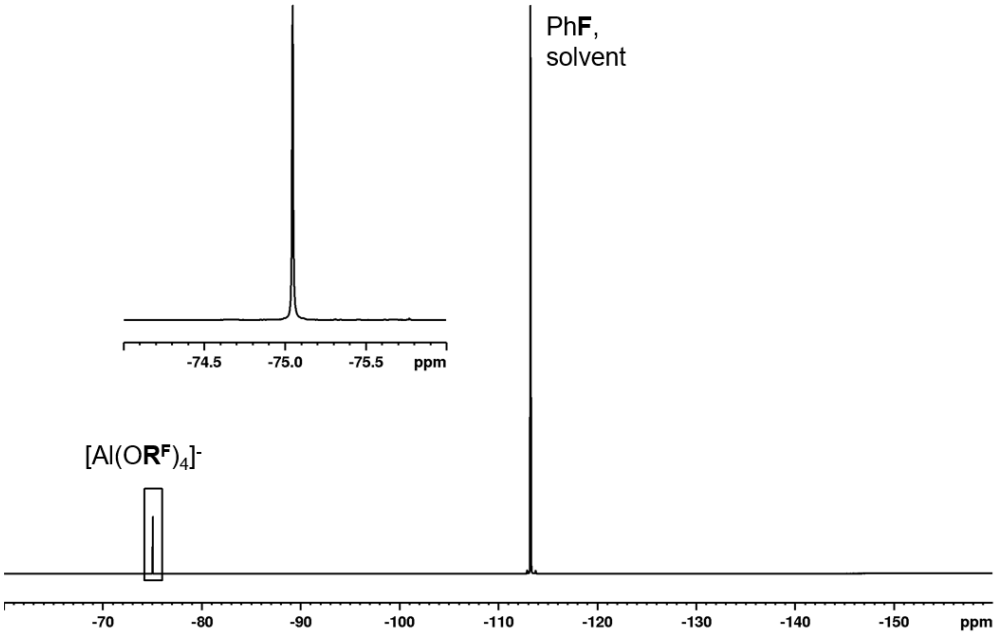
^{1}H{^{27}Al} NMR spectrum (300.18 MHz, PhF, 298 K): δ= 6.45 (s, 10H, $[Al\mathbf{Cp}_2]^+$) ppm.

^{19}F NMR spectrum (282.45 MHz, PhF, 298 K): δ = −75.05 (s, 36 F, $[Al(O\mathbf{R^F})_4]^-$) ppm

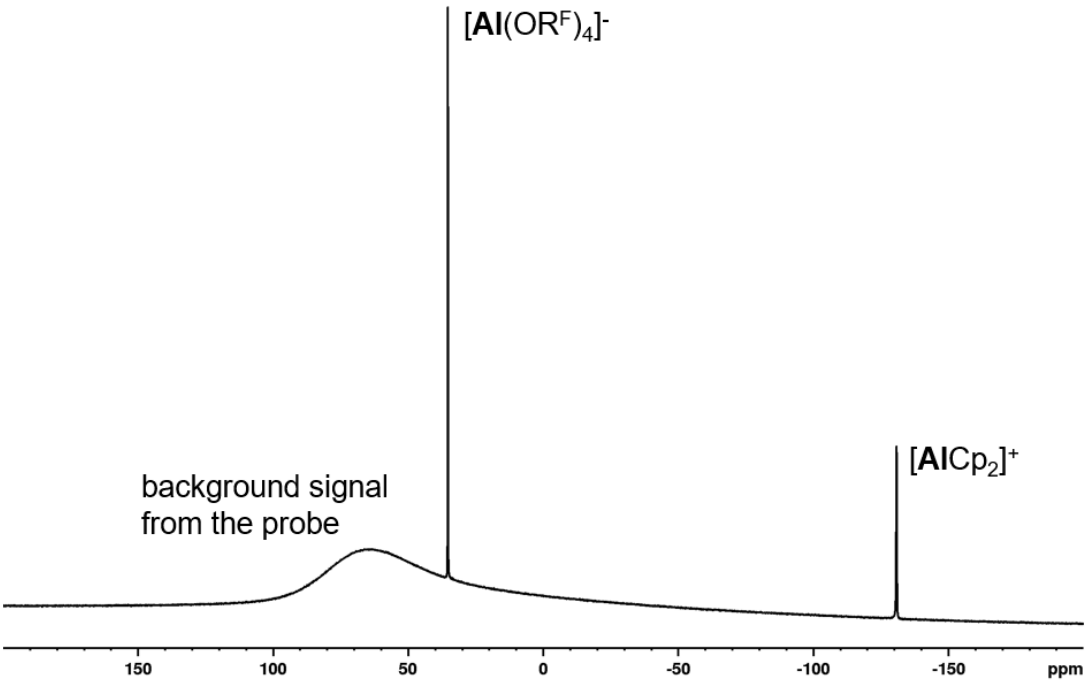
^{27}Al NMR spectrum (78.22 MHz, PhF, 298 K): δ= −130.9 (s, 1Al, $[Al(OR^F)_4]^-$), 35.3 (s, 1Al, $[AlCp_2]^+$) ppm.



S-Figure 11: ^{1}H{^{27}Al} NMR spectrum (300.18 MHz, PhF, 298 K) of $[AlCp_2][Al(OR^F)_4]$ **3**.



S-Figure 12: ^{19}F NMR spectrum (282.45 MHz, PhF, 298 K) of $[AlCp_2][Al(OR^F)_4]$ **3**.



S-Figure 13: ^{27}Al NMR spectrum (78.22 MHz, PhF, 298 K) of $[AlCp_2][Al(OR^F)_4]$ **3**.

S-1.5 Experimental data for the preparation of $[Cp(AlCp)(AlCp^*)][Al(OR^F)_4]$ **4**

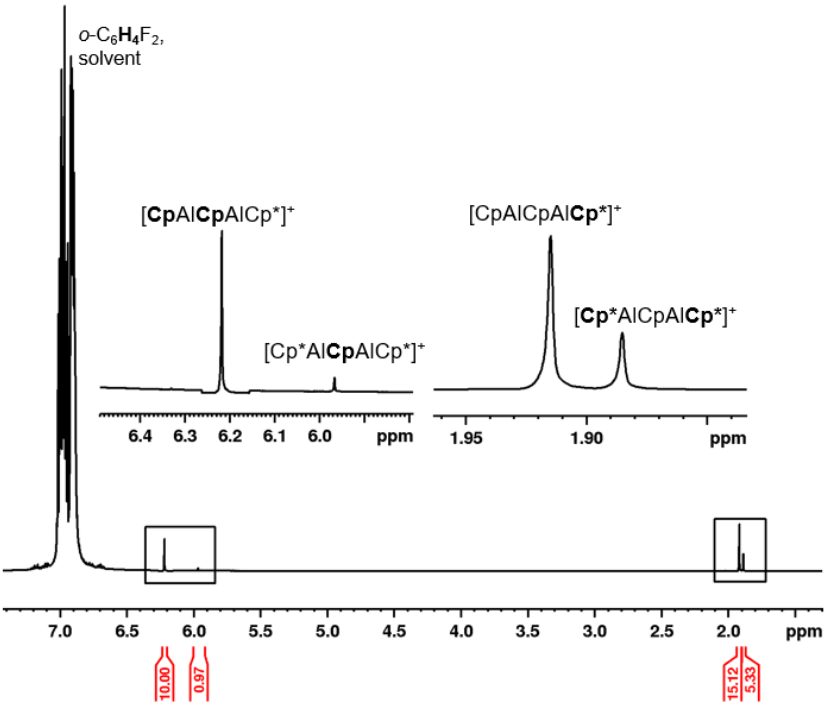
Procedure 1: $[AlCp_2][Al(OR^F)_4]$ (50 mg, 44 μmol) was dissolved in 1,2-DFB (1 mL), cooled to –40°C and canulated onto $[(AlCp^*)_4]$ (7.2 mg, 44 μmol, 1 equiv.). The slightly yellow solution was stirred for 30 min at –40°C and then *n*-pentane (5 mL) was added. The title compound (30 mg, 23 μmol, 52 %, 81 % of the isolated powder) was obtained as off-white powder (in total: 37 mg), which with the symmetric dialane (7.3 mg, 5.4 μmol, 19 % of the isolated powder). scXRD-quality was contaminated crystals could be grown by layering a solution in 1,2-DFB with *n*-pentane at –30°C.

^{1}H NMR spectrum (400.16 MHz, 1,2-DFB, 298 K): δ = 1.89 (s, 30 H, $[Cp(Al\mathbf{Cp^*})_2]^+$), 1.92 (s, 15 H, $[Cp(AlCp)(Al\mathbf{Cp^*})]^+$), 5.97 (s, 5 H, $[Cp(Al\mathbf{Cp^*})_2]^+$), 6.22 (s, 10 H, $[\mathbf{Cp}(Al\mathbf{Cp})(AlCp^*)]^+$) ppm.

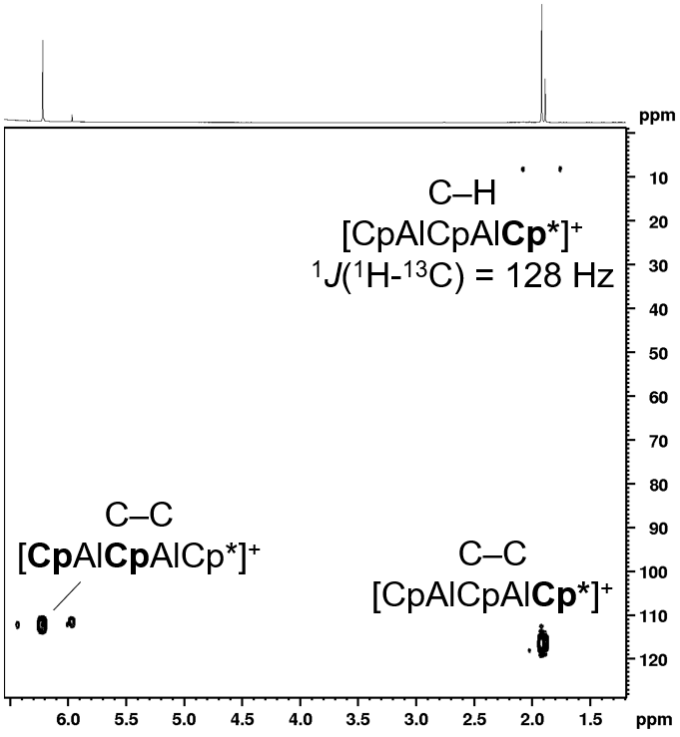
^{1}H, ^{13}C HMBC spectrum (400.16 MHz, 100.6 MHz, 1,2-DFB, 298 K): δ(^{13}C) = 111.6 ($[\mathbf{Cp}(AlCp^*)_2]^+$), 112.3 ($[\mathbf{Cp}(Al\mathbf{Cp})(AlCp^*)]^+$), 116.2 ($[Cp(Al\mathbf{Cp^*})_2]^+$, $\mathbf{C}_5Me_5$), 116.5 ($[Cp(AlCp)(Al\mathbf{Cp^*})]^+$, $\mathbf{C}_5Me_5$) ppm.

^{19}F NMR spectrum (376.54 MHz, 1,2-DFB, 298 K): δ = –75.44 (s, 36 F, $[Al(OC_4F_9)_4]^-$) ppm.

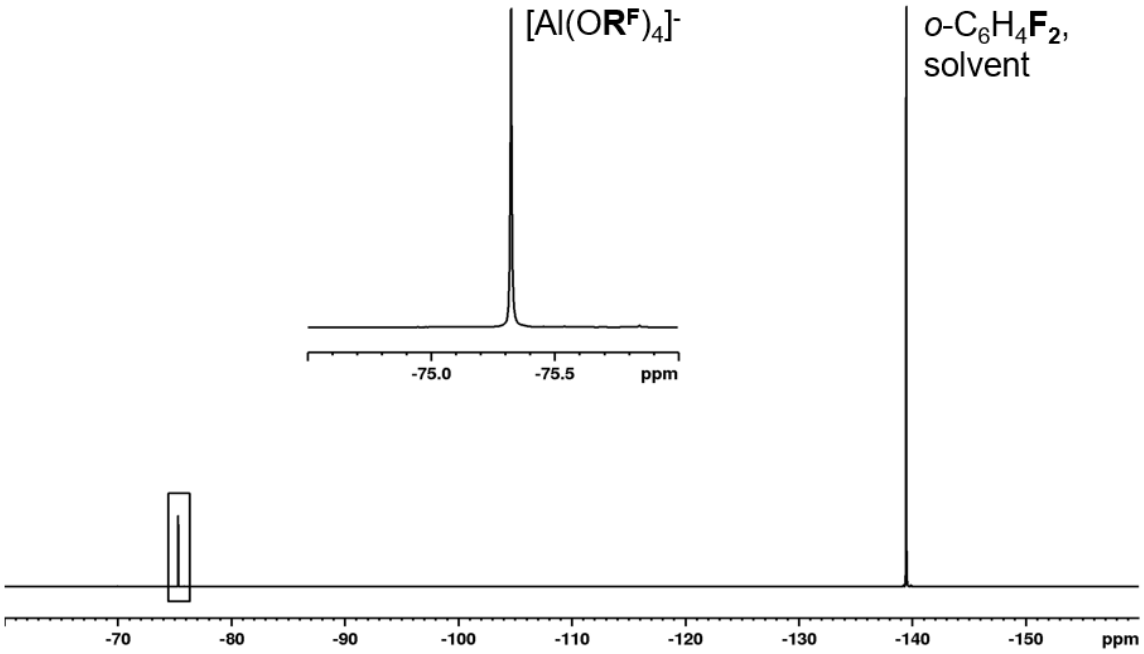
^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 298 K): δ = 35.0 (s, $[Al(OC_4F_9)_4]^-$), –113.9 (s, $[Al(Cp)(Cp^*)]^+$) ppm.



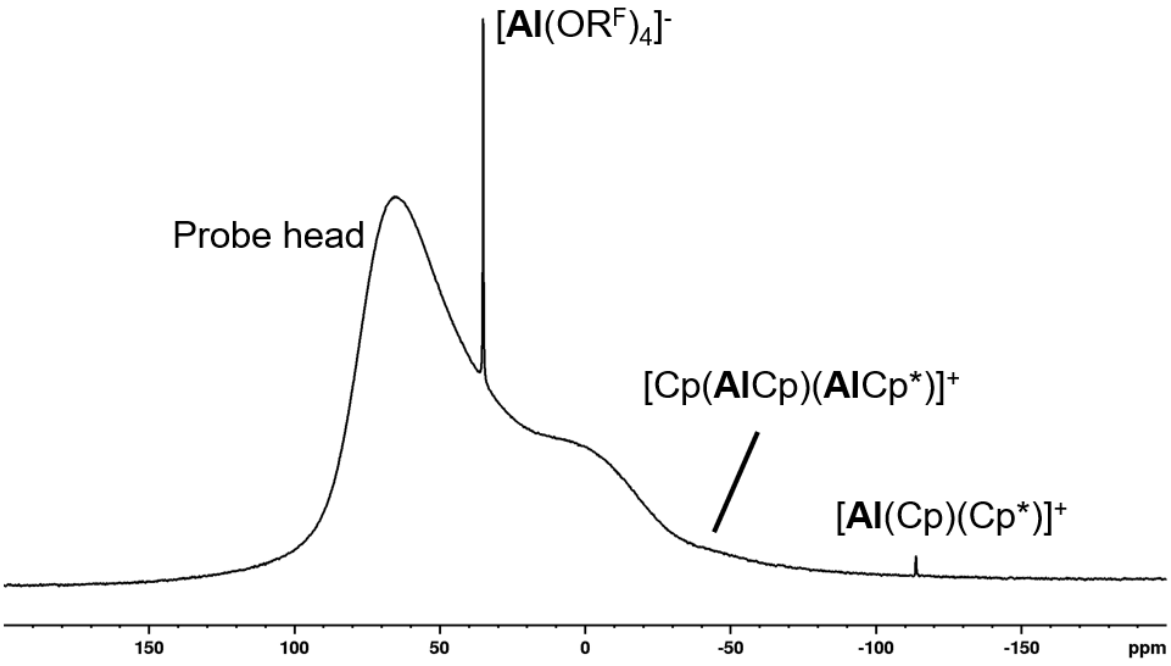
S-Figure 14: ^{1}H NMR spectrum (400.17 MHz, 1,2-DFB, 300K) of [Cp(AlCp)(AlCp*)][Al(OR^{F})$_4$] **4**.



S-Figure 15: ^{1}H-^{13}C HMBC spectrum (400.17 MHz, 100.61 MHz, 1,2-DFB, 300K) of [Cp(AlCp)(AlCp*)][Al(OR^{F})$_4$] **4**.



S-Figure 16: ^{19}F NMR spectrum (376.50 MHz, 1,2-DFB, 300K) of [Cp(AlCp)(AlCp*)][Al(OR^F)$_4$] **4**.



S-Figure 17: ^{27}Al NMR spectrum (104.3 MHz, PhF, 300K) of [Cp(AlCp)(AlCp*)][Al(OR^F)$_4$] **4**.

Procedure 2: $[AlCp_2][Al(OR^F)_4]$ (200 mg, 178 μmol) and $[(AlCp^*)_4]$ (28.86 mg, 178 μmol, 1 equiv.) were dissolved in 1,2-DFB (1 mL) at room temperature. The $[(AlCp^*)_4]$ suspension was added to the $[AlCp_2][Al(OR^F)_4]$ solution and the canula was washed with 1,2-DFB (2×0.5mL). The yellow solution was layered with *n*-pentane at room temperature. The title compound was isolated as off-white powder (170 mg, 132 μmol, 74 %). NMR did show already small beginning signals of the decomposition product and traces of the symmetric dialane **1B**.

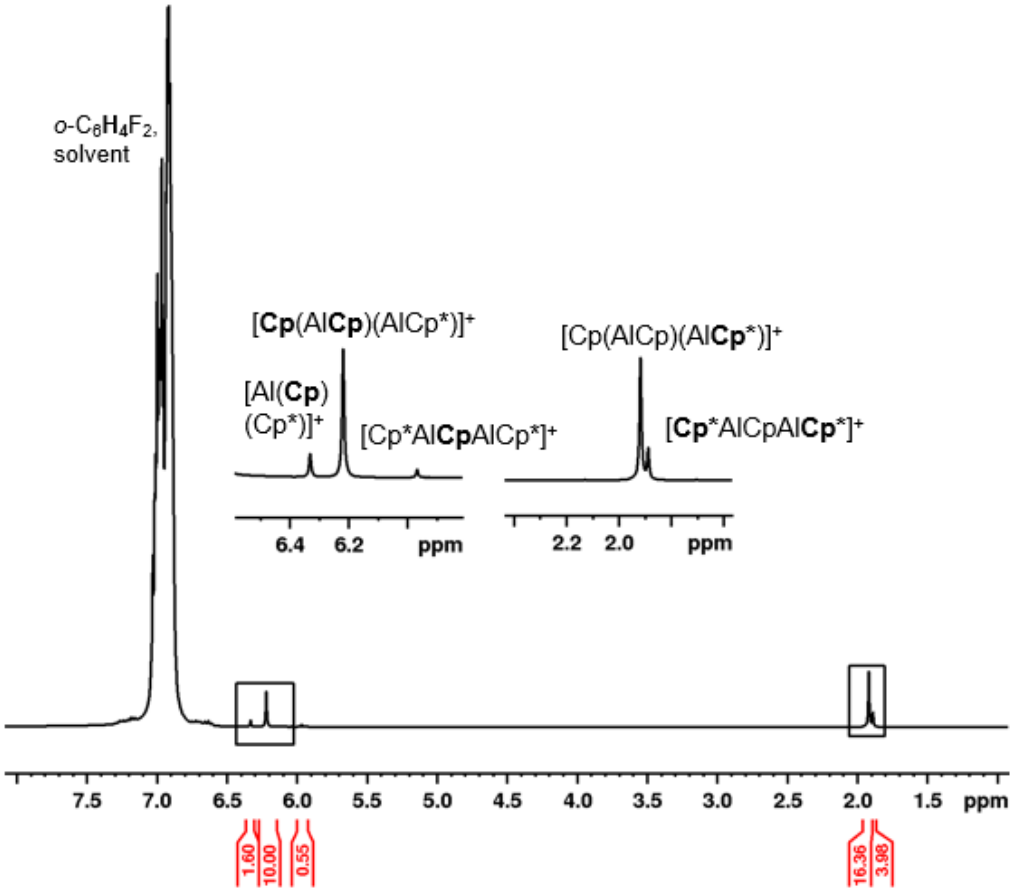
^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 298 K): δ = 1.89 (s, 30 H, $[Cp(Al\mathbf{Cp^*})_2]^+$), 1.92 (s, 15 H, $[Cp(AlCp)(Al\mathbf{Cp^*})]^+$), 5.97 (s, 5 H, $[Cp(Al\mathbf{Cp^*})_2]^+$), 6.22 (s, 10 H, $[\mathbf{Cp}(Al\mathbf{Cp})(AlCp^*)]^+$), 6.33 (s, 5H, $[Al(\mathbf{Cp})(AlCp^*)]^+$ ppm.

^{19}F NMR spectrum (282.45 MHz, 1,2-DFB, 298 K): δ = –75.38 (s, 36 F, $[Al(OC_4F_9)_4]^-$) ppm.

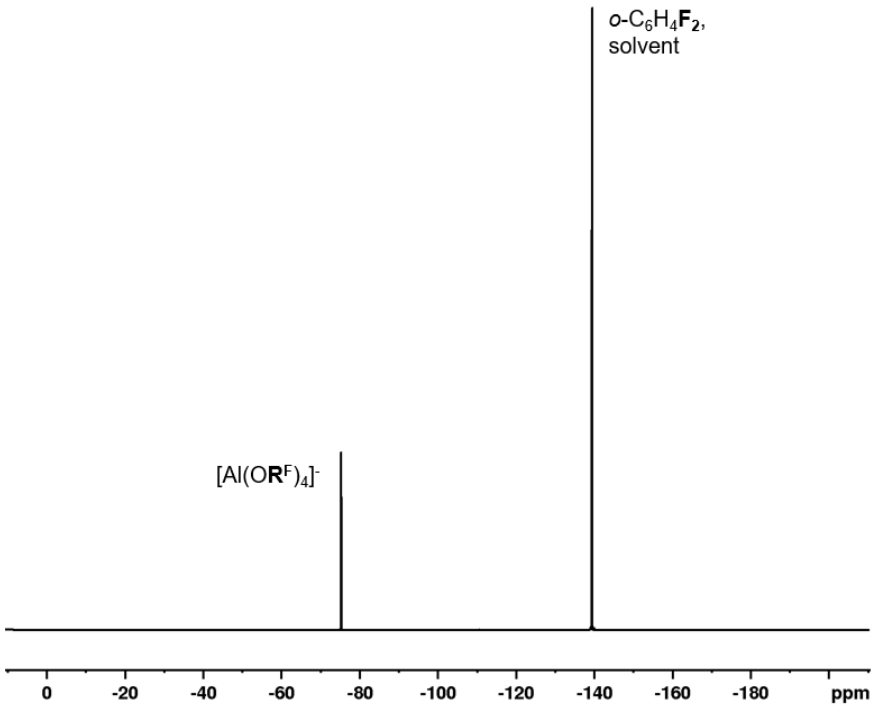
^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 298 K): δ = –113.9 (s, $[Al(Cp)(Cp^*)]^+$), = –47.0 (s, $[Cp(\mathbf{Al}Cp)(\mathbf{Al}Cp^*)]^+$), 35.0 (s, $[Al(OC_4F_9)_4]^-$), ppm.

FTIR spectrum (ZnSe-ATR): $\tilde{\nu}$ = 559 (m), 726 (vs), 755 (w), 795 (m), 821 (w), 835 (w), 846 (w), 969 (vs), 1016 (vw), 1113 (w), 1168 (m), 1210 (vs), 1238 (s), 1273 (m), 1297 (w), 1351 (vw), 2929 (vw) cm^{-1}.

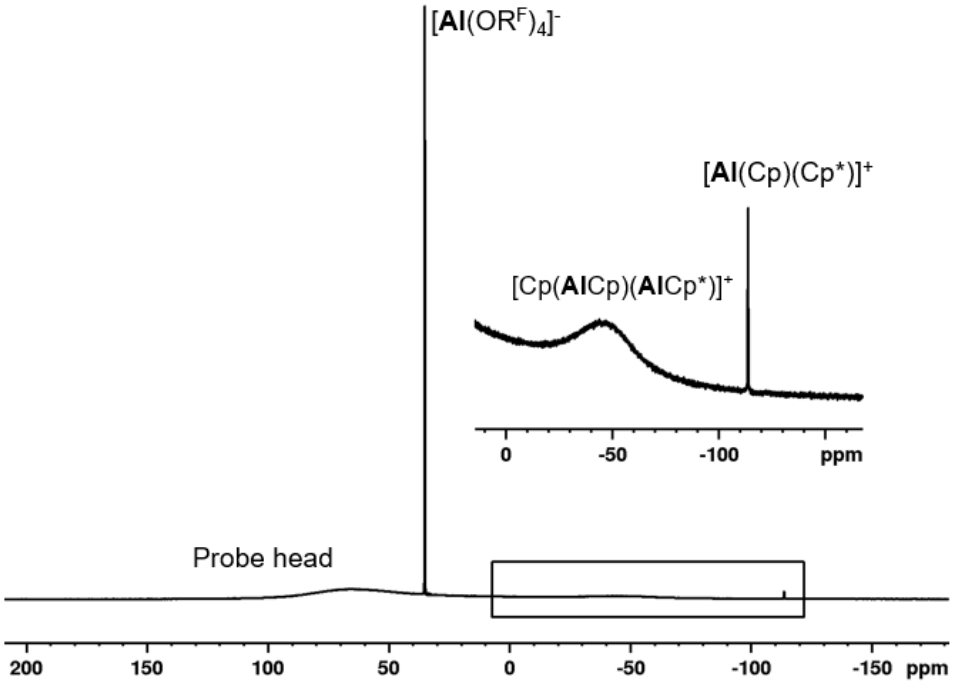
Raman (50 mW, 5000 scans): $\tilde{\nu}$ = 174 (s), 234 (m), 265 (w), 287 (w), 321 (w), 399 (vw), 522 (vw), 538 (vw), 555 (w), 555 (w), 589 (w), 555 (w), 572 (w), 589 (w), 555 (w), 555 (w), 555 (w), 589 (w), 555 (w), 745 (w), 798 (w), 1117 (vs), 1069 (vw), 1394 (w), 1419 (w), 2932 (m), 2877 (vw), 3110 (vw), 3131 (vw) cm^{-1}.



S-Figure 18: ^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 300K) of [Cp(AlCp)(AlCp*)][Al(OR^{F})$_4$] **4**.

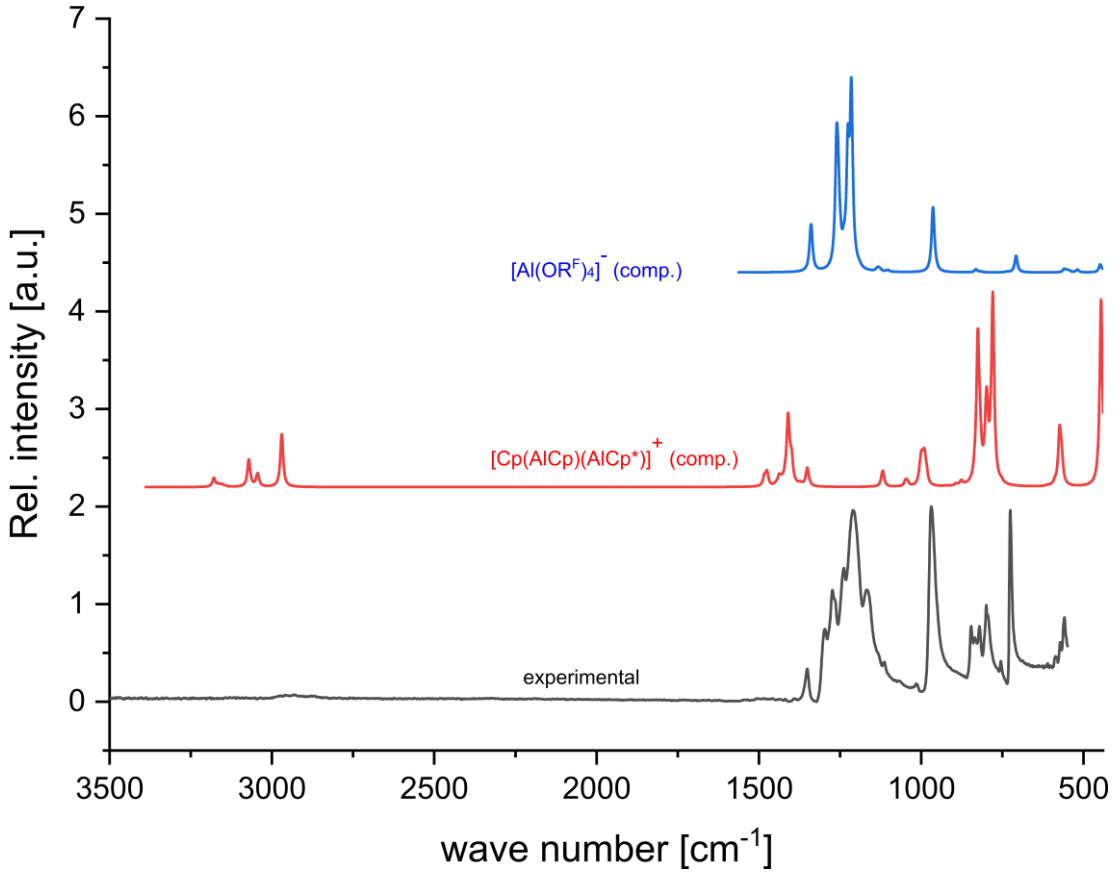


S-Figure 19: ^{19}F NMR spectrum (282.45 MHz, 1,2-DFB, 300K) of [Cp(AlCp)(AlCp*)]-[Al(OR^{F})$_4$] **4**.

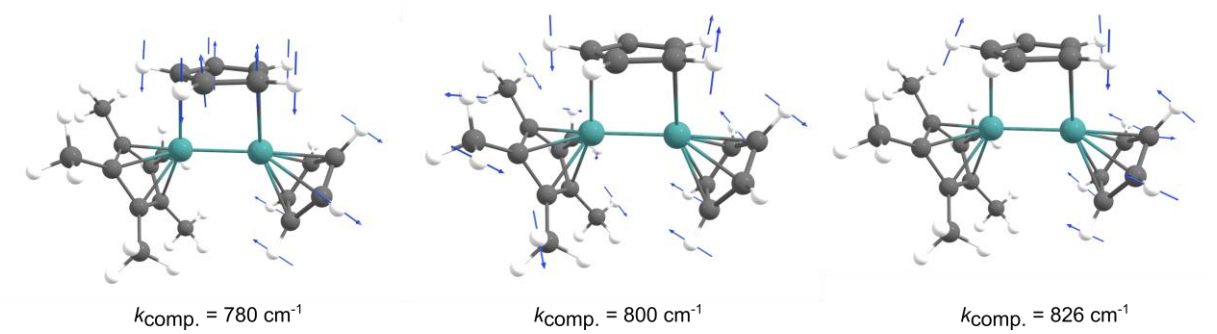


S-Figure 20: ^{27}Al NMR spectrum (78.22 MHz, PhF, 300K) of [Cp(AlCp)(AlCp*)][Al(OR^F)$_4$] **4**.

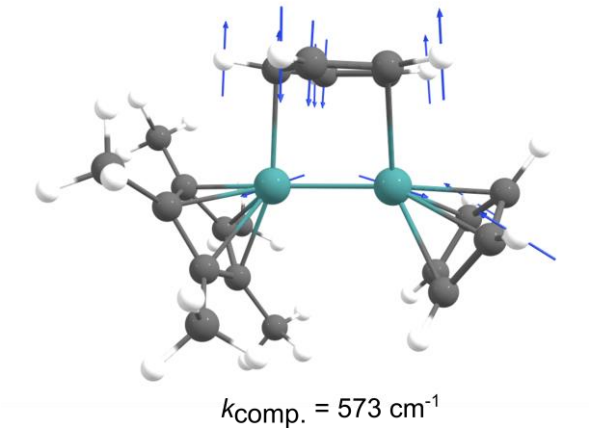
The **IR spectrum** predominantly shows the bands assigned to the [*pf*]$^-$ anion, which matches previously reported IR spectra.[11] Between 790 and 830 cm^{-1}, bending vibrations characteristic for the Cp-ligands in **4** are observed (**S-Figure 22**). Intriguingly, an asymmetric Al–Al bond stretching mode combined with bending of the bridged Cp-ligand is observed at 556 cm^{-1} (comp. 573 cm^{-1}, **S-Figure 23**).



S-Figure 21: Experimental IR spectrum of **4** and computed IR spectra for the [Cp(AlCp)(AlCp*)]$^+$ cation and the [Al(OR^F)$_4$]$^-$ anion (bp86-d3bj/def2-svp).

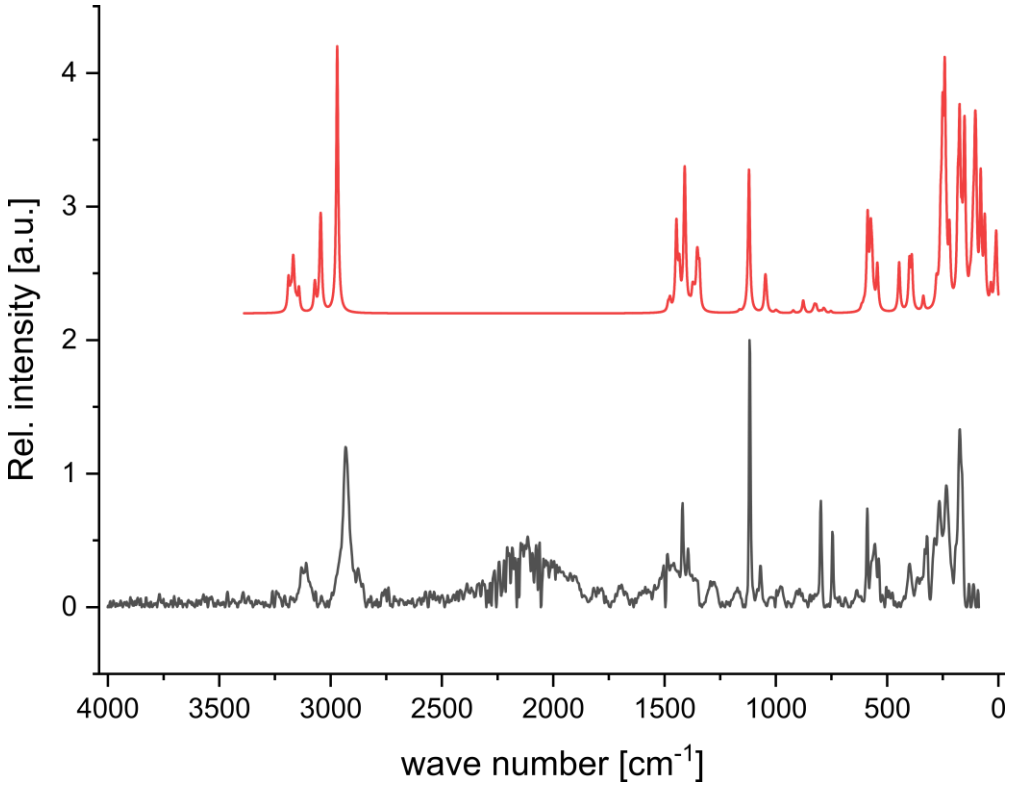


S-Figure 22: Computed IR-active vibrations in the [Cp(AlCp)(AlCp*)]$^{+}$ cation along with displacement vectors (bp86-d3bj/def2-svp).

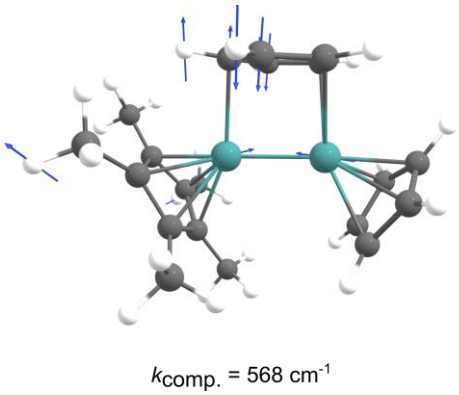


S-Figure 23: Computed IR-active vibration of the Al–Al bond in the [Cp(AlCp)(AlCp*)]$^{+}$ cation along with displacement vectors (bp86-d3bj/def2-svp).

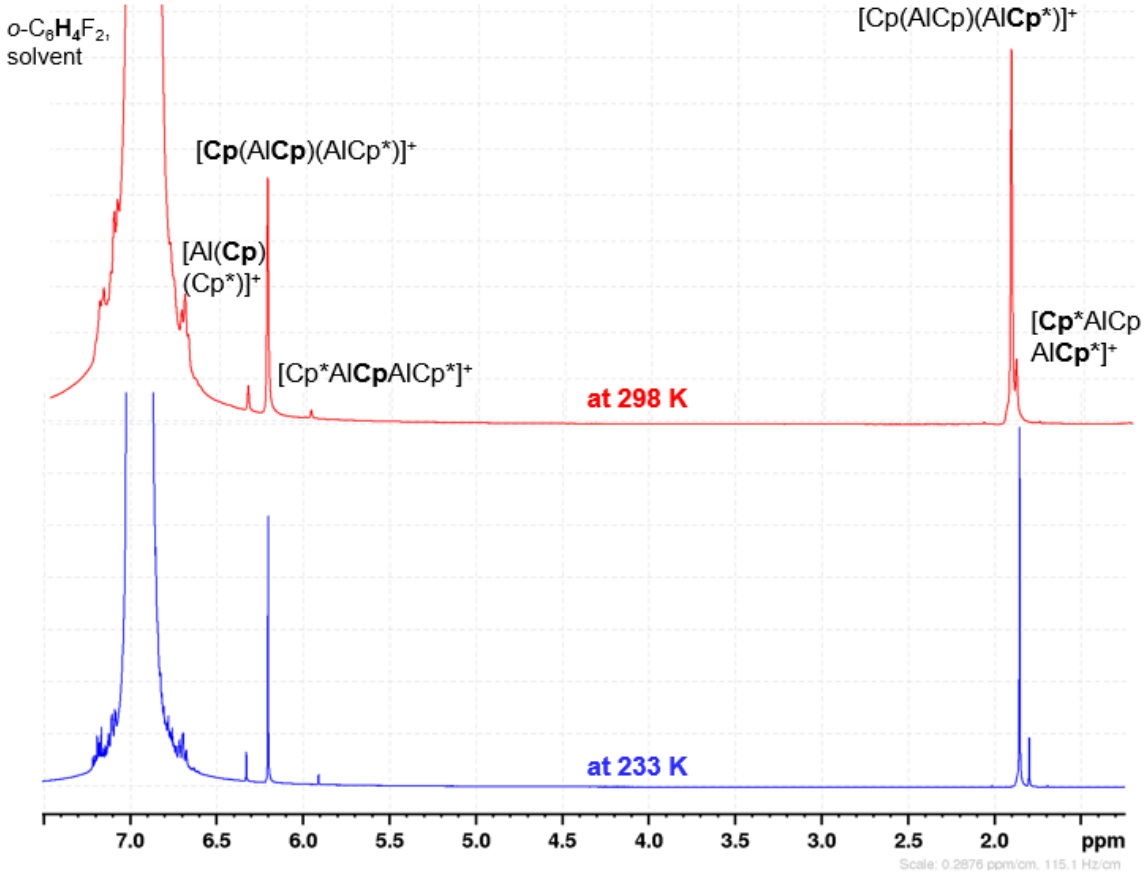
The Raman spectrum of **4** fits to the computed spectrum (**S-Figure 24**). Here, bands at 745 cm^{-1} and 798 cm^{-1} can be assigned to the anion.[11] The symmetric Al–Al stretching vibrations shows as shoulder at 572 cm^{-1} (**S-Figure 25**).



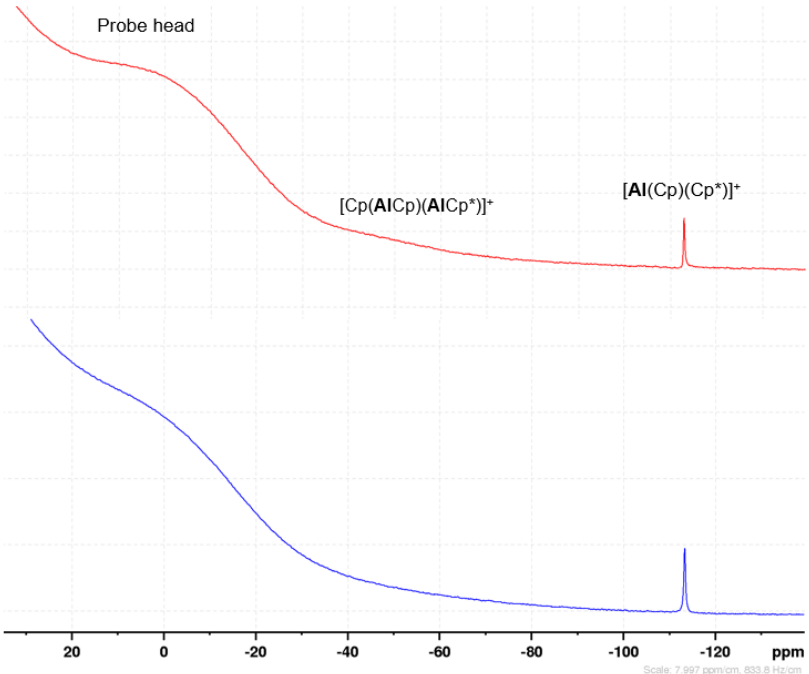
S-Figure 24: Comparison of experimental Raman spectrum (50 mW, 4000 scans, bottom) of **4** with computed spectrum for the cation in **4** (top).



S-Figure 25: Raman-active Al–Al stretching vibration with displacement vectors (bp86-d3bj/def2-svp).



S-Figure 26: ^{1}H NMR spectrum (400.17 MHz, 1,2-DFB) of [Cp(AlCp)(AlCp*)][Al(OR^{F})$_4$] **4** at 298 and 233 K.



S-Figure 27: ^{27}Al NMR spectrum (104.26 MHz, 1,2-DFB) of [Cp(AlCp)(AlCp*)][Al(OR^{F})$_4$] **4** at 298 and 233 K.

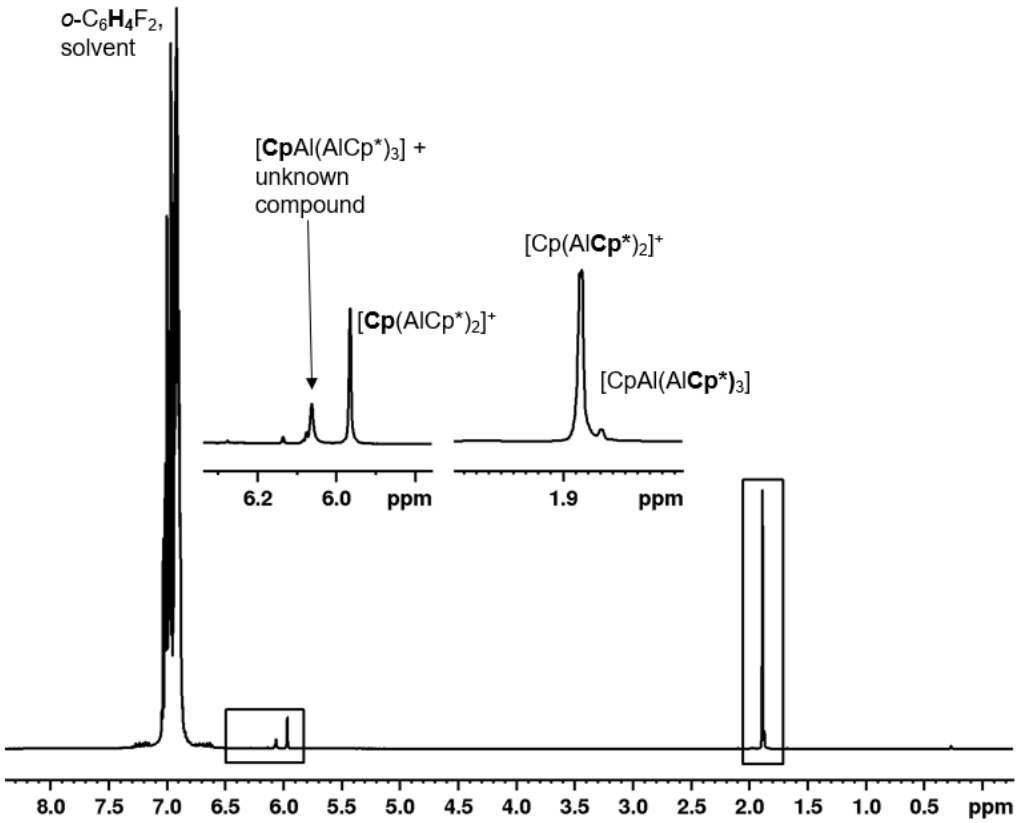
S-1.6 Experimental data for the reaction of $[AlCp_2][Al(OR^F)_4]$ **2** with 0.5 $[(AlCp^*)_4]$

2 (50 mg, 45 μmol) and $[(AlCp^*)_4]$ (14 mg, 22 μmol, 0.5 equiv.) were dissolved in 1,2-DFB (3 mL) at room temperature. The formation of a metallic precipitate and colourless solution was observed in the course of 5 min. The reaction mixture was stirred for 15 more minutes at room temperature and then filter cannulated. The solution was layered with *n*-heptane at −30°C. scXRD quality crystals of $[Cp(AlCp^*)_2][Al(OR^F)_4]$ **1B** could be obtained accompanied with formation of slightly yellow powder. NMR analysis, however, showed contamination of **1B** with $[CpAl(AlCp^*)_3]$ and unknown compounds.

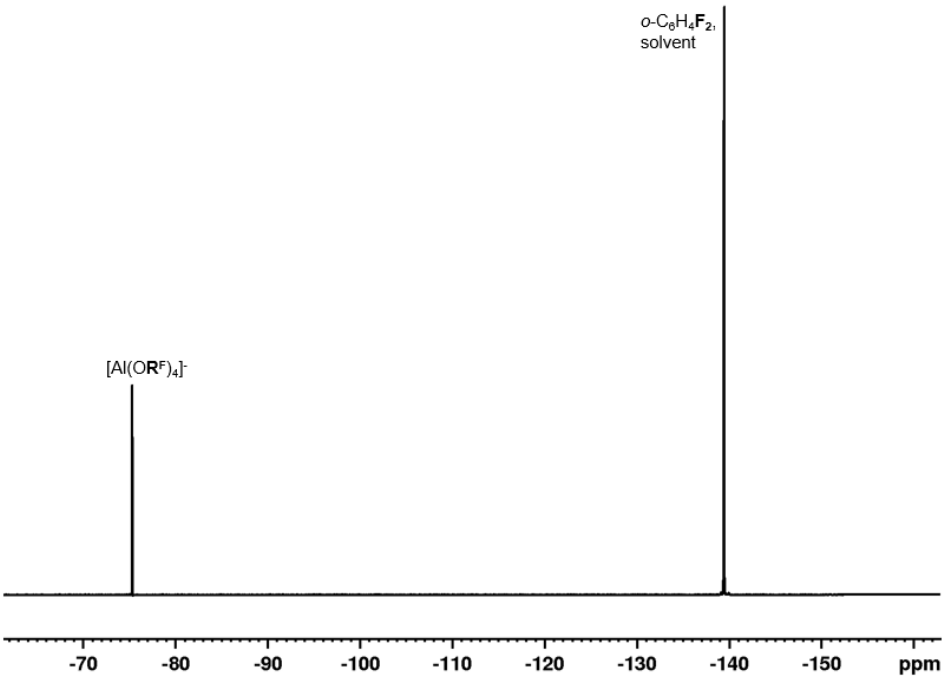
^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 298 K): δ = 1.87 (s, 45 H, $[CpAl(Al\mathbf{Cp^*})_3]$), 1.89 (s, 30 H, $[Cp(Al\mathbf{Cp^*})_2]^+$), 5.96 (s, 5 H, $[Cp(Al\mathbf{Cp^*})_2]^+$), 6.06 (br s, 5H, $[\mathbf{Cp}Al(AlCp^*)_3]$ + unknown compound), 6.08 (s, unknown compound), 6.13 (unknown compound) ppm.

^{19}F NMR spectrum (282.45 MHz, 1,2-DFB, 298 K): δ = −75.32 (s, 36 F, $[Al(OC_4F_9)_4]^-$) ppm.

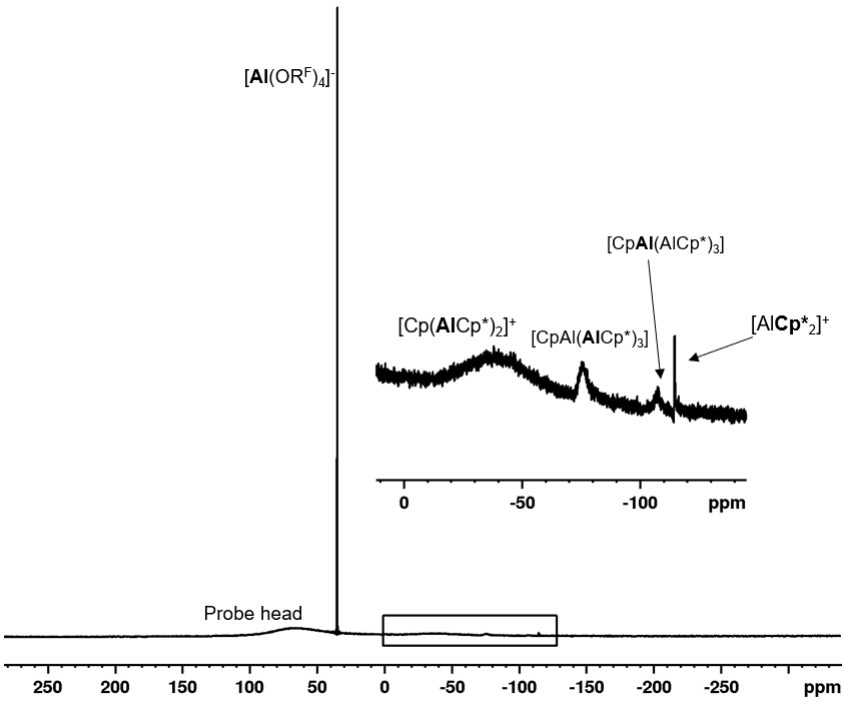
^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 298 K): δ = 35.0 (s, $[Al(OC_4F_9)_4]^-$), −40.0 (s, $[Cp(Al\mathbf{Cp^*})_2]^+$), −75.3 (s, $[CpAl(\mathbf{Al}Cp^*)_3]$), −107.2 (s, $[Cp\mathbf{Al}(AlCp^*)_3]$), −114.7 (s, $[AlCp^*_2]^+$) ppm.



S-Figure 28: ^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 300K) of the reaction between $[AlCp_2][Al(OR^F)_4]$ **2** with 0.5 $[(AlCp^*)_4]$.



S-Figure 29: ^{19}F NMR spectrum (282.45 MHz, 1,2-DFB, 298 K) of the reaction between $[AlCp_2][Al(OR^F)_4]$ **2** with 0.5 $[(AlCp^*)_4]$.



S-Figure 30: ^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 298 K) of the reaction between $[AlCp_2][Al(OR^F)_4]$ **2** with 0.5 $[(AlCp^*)_4]$.

S-1.7 Experimental data for the preparation of $[Cp(AlCp^*)_2][Al(OR^F)_4]$ **1B**

Procedure 1 starting from $[AlCp_2]^+$: $[AlCp_2][Al(OR^F)_4]$ (100 mg, 88.9 μmol) and $[(AlCp^*)_4]$ (72.1 mg, 445 μmol, 5 equiv.) were separately dissolved in 1,2-DFB (1mL and 3 mL). Both mixtures were cooled to –50°C and the $[AlCp_2][Al(OR^F)_4]$ solution was canulated onto the $[(AlCp^*)_4]$ solution. The reaction mixture was allowed to warm to room temperature over night. The reaction mixture was filtered from minor metal precipitate to yield a yellow solution. To this solution, *n*-pentane (approx. 15 mL) was added until a precipitation was observed. Then, the flask was cooled to –30°C for 30 min and the off-white precipitate was separated from the yellow solution by filter cannulation. The title compound **1B** was isolated as off-white powder (70 mg, 52 μmol, 58 %). The yellow solution was removed in vacuo to yield a yellow powder, which was identified as $[CpAl(AlCp^*)_3]$ (34 mg, 58 μmol, 66 %) with only minor contamination of **1B**.[12]

^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 298 K): δ = 1.89 (s, 30 H, $[Cp(Al\mathbf{Cp^*})_2]^+$), 5.97 (s, 5 H, $[Cp(Al\mathbf{Cp^*})_2]^+$) ppm.

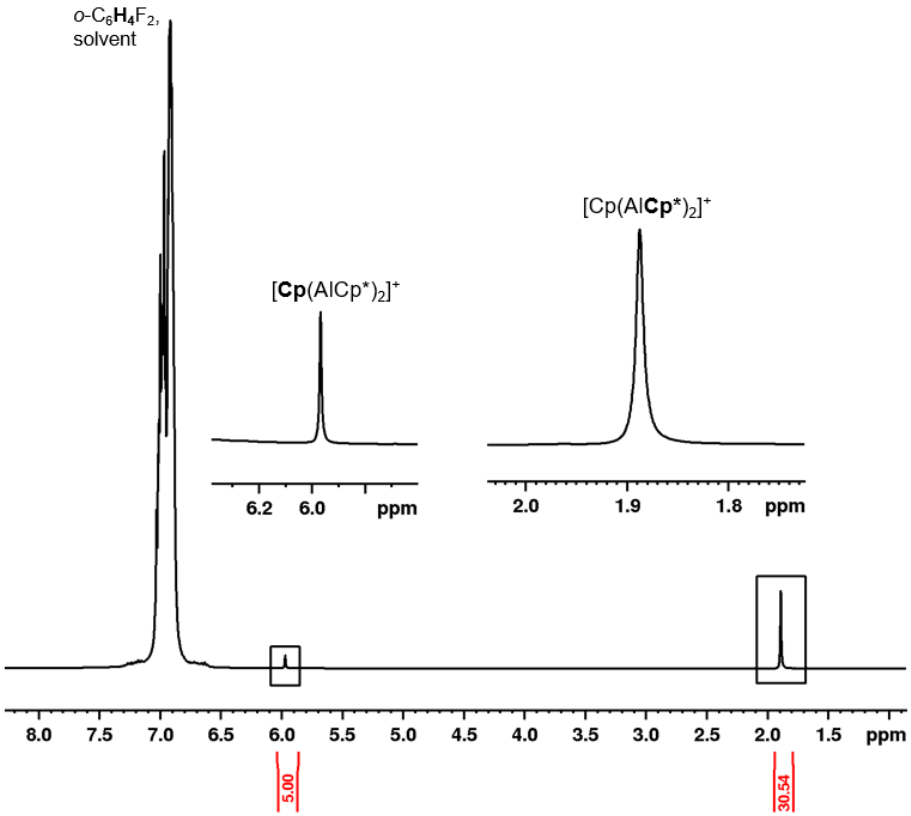
^{1}H, ^{13}C HMBC spectrum (300.18 MHz, 75.48 MHz, 1,2-DFB, 298 K): δ(^{13}C) = 111.6 ($[\mathbf{Cp}(AlCp^*)_2]^+$), 116.7 ($[Cp(Al\mathbf{Cp^*})_2]^+$, $\mathbf{C}_5Me_5$) ppm.

^{19}F NMR spectrum (282.45 MHz, 1,2-DFB, 298 K): δ = –75.32 (s, 36 F, $[Al(OC_4F_9)_4]^-$) ppm.

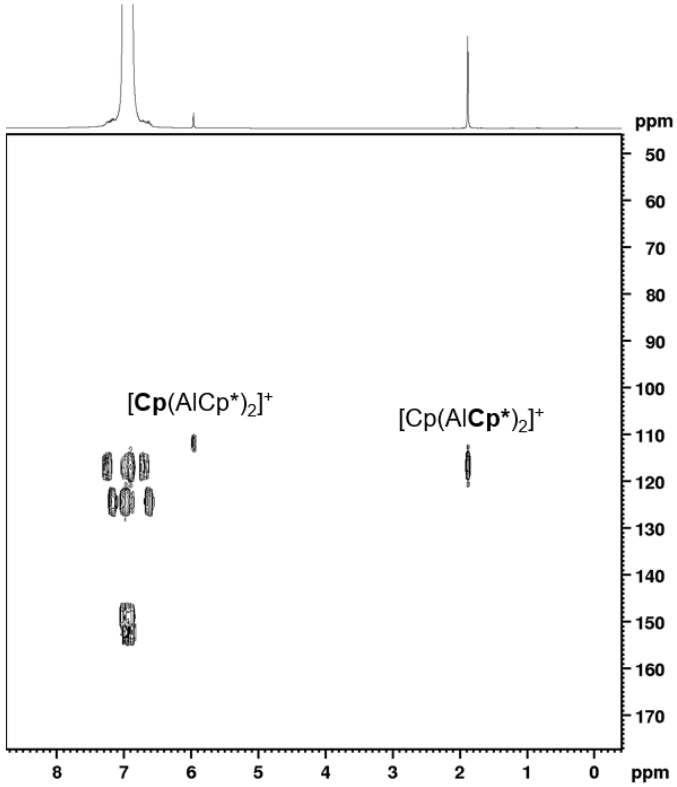
^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 298 K): δ = 35.0 (s, $[Al(OC_4F_9)_4]^-$), –40.0 (s, $[Cp(Al\mathbf{Cp^*})_2]^+$) ppm.

FTIR spectrum (ZnSe-ATR): $\tilde{\nu}$ = 560 (w), 726 (vs), 752 (w), 796 (w), 831 (vw), 971 (vs), 1162 (m), 1212 (vs), 1240 (m), 1274 (m), 1297 (w), 1351 (vw), 1394 (vw), 1509 (vw), 1517 (vw), 2919 (vw) cm^{-1}.

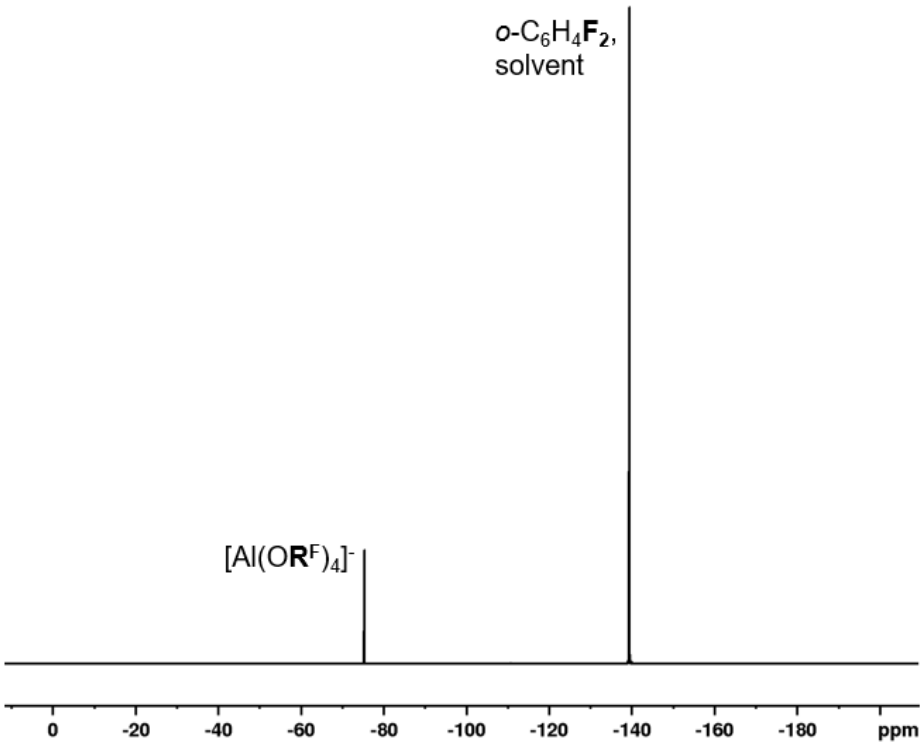
Raman (50 mW, 10000 scans): $\tilde{\nu}$ = 163 (w), 266 (w), 281 (w), 395 (w), 551 (w), 567 (w), 590 (m), 745 (w), 796 (m), 887 (w), 1057 (w), 1098 (w), 1116 (s), 1395 (w), 1419 (s), 1436 (vw) 2936 (vs) cm^{-1}.



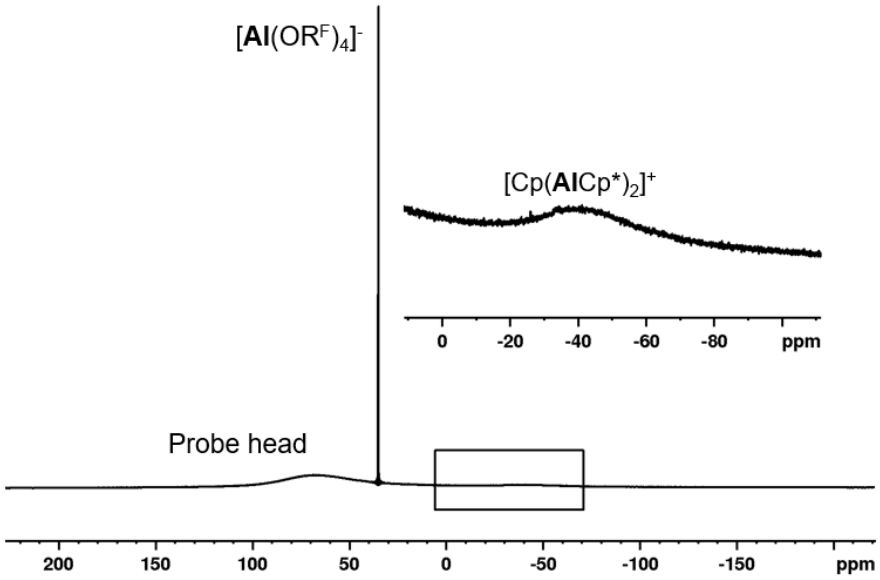
S-Figure 31: ^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 300K) of $[Cp(AlCp^*)_2][Al(OR^F)_4]$ **1B**.



S-Figure 32: ^{1}H-^{13}C HMBC spectrum (300.18 MHz, 75.48 MHz, 1,2-DFB, 300K) of $[Cp(AlCp^*)_2][Al(OR^F)_4]$ **1B**.

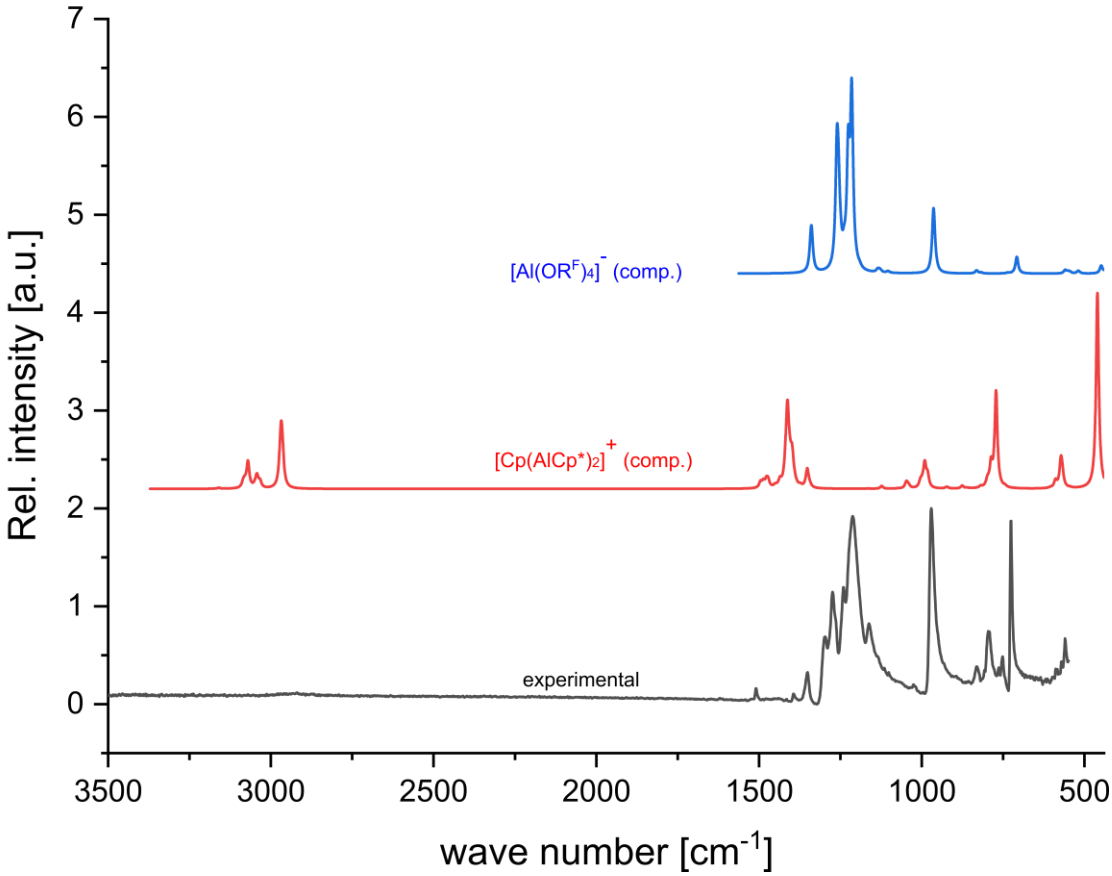


S-Figure 33: ^{11}F NMR spectrum (282.45 MHz, 1,2-DFB, 300K) of $[Cp(AlCp^*)_2][Al(OR^F)_4]$ **1B**.

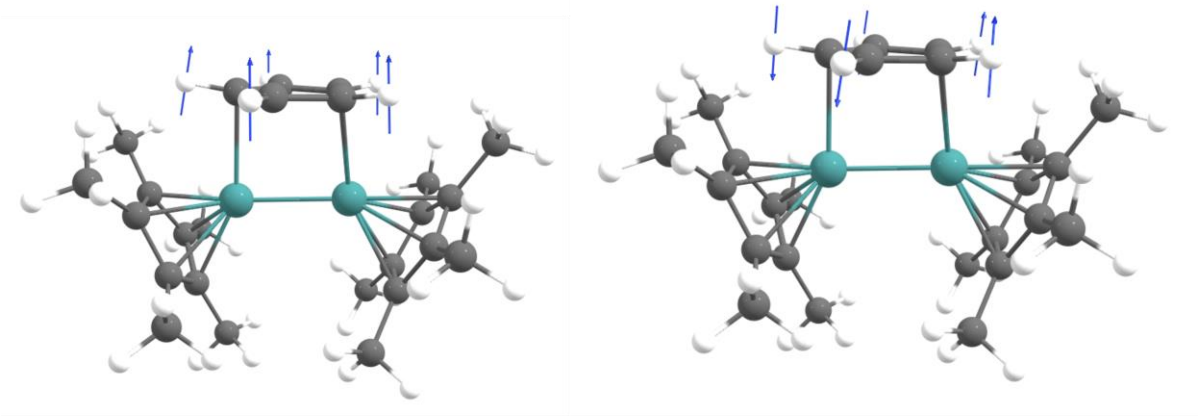


S-Figure 34: ^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 300K) of $[Cp(AlCp^*)_2][Al(OR^F)_4]$ **1B**.

The **IR spectrum** predominantly shows the bands assigned to the $[Al(OR^F)_4]^-$ anion, which matches previously reported IR spectra.[11] Fitting to the computed spectrum, IR-active vibrations of the Cp-ligand in **1B** are less intense compared to **4** (**S-Figure 36**). The asymmetric Al–Al bond stretching mode combined with bending of the bridged Cp-ligand, however, is also observed as band at 573 cm^{-1}.

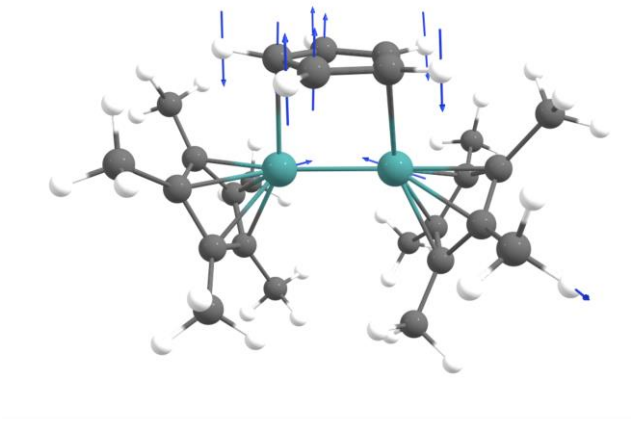


S-Figure 35: Experimental IR spectrum of **1B** and computed IR spectra for the $[Cp(AlCp^*)_2]^+$ cation and the $[Al(OR^F)_4]^-$ anion (bp86-d3bj/def2-svp).



$k_{comp.}$ = 772 cm^{-1} $k_{comp.}$ = 787 cm^{-1}

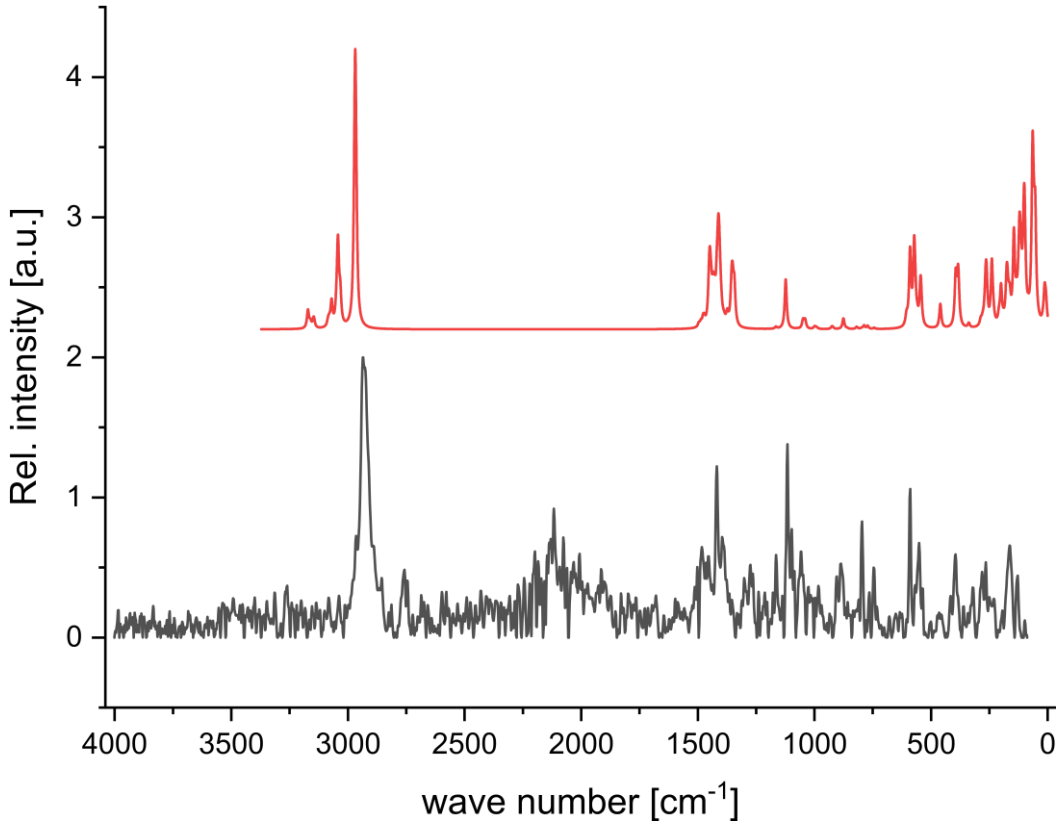
S-Figure 36: Computed IR-active vibrations in the $[Cp(AlCp^*)_2]^+$ cation along with displacement vectors (bp86-d3bj/def2-svp).



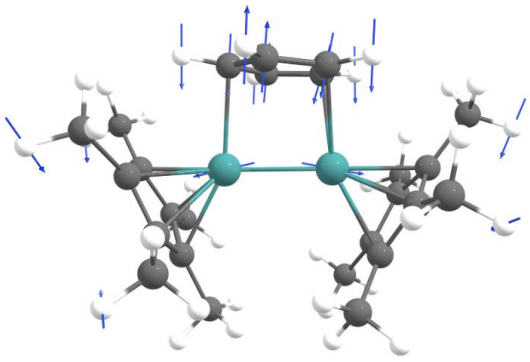
$k_{comp.}$ = 573 cm^{-1}

S-Figure 37: Computed IR-active vibration of the Al–Al bond in the $[Cp(AlCp^*)_2]^+$ cation along with displacement vectors (bp86-d3bj/def2-svp).

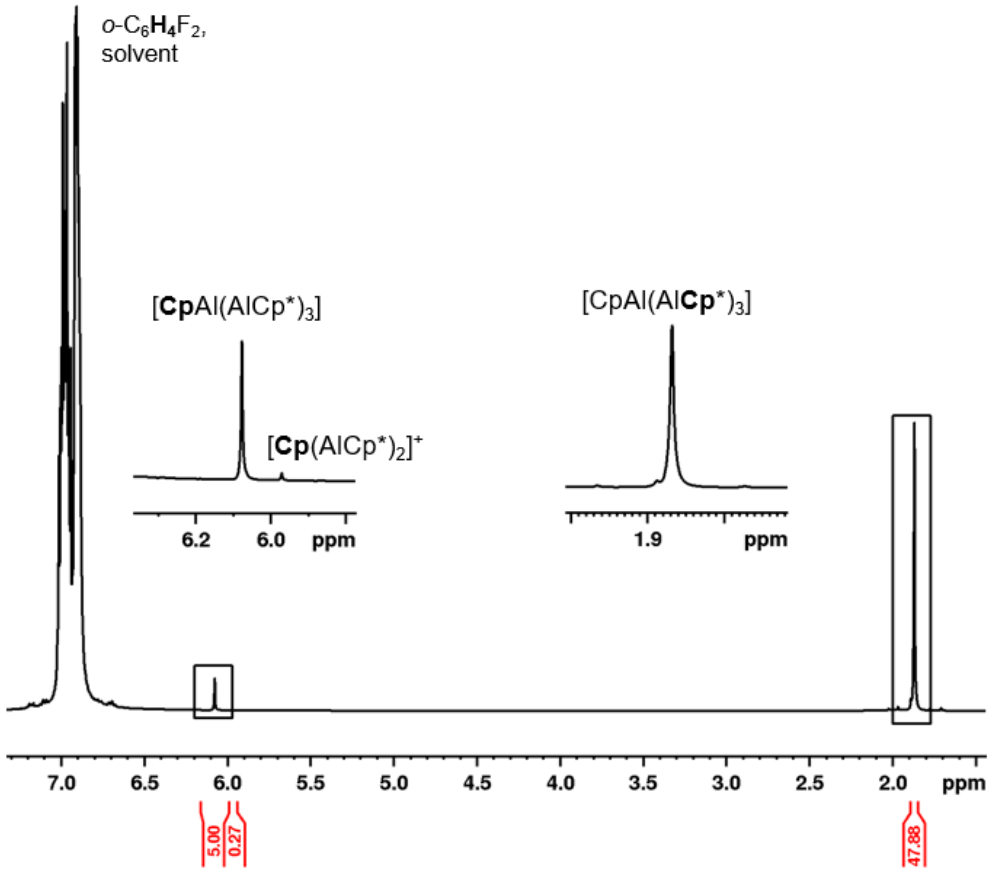
The Raman spectrum of **1** fits to the computed spectrum (**S-Figure 38**). Here, bands at 745 cm^{-1} and 798 cm^{-1} can be assigned to the anion.[11] The symmetric Al–Al stretching vibrations shows as shoulder at 569 cm^{-1} (**S-Figure 39**).



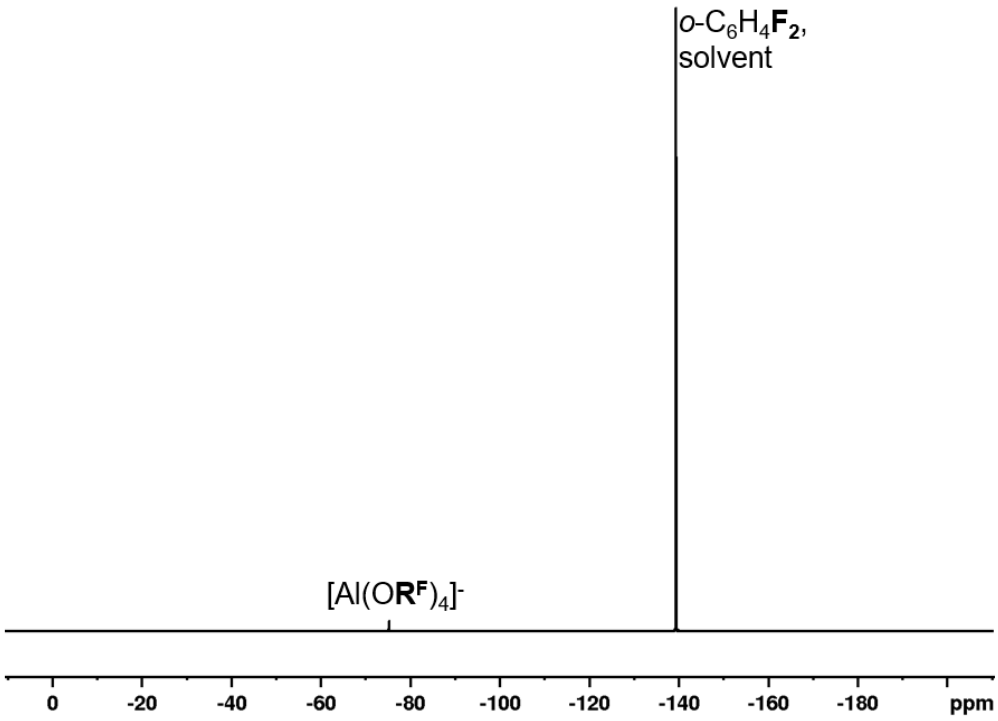
S-Figure 38: Comparison of experimental Raman spectrum (50 mW, 10000 scans, bottom) of **1** with computed spectrum for the cation in **1** (top).



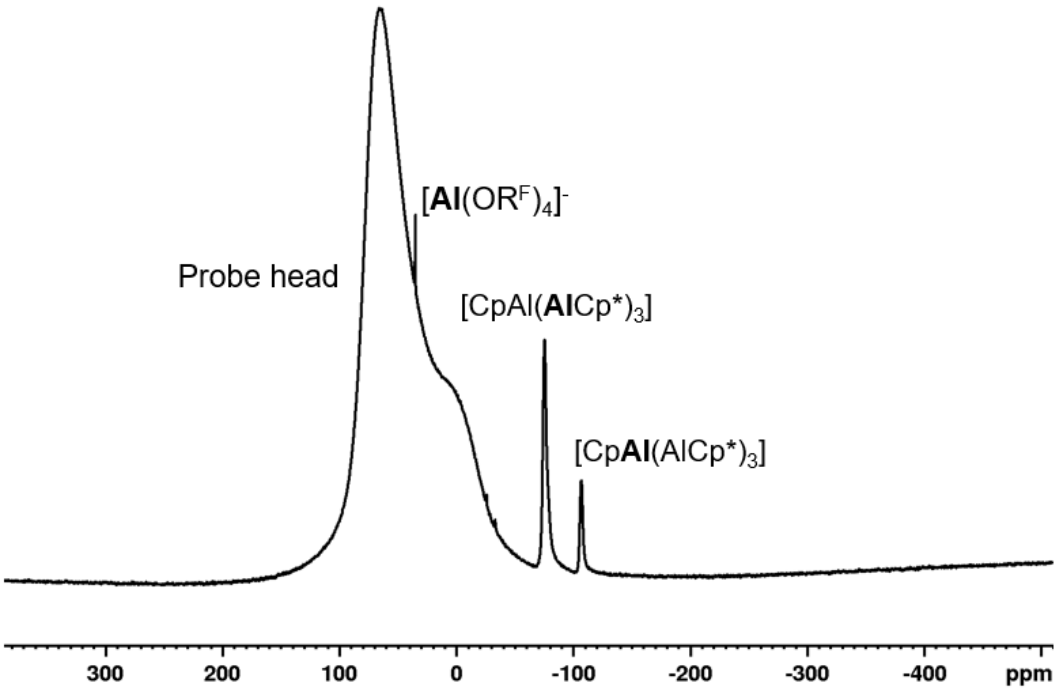
S-Figure 39: Raman-active Al–Al stretching vibration with displacement vectors (bp86-d3bj/def2-svp).



S-Figure 40: ^{1}H NMR spectrum (400.17 MHz, 1,2-DFB, 300K) of [CpAl(AlCp*)$_3$].



S-Figure 41: ^{11}F NMR spectrum (376.54 MHz, 1,2-DFB, 300K) of of [CpAl(AlCp*)$_3$].



S-Figure 42: ^{27}Al NMR spectrum (104.27 MHz, 1,2-DFB, 300K) of [CpAl(AlCp*)$_3$].

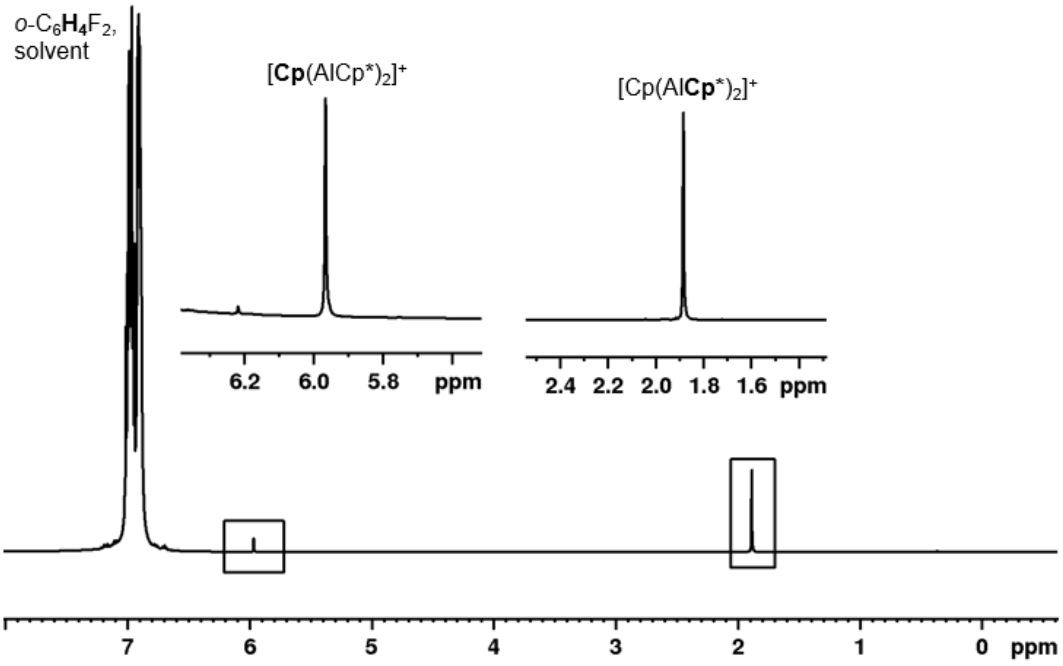
Procedure 2 starting from 4:

4 (10 mg, 7.8 μmol) and $[Al(AlCp^*)_3][Al(OR^F)_4]$ (12 mg, 7.8 μmol, 1 equiv.) were dissolved in 1,2-DFB (0.7 mL) at room temperature in a J. Young NMR tube. NMR analysis showed a clean conversion to **1B** (*vide infra*).

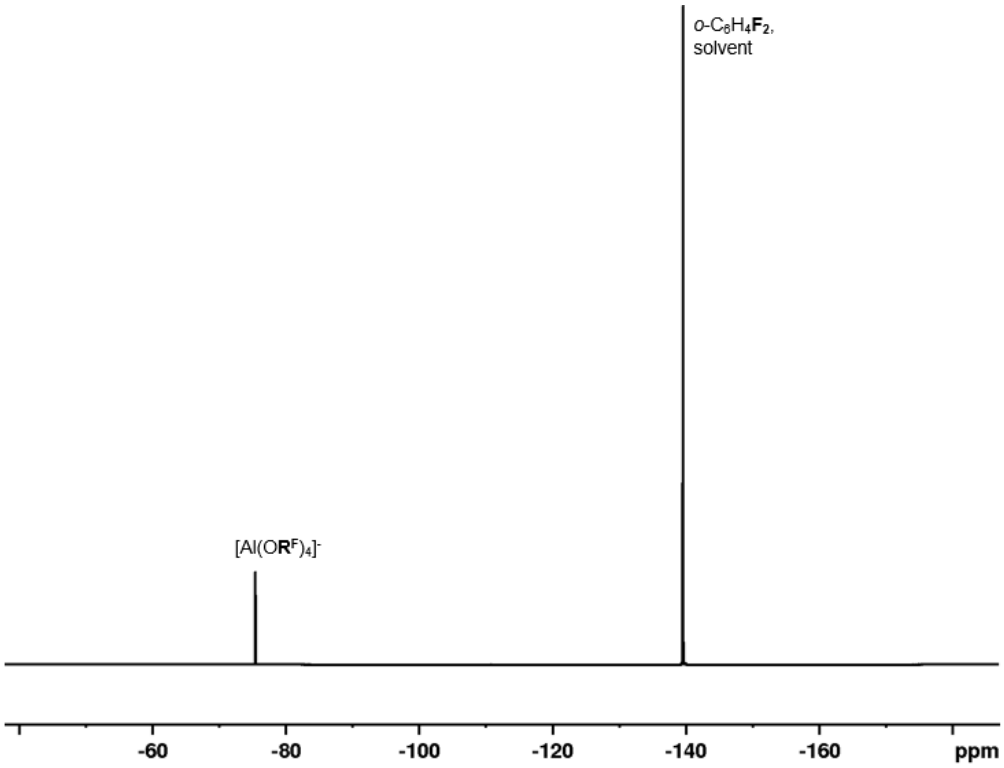
^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 298 K): δ = 1.89 (s, 30 H, $[Cp(Al\mathbf{Cp^*})_2]^+$), 5.97 (s, 5 H, $[Cp(Al\mathbf{Cp^*})_2]^+$) ppm.

^{19}F NMR spectrum (282.45 MHz, 1,2-DFB, 298 K): δ = −75.3 (s, 36 F, $[Al(OC_4F_9)_4]^-$) ppm.

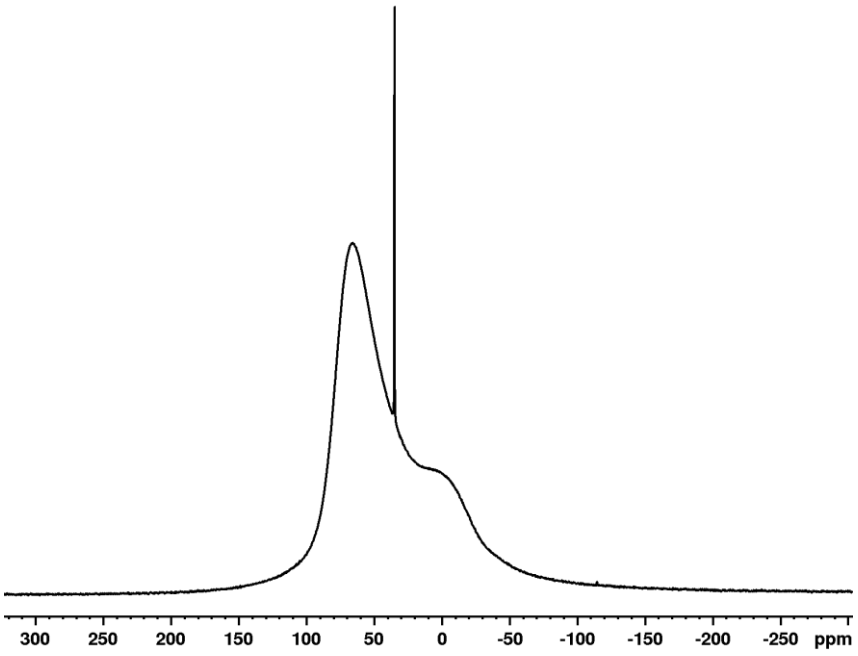
^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 298 K): δ = 35.0 (s, $[Al(OC_4F_9)_4]^-$) ppm.



S-Figure 43: ^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 300K) of $[Cp(AlCp^*)_2][Al(OR^F)_4]$ **1B**.



S-Figure 44: ^{11}F NMR spectrum (282.45 MHz, 1,2-DFB, 300K) of [Cp(AlCp*)$_2$][Al(OR^F)$_4$] **1B**.



S-Figure 45: ^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 298 K) of [Cp(AlCp*)$_2$][Al(OR^F)$_4$] **1B**.

S-2 Supporting quantum-chemical calculations

S-2.1 Computational details

Geometry optimizations were performed with the TURBOMOLE software[13] (v7.2 or v7.5) using DFT functionals bp86[14] with the def2-svp[15] basis set, the resolution-of-identity (RI) approximation[16], dispersion correction (d3bj)[17], a fine integration grid (m4 and 5 for NMR) and the default SCF convergence criteria (10^{-6} a.u.). All structures were checked for imaginary frequencies with the integrated *AOFORCE* module[18]. Thermal and entropic contributions to the Gibbs energy were calculated at the bp86-d3bj/def2-svp level of theory without scaling factor at standard conditions with the *FREEH* module. IR and Raman spectra were simulated on bp86-d3bj/def2-svp level without scaling factor and a FWHM of 10 cm^{-1}. Computed NMR shifts were referenced against the experimental magnetic shielding of $[(AlCp^*)_4]$ ($\delta = -79.9$ ppm) and computed with grid5 and on pbe0[19,20]-d3bj/def2-tzvpp level of DFT using TURBOMOLE.

Gibbs free energies of solvation were calculated with the COSMO-RS model[21] at the bp86-d3/def2-tzvpd//bp86-d3/def2-tzvp[22] level of theory using the CosmoThermX[23] software (v C39_1501). Single-point calculations with the pbe0[19,20]-d3bj/def2-tzvpp method were performed based on bp86-d3bj/def2-svp structures using TURBOMOLE.

QTAIM calculations were performed with the AIMALL[24] on bp86-d3bj/def2-svp structures. EDA-NOCV analysis[25] of the compounds was performed as implemented in the ADF program package (2019.304)[26]. All EDA-NOCV calculations were performed on bp86-d3bj/tz2p//bp86-d3bj/def2-svp level of DFT (numerical quality verygood, nosym).

FIAs and HIAs were computed on DLPNO-CCSD(T)[27]/aug-cc-pVQZ[28]//PBEh-3c[29]/def2-mSVP level of DFT with CPCM for solvation according to the benchmark studies by Greb.[30] Computations performed with Orca (v. 4.2.1).[31]

S-2.2 Short introduction to DFT methods: QTAIM and EDA-NOCV

In the quantum theory of atoms in molecule analysis (**QTAIM**), the values computed at bond critical points (BCP) reflect the nature of interactions between the atoms. The most important values for description of the interaction are the electron density ρ(r) and the Laplacian of the electron density Δ_ρ(r). In general, large values of the electron density ρ(r) indicate a strong bonding interaction. Moreover, a negative Δ_ρ(r) value is indicative of a covalent, shared-shell interaction[32]. The ellipticity of electron density ε at the BCP reflects the anisotropy of the curvature of the electron density orthogonal to the bond. Hence, ε-values below 0.1 indicate no anisotropy (*e.g.* in σ-bonds or triple bonds) and values higher than 0.25 are typically calculated for double bonds[33].

EDA-NOCV analysis (energy decomposition analysis with natural orbitals for chemical valence) of the compounds was performed as implemented in the ADF program package. All EDA-NOCV calculations were performed at the bp86-d3bj/tz2p//bp86-d3bj/def2-svp level of DFT. In the EDA-NOCV approach, the intrinsic interaction energy (ΔE_{int}) is broken down into the Pauli repulsion ΔE_{Pauli}, the quasi-classical electrostatic interaction $\Delta E_{elstat.}$, the dispersion energy ΔE_{disp} and orbital energy ΔE_{orb} as described by equation (2).

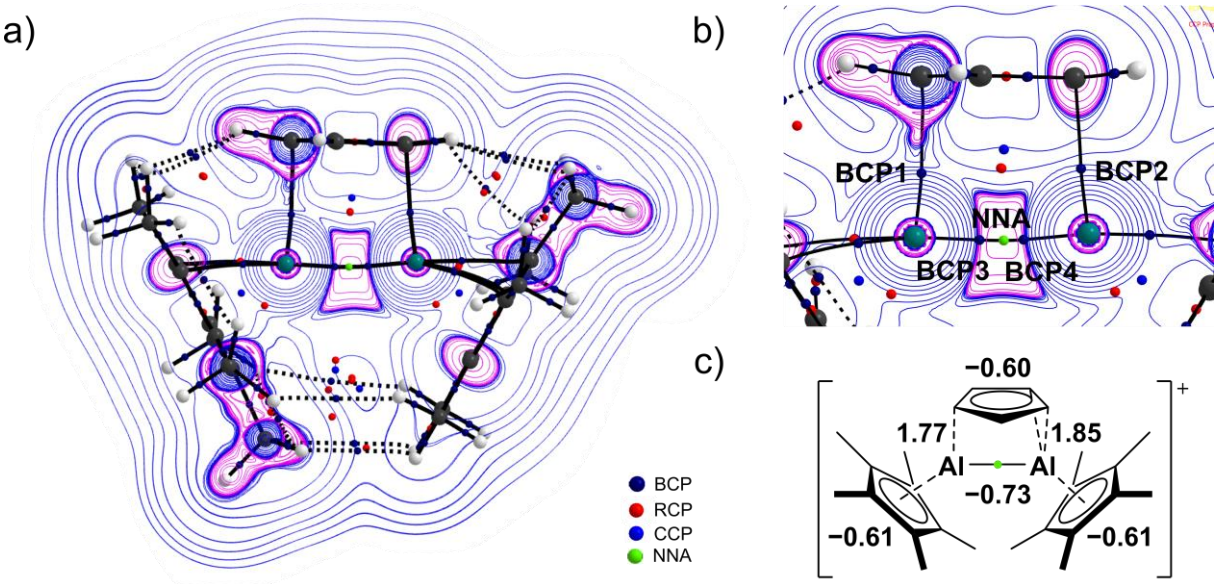
$$\boldsymbol{\Delta E_{int} = \Delta E_{elstat.} + \Delta E_{Pauli} + \Delta E_{disp} + \Delta E_{orb}.} \quad (2)$$

Moreover, the orbital interaction term ΔE_{orb} is further divided in the NOCV procedure into pairwise contributions $\Delta E^k{}_{orb}$. These $\Delta E^k{}_{orb}$ terms can be assigned to plots of deformation density $\Delta\varrho_k(r)$, which illustrate the orbital contributions to the bonding and the change in electron distribution in the molecule compared to the two fragments. More detailed information on the EDA-NOCV method can be found in recent reviews[34,35]. The EDA-NOCV method depends significantly on the charge and multiplicity of the fragments chosen. Here, the fragment combination leading to the lowest ΔE_{orb} is considered as the best bonding representation[35].

S-2.3 Computational analysis of $[Cp(AlCp^*)_2]^+$

S-2.3.1 $[Cp(AlCp^*)_2]^+$: QTAIM analysis

A non-nuclear attractor (NNA) is computed between the Al atoms in the cation (S-Figure 46). Discovered theoretically for Li_2,[36] first experimental evidence for NNAs was found in isolable Mg–Mg dimers.[37,38] NNAs have shown to be observed at Atom-specific internuclear distances due to overlap of specific electron shells.[39] Similarly to isoelectronic Na_2 and $[Mg–Mg]^{2+}$ fragments, NNAs in the discussed $[Al–Al]^{4+}$ dimers originate from significant build-up of electron density upon bonding of Al atoms with high *s* character.[37]



S-Figure 46: Visualization of the Laplacian $\Delta_r\rho$ in the plane including BCP1, BCP2 and the centroid of the bridging Cp ligand (a) along with a zoom (b) and the QTAIM charges for the complex (c)

S-Table 1: Computed values for electron density ρ_r, Laplacian of electron density $\Delta_r\rho$ and ellipticity ε for cricital points in $[Cp(AlCp^*)_2]^+$

CP	ρ_r [Å^{-3}]	$\Delta_r\rho$ [Å^{-5}]	ε
BCP1	0.25	-0.56	0.02
BCP2	0.26	-0.67	4.02
BCP3	0.39	-1.05	0.15
BCP4	0.38	-1.096	0.16
NNA	0.40	-1.09	

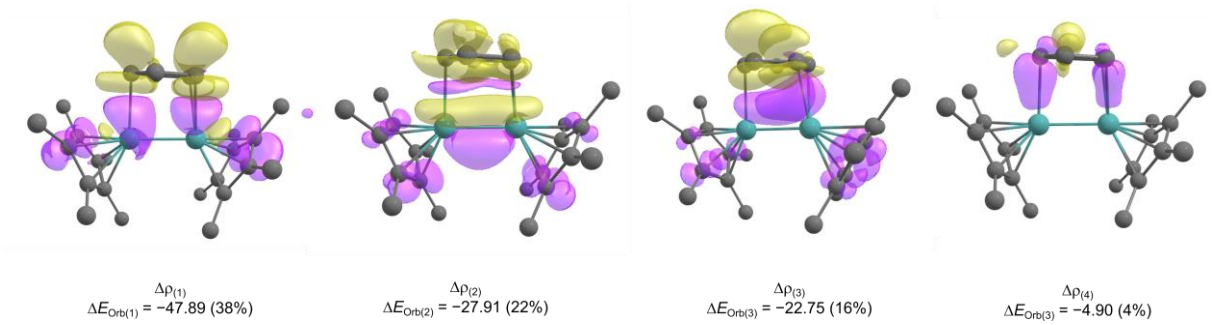
S-2.3.2 $[Cp(AlCp^*)_2]^+$: EDA-NOCV analysis on Cp interaction

In the EDA-NOCV analysis, the interaction of the bridging Cp-ligand in **1** is best described by splitting into an anionic Cp^- and a dicationic $[(AlCp^*)_2]^{2+}$ fragment (**S-Table 2**). Here, the electrostatic interaction energy represents the major contribution to the attractive bonding interaction. Moreover, the orbital interaction is dominated by electron-donation from the HOMO of the Cp^- fragment into the LUMO of the $[(AlCp^*)_2]^{2+}$ fragment, which represents the σ* orbital of the Al–Al bond. A side-on π donation into the π-orbital of the Al–Al bond accounts for 16 % of the orbital interaction energy. Nevertheless, the orbital interaction energy into a Cp radical and $[Cp^*AlAlCp^*]^{+\bullet}$ radical cation is only 16 kcal/mol larger compared to the ionic fragmentation. Here, similar plots of the deformation density are computed (**S-Figure 48**).

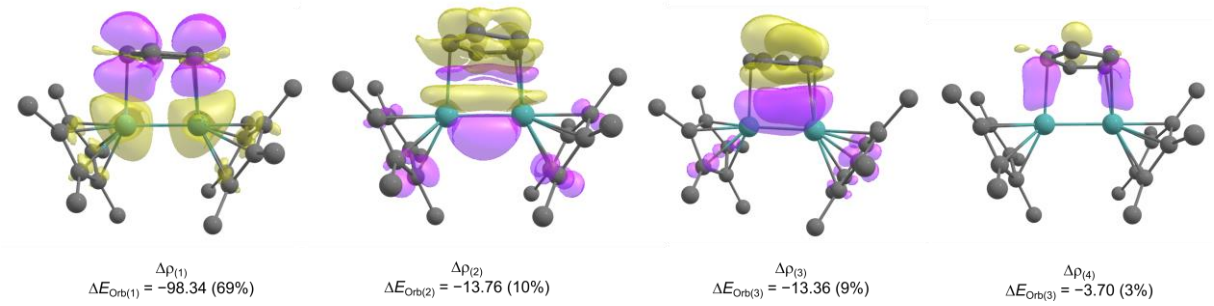
S-Table 2: Results of the EDA-NOCV analysis for the interaction of the bridging Cp ligand with the $[(AlCp^*)_2]$ fragment (S) in **1** (values given in kcal/mol)

		$[Cp(AlCp^*)_2]^+$			
Energy terms	$[Cp]^-$ (S) + $[Cp^*AlAlCp^*]^{2+}$ (S)		$[Cp]^\bullet$ (D) + $[Cp^*AlAlCp^*]^{+\bullet}$ (D)		$[Cp]^+$ (T) + $[Cp^*AlAlCp^*]$ (T)
ΔE_{int}		**-246.45**		-94.37	-196.16
ΔE_{Pauli}		165.44		164.92	192.13
ΔE_{elstat}		-268.70		-100.03	-114.53
ΔE_{Orb}	Orbital interaction	-126.49	Orbital interaction	-142.57	-257.06
$\Delta E_{Orb(1)}$	σ-donation HOMO(Cp^-) →σ*(Al–Al)	-47.89 (38%)	σ-donation σ*(Al–Al) →SOMO(Cp)	-98.34 (69%)	
$\Delta E_{Orb(2)}$	σ-donation HOMO-2(Cp^-) →π(Al–Al)	-27.91 (22%)	σ-donation HOMO-2(Cp) →π(Al–Al)	-13.76 (10%)	

$\Delta E_{Orb(3)}$	π-donation HOMO-1(Cp^-) →π(Al–Al)	-20.75 (16%)	π-donation HOMO-1(Cp) →π(Al–Al)	-13.36 (9%)	
$\Delta E_{Orb(4)}$		-4.90 (4%)		-3.7 (3%)	
ΔE_{Rest}		-25.03 (20%)		-11.50 (8%)	
ΔE_{Disp}		-16.70		-16.70	-16.70



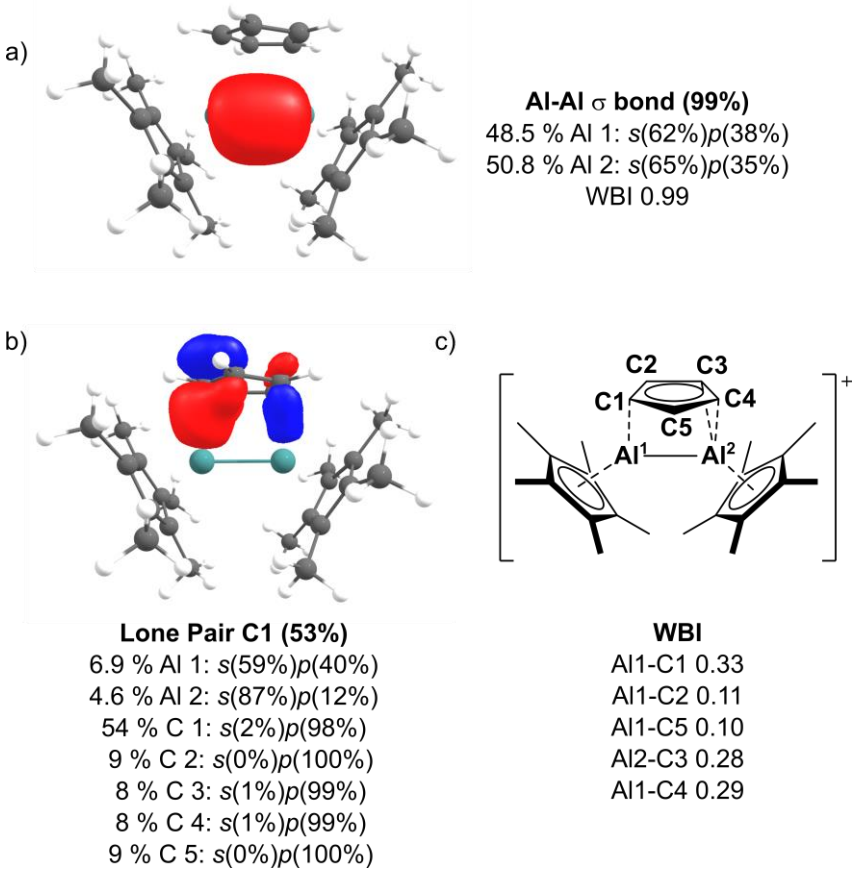
S-Figure 47: Plots of deformation densities $\Delta\rho_{(1)-(4)}$ of the pairwise orbital interaction between $[Cp]^-$ and $[Cp^*Al–AlCp^*]^{2+}$ in **1** associated with energy terms $\Delta E_{Orb(1)-Orb(4)}$ (values in kcal/mol, isovalues 0.001 for $\Delta\rho_{(1)-(4)}$). Charge flows from yellow to purple.



S-Figure 48: Plots of deformation densities $\Delta\rho_{(1)-(4)}$ of the pairwise orbital interaction between $[Cp]^{\bullet}$ and $[Cp^*Al–AlCp^*]^{\bullet+}$ in **1** associated with energy terms $\Delta E_{Orb(1)-Orb(4)}$ (values in kcal/mol, isovalues 0.001 for $\Delta\rho_{(1)-(4)}$). Charge flows from yellow to purple.

S-2.3.3 $[Cp(AlCp^*)_2]^+$: NBO analysis

The NLMO (natural localized molecular orbital) of the cation in **1** shows the Al–Al bond with a high *s* character of the Al atoms (**S-Figure 49**). Moreover, in accordance with the major orbital interaction in the EDA-NOCV analysis, the LNMO assigned to the lone-pair at C1 displays an interaction of the HOMO of the Cp ligand with the σ*-orbital of the Al–Al bond.

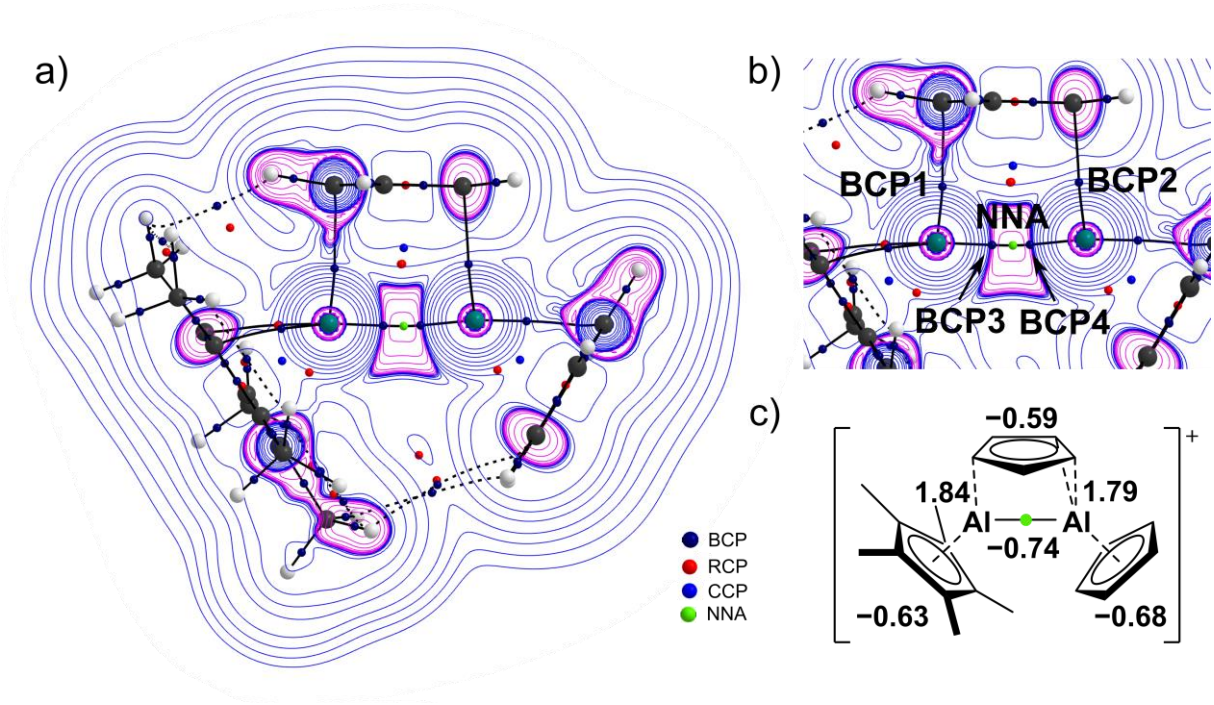


S-Figure 49: a) NLMO displaying the Al–Al s bond (isovalue 0.05). b) NLMO partially describing the NBO of the C1 lone-pair, which shows the interaction between Cp and Al–Al σ* orbital (isovalue 0.05). c) WBI values for interaction between Al atoms and bridging Cp ligand.

S-2.4 Computational analysis of $[Cp(AlCp)(AlCp^*)]^+$

S-2.4.1 $[Cp(AlCp)(AlCp^*)]^+$: QTAIM analysis

The contour plot of the Laplacian of $[Cp(AlCp)(AlCp^*)]^+$ resembles the contour plot computed for the symmetric dialane in **1**. A marginal increase in electron density at the BCPs of the Al–Al bond and the NNA indicate a stronger Al–Al bonding interaction in the cation in **4**, which matches the smaller Al–Al bond distances observed in the molecular structure.



S-Figure 50: Visualization of the Laplacian $\Delta_r\rho$ in the plane including BCP1, BCP2 and the centroid of the bridging Cp ligand (a) along with a zoom (b) and the QTAIM charges for the complex (c)

S-Table 3: Computed values for electron density ρ_r, Laplacian of electron density $\Delta_r\rho$ and ellipticity ε for cricital points in $[Cp(AlCp)(AlCp^*)]^+$

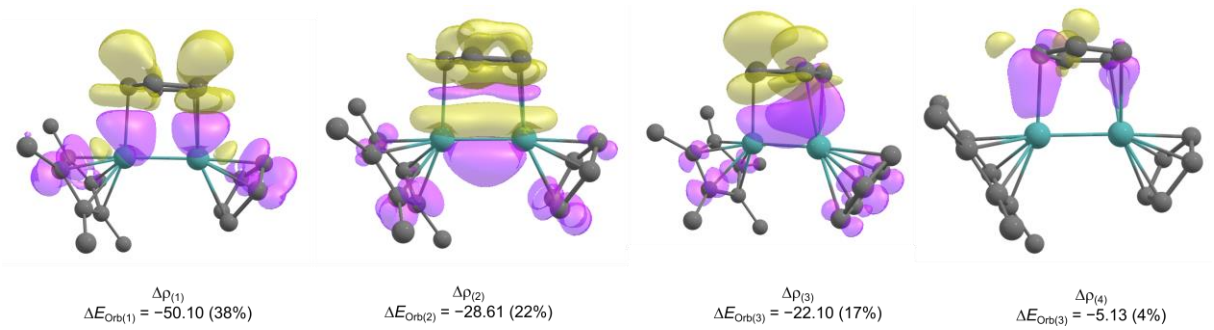
CP	ρ_r [Å^{-3}]	$\Delta_r\rho$ [Å^{-5}]	ε
BCP1	0.26	-0.62	0.01
BCP2	0.26	-0.67	4.01
BCP3	0.40	-1.09	0.14
BCP4	0.40	-1.11	0.17
NNA	0.41	-1.03	

S-2.4.2 [Cp(AlCp)(AlCp*)]$^+$: EDA-NOCV analysis on Cp interaction

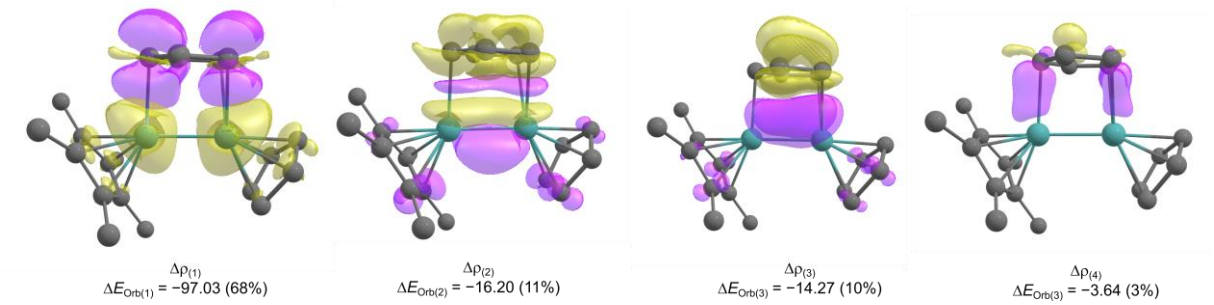
EDA-NOCV results for [Cp(AlCp)(AlCp*)]$^+$ strongly resemble the values obtained for the symmetric dialane. Yet, the difference between the orbital interaction energies computed for a fragmentation into a Cp-anion and [CpAlAlCp*]$^{2+}$ dication compared to fragmentation into a Cp-radical and [CpAlAlCp*]$^{+\bullet}$ radical cation is with 11.03 kcal/mol even smaller than in **1**. This indicates a more significant orbital contribution, which is underestimated in the ionic fragmentation.

S-Table 4: Results of the EDA-NOCV analysis for the interaction of the bridging Cp ligand with the [(AlCp*)$_2$] fragment (S) in **4** (values given in kcal/mol)

	[Cp(AlCp)(AlCp*)]$^+$				
Energy terms	[Cp]$^-$ (S) + [CpAlAlCp*]$^{2+}$ (S)		[Cp]$^\bullet$ (D) + [CpAlAlCp*]$^{+\bullet}$ (D)		[Cp]$^+$ (T) + [CpAlAlCp*] (T)
ΔE_{int}		**-259.51**		-94.23	-192.09
ΔE_{Pauli}		159.89		159.47	187.87
ΔE_{elstat}		-274.88		-98.15	-112.62
ΔE_{Orb}	Orbital interaction	-130.69	Orbital interaction	-141.72	-253.51
$\Delta E_{Orb(1)}$	σ-donation HOMO(Cp$^-$) →σ*(Al–Al)	-50.10 (38%)	σ-donation σ*(Al–Al) →SOMO(Cp)	-97.03 (68%)	
$\Delta E_{Orb(2)}$	σ-donation HOMO-2(Cp$^-$) →π(Al–Al)	-28.61 (22%)	σ-donation HOMO-2(Cp) →π(Al–Al)	-16.20 (11%)	
$\Delta E_{Orb(3)}$	π-donation HOMO-1(Cp$^-$) →π(Al–Al)	-22.10 (17%)	π-donation HOMO-1(Cp) →π(Al–Al)	-14.27 (10%)	
$\Delta E_{Orb(4)}$		-5.13 (4%)		-3.64 (3%)	
ΔE_{Rest}		-24.6 (19%)		-10.59 (7%)	
ΔE_{Disp}		-13.84		-13.84	-13.84



S-Figure 51: Plots of deformation densities $\Delta\rho_{(1)-(4)}$ of the pairwise orbital interaction between $[Cp]^-$ and $[CpAl–AlCp^*]^{2+}$ in **4** associated with energy terms $\Delta E_{Orb(1)-Orb(4)}$ (values in kcal/mol, isovalues 0.001 for $\Delta\rho_{(1)-(4)}$). Charge flows from yellow to purple.



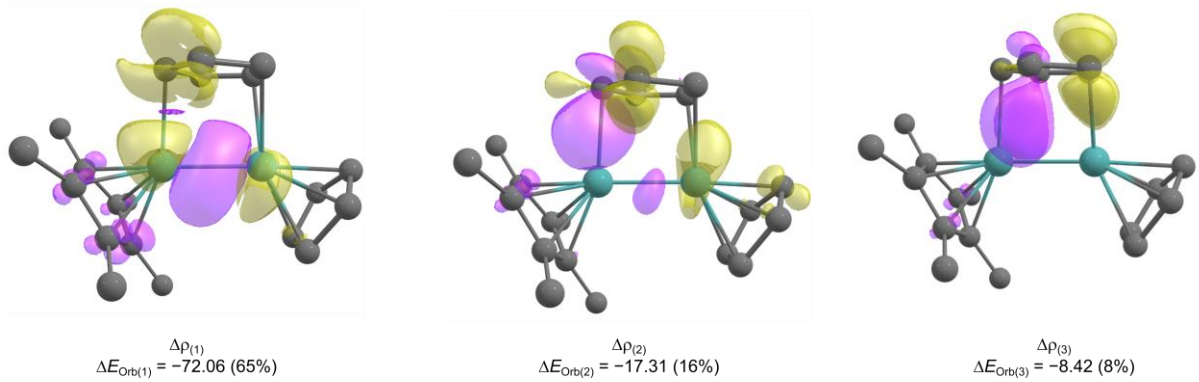
S-Figure 52: Plots of deformation densities $\Delta\rho_{(1)-(4)}$ of the pairwise orbital interaction between $[Cp]^{\bullet}$ and $[CpAl–AlCp^*]^{+\bullet}$ in **4** associated with energy terms $\Delta E_{Orb(1)-Orb(4)}$ (values in kcal/mol, isovalues 0.001 for $\Delta\rho_{(1)-(4)}$). Charge flows from yellow to purple.

S-2.4.3 [Cp(AlCp)(AlCp*)]$^{+}$: EDA-NOCV analysis on Al–Al bond

In the EDA-NOCV analysis, the Al–Al bond in **4** is best described as covalent bond by interaction of two Al radicals (**S-Table 5**). Here, the interaction between the Al atoms represents a σ-bond with no π-bonding observed (**S-Figure 53**). However, the plots of deformation electron densitiy also display an interaction between an Al atom and the Cp-ligand, which is divided into a σ- and π-donation.

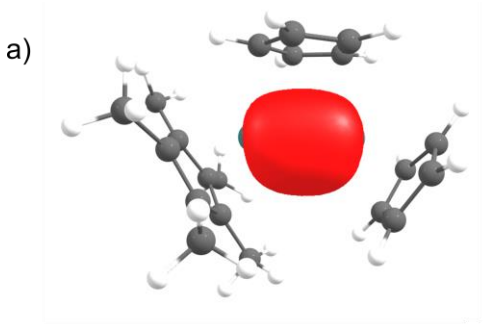
S-Table 5: Results of the EDA-NOCV analysis for the interaction of the AlCp* unit with the $AlCp_2$ fragment in **4** (values given in kcal/mol)

		[Cp(AlCp)(AlCp*)]$^{+}$	
Energy terms	Orbital interaction	$[AlCp^*]^{\bullet+}$ (D) + $[AlCp_2]^{\bullet}$ (D)	AlCp* (S) + $[AlCp_2]^{+}$ (D)
ΔE_{int}		**-101.16**	-95.25
ΔE_{Pauli}		118.77	168.24
ΔE_{elstat}		-94.76	-117.82
ΔE_{Orb}		-110.27	-130.87
$\Delta E_{Orb(1)}$	Al–Al σ-bond	-72.06 (65%)	
$\Delta E_{Orb(2)}$	$C(Cp_{brid})$-Al σ-bonds	-17.31 (16%)	
$\Delta E_{Orb(3)}$	π-donation Cp^{-} → Al (*p*-orbital)	-8.42 (8%)	
$\Delta E_{Orb(4)}$		-2.54 (2%)	
ΔE_{Rest}		-9.96 (9%)	
ΔE_{Disp}		-14.90	-14.90

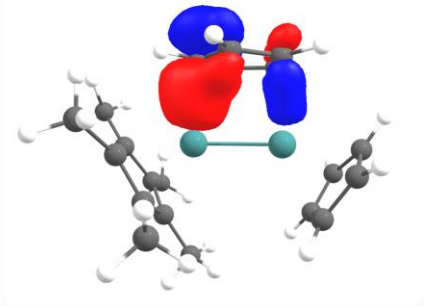


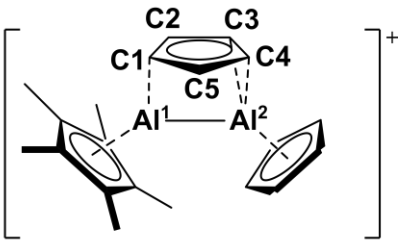
S-Figure 53: Plots of deformation densities $\Delta\rho_{(1)-(3)}$ of the pairwise orbital interaction between $[AlCp^*]^{\bullet+}$ and $[AlCp_2]^{\bullet}$ in **4** associated with energy terms $\Delta E_{Orb(1)-Orb(3)}$ (values in kcal/mol, isovalues 0.001 for $\Delta\rho_{(1)-(3)}$). Charge flows from yellow to purple.

S-2.4.4 [Cp(AlCp)(AlCp*)]$^{+}$: NBO analysis



Al-Al σ bond (99%)
48.2 % Al 1: *s*(63%)*p*(36%)
51.1 % Al 2: *s*(65%)*p*(35%)
WBI 0.96





Lone Pair C1 (54%)
7.3 % Al 1: *s*(60%)*p*(40%)
4.8 % Al 2: *s*(86%)*p*(13%)
54 % C 1: *s*(2%)*p*(98%)
9 % C 2: *s*(0%)*p*(100%)
8 % C 3: *s*(1%)*p*(99%)
8 % C 4: *s*(1%)*p*(99%)
9 % C 5: *s*(0%)*p*(100%)

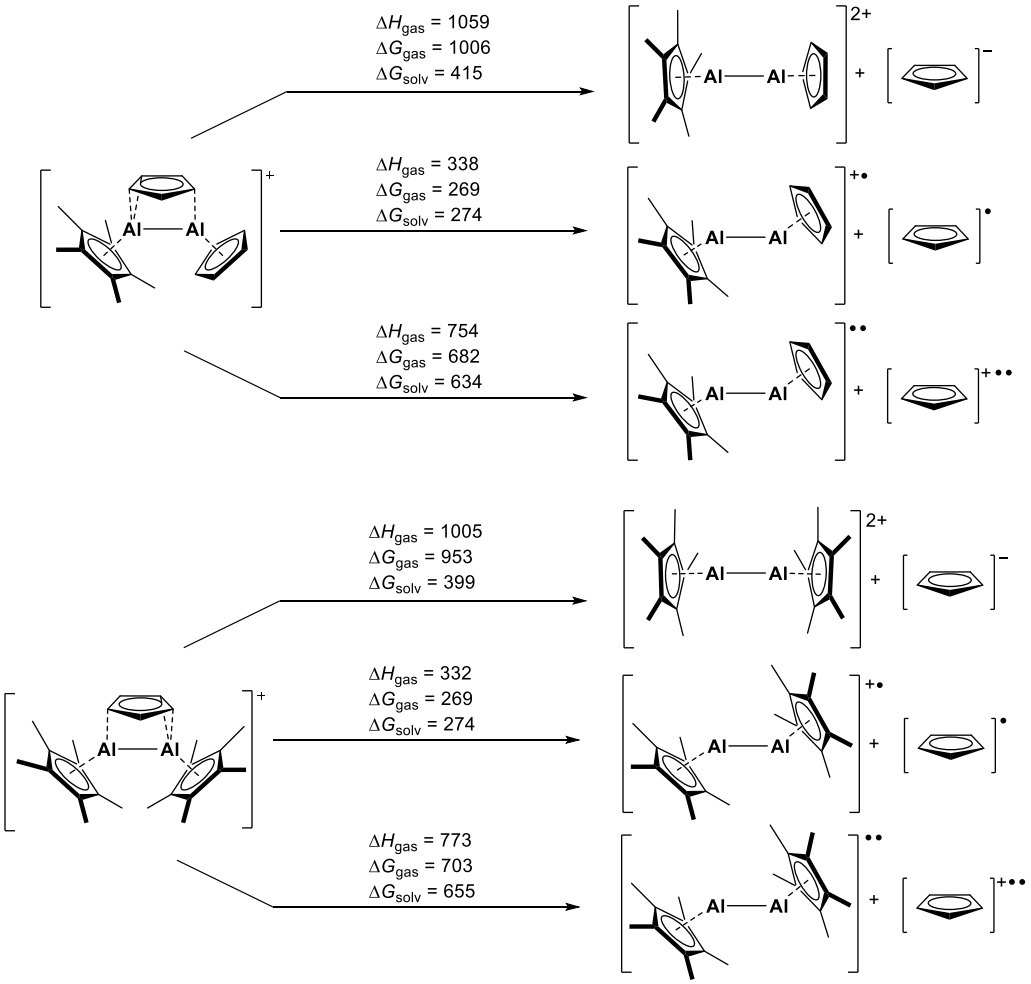
WBI
Al1-C1 0.35
Al1-C2 0.12
Al1-C5 0.11
Al2-C3 0.27
Al2-C4 0.29

S-Figure 54: a) NLMO displaying the Al–Al s bond (isovalue 0.05). b) NLMO partially describing the NBO of the C1 lone-pair, which shows the interaction between Cp and Al–Al σ* orbital (isovalue 0.05). c) WBI values for interaction between Al atoms and bridging Cp ligand.

S-2.5 $[Cp(AlCp^*)_2]^+$ and $[Cp(AlCp)(AlCp^*)]^+$: thermodynamics for dissociation of the briding Cp ligand

The EDA-NOCV study on the coordination of the bridged Cp ligand in the reported dialanes resulted in a preferential fragmentation into an anionic Cp^- and dicationic $[Cp^*Al–AlCp/Cp^*]^{2+}$. The orbital interaction energy for fragmentation into two radicals, however, was computed to be only 16 kcal/mol higher in **1** and 11 kcal/mol in **4**. Here, the ionic fragmentation significantly overestimates the electrostatic contribution to the total attractive bonding energy, while the electrostatic term is underestimated in the fragmentation into two radicals. Hence, the best description of the bonding in the dialanes lies in between the two extremes.

To further investigate the bonding, the thermodynamics of the dissocaiation of the bridging Cp ligand was computed in the gas phase and in 1,2-DFB solution (**S-Figure 55**). Here, the formation of two radicals is favored over the ionic dissociation, which results in a significant charge separation. Yet, the strong solvation levels this to more comparable values of +274 vs. 415 kJ/mol.

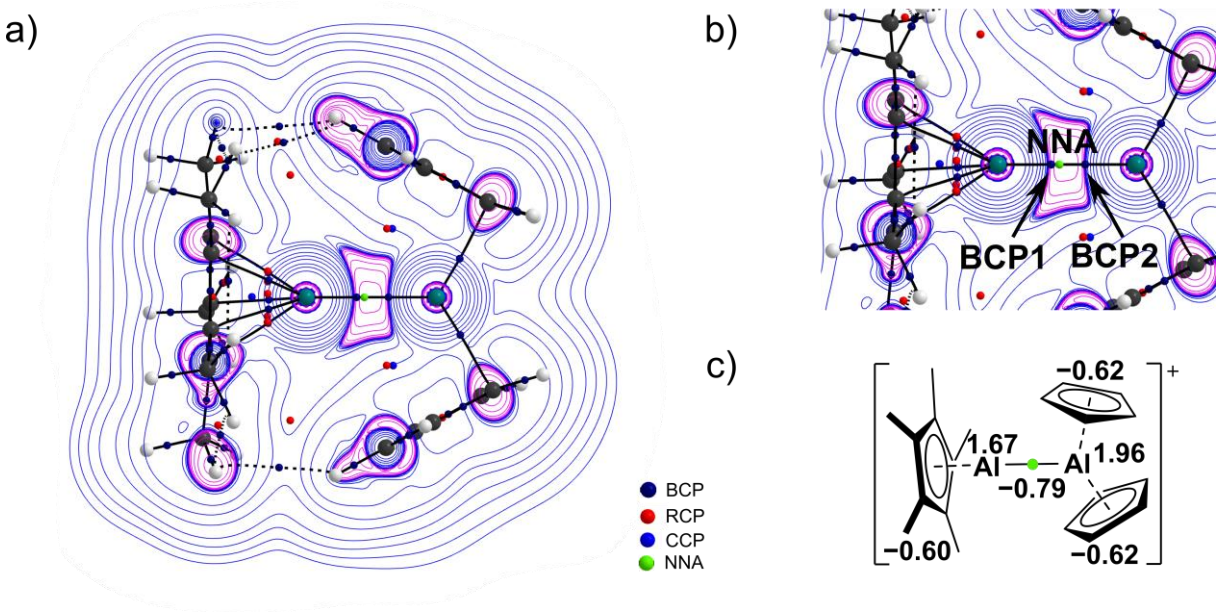


S-Figure 55: Thermodynamics for dissociation reactions of the bridging Cp-ligand into a Cp anion, radical or cation in the gas phase and in 1,2-DFB. All values in kJ/mol. Computed at bp86-d3bj/def2-svp level of DFT with cosmo-rs.

S-2.6 Computational analysis of the transition states $\mathbf{TS_I}$ and $\mathbf{TS_I}$

S-2.6.1 [Cp(AlCp)(AlCp*)]$^+$: QTAIM analysis of $\mathbf{TS_I}$ (Cp switch)

Similar to **1** and **4**, the QTAIM analysis of $\mathbf{TS_I}$ reveals an NNA between the two Al atoms. The Laplacian, however, already displays an asymmetry in the bonding interaction (**S-Figure 56**). Here, a slightly higher electron density is computed for the BCP between the AlCp* fragment and the NNA. This indicates a minor charge accumulation at the AlCp* unit, which reflects a polarization of the Al–Al bond. The asymmetry is also shown in the lower QTAIM charges at the Cp*-coordinated Al atom. The NNA impedes the discussion of the asymmetry in bonding.



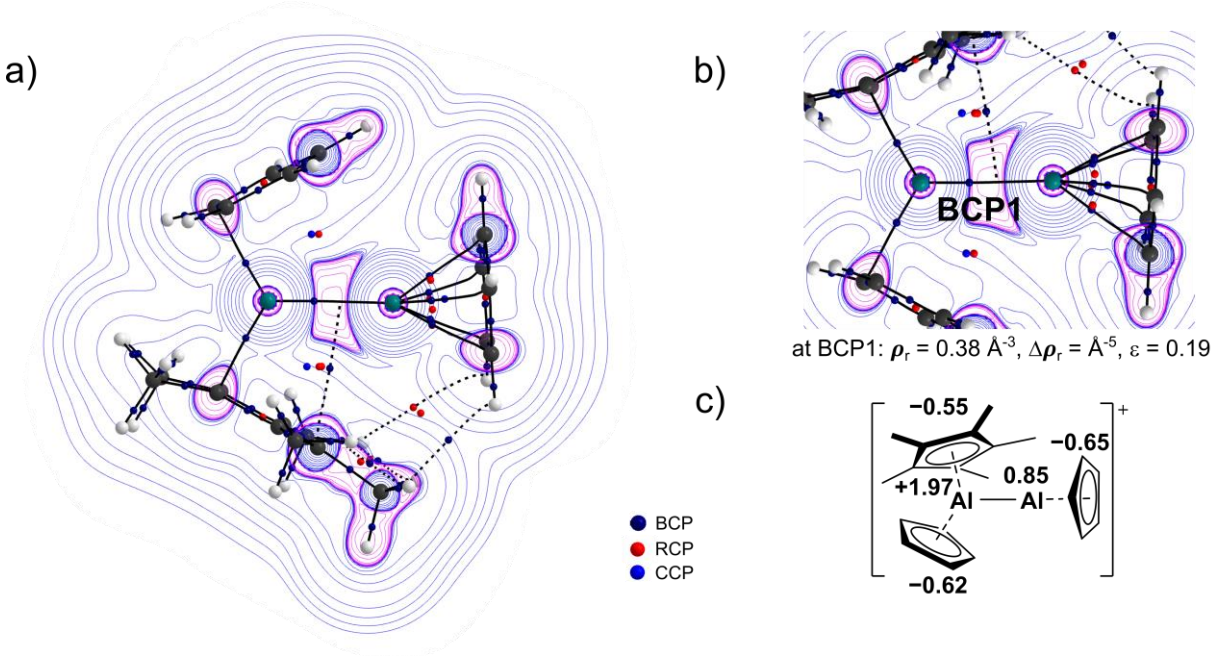
S-Figure 56: Visualization of the Laplacian $\Delta_r\rho$ in the plane including BCP1, BCP2 and the centroid of a Cp ligand (a) along with a zoom (b) and the QTAIM charges for the complex (c)

S-Table 6: Computed values for electron density ρ_r, Laplacian of electron density $\Delta_r\rho$ and ellipticity ε for cricital points in TS_I

CP	ρ_r [Å^{-3}]	$\Delta_r\rho$ [Å^{-5}]	ε
BCP1	0.42	-1.08	0.079
BCP2	0.39	-1.15	0.017
NNA	0.42	-1.16	

S-2.6.2 [Cp(AlCp)(AlCp*)]$^{+}$: QTAIM analysis of $\mathbf{TS_{II}}$ (Cp* switch)

In contrast, to the previously observed Al–Al bonds no NNA is computed for the Al–Al bond in $\mathbf{TS_{II}}$ (**S-Figure 57**). This is caused by disappearance of the BCP next to the Al(η^5-Cp) fragment. Yet, the Laplacian clearly shows a significant charge accumulation between the Al atoms. Unfortunately, the comparison of the QTAIM charges computed for the Al atoms in $\mathbf{TS_{I}}$ and $\mathbf{TS_{II}}$ is not meaningful, due to the disappearance of the NNA. Here, the sattle-point in the electron density next to the Al(η^5-Cp) fragment was not detect as boundary, since it decreases significantly. Hence, no NNA is detected and the charge from the basin is added quantitatively to the respective Al atom of the fragment.



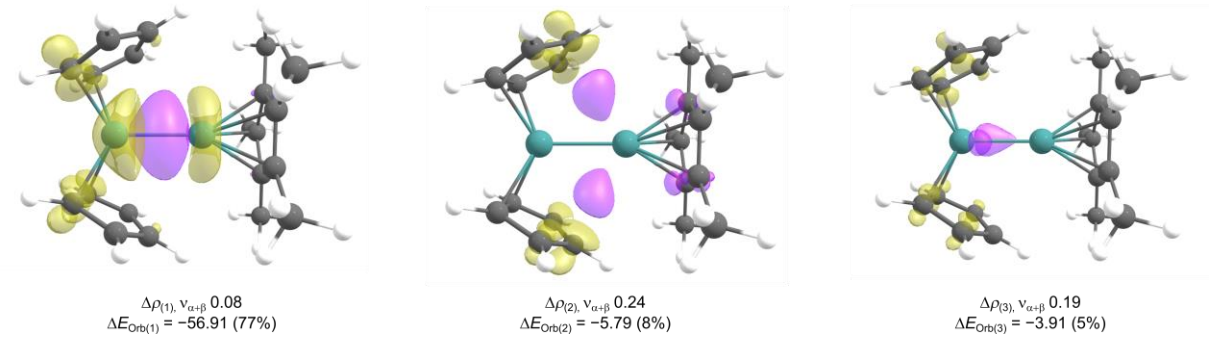
S-Figure 57: Visualization of the Laplacian $\Delta_r\rho$ in the plane including BCP1, BCP2 and the centroid of a Cp ligand (a) along with a zoom (b) and the QTAIM charges for the complex (c).

S-2.6.3 [Cp(AlCp)(AlCp*)]$^+$: EDA-NOCV of the Al–Al bond in **TS$_I$**

In the EDA-NOCV analysis, the Al–Al bond in **TS$_I$** is best described by interaction of a $[AlCp^*]^{\bullet+}$ radical cation with an $[AlCp_2]^\bullet$ radical (**S-Table 7**). Here, the interaction is best described as polarized Al–Al σ-bond with a minor charge accumulation at the Cp*-coordinated Al atom. Intriguingly, the high electrophilicity of the unsaturated Cp*-coordinated Al induces a weak electron donation from the Cp-ligands into the *p*-orbital at the Al atom (**S-Figure 58**).

S-Table 7: Results of the EDA-NOCV analysis for the interaction of the AlCp* unit with the $AlCp_2$ fragment in **TS$_I$** (values given in kcal/mol)

		TS$_I$	
Energy terms	Orbital interaction	$[AlCp^*]^{\bullet+}$ (D) + $[AlCp_2]^\bullet$ (D)	AlCp* (S) + $[AlCp_2]^+$ (S)
ΔE_{int}		**-92.80**	-97.04
ΔE_{Pauli}		70.30	102.97
ΔE_{elstat}		-73.23	-80.93
ΔE_{Orb}		-74.05	-103.27
$\Delta E_{Orb(1)}$	Al–Al σ-bond	-56.91 (77%)	
$\Delta E_{Orb(2)}$	π-donation Cp-ligands → AlCp*	-5.79 (8%)	
$\Delta E_{Orb(3)}$		-3.91 (5%)	
ΔE_{Rest}		-7.47 (10%)	
ΔE_{Disp}		-15.81	-15.81



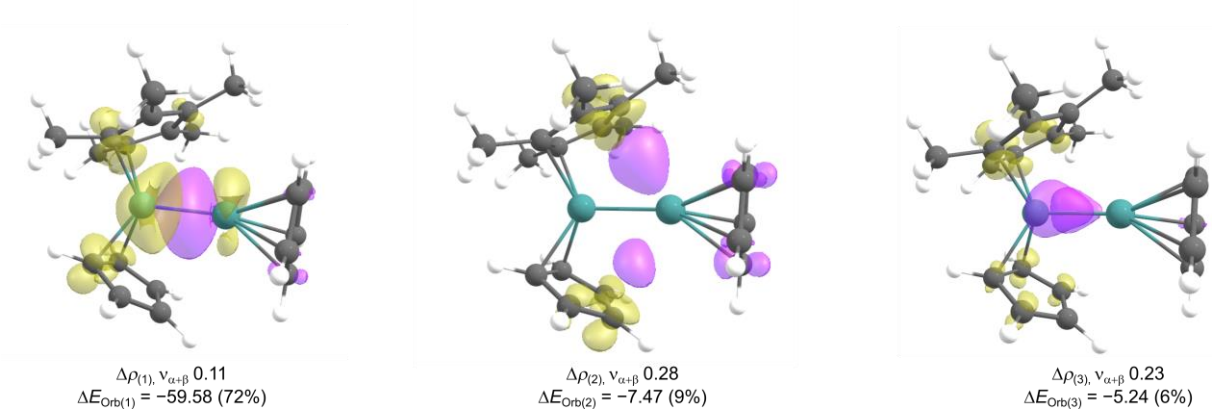
S-Figure 58: Plots of deformation densities $\Delta\rho_{(1)-(3)}$ of the pairwise orbital interaction between $[AlCp^*]^{\bullet+}$ and $[AlCp_2]^{\bullet}$ in **TS$_I$** associated with energy terms $\Delta E_{Orb(1)-Orb(3)}$ (values in kcal/mol, isovalues 0.001 for $\Delta\rho_{(1)-(3)}$). Charge flows from yellow to purple.

S-2.6.4 [Cp(AlCp)(AlCp*)]$^{+}$: EDA-NOCV of the Al–Al bond in **TS$_{II}$**

Similar to **TS$_{I}$**, the Al–Al bond in **TS$_{II}$** is best described by interaction of a [AlCp*]$^{\bullet+}$ radical cation with an [AlCp$_2$]$^{\bullet}$ radical (**S-Table 8**). The polarization of the σ-bond, however, is intensified as shown by the higher eigenvalue of the respective NOCV orbital $\Delta\rho_{(1)}$ (**S-Figure 59**). Moreover, the splitting into singlet AlCp* and [Al(Cp)(Cp*)]$^{+}$ fragments, which would describe a dative Al(I)→Al(III) interaction, is only 8.34 kcal/mol higher energy (ΔE_{Orb}).

S-Table 8: Results of the EDA-NOCV analysis for the interaction of the AlCp* unit with the AlCp$_2$ fragment in **TS$_{II}$** (values given in kcal/mol)

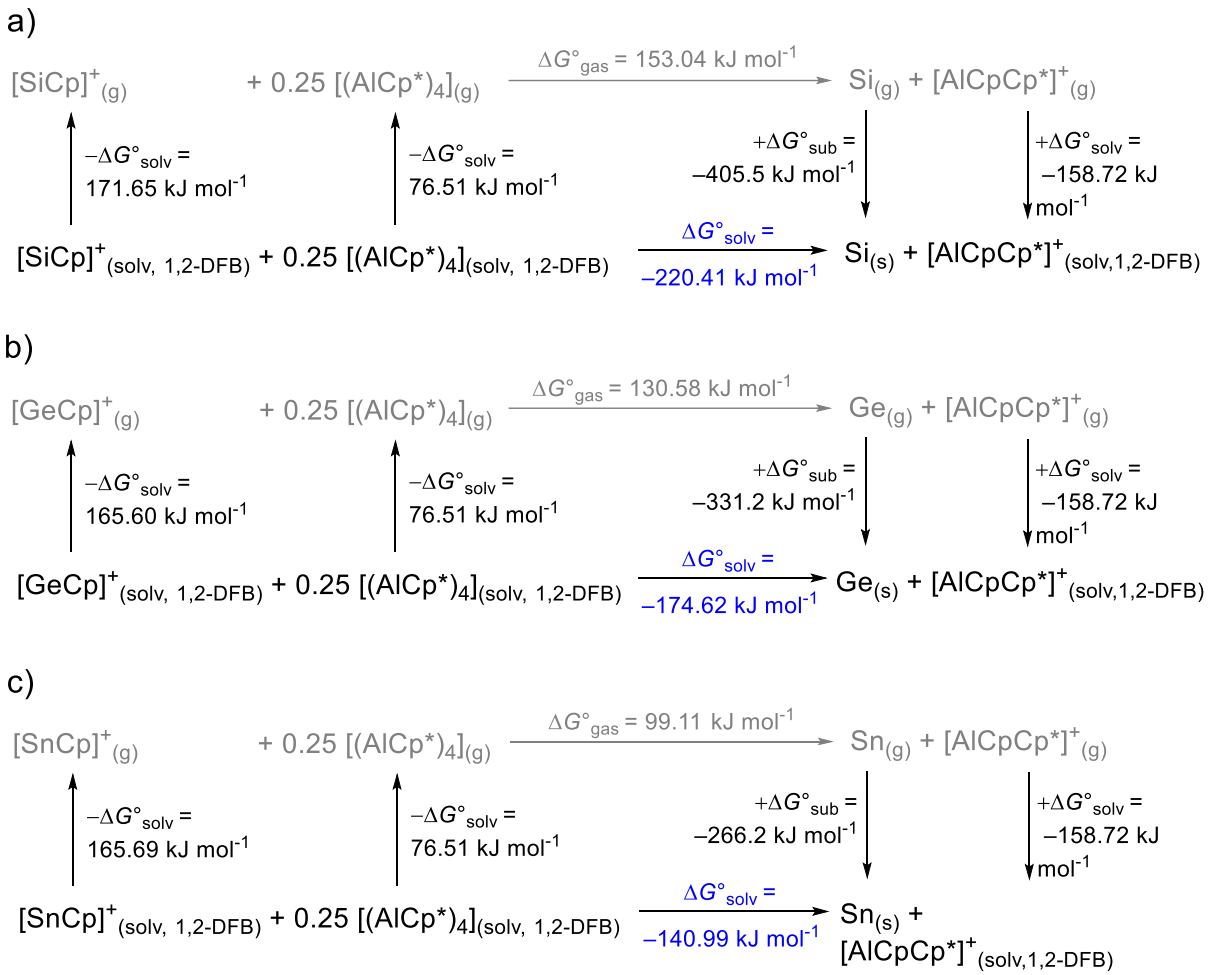
		TS$_{IP}$	
Energy terms	Orbital interaction	[AlCp]$^{\bullet+}$ (D) + [Al(Cp)(Cp*)]$^{\bullet}$ (D)	AlCp (S) + [Al(Cp)(Cp*)]$^{+}$ (S)
ΔE_{int}		**-104.20**	-79.00
ΔE_{Pauli}		69.66	100.85
ΔE_{elstat}		-76.46	-74.09
ΔE_{Orb}		-82.49	-90.83
$\Delta E_{Orb(1)}$	Al–Al σ-bond	-59.58 (72%)	
$\Delta E_{Orb(2)}$	π-donation Cp/Cp*-ligands → AlCp	-7.47 (9%)	
$\Delta E_{Orb(3)}$		-5.24 (6%)	
ΔE_{Rest}		-7.47 (9%)	
ΔE_{Disp}		-14.92	-14.90



S-Figure 59: Plots of deformation densities $\Delta\rho_{(1)\text{-}(3)}$ of the pairwise orbital interaction between $[AlCp]^{\bullet+}$ and $[Al(Cp)(Cp^*)]^{\bullet}$ in **TS_{II}** associated with energy terms $\Delta E_{Orb(1)\text{-}Orb(3)}$ (values in kcal/mol, isovalues 0.001 for $\Delta\rho_{(1)\text{-}(3)}$). Charge flows from yellow to purple.

S-2.8 Born-Fajans-Haber cycle for $[MCp]^+$ (M = Si, Ge, Sn) reduction by $[(AlCp^*)_4]$

The Born-Fajans-Haber cycles support the findings, that $[GeCp]^+$ and $[SnCp]^+$ are readily reduced to the metal by $[(AlCp^*)_4]$ to form the asymmetric aluminocenium cation $[Al(Cp)(Cp^*)]^+$ (**S-Figure 60**). For the unknown $[SiCp]^+$ cation the reduction was computed to be even more exergonic.



S-Figure 60: Born-Fajans-Haber cycles for reduction of $[MCp^+]$ (Si (a), Ge (b), Sn (c)) by $[(AlCp^*)_4]$ to form an aluminocenium cation and the respective metal. Thermodynamics computed on BP86-D3BJ/def2-SVP level of DFT with cosmo-rs. The values for $\Delta G°_{sub}$ were taken from the literature.[40]

S-2.9 Thermodynamic data for computed molecules

S-Table 9: Thermodynamic data of computed molecules (pbe0-d3bj/def2-tzvpp//bp86-d3bj/def2-svp)

Compound	E(SCF) [Eh]	FreeH Energy [kJmol^{-1}]	FreeH entropy at 298 K [kJmol^{-1}]	COSMO-RS (in 1,2-DFB) [kJmol^{-1}]
[AlCp$_2$]$^+$	-628.8816277	457.05	0.40853	-157.276029
[Al(Cp)(Cp*)]$^+$	-825.3245604	830.83	0.59822	-158.541254
[Cp(AlCp)(AlCp*)]$^+$	-1261.075701	1064.72	0.73189	-162.090132
AlCp*	-1457.512274	1438.81	0.9067	-161.880675
AlCp	-632.1286258	600.57	0.481	-15.2055144
[(AlCp*)$_4$]	-435.7031928	227.04	0.30664	-15.2050126
[(AlCp)$_4$]	-2528.623658	2426.51	1.37152	-75.2805268
[CpAl(AlCp*)$_3$]	-1742.905035	929.86	0.84034	-38.3108981

S-Table 10: SCF energies of various conformations of **4** and the transition states **TS$_I$** and **TS$_{II}$** (bp86-d3bj/def2-svp)

Compound	E(SCF) [Eh]	FreeH Energy [kJmol^{-1}]	FreeH entropy at 298 K [kJmol^{-1}]	COSMO-RS (in 1,2-DFB) [kJmol^{-1}]
4$_I$	-628.8816277	457.05	0.40853	-157.276029
TS$_I$	-825.3245604	830.83	0.59822	-158.541254
4$_{II}$	-1261.075701	1064.72	0.73189	-162.090132
TS$_{II}$	-1457.512274	1438.81	0.9067	-161.880675
4$_{III}$	-632.1286258	600.57	0.481	-15.2055144

S-Table 11: Thermodynamic data of computed molecules for Born-Fajans-haber cycles (bp86-d3bj/def2-svp)

Compound	E(SCF) [Eh]	FreeH Energy [kJmol^{-1}]	FreeH entropy at 298 K [kJmol^{-1}]	COSMO-RS (in 1,2-DFB) [kJmol^{-1}]
AlCp*	-632.2715013	600.57	0.48099	-15.403164
[(AlCp*)$_4$]	-2529.207616	2426.76	1.37541	-76.510616
[Al(Cp)(Cp*)]$^+$	-825.5015954	830.83	0.59822	-158.72134
[SnCp]$^+$	-407.6304541	227.31	0.30785	-165.69459
Sn(0)	-214.3808798	3.716	0.1684	
[GeCp]$^+$	-2270.199504	228.37	0.31223	-165.5971
Ge(0)	-2076.938731	3.716	0.162303	
Si(0)	-289.306554	3.716	0.150451586	
[SiCp]$^+$	-482.5780354	229.69	0.28586	-171.64539

S-Table 12: Thermodynamic data of computed molecules for XIA calculations DLPNO-CCSD(T)/aug-cc-pVQZ//PBEh-3c/def2-mSVP

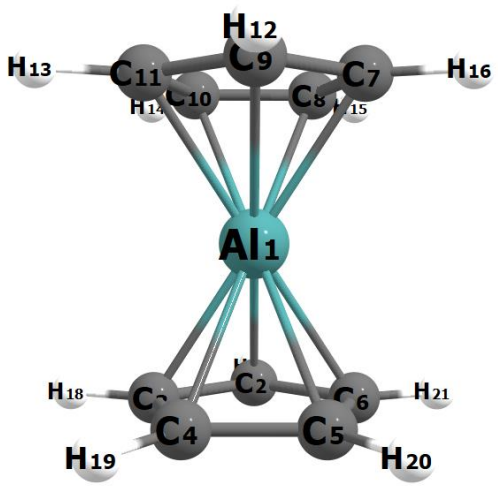
Compound	E(SCF) [Eh]	Enthalpy [Eh]	Entropy at 298 K [kcalmol^{-1}]	CPCM (in DCM) [Eh]
TMS-F	-508.5071263	0.12525902	24.92	-0.00049383
TMS$^+$	-408.3657995	0.11999623	24.25	-0.08184819
TMS-H	-409.2541248	0.12991798	23.52	0.00415036
[AlCp$_2$]$^+$	-628.2528461	0.18329459	26.94	-0.06631178
AlCp$_2$F	-728.3130653	0.18595537	30.49	-0.00780796
AlCp$_2$H	-629.0544916	0.18931646	29.72	-0.00606931

S-Table 13: Thermodynamic data of computed molecules for Cp dissociation (bp86-d3bj/def2-svp)

Compound	E(SCF) [Eh]	FreeH Energy [kJmol^{-1}]	FreeH entropy at 298 K [kJmol^{-1}]	COSMO-RS (in 1,2-DFB) [kJmol^{-1}]
[Cp(AlCp*)$_2$]$^+$	-1457.840842	1438.81	0.9067	-161.861371
[Cp*Al–AlCp*]$^{2+}$	-1264.054636	1213.64	0.80315	-509.161661
[Cp*Al–AlCp*]$^+$	-1264.366731	1211.6	0.81647	-155.138378
[Cp*Al–AlCp*]	-1264.501899	1207.22	0.86233	-31.2708896
[Cp(AlCp)(AlCP*)]$^+$	-1261.354395	1064.59	0.73569	-161.836348
[CpAl–AlCp*]$^{2+}$	-1067.548102	839.36	0.63166	-545.756595
[CpAl–AlCp*]$^+$	-1067.878178	838.04	0.66509	-155.146983
[CpAl–AlCp*]	-1068.022823	833.94	0.69932	-31.6858006
[Cp]$^+$	-193.0398475	216.79	0.28013	-178.223587
Cp	-193.3426426	211.78	0.30296	-1.88352935
[Cp]$^-$	-193.3989963	211.27	0.27804	-207.095706

S-2.10 Optimized structures

$[AlCp_2]^+$



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

Al	-0.0016020	0.0068652	0.0199067
C	-1.1166418	-0.4563599	1.8334300
C	-0.7934549	0.9441504	1.8202315
C	0.6384431	1.0694933	1.8108785
C	1.2001623	-0.2535777	1.8182541
C	0.1154491	-1.1965841	1.8322120
C	0.7841543	-0.9358308	-1.7801978
C	-0.6485123	-1.0519395	-1.7708295
C	1.1163639	0.4625703	-1.7937020
C	-1.2017060	0.2747233	-1.7785010
C	-0.1109372	1.2107180	-1.7926586
H	2.1290819	0.8848523	-1.7990442
H	-0.1995952	2.3043219	-1.7970841
H	-2.2691458	0.5284372	-1.7701016
H	-1.2195269	-1.9887647	-1.7554248
H	1.4987866	-1.7684154	-1.7731881
H	-2.1266246	-0.8851515	1.8385403
H	-1.5133897	1.7721535	1.8134674
H	1.2033951	2.0099902	1.7957673
H	2.2692081	-0.5004733	1.8097012
H	0.2111418	-2.2895887	1.8362327

SCF energy GEOOPT = -629.0087886660 H

ZPE = 432.1 kJ/mol

FREEH energy = 457.05 kJ/mol

FREEH entropy = 0.40853 kJ/mol/K

$vibrational spectrum

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6		0.00	0.00000	- -
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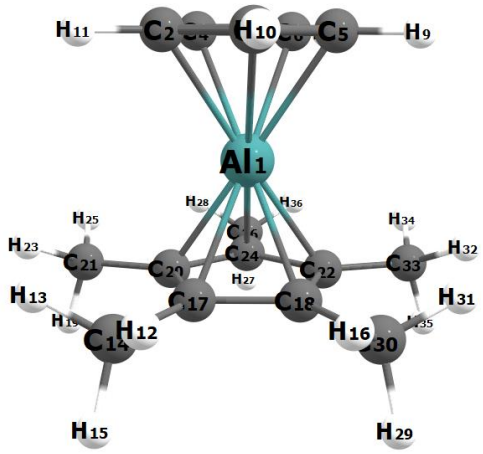
9	a	130.85	3.47335	YES YES
10	a	198.98	0.00000	YES YES
11	a	199.16	0.00000	YES YES
12	a	287.39	0.00000	YES YES
13	a	342.97	0.02906	YES YES
14	a	343.77	0.03160	YES YES
15	a	599.50	0.00294	YES YES
16	a	599.77	0.02942	YES YES
17	a	601.72	74.91196	YES YES
18	a	607.09	0.00001	YES YES
19	a	607.37	0.00001	YES YES
20	a	800.17	0.00018	YES YES
21	a	800.94	0.00003	YES YES
22	a	829.62	1.35658	YES YES
23	a	830.29	0.15607	YES YES
24	a	836.38	0.00629	YES YES
25	a	836.51	0.00046	YES YES
26	a	837.88	0.00011	YES YES
27	a	837.98	0.00018	YES YES
28	a	838.02	0.00017	YES YES
29	a	847.63	537.36688	YES YES
30	a	899.78	0.01698	YES YES
31	a	901.00	0.02307	YES YES
32	a	907.76	0.00001	YES YES
33	a	908.97	0.00003	YES YES
34	a	993.74	0.00005	YES YES
35	a	993.81	0.00017	YES YES
36	a	998.83	35.10253	YES YES
37	a	998.89	35.08963	YES YES
38	a	1044.67	0.00047	YES YES
39	a	1044.94	0.00074	YES YES
40	a	1047.81	0.00000	YES YES
41	a	1048.11	0.00001	YES YES
42	a	1107.04	11.62520	YES YES
43	a	1111.93	0.00002	YES YES
44	a	1229.75	0.00000	YES YES
45	a	1229.99	0.00080	YES YES
46	a	1351.58	0.00001	YES YES

47	a	1351.66	0.00002	YES	YES
48	a	1353.37	0.00000	YES	YES
49	a	1353.45	0.00000	YES	YES
50	a	1404.47	0.00000	YES	YES
51	a	1404.49	0.00001	YES	YES
52	a	1415.55	10.90453	YES	YES
53	a	1415.57	10.91422	YES	YES
54	a	3167.66	0.00364	YES	YES
55	a	3167.92	0.01211	YES	YES
56	a	3168.04	0.00027	YES	YES
57	a	3168.30	0.00021	YES	YES
58	a	3178.08	0.06132	YES	YES
59	a	3178.23	0.07409	YES	YES
60	a	3178.52	44.20921	YES	YES
61	a	3178.67	44.22192	YES	YES
62	a	3186.67	1.67297	YES	YES
63	a	3187.51	0.00004	YES	YES

[Al(Cp)(Cp*)]$^+$



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

Al	-0.0206476	0.0150332	-0.7531101
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C	-1.2282804	-0.3435782	-2.5431795
C	1.0943332	-0.3063274	-2.6088351
C	-0.8058340	1.0290027	-2.5273261
C	0.6296038	1.0520424	-2.5679104
H	2.1424029	-0.6286004	-2.6379544
H	1.2605610	1.9492856	-2.5601610
H	-1.4636720	1.9056257	-2.4830197
H	-2.2655183	-0.6991823	-2.5133113
H	-0.0369306	-2.2655034	-2.6087743
H	-2.4274458	-2.2122154	0.5855553
H	-0.9121380	-3.1656078	0.5230613
C	-1.4271347	-2.3353504	1.0432844
H	-1.5873938	-2.6588518	2.0928073
H	-3.2698605	-0.1061760	0.6539467
C	-0.6290036	-1.0647764	1.0057599
C	-1.1671326	0.2816896	1.0481944
H	2.0335598	-2.4188205	1.9964375
C	0.8179422	-0.9682453	0.9671111
C	1.7785327	-2.1215782	0.9579360
C	-0.0528139	1.2104412	1.0357008
H	1.3526140	-3.0140316	0.4605327
C	1.1740972	0.4379439	0.9855721
H	2.7289293	-1.8673963	0.4505968
C	2.5678286	0.9948257	0.9986222
H	2.9279385	1.1076182	2.0424090
H	3.2853874	0.3323197	0.4776408
H	-2.9357268	0.7183128	2.1984917
C	-2.6198983	0.6486132	1.1367740
H	-2.8304038	1.6303950	0.6707152
H	-1.0871505	3.0847443	0.6567645
C	-0.1505949	2.7064074	1.1094707
H	0.6994969	3.2042627	0.6047914
H	-0.1422810	3.0415176	2.1675711
H	2.6205862	1.9950443	0.5274030

SCF energy GEOOPT = -825.5015953942 H

ZPE = 781.6 kJ/mol

FREEH energy = 830.83 kJ/mol

FREEH entropy = 0.59822 kJ/mol/K

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6			0.00	0.00000	- -
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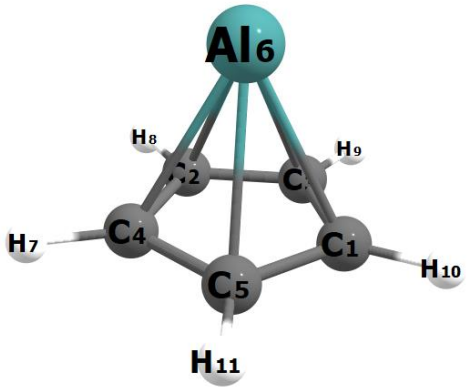
8		a	69.14	0.70541	YES YES
9		a	70.19	0.69020	YES YES
10		a	89.07	0.04372	YES YES
11		a	92.74	0.01013	YES YES
12		a	101.51	0.15555	YES YES
13		a	104.69	0.14309	YES YES
14		a	110.70	0.10221	YES YES
15		a	146.97	0.01008	YES YES

16	a	147.74	0.14079	YES	YES
17	a	150.73	1.24916	YES	YES
18	a	172.22	1.65509	YES	YES
19	a	172.58	1.64662	YES	YES
20	a	266.54	0.19071	YES	YES
21	a	267.00	0.19138	YES	YES
22	a	272.93	0.00139	YES	YES
23	a	274.74	0.00090	YES	YES
24	a	304.03	1.98950	YES	YES
25	a	304.70	1.98847	YES	YES
26	a	331.61	3.78127	YES	YES
27	a	403.10	0.07447	YES	YES
28	a	404.00	0.08113	YES	YES
29	a	542.78	0.00050	YES	YES
30	a	544.47	0.00002	YES	YES
31	a	544.65	0.00003	YES	YES
32	a	582.67	15.96058	YES	YES
33	a	603.15	0.00051	YES	YES
34	a	603.33	0.00025	YES	YES
35	a	622.69	0.10139	YES	YES
36	a	622.97	0.58695	YES	YES
37	a	626.46	144.11400	YES	YES
38	a	789.68	1.49869	YES	YES
39	a	790.10	1.54145	YES	YES
40	a	808.90	2.68985	YES	YES
41	a	809.17	1.07905	YES	YES
42	a	834.83	304.73673	YES	YES
43	a	836.70	0.11845	YES	YES
44	a	836.84	3.05150	YES	YES
45	a	896.93	0.00152	YES	YES
46	a	899.80	0.00151	YES	YES
47	a	918.12	0.00163	YES	YES
48	a	919.95	0.00180	YES	YES
49	a	989.19	6.73099	YES	YES
50	a	990.45	5.36833	YES	YES
51	a	996.61	23.39904	YES	YES
52	a	996.70	18.27872	YES	YES
53	a	997.00	4.68866	YES	YES
54	a	997.56	2.05304	YES	YES
55	a	1002.04	0.53810	YES	YES
56	a	1044.99	0.00030	YES	YES
57	a	1045.12	0.00097	YES	YES
58	a	1047.18	3.67557	YES	YES
59	a	1047.80	3.69623	YES	YES
60	a	1073.07	0.00312	YES	YES
61	a	1111.24	6.25409	YES	YES
62	a	1160.42	0.00049	YES	YES
63	a	1160.64	0.00008	YES	YES
64	a	1229.80	0.00147	YES	YES
65	a	1342.74	0.07903	YES	YES
66	a	1344.30	0.14004	YES	YES
67	a	1351.37	10.11204	YES	YES
68	a	1353.34	10.18481	YES	YES
69	a	1354.68	0.02307	YES	YES
70	a	1354.74	0.00098	YES	YES
71	a	1357.41	0.65326	YES	YES
72	a	1382.74	0.00256	YES	YES
73	a	1382.94	0.00297	YES	YES
74	a	1394.58	12.34815	YES	YES
75	a	1395.56	12.58350	YES	YES
76	a	1402.90	0.06257	YES	YES
77	a	1403.16	1.08206	YES	YES
78	a	1404.06	42.32003	YES	YES
79	a	1405.22	0.99662	YES	YES
80	a	1407.61	2.10695	YES	YES
81	a	1407.77	2.19124	YES	YES
82	a	1412.12	1.85677	YES	YES
83	a	1412.24	1.82664	YES	YES
84	a	1429.67	14.30451	YES	YES
85	a	1442.11	0.00981	YES	YES
86	a	1442.22	0.00056	YES	YES
87	a	1466.33	16.80068	YES	YES
88	a	1466.78	16.90659	YES	YES
89	a	2973.02	16.72467	YES	YES
90	a	2973.17	12.04601	YES	YES
91	a	2973.25	4.79683	YES	YES
92	a	2973.41	1.60346	YES	YES
93	a	2973.57	2.17600	YES	YES
94	a	3049.14	3.30704	YES	YES
95	a	3049.27	3.71174	YES	YES
96	a	3049.38	3.83730	YES	YES
97	a	3050.36	0.01299	YES	YES
98	a	3050.41	0.06646	YES	YES
99	a	3074.19	0.38141	YES	YES
100	a	3074.29	1.36626	YES	YES
101	a	3074.72	0.06378	YES	YES
102	a	3074.95	10.12424	YES	YES
103	a	3075.16	11.19240	YES	YES
104	a	3168.54	0.00299	YES	YES
105	a	3168.83	0.00304	YES	YES
106	a	3179.53	12.94229	YES	YES
107	a	3179.74	12.92302	YES	YES
108	a	3188.49	0.82419	YES	YES

AlCp



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

C	0.0215873	0.3890070	10.6951015
C	2.1824375	1.1980054	10.8140019
C	1.3307812	0.1175519	11.1963738
C	1.3996225	2.1372164	10.0764343
C	0.0641334	1.6372331	10.0029460
Al	0.5358194	2.0784053	12.3004965
H	1.7597399	3.0800714	9.6466187
H	3.2494971	1.2926779	11.0502918
H	1.6286667	-0.7635848	11.7779766
H	-0.8629398	-0.2469085	10.8240683
H	-0.7819352	2.1285149	9.5067407

SCF energy GEOOPT = -435.7985370735 H

ZPE = 213.2 kJ/mol

FREEH energy = 227.04 kJ/mol

FREEH entropy = 0.30664 kJ/mol/K

$vibrational spectrum

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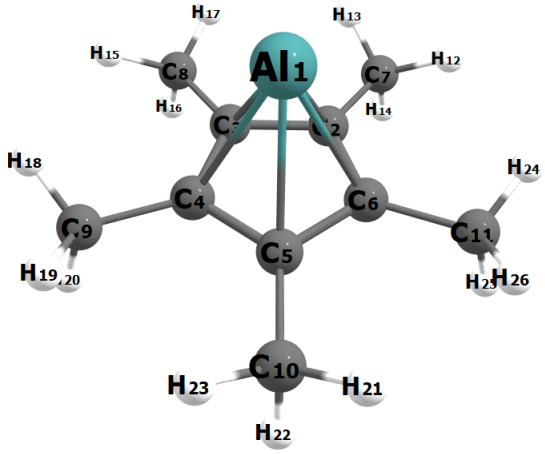
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	241.36	3.42805	YES	YES
8		a	241.56	3.42579	YES	YES
9		a	344.42	68.84934	YES	YES
10		a	563.08	0.00000	YES	YES
11		a	563.18	0.00000	YES	YES
12		a	790.76	4.87900	YES	YES
13		a	790.80	4.89453	YES	YES
14		a	799.28	196.81835	YES	YES
15		a	823.57	0.00019	YES	YES
16		a	823.70	0.00032	YES	YES
17		a	879.21	0.00001	YES	YES
18		a	879.33	0.00004	YES	YES
19		a	999.56	12.00989	YES	YES
20		a	999.66	12.01688	YES	YES
21		a	1045.41	0.00001	YES	YES
22		a	1045.46	0.00003	YES	YES
23		a	1125.18	5.26178	YES	YES
24		a	1233.63	0.00000	YES	YES
25		a	1378.72	0.00001	YES	YES
26		a	1378.74	0.00000	YES	YES
27		a	1431.10	7.79849	YES	YES
28		a	1431.20	7.80936	YES	YES
29		a	3157.16	0.00000	YES	YES
30		a	3157.17	0.00000	YES	YES
31		a	3171.77	0.24050	YES	YES
32		a	3171.79	0.24063	YES	YES
33		a	3182.26	1.74641	YES	YES

$end

AlCp*



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

Al	4.7942950	5.0790550	7.2666824
C	3.4937503	5.5197319	9.1696205
C	3.2094391	6.5387150	8.1963420
C	4.4165175	7.2857355	7.9697539
C	5.4468136	6.7285630	8.8029617
C	4.8766314	5.6369876	9.5443613
C	2.5047481	4.5438781	9.7408564
C	1.8712026	6.8141755	7.5717900

C	4.5597504	8.4781094	7.0673427
C	6.8552496	7.2368473	8.9238032
C	5.5849219	4.8048530	10.5752064
H	2.9898462	3.5953492	10.0446605
H	1.7072420	4.2922856	9.0142937
H	2.0062888	4.9604880	10.6431677
H	1.9709762	7.2473640	6.5570060
H	1.2862263	7.5375043	8.1806587
H	1.2606496	5.8940985	7.4822615
H	3.8718095	8.4243951	6.2006001
H	5.5893944	8.5729624	6.6696594
H	4.3301681	9.4210080	7.6098794
H	7.5641102	6.4281417	9.1900203
H	6.9339875	8.0147413	9.7142500
H	7.2111463	7.6938923	7.9794716
H	5.1659618	3.7811542	10.6375342
H	5.4949269	5.2578544	11.5865419
H	6.6665670	4.7090897	10.3556545

SCF energy GEOOPT = -632.2715013140 H

ZPE = 563.5 kJ/mol

FREEH energy = 600.57 kJ/mol

FREEH entropy = 0.48100 kJ/mol/K

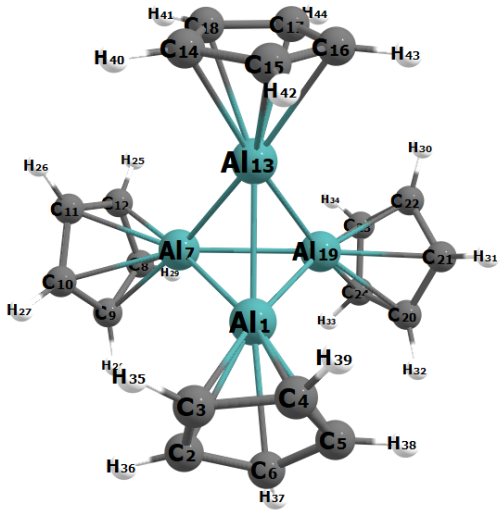
$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		-0.00	0.00000	- -
2		-0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	93.85	0.00098	YES YES
8	a	95.73	0.00075	YES YES
9	a	110.60	0.08440	YES YES
10	a	114.26	0.08981	YES YES
11	a	117.50	0.00230	YES YES
12	a	150.18	0.00005	YES YES
13	a	150.35	0.00007	YES YES
14	a	169.23	0.05382	YES YES
15	a	169.99	0.05312	YES YES
16	a	178.31	1.61169	YES YES
17	a	271.86	0.10475	YES YES
18	a	274.84	0.06538	YES YES
19	a	277.00	0.43208	YES YES
20	a	277.12	0.51002	YES YES
21	a	379.95	3.40203	YES YES
22	a	380.09	3.39259	YES YES
23	a	399.72	114.44140	YES YES
24	a	542.39	0.00004	YES YES
25	a	542.54	0.00001	YES YES
26	a	544.07	0.00012	YES YES
27	a	577.25	0.00000	YES YES
28	a	577.32	0.00004	YES YES
29	a	590.72	2.79551	YES YES
30	a	799.98	3.83572	YES YES
31	a	801.13	3.81134	YES YES
32	a	922.45	0.00060	YES YES
33	a	924.03	0.00006	YES YES
34	a	993.91	7.15065	YES YES
35	a	994.11	7.15438	YES YES
36	a	1000.54	0.01489	YES YES
37	a	1000.60	0.00621	YES YES
38	a	1001.10	0.05180	YES YES
39	a	1046.07	1.79150	YES YES
40	a	1046.96	1.80373	YES YES
41	a	1073.46	0.00091	YES YES
42	a	1164.10	0.00001	YES YES
43	a	1164.36	0.00008	YES YES
44	a	1340.17	0.16384	YES YES
45	a	1341.45	0.00155	YES YES
46	a	1346.21	1.46406	YES YES
47	a	1347.46	1.44571	YES YES
48	a	1350.80	5.69176	YES YES
49	a	1391.01	0.00038	YES YES
50	a	1391.12	0.00120	YES YES
51	a	1401.42	9.81779	YES YES
52	a	1401.79	9.74744	YES YES
53	a	1403.42	0.23077	YES YES
54	a	1403.94	0.04765	YES YES
55	a	1405.83	0.00103	YES YES
56	a	1407.80	0.19744	YES YES
57	a	1408.85	0.07348	YES YES
58	a	1414.41	38.92017	YES YES
59	a	1442.19	0.03081	YES YES
60	a	1452.91	0.00086	YES YES
61	a	1452.99	0.00038	YES YES
62	a	1492.00	13.61848	YES YES
63	a	1492.26	13.58872	YES YES
64	a	2952.64	33.37904	YES YES
65	a	2952.84	33.32803	YES YES
66	a	2952.87	70.15541	YES YES
67	a	2952.97	47.07046	YES YES
68	a	2954.27	26.44482	YES YES
69	a	3026.79	28.06994	YES YES

70	a	3027.10	5.14003	YES	YES
71	a	3027.25	4.32737	YES	YES
72	a	3028.46	0.15283	YES	YES
73	a	3028.70	0.03439	YES	YES
74	a	3058.52	2.22196	YES	YES
75	a	3058.85	2.69835	YES	YES
76	a	3059.08	4.32815	YES	YES
77	a	3059.51	22.71835	YES	YES
78	a	3059.85	22.98720	YES	YES

$end

$AlCp_4$



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

Al	0.9317744	-0.8110201	-1.0819487
C	1.3015622	-2.7394268	-2.4038272
C	2.4381344	-2.5734268	-1.5549137
C	3.0815356	-1.3494840	-1.9137499
C	2.3425462	-0.7596093	-2.9839656
C	1.2423345	-1.6185682	-3.2869581
Al	-1.3214092	-0.9010334	0.3655092
C	-3.6711665	-1.1805823	0.2947241
C	-3.0830656	-2.3092753	-0.3534133
C	-2.3245683	-3.0305181	0.6187883
C	-2.4440116	-2.3474240	1.8672329
C	-3.2762686	-1.2039361	1.6671762
Al	0.8666029	0.2745985	1.3681182
C	1.9826731	-0.5755412	3.2758986
C	2.9297239	0.1857943	2.5251305
C	2.4971643	1.5469672	2.5192590
C	1.2824592	1.6269322	3.2667307
C	0.9646908	0.3154478	3.7341771
Al	-0.4706618	1.4291081	-0.6470845
C	-0.7175465	2.8103986	-2.5543763
C	0.1039813	3.5100862	-1.6186024
C	-0.6819325	3.7788785	-0.4565336
C	-1.9887742	3.2454744	-0.6740556
C	-2.0107224	2.6468614	-1.9708977
H	-3.5435550	-0.4601315	2.4275171
H	-1.9602961	-2.6357517	2.8082994
H	-1.7331852	-3.9353033	0.4333693
H	-3.1759186	-2.5630170	-1.4163112
H	-4.2949958	-0.4157106	-0.1832181
H	-0.3349373	4.2835518	0.4531484
H	1.1599215	3.7718720	-1.7573387
H	-0.4027753	2.4404158	-3.5376090
H	-2.8629842	2.1293239	-2.4276048
H	-2.8211819	3.2679321	0.0396498
H	2.7475644	-3.2529221	-0.7516224
H	0.5851388	-3.5688716	-2.3666614
H	0.4722011	-1.4362428	-4.0462512
H	2.5653353	0.1979621	-3.4699350
H	3.9717659	-0.9246125	-1.4345391
H	2.0173138	-1.6581031	3.4481165
H	0.0803375	0.0368990	4.3198623
H	3.8194222	-0.2099703	2.0206260
H	2.9956343	2.3796080	2.0084264
H	0.6848581	2.5317553	3.4306048

SCF energy GEOOPT = -1743.287977613 H

ZPE = 859.0 kJ/mol

FREEH energy = 929.86 kJ/mol

FREEH entropy = 0.84034 kJ/mol/K

$vibrational spectrum

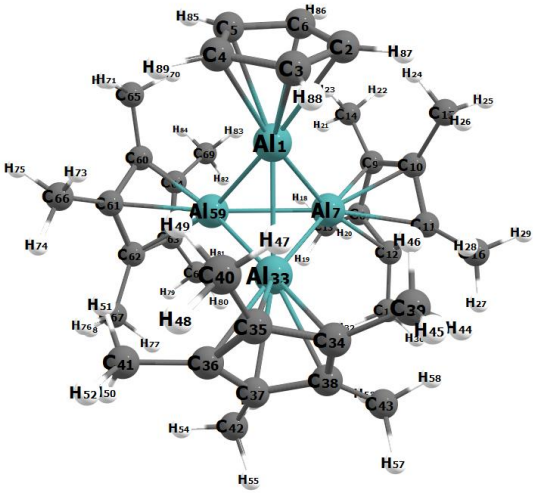
# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		-0.00	0.00000	- -
2		-0.00	0.00000	- -
3		-0.00	0.00000	- -
4		-0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	5.24	0.00086	YES YES
8	a	9.52	0.00011	YES YES
9	a	10.41	0.00060	YES YES
10	a	13.92	0.00094	YES YES
11	a	22.37	0.00008	YES YES
12	a	22.65	0.00030	YES YES

13	a	27.33	0.08589	YES	YES
14	a	28.21	0.08628	YES	YES
15	a	28.72	0.08334	YES	YES
16	a	96.64	0.00020	YES	YES
17	a	96.99	0.00038	YES	YES
18	a	97.39	0.00065	YES	YES
19	a	134.66	0.00003	YES	YES
20	a	157.72	0.14659	YES	YES
21	a	157.87	0.16093	YES	YES
22	a	158.11	0.14498	YES	YES
23	a	162.64	0.00252	YES	YES
24	a	162.94	0.00150	YES	YES
25	a	163.39	0.00217	YES	YES
26	a	176.68	0.00043	YES	YES
27	a	176.98	0.00684	YES	YES
28	a	214.28	22.54460	YES	YES
29	a	214.48	22.20609	YES	YES
30	a	214.66	22.97185	YES	YES
31	a	254.15	0.00652	YES	YES
32	a	254.78	0.00163	YES	YES
33	a	352.52	310.91391	YES	YES
34	a	352.78	310.96345	YES	YES
35	a	353.41	311.63287	YES	YES
36	a	477.99	0.00742	YES	YES
37	a	571.51	0.00679	YES	YES
38	a	571.56	0.00378	YES	YES
39	a	571.75	0.00264	YES	YES
40	a	572.42	0.13619	YES	YES
41	a	572.52	0.18317	YES	YES
42	a	572.56	0.18400	YES	YES
43	a	572.70	0.06682	YES	YES
44	a	572.75	0.02622	YES	YES
45	a	769.29	0.49308	YES	YES
46	a	769.67	0.45396	YES	YES
47	a	769.96	0.26798	YES	YES
48	a	773.70	30.82503	YES	YES
49	a	774.30	35.92874	YES	YES
50	a	774.87	25.31002	YES	YES
51	a	779.99	3.89582	YES	YES
52	a	780.55	0.08580	YES	YES
53	a	784.44	437.19871	YES	YES
54	a	785.07	427.16476	YES	YES
55	a	785.59	427.25144	YES	YES
56	a	800.31	0.50909	YES	YES
57	a	824.43	0.03446	YES	YES
58	a	824.69	0.01940	YES	YES
59	a	824.83	0.02865	YES	YES
60	a	825.02	0.01210	YES	YES
61	a	825.22	0.05163	YES	YES
62	a	825.40	0.08399	YES	YES
63	a	825.46	0.07168	YES	YES
64	a	825.78	0.00417	YES	YES
65	a	867.04	0.12212	YES	YES
66	a	868.02	0.03759	YES	YES
67	a	868.19	0.02531	YES	YES
68	a	869.27	0.19757	YES	YES
69	a	869.80	0.03491	YES	YES
70	a	870.06	0.16409	YES	YES
71	a	870.40	0.10942	YES	YES
72	a	870.95	0.00537	YES	YES
73	a	998.08	4.81580	YES	YES
74	a	998.41	9.50267	YES	YES
75	a	998.50	9.28998	YES	YES
76	a	998.65	11.12346	YES	YES
77	a	998.68	15.10544	YES	YES
78	a	998.87	23.82142	YES	YES
79	a	999.35	0.10815	YES	YES
80	a	999.80	0.34322	YES	YES
81	a	1041.88	0.01282	YES	YES
82	a	1041.99	0.00783	YES	YES
83	a	1042.36	0.00587	YES	YES
84	a	1043.33	0.04106	YES	YES
85	a	1043.87	0.00668	YES	YES
86	a	1044.34	0.00241	YES	YES
87	a	1044.44	0.01692	YES	YES
88	a	1044.51	0.01291	YES	YES
89	a	1123.51	17.07322	YES	YES
90	a	1123.52	17.13425	YES	YES
91	a	1123.59	17.07069	YES	YES
92	a	1125.34	0.00857	YES	YES
93	a	1232.03	0.00058	YES	YES
94	a	1232.16	0.00032	YES	YES
95	a	1232.35	0.00004	YES	YES
96	a	1232.59	0.00018	YES	YES
97	a	1373.68	0.03476	YES	YES
98	a	1373.76	0.06062	YES	YES
99	a	1373.93	0.01858	YES	YES
100	a	1374.30	0.05156	YES	YES
101	a	1374.43	0.15539	YES	YES
102	a	1374.47	0.15191	YES	YES
103	a	1375.23	0.17266	YES	YES
104	a	1375.32	0.04861	YES	YES
105	a	1427.87	0.23512	YES	YES
106	a	1428.02	0.07663	YES	YES
107	a	1428.06	0.00475	YES	YES
108	a	1428.64	10.26511	YES	YES

109	a	1428.74	10.53366	YES	YES
110	a	1428.85	10.62106	YES	YES
111	a	1430.05	0.00302	YES	YES
112	a	1430.17	0.07387	YES	YES
113	a	3156.30	0.00106	YES	YES
114	a	3156.41	0.00238	YES	YES
115	a	3156.45	0.00561	YES	YES
116	a	3156.47	0.01009	YES	YES
117	a	3156.62	0.00782	YES	YES
118	a	3156.69	0.00713	YES	YES
119	a	3156.72	0.01947	YES	YES
120	a	3156.76	0.00825	YES	YES
121	a	3171.18	0.08320	YES	YES
122	a	3171.27	0.09725	YES	YES
123	a	3171.32	0.09384	YES	YES
124	a	3171.35	1.14928	YES	YES
125	a	3171.43	1.18633	YES	YES
126	a	3171.45	0.59122	YES	YES
127	a	3171.48	1.10167	YES	YES
128	a	3171.54	0.51056	YES	YES
129	a	3182.32	2.18352	YES	YES
130	a	3182.35	2.22064	YES	YES
131	a	3182.37	2.23096	YES	YES
132	a	3182.45	0.09117	YES	YES

$end

CpAl(AlCp*)$_3$



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

Al	0.0375329	0.1025196	1.9793412
C	-1.0966738	0.3255193	4.0802978
C	-0.1181375	1.3609578	4.0118966
C	1.1717277	0.7492960	3.9725017
C	0.9888447	-0.6662120	4.0201569
C	-0.4134424	-0.9282450	4.0833661
Al	-1.4271734	-0.6975716	-0.0894289
C	-2.5618878	-2.3545196	-1.2302718
C	-2.7325160	-2.6055045	0.1731898
C	-3.4470263	-1.4934302	0.7343076
C	-3.7444189	-0.5681385	-0.3231896
C	-3.1886008	-1.0939886	-1.5383820
C	-1.9060474	-3.2486405	-2.2406037
C	-2.2163001	-3.7809036	0.9517338
C	-3.8528662	-1.3375394	2.1707106
C	-4.4774005	0.7291637	-0.1414136
C	-3.2467639	-0.4848773	-2.9095851
H	-1.2316463	-3.9830358	-1.7609467
H	-1.3006126	-2.6687369	-2.9653284
H	-2.6590158	-3.8201334	-2.8258934
H	-1.6860305	-4.4987427	0.2975810
H	-3.0389085	-4.3328925	1.4526206
H	-1.5006827	-3.4661111	1.7428365
H	-3.1502532	-1.8553314	2.8523235
H	-4.8646494	-1.7602131	2.3569358
H	-3.8830723	-0.2712647	2.4703013
H	-4.6310968	1.2467948	-1.1071432
H	-3.9217682	1.4265414	0.5222920
H	-5.4772678	0.5692229	0.3129902
H	-3.7655797	0.4921395	-2.8981150
H	-3.7883939	-1.1419511	-3.6225208
H	-2.2325020	-0.3132717	-3.3311195
Al	-0.0583303	1.6057660	-0.2114205
C	-0.9898701	3.7173433	0.0717378
C	0.3993524	3.7979687	0.4249409
C	1.1799661	3.5105958	-0.7454840
C	0.2747132	3.2308084	-1.8238351
C	-1.0684757	3.3569354	-1.3172984
C	-2.1410343	3.9122537	1.0169835
C	0.9699568	4.1371715	1.7713770
C	2.6796263	3.4982884	-0.7772183
C	0.6223852	2.8909263	-3.2444205
C	-2.3078090	3.1962120	-2.1471989
H	-3.1118521	3.8013787	0.4975008
H	-2.1271231	4.9219731	1.4779246
H	-2.1242925	3.1688409	1.8435457
H	0.1744828	4.2472698	2.5326392
H	1.5354908	5.0933564	1.7425553
H	1.6706821	3.3547503	2.1317955
H	3.0657539	3.2859412	-1.7919953
H	3.0979559	2.7286317	-0.0936317
H	3.0965184	4.4771306	-0.4593648
H	0.1894822	1.9158431	-3.5564825

H	1.7174022	2.8251761	-3.3896033
H	0.2386215	3.6575454	-3.9505381
H	-2.2325192	2.3248591	-2.8279283
H	-2.4899408	4.0916109	-2.7805557
H	-3.2055305	3.0466187	-1.5184500
Al	1.2501809	-0.7329754	-0.2434636
C	3.0158164	-2.1290943	0.3099642
C	3.5690656	-0.9234722	-0.2417757
C	3.1212708	-0.8189229	-1.6021558
C	2.3059186	-1.9699235	-1.8946936
C	2.2509012	-2.7844384	-0.7141654
C	3.2255285	-2.6506628	1.7016364
C	4.4124309	0.0649590	0.5113610
C	3.4553361	0.2537288	-2.5960814
C	1.6648077	-2.2388390	-3.2250178
C	1.5146977	-4.0787764	-0.5287243
H	2.2922319	-3.0759298	2.1240567
H	3.5695850	-1.8514403	2.3862803
H	3.9915351	-3.4565320	1.7236132
H	3.8647556	0.4966479	1.3777183
H	4.7192759	0.9093540	-0.1349072
H	5.3383403	-0.4031483	0.9057851
H	3.9444626	1.1203427	-2.1136803
H	2.5485452	0.6310480	-3.1114102
H	4.1444434	-0.1241369	-3.3820564
H	2.4259703	-2.3473791	-4.0267293
H	0.9858749	-1.4137522	-3.5316257
H	1.0648607	-3.1680423	-3.2075412
H	1.0213090	-4.4040797	-1.4644634
H	0.7264803	-3.9955300	0.2501555
H	2.2007459	-4.8929146	-0.2143090
H	1.7832380	-1.4198448	3.9894407
H	-0.8816508	-1.9194800	4.1117846
H	-2.1832185	0.4665480	4.0986143
H	-0.3210437	2.4368863	3.9703608
H	2.1325818	1.2727151	3.9001934

SCF energy GEOOPT = -2332.733028891 H

ZPE = 1911. kJ/mol

FREEH energy = 2048.56 kJ/mol

FREEH entropy = 1.23732 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-6.32	0.00000	YES	YES
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	16.50	0.02691	YES	YES
9	a	18.08	0.00721	YES	YES
10	a	28.72	0.01433	YES	YES
11	a	32.71	0.01022	YES	YES
12	a	47.05	0.00543	YES	YES
13	a	48.64	0.02670	YES	YES
14	a	51.91	0.06348	YES	YES
15	a	54.60	0.00711	YES	YES
16	a	59.14	0.03401	YES	YES
17	a	60.78	0.05096	YES	YES
18	a	62.04	0.04896	YES	YES
19	a	70.58	0.06506	YES	YES
20	a	74.02	0.20469	YES	YES
21	a	78.95	0.04547	YES	YES
22	a	79.56	0.17040	YES	YES
23	a	86.31	0.10373	YES	YES
24	a	93.46	1.39779	YES	YES
25	a	96.40	0.78867	YES	YES
26	a	98.72	0.33977	YES	YES
27	a	99.97	1.09534	YES	YES
28	a	101.45	0.16238	YES	YES
29	a	104.01	0.45427	YES	YES
30	a	109.11	0.23824	YES	YES
31	a	116.30	0.20855	YES	YES
32	a	119.66	0.11716	YES	YES
33	a	123.26	0.25436	YES	YES
34	a	126.13	0.19436	YES	YES
35	a	128.13	0.23797	YES	YES
36	a	133.36	0.10627	YES	YES
37	a	136.83	0.37082	YES	YES
38	a	140.38	0.23786	YES	YES
39	a	142.25	0.22429	YES	YES
40	a	153.72	0.75819	YES	YES
41	a	154.64	0.85039	YES	YES
42	a	163.53	0.00523	YES	YES
43	a	166.66	0.07452	YES	YES
44	a	167.62	0.03213	YES	YES
45	a	169.50	0.06183	YES	YES
46	a	171.40	0.03489	YES	YES
47	a	173.70	0.13416	YES	YES
48	a	175.98	0.12209	YES	YES
49	a	176.52	0.32232	YES	YES
50	a	178.80	0.51014	YES	YES
51	a	205.88	12.16219	YES	YES

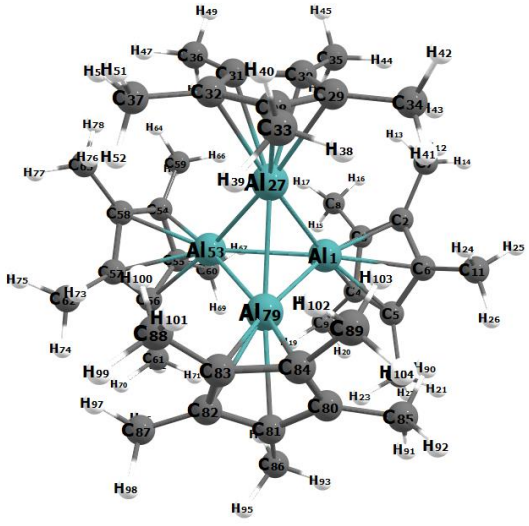
52	a	244.88	0.75366	YES	YES
53	a	245.66	1.19296	YES	YES
54	a	249.67	3.15325	YES	YES
55	a	251.74	0.48055	YES	YES
56	a	254.78	6.08583	YES	YES
57	a	257.33	5.84664	YES	YES
58	a	262.12	3.03154	YES	YES
59	a	262.38	4.52654	YES	YES
60	a	263.14	5.58598	YES	YES
61	a	264.56	0.67629	YES	YES
62	a	266.89	2.23199	YES	YES
63	a	274.40	1.61538	YES	YES
64	a	277.18	1.96901	YES	YES
65	a	278.85	2.32973	YES	YES
66	a	286.27	0.33142	YES	YES
67	a	288.72	1.27766	YES	YES
68	a	289.39	1.35044	YES	YES
69	a	340.39	4.04423	YES	YES
70	a	343.30	18.68690	YES	YES
71	a	345.03	10.17892	YES	YES
72	a	347.45	235.96914	YES	YES
73	a	363.39	0.30769	YES	YES
74	a	377.43	0.70311	YES	YES
75	a	379.54	1.87122	YES	YES
76	a	391.82	447.11508	YES	YES
77	a	393.21	443.29041	YES	YES
78	a	508.49	7.84010	YES	YES
79	a	543.88	0.02009	YES	YES
80	a	544.44	0.06192	YES	YES
81	a	544.86	0.04319	YES	YES
82	a	546.09	0.03211	YES	YES
83	a	546.45	0.00116	YES	YES
84	a	546.60	0.02691	YES	YES
85	a	548.96	0.01617	YES	YES
86	a	549.29	0.01334	YES	YES
87	a	549.63	0.03085	YES	YES
88	a	570.21	0.05134	YES	YES
89	a	570.97	0.02492	YES	YES
90	a	578.66	1.26662	YES	YES
91	a	579.64	1.71787	YES	YES
92	a	580.08	3.00699	YES	YES
93	a	582.26	1.07112	YES	YES
94	a	582.42	1.57369	YES	YES
95	a	583.70	0.49857	YES	YES
96	a	593.85	3.33419	YES	YES
97	a	594.35	3.10520	YES	YES
98	a	595.97	1.35486	YES	YES
99	a	765.17	12.37354	YES	YES
100	a	768.14	14.03161	YES	YES
101	a	784.97	319.45088	YES	YES
102	a	796.70	0.64806	YES	YES
103	a	797.33	1.97042	YES	YES
104	a	797.94	1.50980	YES	YES
105	a	806.14	7.34656	YES	YES
106	a	807.08	0.43680	YES	YES
107	a	807.83	1.05120	YES	YES
108	a	823.72	0.15447	YES	YES
109	a	824.34	0.25797	YES	YES
110	a	861.89	0.82321	YES	YES
111	a	867.32	0.67016	YES	YES
112	a	924.10	2.39476	YES	YES
113	a	924.95	0.15340	YES	YES
114	a	925.27	0.32556	YES	YES
115	a	932.06	3.71379	YES	YES
116	a	932.54	1.70035	YES	YES
117	a	933.53	2.00588	YES	YES
118	a	987.24	3.36409	YES	YES
119	a	987.96	2.68912	YES	YES
120	a	988.38	0.78138	YES	YES
121	a	996.30	1.07914	YES	YES
122	a	996.80	0.41631	YES	YES
123	a	997.16	1.31249	YES	YES
124	a	997.64	1.94014	YES	YES
125	a	998.08	3.66885	YES	YES
126	a	998.50	0.94869	YES	YES
127	a	998.91	2.18045	YES	YES
128	a	1000.07	8.27627	YES	YES
129	a	1004.48	0.11867	YES	YES
130	a	1005.19	0.15487	YES	YES
131	a	1007.29	0.12263	YES	YES
132	a	1008.30	0.59711	YES	YES
133	a	1009.15	0.41324	YES	YES
134	a	1010.36	0.14097	YES	YES
135	a	1041.87	0.89563	YES	YES
136	a	1041.96	0.21143	YES	YES
137	a	1045.40	1.39230	YES	YES
138	a	1046.30	4.59233	YES	YES
139	a	1047.24	0.44150	YES	YES
140	a	1047.92	1.21766	YES	YES
141	a	1049.16	0.42043	YES	YES
142	a	1049.92	0.24303	YES	YES
143	a	1070.63	0.38733	YES	YES
144	a	1071.02	0.66160	YES	YES
145	a	1073.46	0.13495	YES	YES
146	a	1124.57	9.79789	YES	YES
147	a	1166.31	0.11986	YES	YES

148	a	1166.54	0.01173	YES	YES
149	a	1166.87	0.07235	YES	YES
150	a	1167.50	0.31608	YES	YES
151	a	1167.68	0.12851	YES	YES
152	a	1168.01	0.50937	YES	YES
153	a	1231.41	0.10072	YES	YES
154	a	1335.71	1.13743	YES	YES
155	a	1337.68	0.50204	YES	YES
156	a	1338.13	0.96531	YES	YES
157	a	1338.46	1.91324	YES	YES
158	a	1339.73	4.07238	YES	YES
159	a	1340.25	2.84994	YES	YES
160	a	1341.68	2.81788	YES	YES
161	a	1342.50	3.55512	YES	YES
162	a	1343.25	1.96590	YES	YES
163	a	1344.02	1.16764	YES	YES
164	a	1344.87	0.76110	YES	YES
165	a	1345.21	1.65489	YES	YES
166	a	1348.32	0.23748	YES	YES
167	a	1348.83	0.24643	YES	YES
168	a	1350.53	0.15736	YES	YES
169	a	1375.09	0.07703	YES	YES
170	a	1375.32	0.25668	YES	YES
171	a	1387.20	3.04169	YES	YES
172	a	1387.61	1.87997	YES	YES
173	a	1388.09	2.93253	YES	YES
174	a	1389.84	2.34022	YES	YES
175	a	1391.78	4.03028	YES	YES
176	a	1391.95	3.00243	YES	YES
177	a	1393.72	4.03520	YES	YES
178	a	1394.86	3.18057	YES	YES
179	a	1396.25	1.34804	YES	YES
180	a	1396.77	8.64770	YES	YES
181	a	1398.40	3.83191	YES	YES
182	a	1399.77	6.50106	YES	YES
183	a	1400.12	2.70952	YES	YES
184	a	1401.79	5.38219	YES	YES
185	a	1403.43	16.60209	YES	YES
186	a	1403.89	14.46222	YES	YES
187	a	1404.81	21.41024	YES	YES
188	a	1405.71	11.95424	YES	YES
189	a	1407.04	0.93268	YES	YES
190	a	1407.87	2.73906	YES	YES
191	a	1409.33	4.50091	YES	YES
192	a	1411.83	2.50910	YES	YES
193	a	1412.96	7.58965	YES	YES
194	a	1413.37	3.21384	YES	YES
195	a	1415.37	10.39039	YES	YES
196	a	1416.74	6.38221	YES	YES
197	a	1417.29	37.98378	YES	YES
198	a	1419.02	39.16795	YES	YES
199	a	1419.45	19.01767	YES	YES
200	a	1420.81	16.24322	YES	YES
201	a	1428.72	0.55854	YES	YES
202	a	1429.59	6.41099	YES	YES
203	a	1433.26	2.83475	YES	YES
204	a	1433.31	2.68143	YES	YES
205	a	1435.14	1.39502	YES	YES
206	a	1443.95	0.16615	YES	YES
207	a	1444.13	0.09710	YES	YES
208	a	1444.51	0.14867	YES	YES
209	a	1454.62	0.55829	YES	YES
210	a	1455.26	1.06182	YES	YES
211	a	1455.93	1.50858	YES	YES
212	a	1487.34	3.34003	YES	YES
213	a	1487.96	1.03070	YES	YES
214	a	1488.85	1.70815	YES	YES
215	a	1501.73	5.30535	YES	YES
216	a	1502.52	6.14581	YES	YES
217	a	1503.28	6.39953	YES	YES
218	a	2942.80	44.77931	YES	YES
219	a	2943.12	52.37642	YES	YES
220	a	2944.50	119.15714	YES	YES
221	a	2944.63	11.32052	YES	YES
222	a	2944.83	5.02992	YES	YES
223	a	2945.59	31.05893	YES	YES
224	a	2946.86	45.44738	YES	YES
225	a	2947.98	60.75895	YES	YES
226	a	2948.34	57.92494	YES	YES
227	a	2948.74	28.49288	YES	YES
228	a	2949.26	29.10280	YES	YES
229	a	2949.29	30.09618	YES	YES
230	a	2951.95	34.56559	YES	YES
231	a	2952.06	37.77278	YES	YES
232	a	2952.33	48.89881	YES	YES
233	a	3008.13	12.56041	YES	YES
234	a	3009.00	12.94757	YES	YES
235	a	3009.41	16.04136	YES	YES
236	a	3011.47	20.51092	YES	YES
237	a	3011.88	21.76860	YES	YES
238	a	3012.68	16.64725	YES	YES
239	a	3014.55	12.19223	YES	YES
240	a	3015.53	19.60844	YES	YES
241	a	3016.12	3.61415	YES	YES
242	a	3016.68	15.41701	YES	YES
243	a	3019.13	1.04693	YES	YES

244	a	3022.13	6.44963	YES	YES
245	a	3024.45	5.98528	YES	YES
246	a	3027.37	6.88015	YES	YES
247	a	3027.64	6.92853	YES	YES
248	a	3057.67	10.58548	YES	YES
249	a	3058.92	13.38645	YES	YES
250	a	3059.53	7.49634	YES	YES
251	a	3059.57	2.29775	YES	YES
252	a	3060.26	11.01825	YES	YES
253	a	3061.05	11.44778	YES	YES
254	a	3062.09	7.96005	YES	YES
255	a	3062.40	4.90733	YES	YES
256	a	3062.68	9.41824	YES	YES
257	a	3064.30	8.33511	YES	YES
258	a	3064.37	11.08439	YES	YES
259	a	3064.79	9.51565	YES	YES
260	a	3068.24	4.89962	YES	YES
261	a	3070.05	4.85832	YES	YES
262	a	3070.83	5.07894	YES	YES
263	a	3157.99	0.24583	YES	YES
264	a	3159.35	0.21029	YES	YES
265	a	3172.38	1.20657	YES	YES
266	a	3179.52	0.81303	YES	YES
267	a	3187.08	2.60760	YES	YES

$end

AlCp*$_4$



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

Al	4.2176056	3.7084829	5.7673939
C	2.9849624	4.3103581	7.6430849
C	2.7065745	5.2728577	6.6114077
C	3.9302139	5.9668338	6.3232287
C	4.9539897	5.4457168	7.1870588
C	4.3716763	4.4224505	8.0035829
C	1.9851974	3.4432597	8.3470680
C	1.3712464	5.4826867	5.9562538
C	4.1566756	7.0814410	5.3455263
C	6.3565225	5.9725310	7.2276714
C	5.0488165	3.5954329	9.0580328
H	2.3927291	2.4353535	8.5613285
H	1.0630178	3.3098210	7.7526226
H	1.6909828	3.8879978	9.3232087
H	1.3418722	6.4392203	5.3994154
H	0.5515601	5.5102529	6.7023850
H	1.1287478	4.6743175	5.2302404
H	3.2086038	7.4422343	4.9063527
H	4.8151246	6.7717329	4.5049532
H	4.6473263	7.9466906	5.8388727
H	6.9455975	5.5076253	8.0390408
H	6.3606756	7.0699234	7.3995653
H	6.8962803	5.7924165	6.2758453
H	5.1175606	2.5244317	8.7657268
H	4.4972006	3.6351795	10.0204552
H	6.0790760	3.9496830	9.2532289
Al	3.9378509	1.1583221	4.8976739
C	4.0857835	-1.1253637	5.3738860
C	3.3060160	-0.4874821	6.4007012
C	2.1085183	0.0160196	5.7857748
C	2.1522660	-0.3097287	4.3876365
C	3.3721443	-1.0163715	4.1324930
C	5.3533891	-1.9040267	5.5615389
C	3.6817258	-0.3905586	7.8509607
C	0.9507847	0.7064518	6.4423250
C	1.0532195	0.0135382	3.4211399
C	3.8534246	-1.5664908	2.8216387
H	5.8037960	-1.7211701	6.5540485
H	6.1127847	-1.6553550	4.7947355
H	5.1582052	-2.9963787	5.4857192
H	4.7596961	-0.1597790	7.9796102
H	3.4792995	-1.3372473	8.3964445
H	3.1162386	0.4129338	8.3619082
H	1.0975253	0.8107016	7.5323001
H	0.0114551	0.1336144	6.2878919
H	0.7816455	1.7231329	6.0272709
H	1.2220589	-0.4596302	2.4364748
H	0.9555798	1.1060258	3.2537912
H	0.0733868	-0.3446704	3.8013795
H	3.0405293	-1.6007139	2.0711400
H	4.2442684	-2.5983909	2.9367638

H	4.6765175	-0.9552068	2.3878139
Al	4.0825018	3.1770491	3.1165113
C	2.3208156	3.7032564	1.6377316
C	3.1557277	4.8609968	1.8033285
C	4.4591600	4.5569481	1.2775453
C	4.4313427	3.2003563	0.8049822
C	3.1099231	2.6779763	1.0219833
C	0.8752790	3.6328773	2.0352978
C	2.6760062	6.1883101	2.3097482
C	5.6349579	5.4918889	1.2638951
C	5.5328086	2.4267151	0.1428427
C	2.6694599	1.3138236	0.5835842
H	0.3953370	2.7060205	1.6674088
H	0.3015063	4.4897959	1.6247550
H	0.7445719	3.6562423	3.1399692
H	2.0983962	6.0876674	3.2491831
H	2.0075693	6.6775448	1.5675713
H	3.5146985	6.8803543	2.5068586
H	6.3962545	5.1709293	0.5263763
H	6.1407451	5.5434149	2.2548097
H	5.3312709	6.5238632	0.9965802
H	5.9009386	1.5939995	0.7809906
H	6.4009279	3.0690355	-0.0931701
H	5.1821480	1.9747862	-0.8087733
H	3.2179312	0.5087675	1.1127990
H	2.8530123	1.1702655	-0.5025960
H	1.5900974	1.1550407	0.7610989
Al	6.2738364	2.4789297	4.5459939
C	8.3180298	2.6739023	5.7172648
C	8.4363970	3.4199111	4.4997305
C	8.3003038	2.4990571	3.4043736
C	8.1101940	1.1796446	3.9446810
C	8.1116703	1.2931632	5.3768568
C	8.4479984	3.1743534	7.1243520
C	8.6812628	4.8928045	4.3463571
C	8.4798329	2.8659657	1.9612010
C	7.9120736	-0.0754377	3.1430476
C	7.9829474	0.1975709	6.3924439
H	7.5045687	3.0574170	7.6965710
H	8.7274858	4.2432797	7.1552045
H	9.2308794	2.6091865	7.6733007
H	8.9425159	5.3658592	5.3122558
H	7.7894082	5.4260264	3.9480079
H	9.5162484	5.0913824	3.6426768
H	7.8748025	3.7499341	1.6802504
H	8.1920578	2.0380970	1.2880874
H	9.5418299	3.1165120	1.7460084
H	8.5560758	-0.0887395	2.2410957
H	6.8593889	-0.1902281	2.7980323
H	8.1590078	-0.9763309	3.7381394
H	8.0312204	-0.8031742	5.9255304
H	7.0232097	0.2564668	6.9507234
H	8.7982633	0.2567021	7.1434869

SCF energy GEOOPT = -2529.207598430 H

ZPE = 2267. kJ/mol

FREEH energy = 2426.51 kJ/mol

FREEH entropy = 1.37152 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		-0.00	0.00000	- -
2		-0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	15.19	0.00920	YES YES
8	a	28.65	0.02389	YES YES
9	a	32.49	0.02063	YES YES
10	a	33.00	0.00695	YES YES
11	a	41.62	0.01724	YES YES
12	a	45.88	0.01233	YES YES
13	a	49.20	0.00983	YES YES
14	a	60.70	0.04339	YES YES
15	a	60.90	0.03028	YES YES
16	a	64.54	0.05241	YES YES
17	a	67.08	0.02457	YES YES
18	a	70.30	0.04015	YES YES
19	a	71.87	0.02476	YES YES
20	a	73.97	0.22926	YES YES
21	a	78.41	0.02253	YES YES
22	a	80.71	0.10673	YES YES
23	a	82.47	0.07523	YES YES
24	a	89.50	0.03365	YES YES
25	a	95.94	0.34921	YES YES
26	a	100.86	0.07316	YES YES
27	a	104.64	0.29768	YES YES
28	a	107.93	0.30989	YES YES
29	a	111.47	0.46415	YES YES
30	a	113.10	0.14484	YES YES
31	a	120.94	0.79609	YES YES
32	a	124.29	0.03138	YES YES
33	a	129.63	0.31481	YES YES
34	a	131.64	0.17687	YES YES

35	a	133.39	0.28657	YES	YES
36	a	136.16	0.74638	YES	YES
37	a	140.12	0.34422	YES	YES
38	a	142.85	0.19531	YES	YES
39	a	146.10	0.17348	YES	YES
40	a	153.10	0.15354	YES	YES
41	a	154.91	0.15793	YES	YES
42	a	157.05	0.11772	YES	YES
43	a	158.34	0.16203	YES	YES
44	a	160.11	0.05839	YES	YES
45	a	160.60	0.12758	YES	YES
46	a	163.14	0.37897	YES	YES
47	a	169.81	0.64825	YES	YES
48	a	170.47	0.04884	YES	YES
49	a	171.71	1.44286	YES	YES
50	a	173.25	0.02232	YES	YES
51	a	174.42	0.46502	YES	YES
52	a	177.15	0.51269	YES	YES
53	a	179.16	0.83308	YES	YES
54	a	181.97	0.04504	YES	YES
55	a	193.13	1.27924	YES	YES
56	a	194.82	1.32796	YES	YES
57	a	197.74	0.54213	YES	YES
58	a	198.13	0.29387	YES	YES
59	a	243.70	1.58078	YES	YES
60	a	243.94	1.86773	YES	YES
61	a	244.59	0.73202	YES	YES
62	a	246.97	4.89963	YES	YES
63	a	250.76	3.34477	YES	YES
64	a	252.96	10.37690	YES	YES
65	a	262.68	1.25019	YES	YES
66	a	264.01	1.73933	YES	YES
67	a	265.52	1.00469	YES	YES
68	a	267.39	1.72272	YES	YES
69	a	269.09	1.13986	YES	YES
70	a	271.25	1.03226	YES	YES
71	a	275.37	0.67998	YES	YES
72	a	277.19	0.75301	YES	YES
73	a	278.12	0.56475	YES	YES
74	a	279.11	1.88031	YES	YES
75	a	279.81	0.46884	YES	YES
76	a	281.20	0.96659	YES	YES
77	a	284.34	0.94346	YES	YES
78	a	285.00	0.32242	YES	YES
79	a	287.57	2.42060	YES	YES
80	a	289.46	0.16487	YES	YES
81	a	327.47	0.46979	YES	YES
82	a	328.68	3.77410	YES	YES
83	a	331.31	2.16886	YES	YES
84	a	348.59	30.31407	YES	YES
85	a	359.14	66.25358	YES	YES
86	a	361.06	49.55698	YES	YES
87	a	371.16	155.93349	YES	YES
88	a	373.00	352.13572	YES	YES
89	a	375.98	340.96879	YES	YES
90	a	379.41	7.65257	YES	YES
91	a	382.28	236.52800	YES	YES
92	a	496.04	0.00984	YES	YES
93	a	545.07	0.01343	YES	YES
94	a	545.45	0.05453	YES	YES
95	a	545.81	0.02265	YES	YES
96	a	546.21	0.19276	YES	YES
97	a	546.74	0.10545	YES	YES
98	a	547.07	0.10570	YES	YES
99	a	547.47	0.02468	YES	YES
100	a	548.30	0.04224	YES	YES
101	a	549.96	0.02710	YES	YES
102	a	550.25	0.00792	YES	YES
103	a	551.17	0.00439	YES	YES
104	a	552.11	0.00544	YES	YES
105	a	569.47	5.26419	YES	YES
106	a	570.59	3.48052	YES	YES
107	a	571.17	1.40631	YES	YES
108	a	573.73	0.95487	YES	YES
109	a	577.87	0.46310	YES	YES
110	a	578.45	0.21413	YES	YES
111	a	580.03	1.70072	YES	YES
112	a	580.93	0.07904	YES	YES
113	a	595.02	7.92504	YES	YES
114	a	595.42	7.18437	YES	YES
115	a	595.77	7.08462	YES	YES
116	a	599.64	0.04297	YES	YES
117	a	798.34	1.96222	YES	YES
118	a	798.89	2.16083	YES	YES
119	a	799.37	0.99470	YES	YES
120	a	800.69	1.31473	YES	YES
121	a	809.28	5.13764	YES	YES
122	a	809.95	4.25802	YES	YES
123	a	810.20	3.00750	YES	YES
124	a	812.12	1.84560	YES	YES
125	a	925.15	2.17641	YES	YES
126	a	926.23	1.76756	YES	YES
127	a	926.95	1.66523	YES	YES
128	a	928.43	0.88424	YES	YES
129	a	932.14	2.22377	YES	YES
130	a	933.03	1.88665	YES	YES

131	a	934.02	1.07486	YES	YES
132	a	935.44	0.57263	YES	YES
133	a	988.03	0.41765	YES	YES
134	a	988.51	0.48818	YES	YES
135	a	989.51	0.23991	YES	YES
136	a	989.76	0.67857	YES	YES
137	a	993.71	0.13256	YES	YES
138	a	994.94	0.27160	YES	YES
139	a	995.77	0.18228	YES	YES
140	a	996.46	0.43965	YES	YES
141	a	997.63	0.38426	YES	YES
142	a	998.06	1.70870	YES	YES
143	a	998.91	0.18844	YES	YES
144	a	1000.17	0.20633	YES	YES
145	a	1007.32	0.17341	YES	YES
146	a	1007.67	0.58436	YES	YES
147	a	1008.53	0.56777	YES	YES
148	a	1009.51	0.16970	YES	YES
149	a	1010.46	0.23097	YES	YES
150	a	1011.12	0.58818	YES	YES
151	a	1011.75	0.27315	YES	YES
152	a	1012.04	0.43865	YES	YES
153	a	1045.49	0.73174	YES	YES
154	a	1046.59	0.25438	YES	YES
155	a	1047.39	0.53520	YES	YES
156	a	1047.74	2.16786	YES	YES
157	a	1048.14	2.57498	YES	YES
158	a	1049.06	0.57737	YES	YES
159	a	1049.72	0.43542	YES	YES
160	a	1051.35	1.42221	YES	YES
161	a	1070.33	0.28746	YES	YES
162	a	1070.93	0.32706	YES	YES
163	a	1072.09	0.06109	YES	YES
164	a	1073.43	0.21799	YES	YES
165	a	1165.78	0.23786	YES	YES
166	a	1165.99	0.59986	YES	YES
167	a	1166.88	0.27725	YES	YES
168	a	1167.55	0.33898	YES	YES
169	a	1168.03	0.00539	YES	YES
170	a	1168.50	0.22066	YES	YES
171	a	1168.98	0.03501	YES	YES
172	a	1169.45	0.38474	YES	YES
173	a	1336.68	0.06263	YES	YES
174	a	1337.49	0.73495	YES	YES
175	a	1338.05	0.17540	YES	YES
176	a	1338.82	1.29926	YES	YES
177	a	1339.55	1.29175	YES	YES
178	a	1340.02	2.65068	YES	YES
179	a	1340.76	4.14590	YES	YES
180	a	1341.13	4.21796	YES	YES
181	a	1342.26	1.20407	YES	YES
182	a	1343.28	2.46360	YES	YES
183	a	1344.28	1.38390	YES	YES
184	a	1344.81	0.21013	YES	YES
185	a	1345.82	0.52729	YES	YES
186	a	1346.68	1.62716	YES	YES
187	a	1347.09	0.60539	YES	YES
188	a	1347.50	1.46739	YES	YES
189	a	1349.06	0.48031	YES	YES
190	a	1350.19	0.29351	YES	YES
191	a	1350.61	0.03339	YES	YES
192	a	1352.42	0.19660	YES	YES
193	a	1386.45	5.66584	YES	YES
194	a	1387.31	15.21856	YES	YES
195	a	1388.61	4.00360	YES	YES
196	a	1388.86	5.62326	YES	YES
197	a	1389.70	1.72006	YES	YES
198	a	1390.30	4.69361	YES	YES
199	a	1390.82	12.88139	YES	YES
200	a	1391.52	2.87895	YES	YES
201	a	1393.74	4.20048	YES	YES
202	a	1394.44	2.96370	YES	YES
203	a	1395.62	4.95197	YES	YES
204	a	1397.09	0.65387	YES	YES
205	a	1397.33	6.34695	YES	YES
206	a	1398.71	3.54028	YES	YES
207	a	1399.55	8.28785	YES	YES
208	a	1400.75	6.49866	YES	YES
209	a	1401.52	4.29985	YES	YES
210	a	1402.08	6.92075	YES	YES
211	a	1402.54	17.13023	YES	YES
212	a	1403.53	7.32516	YES	YES
213	a	1403.99	0.56289	YES	YES
214	a	1404.59	9.99579	YES	YES
215	a	1404.97	3.79288	YES	YES
216	a	1405.52	2.46247	YES	YES
217	a	1406.23	1.67864	YES	YES
218	a	1407.13	10.96715	YES	YES
219	a	1407.25	0.34120	YES	YES
220	a	1407.70	3.68583	YES	YES
221	a	1407.80	8.69139	YES	YES
222	a	1408.89	19.33697	YES	YES
223	a	1411.29	4.43947	YES	YES
224	a	1413.13	3.78918	YES	YES
225	a	1415.00	6.16409	YES	YES
226	a	1415.90	2.43351	YES	YES

227	a	1419.52	20.68086	YES	YES
228	a	1420.72	4.40028	YES	YES
229	a	1422.89	13.62831	YES	YES
230	a	1423.75	19.93787	YES	YES
231	a	1424.12	9.55971	YES	YES
232	a	1424.92	1.42263	YES	YES
233	a	1434.28	10.33064	YES	YES
234	a	1434.92	8.44666	YES	YES
235	a	1435.98	11.20084	YES	YES
236	a	1436.35	9.19643	YES	YES
237	a	1445.49	0.80192	YES	YES
238	a	1445.82	0.54356	YES	YES
239	a	1446.55	1.07189	YES	YES
240	a	1449.22	0.21133	YES	YES
241	a	1455.79	1.30475	YES	YES
242	a	1456.35	3.72408	YES	YES
243	a	1457.10	4.34235	YES	YES
244	a	1457.42	3.60166	YES	YES
245	a	1486.42	2.09327	YES	YES
246	a	1487.10	2.47721	YES	YES
247	a	1488.18	1.35679	YES	YES
248	a	1488.72	1.81369	YES	YES
249	a	1505.00	9.66154	YES	YES
250	a	1505.60	3.51706	YES	YES
251	a	1505.98	6.41744	YES	YES
252	a	1506.53	1.59855	YES	YES
253	a	2929.01	66.59484	YES	YES
254	a	2929.60	64.33541	YES	YES
255	a	2932.55	63.46080	YES	YES
256	a	2935.28	10.47539	YES	YES
257	a	2936.84	21.14551	YES	YES
258	a	2939.04	15.32482	YES	YES
259	a	2941.67	41.81159	YES	YES
260	a	2943.08	58.59586	YES	YES
261	a	2944.12	41.40782	YES	YES
262	a	2944.55	38.24461	YES	YES
263	a	2946.20	32.54465	YES	YES
264	a	2948.06	84.83636	YES	YES
265	a	2948.62	7.80880	YES	YES
266	a	2951.41	82.74890	YES	YES
267	a	2951.57	24.32798	YES	YES
268	a	2951.84	44.69555	YES	YES
269	a	2955.74	35.74852	YES	YES
270	a	2957.60	12.36874	YES	YES
271	a	2958.27	101.73920	YES	YES
272	a	2958.49	12.09011	YES	YES
273	a	3007.26	19.16768	YES	YES
274	a	3007.37	11.99430	YES	YES
275	a	3007.95	11.09686	YES	YES
276	a	3009.10	15.65923	YES	YES
277	a	3009.11	18.56143	YES	YES
278	a	3009.30	17.44810	YES	YES
279	a	3009.51	20.43102	YES	YES
280	a	3010.00	16.11715	YES	YES
281	a	3014.54	17.11079	YES	YES
282	a	3014.80	15.53186	YES	YES
283	a	3015.54	13.01733	YES	YES
284	a	3017.75	13.18852	YES	YES
285	a	3022.17	5.63378	YES	YES
286	a	3023.35	6.72504	YES	YES
287	a	3025.26	7.12996	YES	YES
288	a	3027.67	3.73348	YES	YES
289	a	3029.27	3.01722	YES	YES
290	a	3031.12	4.90742	YES	YES
291	a	3032.78	4.28257	YES	YES
292	a	3033.13	5.21202	YES	YES
293	a	3050.60	9.09820	YES	YES
294	a	3054.53	8.92095	YES	YES
295	a	3054.75	8.98399	YES	YES
296	a	3055.89	8.77663	YES	YES
297	a	3057.41	11.28051	YES	YES
298	a	3057.91	11.40952	YES	YES
299	a	3057.94	10.01828	YES	YES
300	a	3058.90	11.07173	YES	YES
301	a	3070.93	8.47492	YES	YES
302	a	3071.73	9.10951	YES	YES
303	a	3072.09	8.37235	YES	YES
304	a	3072.99	9.80171	YES	YES
305	a	3073.97	7.65008	YES	YES
306	a	3076.36	4.31305	YES	YES
307	a	3076.63	6.73378	YES	YES
308	a	3077.98	5.19836	YES	YES
309	a	3078.46	4.39819	YES	YES
310	a	3080.89	5.97406	YES	YES
311	a	3081.49	5.26893	YES	YES
312	a	3082.15	5.00672	YES	YES

$end

$raman spectrum

# mode	symmetry	wave	selection	derivative of	derivative of	raman
#	number	rule	isotropic	polarizability	polarizability	scattering
#					anisotropy	cross sections
#	cm**(-1)		a.u.	a.u.		bohr**2/sr
#					T,T	II,II
1	0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
2	0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00
3	0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00

4		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00		52	a	177.15	YES	-0.004990	0.023214	0.69348D-15	0.34221D-15
5		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00		53	a	179.16	YES	-0.004082	0.027585	0.78771D-15	0.47400D-15
6		0.00	-	0.000000	0.000000	0.00000D+00	0.00000D+00		54	a	181.97	YES	0.013787	0.018836	0.20167D-14	0.21523D-15
7	a	15.19	YES	-0.003330	0.013137	0.25592D-13	0.11142D-13		55	a	193.13	YES	-0.000854	0.016298	0.20020D-15	0.14566D-15
8	a	28.65	YES	0.002021	0.016294	0.77359D-14	0.49460D-14		56	a	194.82	YES	0.004755	0.014451	0.33369D-15	0.11284D-15
9	a	32.49	YES	-0.000413	0.013232	0.34440D-14	0.25550D-14		57	a	197.74	YES	0.004254	0.029288	0.74579D-15	0.45204D-15
10	a	33.00	YES	0.001011	0.018681	0.68054D-14	0.49411D-14		58	a	198.13	YES	-0.005076	0.025799	0.66909D-15	0.34960D-15
11	a	41.62	YES	-0.000887	0.018227	0.41153D-14	0.30064D-14		59	a	243.70	YES	-0.018856	0.004206	0.19964D-14	0.65939D-17
12	a	45.88	YES	-0.001081	0.024734	0.62555D-14	0.45929D-14		60	a	243.94	YES	0.013016	0.006320	0.96532D-15	0.14861D-16
13	a	49.20	YES	0.004727	0.008169	0.27864D-14	0.43845D-15		61	a	244.59	YES	-0.008784	0.009234	0.47093D-15	0.31589D-16
14	a	60.70	YES	0.001368	0.049902	0.14768D-13	0.10983D-13		62	a	246.97	YES	-0.001203	0.003203	0.12905D-16	0.37422D-17
15	a	60.90	YES	0.005711	0.052861	0.18475D-13	0.12248D-13		63	a	250.76	YES	-0.003495	0.008691	0.10100D-15	0.26873D-16
16	a	64.54	YES	-0.000563	0.065152	0.22257D-13	0.16679D-13		64	a	252.96	YES	-0.000670	0.009917	0.48353D-16	0.34495D-16
17	a	67.08	YES	0.003133	0.083650	0.34634D-13	0.25572D-13		65	a	262.68	YES	-0.004441	0.017346	0.23002D-15	0.99295D-16
18	a	70.30	YES	-0.002670	0.096324	0.41767D-13	0.31057D-13		66	a	264.01	YES	0.000829	0.025788	0.29362D-15	0.21768D-15
19	a	71.87	YES	-0.001550	0.049769	0.10724D-13	0.79559D-14		67	a	265.52	YES	-0.002903	0.020939	0.23059D-15	0.14220D-15
20	a	73.97	YES	0.004601	0.073985	0.23182D-13	0.16662D-13		68	a	267.39	YES	0.000627	0.020798	0.18685D-15	0.13872D-15
21	a	78.41	YES	0.006899	0.068689	0.19131D-13	0.12886D-13		69	a	269.09	YES	-0.000329	0.009057	0.35234D-16	0.26038D-16
22	a	80.71	YES	-0.001641	0.052875	0.97539D-14	0.72370D-14		70	a	271.25	YES	-0.000263	0.011634	0.56885D-16	0.42420D-16
23	a	82.47	YES	-0.003147	0.050461	0.88139D-14	0.63334D-14		71	a	275.37	YES	0.001032	0.013729	0.81770D-16	0.57662D-16
24	a	89.50	YES	-0.038314	0.042219	0.52183D-13	0.38127D-14		72	a	277.19	YES	-0.001970	0.018821	0.16061D-15	0.10724D-15
25	a	95.94	YES	0.009031	0.044811	0.73462D-14	0.37815D-14		73	a	278.12	YES	0.001929	0.021057	0.19483D-15	0.13351D-15
26	a	100.86	YES	-0.009239	0.098838	0.24592D-13	0.16793D-13		74	a	279.11	YES	0.001855	0.009517	0.51618D-16	0.27116D-16
27	a	104.64	YES	-0.011895	0.044362	0.76316D-14	0.31643D-14		75	a	279.81	YES	-0.002691	0.011932	0.88999D-16	0.42457D-16
28	a	107.93	YES	-0.015087	0.033307	0.74392D-14	0.16865D-14		76	a	281.20	YES	-0.000420	0.008538	0.29541D-16	0.21568D-16
29	a	111.47	YES	0.016384	0.045939	0.98102D-14	0.30267D-14		77	a	284.34	YES	0.000118	0.014594	0.82608D-16	0.61911D-16
30	a	113.10	YES	-0.021680	0.035102	0.12145D-13	0.17215D-14		78	a	285.00	YES	-0.001101	0.012936	0.69883D-16	0.48463D-16
31	a	120.94	YES	0.018031	0.019870	0.66936D-14	0.48913D-15		79	a	287.57	YES	0.001366	0.020940	0.17491D-15	0.12519D-15
32	a	124.29	YES	0.028480	0.022838	0.15175D-13	0.61536D-15		80	a	289.46	YES	0.000092	0.007630	0.21972D-16	0.16452D-16
33	a	129.63	YES	0.001377	0.026660	0.10685D-14	0.77806D-15		81	a	327.47	YES	-0.003525	0.027532	0.27867D-15	0.17646D-15
34	a	131.64	YES	-0.019095	0.016014	0.61906D-14	0.27318D-15		82	a	328.68	YES	0.001786	0.037742	0.45070D-15	0.32971D-15
35	a	133.39	YES	-0.000153	0.026505	0.97511D-15	0.73106D-15		83	a	331.31	YES	0.000243	0.040016	0.48832D-15	0.36609D-15
36	a	136.16	YES	0.014650	0.022190	0.38894D-14	0.49409D-15		84	a	348.59	YES	0.000222	0.057254	0.92391D-15	0.69281D-15
37	a	140.12	YES	0.006982	0.030870	0.19098D-14	0.90911D-15		85	a	359.14	YES	0.001193	0.096876	0.25307D-14	0.18948D-14
38	a	142.85	YES	-0.009031	0.031721	0.23653D-14	0.92791D-15		86	a	361.06	YES	0.000365	0.092572	0.22886D-14	0.17161D-14
39	a	146.10	YES	-0.005352	0.019462	0.82857D-15	0.33577D-15		87	a	371.16	YES	-0.000416	0.080611	0.16640D-14	0.12477D-14
40	a	153.10	YES	-0.004798	0.021670	0.79355D-15	0.38362D-15		88	a	373.00	YES	-0.000335	0.114444	0.33281D-14	0.24958D-14
41	a	154.91	YES	-0.002075	0.016411	0.33911D-15	0.21555D-15		89	a	375.98	YES	-0.000131	0.113529	0.32354D-14	0.24265D-14
42	a	157.05	YES	0.000947	0.016112	0.28102D-15	0.20289D-15		90	a	379.41	YES	-0.001062	0.099919	0.24750D-14	0.18539D-14
43	a	158.34	YES	-0.000167	0.025592	0.67320D-15	0.50466D-15		91	a	382.28	YES	-0.000855	0.144645	0.51232D-14	0.38409D-14
44	a	160.11	YES	0.001237	0.020372	0.43560D-15	0.31368D-15		92	a	496.04	YES	-0.041056	0.004959	0.31542D-14	0.30644D-17
45	a	160.60	YES	0.000638	0.013338	0.18292D-15	0.13375D-15		93	a	545.07	YES	-0.003987	0.020607	0.87396D-16	0.46121D-16
46	a	163.14	YES	-0.001318	0.006350	0.58399D-16	0.29499D-16		94	a	545.45	YES	0.000145	0.021650	0.67842D-16	0.50856D-16
47	a	169.81	YES	0.001119	0.024324	0.55151D-15	0.40401D-15		95	a	545.81	YES	0.000496	0.039508	0.22599D-15	0.16919D-15
48	a	170.47	YES	-0.002256	0.005935	0.83658D-16	0.23890D-16		96	a	546.21	YES	-0.000592	0.060108	0.52217D-15	0.39120D-15
49	a	171.71	YES	0.003251	0.026325	0.72520D-15	0.46426D-15		97	a	546.74	YES	0.002382	0.033265	0.16874D-15	0.11965D-15
50	a	173.25	YES	-0.000085	0.017414	0.26683D-15	0.20007D-15		98	a	547.07	YES	-0.002550	0.054953	0.44552D-15	0.32624D-15
51	a	174.42	YES	-0.002616	0.024886	0.60548D-15	0.40389D-15		99	a	547.47	YES	0.002925	0.042260	0.27082D-15	0.19273D-15

100	a	548.30	YES	-0.005772	0.045327	0.34879D-15	0.22123D-15
101	a	549.96	YES	0.001865	0.045134	0.29679D-15	0.21840D-15
102	a	550.25	YES	-0.002669	0.041324	0.25537D-15	0.18294D-15
103	a	551.17	YES	-0.001366	0.031983	0.14875D-15	0.10932D-15
104	a	552.11	YES	0.000761	0.036456	0.18984D-15	0.14169D-15
105	a	569.47	YES	-0.002137	0.053754	0.39969D-15	0.29453D-15
106	a	570.59	YES	-0.001512	0.080030	0.87150D-15	0.65101D-15
107	a	571.17	YES	0.015221	0.051535	0.71211D-15	0.26955D-15
108	a	573.73	YES	0.007663	0.041596	0.32147D-15	0.17448D-15
109	a	577.87	YES	-0.001514	0.053404	0.38294D-15	0.28463D-15
110	a	578.45	YES	0.001255	0.057304	0.43868D-15	0.32724D-15
111	a	580.03	YES	-0.002601	0.050390	0.34613D-15	0.25204D-15
112	a	580.93	YES	0.004885	0.033685	0.18530D-15	0.11238D-15
113	a	595.02	YES	0.001498	0.021276	0.60962D-16	0.43307D-16
114	a	595.42	YES	0.001828	0.023328	0.74145D-16	0.52016D-16
115	a	595.77	YES	-0.006175	0.022117	0.11691D-15	0.46715D-16
116	a	599.64	YES	-0.089615	0.004928	0.11400D-13	0.22981D-17
117	a	798.34	YES	0.000693	0.016898	0.24281D-16	0.17873D-16
118	a	798.89	YES	0.000022	0.021685	0.39209D-16	0.29407D-16
119	a	799.37	YES	0.001052	0.033767	0.96021D-16	0.71238D-16
120	a	800.69	YES	0.000207	0.029609	0.72894D-16	0.54641D-16
121	a	809.28	YES	0.000576	0.005245	0.25558D-17	0.16882D-17
122	a	809.95	YES	0.000263	0.005403	0.24498D-17	0.17896D-17
123	a	810.20	YES	-0.000189	0.011267	0.10403D-16	0.77775D-17
124	a	812.12	YES	-0.000334	0.026412	0.56893D-16	0.42593D-16
125	a	925.15	YES	-0.000138	0.019492	0.25545D-16	0.19148D-16
126	a	926.23	YES	0.002269	0.019030	0.28178D-16	0.18220D-16
127	a	926.95	YES	0.002263	0.022443	0.37609D-16	0.25313D-16
128	a	928.43	YES	-0.000898	0.016823	0.19524D-16	0.14188D-16
129	a	932.14	YES	0.000239	0.020528	0.28045D-16	0.21002D-16
130	a	933.03	YES	-0.000276	0.011503	0.88375D-17	0.65854D-17
131	a	934.02	YES	-0.000030	0.019393	0.24917D-16	0.18687D-16
132	a	935.44	YES	0.000456	0.024343	0.39323D-16	0.29376D-16
133	a	988.03	YES	0.002164	0.036093	0.82527D-16	0.59490D-16
134	a	988.51	YES	-0.000662	0.037180	0.84407D-16	0.63080D-16
135	a	989.51	YES	-0.002266	0.054497	0.18394D-15	0.13532D-15
136	a	989.76	YES	-0.001120	0.074581	0.33865D-15	0.25334D-15
137	a	993.71	YES	-0.007211	0.035424	0.11106D-15	0.56812D-16
138	a	994.94	YES	0.010756	0.033640	0.14661D-15	0.51137D-16
139	a	995.77	YES	-0.006537	0.028313	0.77163D-16	0.36179D-16
140	a	996.46	YES	-0.006790	0.024751	0.68007D-16	0.27619D-16
141	a	997.63	YES	-0.011292	0.023650	0.11963D-15	0.25173D-16
142	a	998.06	YES	0.005619	0.040173	0.11808D-15	0.72584D-16
143	a	998.91	YES	0.005045	0.031352	0.76016D-16	0.44151D-16
144	a	1000.17	YES	-0.002291	0.014371	0.15876D-16	0.92590D-17
145	a	1007.32	YES	-0.000138	0.013204	0.10322D-16	0.77322D-17
146	a	1007.67	YES	-0.003610	0.013049	0.18729D-16	0.75482D-17
147	a	1008.53	YES	-0.000564	0.011417	0.79046D-17	0.57699D-17
148	a	1009.51	YES	-0.002479	0.002709	0.45056D-17	0.32427D-18
149	a	1010.46	YES	-0.000940	0.016045	0.15737D-16	0.11364D-16
150	a	1011.12	YES	0.005604	0.006883	0.23561D-16	0.20893D-17
151	a	1011.75	YES	-0.001154	0.010533	0.73963D-17	0.48875D-17
152	a	1012.04	YES	0.004047	0.010181	0.16905D-16	0.45643D-17
153	a	1045.49	YES	-0.000624	0.018527	0.19423D-16	0.14384D-16
154	a	1046.59	YES	-0.000876	0.018235	0.19029D-16	0.13911D-16
155	a	1047.39	YES	-0.001723	0.018029	0.19970D-16	0.13583D-16
156	a	1047.74	YES	0.001168	0.014994	0.13374D-16	0.93900D-17
157	a	1048.14	YES	-0.000135	0.011113	0.68845D-17	0.51549D-17
158	a	1049.06	YES	0.000845	0.040175	0.90152D-16	0.67279D-16
159	a	1049.72	YES	-0.000464	0.028676	0.45792D-16	0.34244D-16
160	a	1051.35	YES	-0.000536	0.039435	0.86320D-16	0.64606D-16
161	a	1070.33	YES	0.000658	0.018381	0.18470D-16	0.13656D-16
162	a	1070.93	YES	-0.000372	0.018171	0.17862D-16	0.13334D-16
163	a	1072.09	YES	0.000599	0.023579	0.30100D-16	0.22413D-16
164	a	1073.43	YES	-0.001145	0.022271	0.27401D-16	0.19957D-16
165	a	1165.78	YES	0.004996	0.007776	0.16087D-16	0.21381D-17

166	a	1165.99	YES	-0.002511	0.007614	0.60758D-17	0.20492D-17
167	a	1166.88	YES	-0.004969	0.012675	0.20637D-16	0.56719D-17
168	a	1167.55	YES	-0.000138	0.025110	0.29665D-16	0.22241D-16
169	a	1168.03	YES	-0.002352	0.017091	0.16654D-16	0.10297D-16
170	a	1168.50	YES	0.003465	0.019187	0.23635D-16	0.12969D-16
171	a	1168.98	YES	0.005916	0.018733	0.34953D-16	0.12354D-16
172	a	1169.45	YES	0.003663	0.022956	0.31804D-16	0.18542D-16
173	a	1336.68	YES	0.000866	0.063879	0.15429D-15	0.11548D-15
174	a	1337.49	YES	-0.000091	0.050467	0.96007D-16	0.72003D-16
175	a	1338.05	YES	0.000671	0.035963	0.48908D-16	0.36538D-16
176	a	1338.82	YES	-0.000301	0.089792	0.30345D-15	0.22756D-15
177	a	1339.55	YES	-0.007572	0.084458	0.29244D-15	0.20114D-15
178	a	1340.02	YES	0.002921	0.097616	0.36166D-15	0.26854D-15
179	a	1340.76	YES	-0.003165	0.103452	0.40600D-15	0.30133D-15
180	a	1341.13	YES	-0.004244	0.082398	0.26237D-15	0.19107D-15
181	a	1342.26	YES	-0.001173	0.101577	0.38719D-15	0.28996D-15
182	a	1343.28	YES	-0.003335	0.048132	0.91378D-16	0.65022D-16
183	a	1344.28	YES	-0.000913	0.114346	0.48904D-15	0.36652D-15
184	a	1344.81	YES	0.005113	0.027730	0.39707D-16	0.21541D-16
185	a	1345.82	YES	-0.005786	0.102932	0.40929D-15	0.29643D-15
186	a	1346.68	YES	-0.003499	0.090284	0.30888D-15	0.22781D-15
187	a	1347.09	YES	0.002937	0.090373	0.30780D-15	0.22814D-15
188	a	1347.50	YES	-0.002526	0.112756	0.47596D-15	0.35497D-15
189	a	1349.06	YES	-0.004934	0.110990	0.46787D-15	0.34327D-15
190	a	1350.19	YES	0.003333	0.152967	0.87278D-15	0.65111D-15
191	a	1350.61	YES	0.000613	0.136470	0.69077D-15	0.51796D-15
192	a	1352.42	YES	0.015244	0.028423	0.12661D-15	0.22418D-16
193	a	1386.45	YES	-0.011354	0.067587	0.21351D-15	0.12154D-15
194	a	1387.31	YES	-0.005863	0.063165	0.15510D-15	0.10605D-15
195	a	1388.61	YES	-0.001294	0.035184	0.44467D-16	0.32850D-16
196	a	1388.86	YES	0.011874	0.058244	0.17610D-15	0.89994D-16
197	a	1389.70	YES	0.003308	0.063926	0.14875D-15	0.10830D-15
198	a	1390.30	YES	-0.000173	0.053523	0.10116D-15	0.75862D-16
199	a	1390.82	YES	-0.004544	0.121553	0.52956D-15	0.39102D-15
200	a	1391.52	YES	0.002034	0.036009	0.47356D-16	0.34286D-16
201	a	1393.74	YES	-0.002424	0.104527	0.38648D-15	0.28812D-15
202	a	1394.44	YES	0.001029	0.064356	0.14592D-15	0.10913D-15
203	a	1395.62	YES	0.002921	0.116558	0.47995D-15	0.35744D-15
204	a	1397.09	YES	-0.000102	0.064246	0.14454D-15	0.10840D-15
205	a	1397.33	YES	0.011146	0.078636	0.26540D-15	0.16235D-15
206	a	1398.71	YES	-0.005648	0.049574	0.98430D-16	0.64416D-16
207	a	1399.55	YES	0.007424	0.030709	0.54570D-16	0.24693D-16
208	a	1400.75	YES	-0.000935	0.076449	0.20408D-15	0.15281D-15
209	a	1401.52	YES	-0.003635	0.049808	0.91580D-16	0.64803D-16
210	a	1402.08	YES	-0.009002	0.041280	0.91037D-16	0.44482D-16
211	a	1402.54	YES	0.001913	0.076453	0.20475D-15	0.15249D-15
212	a	1403.53	YES	-0.010298	0.106398	0.43476D-15	0.29498D-15
213	a	1403.99	YES	0.012113	0.035705	0.10158D-15	0.33201D-16
214	a	1404.59	YES	0.002206	0.037378	0.50377D-16	0.36358D-16
215	a	1404.97	YES	-0.008269	0.061800	0.15914D-15	0.99345D-16
216	a	1405.52	YES	-0.003899	0.081875	0.23826D-15	0.17425D-15
217	a	1406.23	YES	-0.022492	0.119064	0.68799D-15	0.36818D-15
218	a	1407.13	YES	0.006290	0.104369	0.39219D-15	0.28260D-15
219	a	1407.25	YES	-0.003142	0.082655	0.24013D-15	0.17722D-15
220	a	1407.70	YES	-0.005992	0.075666	0.21187D-15	0.14843D-15
221	a	1407.80	YES	-0.001033	0.056281	0.10990D-15	0.82111D-16
222	a	1408.89	YES	0.007268	0.081178	0.24798D-15	0.17060D-15
223	a	1411.29	YES	-0.000309	0.057412	0.11348D-15	0.85081D-16
224	a	1413.13	YES	0.004593	0.119636	0.49965D-15	0.36862D-15
225	a	1415.00	YES	-0.000059	0.127129	0.55374D-15	0.41530D-15
226	a	1415.90	YES	0.009497	0.118863	0.51827D-15	0.36265D-15
227	a	1419.52	YES	0.005446	0.119367	0.49688D-15	0.36413D-15
228	a	1420.72	YES	0.003216	0.193253	0.12747D-14	0.95305D-15
229	a	1422.89	YES	0.014675	0.130641	0.66140D-15	0.43439D-15
230	a	1423.75	YES	0.013477	0.070960	0.23997D-15	0.12803D-15
231	a	1424.12	YES	-0.002957	0.164276	0.91779D-15	0.68584D-15

232	a	1424.92	YES	-0.038632	0.045860	0.63959D-15	0.53397D-16
233	a	1434.28	YES	0.084859	0.144012	0.34059D-14	0.52066D-15
234	a	1434.92	YES	0.092431	0.129124	0.37724D-14	0.41824D-15
235	a	1435.98	YES	0.056162	0.136076	0.18039D-14	0.46390D-15
236	a	1436.35	YES	-0.078973	0.115619	0.27891D-14	0.33476D-15
237	a	1445.49	YES	-0.015423	0.143439	0.76785D-15	0.50961D-15
238	a	1445.82	YES	0.001903	0.145604	0.70121D-15	0.52490D-15
239	a	1446.55	YES	-0.000214	0.156461	0.80745D-15	0.60557D-15
240	a	1449.22	YES	0.008102	0.139741	0.66630D-15	0.48152D-15
241	a	1455.79	YES	0.126013	0.066593	0.59720D-14	0.10849D-15
242	a	1456.35	YES	-0.046535	0.149041	0.15183D-14	0.54309D-15
243	a	1457.10	YES	0.038663	0.105955	0.91336D-15	0.27423D-15
244	a	1457.42	YES	0.009989	0.127410	0.56505D-15	0.39638D-15
245	a	1486.42	YES	0.004853	0.071936	0.17110D-15	0.12208D-15
246	a	1487.10	YES	0.002721	0.076299	0.18558D-15	0.13722D-15
247	a	1488.18	YES	-0.007174	0.074352	0.19170D-15	0.13014D-15
248	a	1488.72	YES	-0.002265	0.146219	0.67248D-15	0.50300D-15
249	a	1505.00	YES	0.002797	0.078273	0.19124D-15	0.14140D-15
250	a	1505.60	YES	0.007121	0.080588	0.21726D-15	0.14979D-15
251	a	1505.98	YES	-0.004168	0.091143	0.26135D-15	0.19151D-15
252	a	1506.53	YES	0.008819	0.139845	0.62762D-15	0.45056D-15
253	a	2929.01	YES	0.152158	0.229863	0.22338D-14	0.28254D-15
254	a	2929.60	YES	0.196333	0.195065	0.33613D-14	0.20336D-15
255	a	2932.55	YES	-0.209820	0.231011	0.38985D-14	0.28440D-15
256	a	2935.28	YES	0.069046	0.144192	0.52746D-15	0.11051D-15
257	a	2936.84	YES	-0.106706	0.173177	0.11187D-14	0.15917D-15
258	a	2939.04	YES	-0.081151	0.167128	0.72042D-15	0.14793D-15
259	a	2941.67	YES	-0.120940	0.218271	0.14946D-14	0.25169D-15
260	a	2943.08	YES	0.181425	0.224452	0.29591D-14	0.26578D-15
261	a	2944.12	YES	-0.157672	0.220183	0.23061D-14	0.25551D-15
262	a	2944.55	YES	-0.157645	0.208902	0.22705D-14	0.22991D-15
263	a	2946.20	YES	0.087777	0.266676	0.11067D-14	0.37407D-15
264	a	2948.06	YES	0.263083	0.343666	0.62779D-14	0.62013D-15
265	a	2948.62	YES	0.019750	0.279018	0.57543D-15	0.40854D-15
266	a	2951.41	YES	-0.089571	0.268163	0.11317D-14	0.37637D-15
267	a	2951.57	YES	0.196504	0.445426	0.44153D-14	0.10382D-14
268	a	2951.84	YES	-0.231194	0.304876	0.48428D-14	0.48627D-15
269	a	2955.74	YES	-0.149268	0.232752	0.21184D-14	0.28236D-15
270	a	2957.60	YES	0.052146	0.247681	0.63777D-15	0.31917D-15
271	a	2958.27	YES	-0.037294	0.170929	0.31102D-15	0.15191D-15
272	a	2958.49	YES	0.304871	0.294229	0.78475D-14	0.45002D-15
273	a	3007.26	YES	-0.037119	0.354061	0.93171D-15	0.62189D-15
274	a	3007.37	YES	-0.083682	0.236395	0.89063D-15	0.27720D-15
275	a	3007.95	YES	0.035969	0.327287	0.80426D-15	0.53104D-15
276	a	3009.10	YES	0.015796	0.309296	0.65019D-15	0.47374D-15
277	a	3009.11	YES	-0.057166	0.275657	0.74447D-15	0.37629D-15
278	a	3009.30	YES	0.066687	0.240801	0.71307D-15	0.28709D-15
279	a	3009.51	YES	0.087497	0.273079	0.10606D-14	0.36914D-15
280	a	3010.00	YES	0.077788	0.259180	0.89225D-15	0.33237D-15
281	a	3014.54	YES	0.070588	0.254579	0.79391D-15	0.31928D-15
282	a	3014.80	YES	-0.064311	0.219878	0.62303D-15	0.23811D-15
283	a	3015.54	YES	0.066529	0.223800	0.65543D-15	0.24651D-15
284	a	3017.75	YES	-0.037099	0.319726	0.77079D-15	0.50205D-15
285	a	3022.17	YES	0.014264	0.205320	0.28981D-15	0.20616D-15
286	a	3023.35	YES	-0.007663	0.250041	0.41152D-15	0.30541D-15
287	a	3025.26	YES	-0.014115	0.216882	0.32038D-15	0.22936D-15
288	a	3027.67	YES	-0.007748	0.216944	0.30966D-15	0.22896D-15
289	a	3029.27	YES	-0.005377	0.228878	0.34137D-15	0.25445D-15
290	a	3031.12	YES	-0.002809	0.244487	0.38701D-15	0.28983D-15
291	a	3032.78	YES	-0.004645	0.240058	0.37353D-15	0.27898D-15
292	a	3033.13	YES	-0.003905	0.262584	0.44601D-15	0.33368D-15
293	a	3050.60	YES	0.005660	0.190584	0.23277D-15	0.17286D-15
294	a	3054.53	YES	-0.010745	0.114532	0.91134D-16	0.62193D-16
295	a	3054.75	YES	0.003584	0.292765	0.54263D-15	0.40629D-15
296	a	3055.89	YES	0.006311	0.234021	0.34859D-15	0.25932D-15
297	a	3057.41	YES	-0.002398	0.206639	0.26959D-15	0.20189D-15

298 a 3057.91 YES 0.001058 0.191082 0.23015D-15 0.17255D-15

299 a 3057.94 YES 0.002801 0.218081 0.30023D-15 0.22475D-15

300 a 3058.90 YES 0.002266 0.204194 0.26284D-15 0.19686D-15

301 a 3070.93 YES -0.008336 0.154757 0.15391D-15 0.11178D-15

302 a 3071.73 YES 0.005325 0.159490 0.16016D-15 0.11863D-15

303 a 3072.09 YES 0.009315 0.149404 0.14482D-15 0.10407D-15

304 a 3072.99 YES 0.001719 0.213265 0.28268D-15 0.21186D-15

305 a 3073.97 YES 0.003959 0.231546 0.33376D-15 0.24950D-15

306 a 3076.36 YES -0.004546 0.116885 0.86019D-16 0.63434D-16

307 a 3076.63 YES 0.000074 0.159136 0.15674D-15 0.11755D-15

308 a 3077.98 YES -0.007109 0.112334 0.81514D-16 0.58500D-16

309 a 3078.46 YES 0.010168 0.149128 0.14459D-15 0.10305D-15

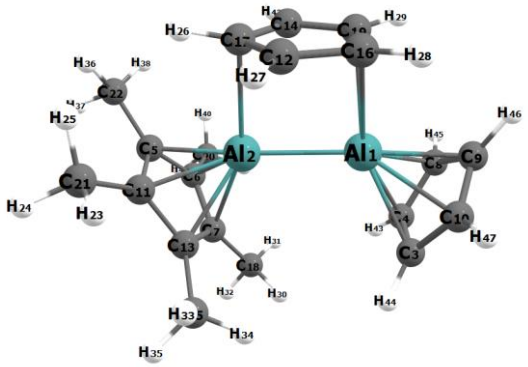
310 a 3080.89 YES 0.002673 0.142230 0.12519D-15 0.93520D-16

311 a 3081.49 YES 0.000939 0.138089 0.11753D-15 0.88103D-16

312 a 3082.15 YES 0.001192 0.136331 0.11452D-15 0.85819D-16

$end

[Cp(AlCp)(AlCp*)]$^{+}$



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

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Al 3.1007867 6.8161640 14.6753197

C 2.1870319 2.8770634 14.2896553

C 2.4102487 2.9523485 15.6917311

C 4.6266638 8.3579784 14.8708360

C 5.0753261 7.1871057 15.5968233

C 5.2486101 6.1153153 14.6478738

C 1.1529181 3.2004946 16.3330722

C 0.1420859 3.2558765 15.3153504

C 0.7882206 3.0758609 14.0465342

C 4.4891862 7.9912889 13.4784071

C 0.5525468 7.5500496 13.7932734

C 4.8744097 6.5992725 13.3474390

C 0.8820479 7.7192079 16.0878611

C 4.9199696 5.8176216 12.0663801

C -0.2163402 6.5405337 14.4216656

C 1.2607808 8.2627816 14.8154440

C 5.7274944 4.7304174 14.9674536

C -0.0107018 6.6465018 15.8532762

C 5.3997631 7.1386214 17.0625120

C 4.1071515 8.9114412 12.3549906

C 4.4350180 9.7277287 15.4521918

H 3.6347732 8.3661950 11.5155409

H 5.0052118 9.4220266 11.9485487

H 3.4059564 9.7036706 12.6822623

H 1.8031734 9.2066998 14.6691688

H 0.5915335 7.7553552 12.7158730

H -0.9552066 5.8981019 13.9230071

H -0.5615209 6.0932849 16.6262794

H 5.2817949 3.9720851 14.2949913

H 5.4950971 4.4447586 16.0114997

H 6.8292482 4.6593641 14.8501122

H 4.1650318 6.1690760 11.3370173

H 4.7503950 4.7368527 12.2367222

H 5.9138638 5.9187271 11.5821863

H 3.7855188 10.3622902 14.8191762

H 5.4111773 10.2503493 15.5330954

H 3.9993660 9.6967859 16.4700003

H 5.2567784 6.1259644 17.4859253

H 4.7786184 7.8426413 17.6488796

H 6.4603850 7.4181447 17.2346578

H 1.2159621 8.0773091 17.0700792

H 3.3799906 2.8740483 16.1964968

H 2.9521486 2.7269832 13.5188232

H 0.9845530 3.2978905 17.4127526

H -0.9323441 3.4050962 15.4785914

H 0.2925065 3.0604165 13.0680093

SCF energy GEOOPT = -1261.354398072 H

ZPE = 997.6 kJ/mol

FREEH energy = 1064.72 kJ/mol

FREEH entropy = 0.73189 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules
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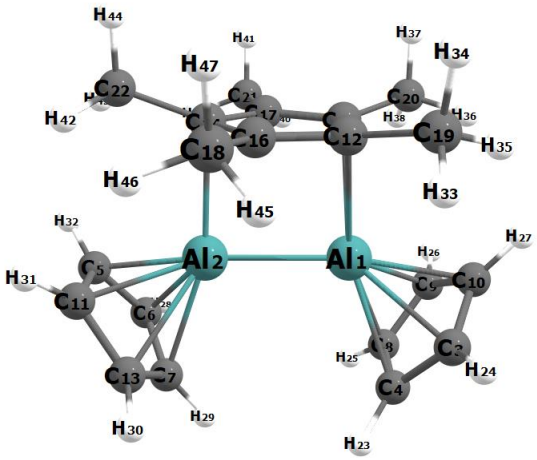
1		-0.00	0.00000	- -
2		-0.00	0.00000	- -

3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	13.26	0.01671	YES	YES
8	a	19.01	0.15514	YES	YES
9	a	34.96	0.10722	YES	YES
10	a	61.61	0.09136	YES	YES
11	a	65.22	0.26618	YES	YES
12	a	80.36	0.73937	YES	YES
13	a	96.13	0.02349	YES	YES
14	a	103.47	0.62963	YES	YES
15	a	108.17	1.63657	YES	YES
16	a	112.35	0.82778	YES	YES
17	a	115.56	0.14559	YES	YES
18	a	118.22	0.09325	YES	YES
19	a	131.68	0.27267	YES	YES
20	a	150.12	0.02261	YES	YES
21	a	154.30	0.02401	YES	YES
22	a	164.95	0.02500	YES	YES
23	a	174.93	2.77835	YES	YES
24	a	182.54	0.37201	YES	YES
25	a	220.29	10.62257	YES	YES
26	a	233.78	0.43381	YES	YES
27	a	241.41	0.03380	YES	YES
28	a	251.49	2.25677	YES	YES
29	a	260.24	0.23856	YES	YES
30	a	272.92	0.12498	YES	YES
31	a	277.65	0.19366	YES	YES
32	a	279.45	1.86374	YES	YES
33	a	289.02	1.16169	YES	YES
34	a	337.54	77.83729	YES	YES
35	a	388.93	14.97673	YES	YES
36	a	399.59	0.01383	YES	YES
37	a	445.94	202.37157	YES	YES
38	a	542.77	0.01457	YES	YES
39	a	543.84	0.04286	YES	YES
40	a	544.72	0.07099	YES	YES
41	a	557.49	0.12278	YES	YES
42	a	567.51	26.06923	YES	YES
43	a	573.94	56.17505	YES	YES
44	a	587.58	2.24837	YES	YES
45	a	590.37	0.86453	YES	YES
46	a	591.61	0.21030	YES	YES
47	a	604.83	0.34312	YES	YES
48	a	613.49	0.59311	YES	YES
49	a	753.62	2.50649	YES	YES
50	a	780.92	202.03453	YES	YES
51	a	787.64	7.17205	YES	YES
52	a	795.55	2.97458	YES	YES
53	a	797.84	9.32524	YES	YES
54	a	803.16	78.63153	YES	YES
55	a	807.97	1.29621	YES	YES
56	a	816.92	0.74133	YES	YES
57	a	819.22	30.48822	YES	YES
58	a	826.72	152.10760	YES	YES
59	a	829.75	0.17354	YES	YES
60	a	834.29	10.74649	YES	YES
61	a	870.22	0.21236	YES	YES
62	a	877.76	5.38733	YES	YES
63	a	891.54	0.17895	YES	YES
64	a	896.07	1.80157	YES	YES
65	a	919.74	0.36200	YES	YES
66	a	924.71	0.17884	YES	YES
67	a	984.26	10.76901	YES	YES
68	a	989.64	15.98644	YES	YES
69	a	991.51	12.75909	YES	YES
70	a	996.72	1.18672	YES	YES
71	a	997.54	15.12880	YES	YES
72	a	998.01	1.33172	YES	YES
73	a	1000.39	0.72030	YES	YES
74	a	1001.38	15.98756	YES	YES
75	a	1006.46	4.80026	YES	YES
76	a	1042.17	2.35854	YES	YES
77	a	1044.52	1.86209	YES	YES
78	a	1045.96	0.00676	YES	YES
79	a	1047.42	1.60098	YES	YES
80	a	1047.99	2.17081	YES	YES
81	a	1049.01	2.05715	YES	YES
82	a	1074.10	0.04944	YES	YES
83	a	1118.02	12.68477	YES	YES
84	a	1120.65	5.58374	YES	YES
85	a	1162.24	0.18292	YES	YES
86	a	1163.20	0.05686	YES	YES
87	a	1228.85	0.05140	YES	YES
88	a	1232.11	0.02970	YES	YES
89	a	1342.52	0.27094	YES	YES
90	a	1343.92	0.64195	YES	YES
91	a	1350.21	9.93637	YES	YES
92	a	1351.86	8.54395	YES	YES
93	a	1355.02	1.75068	YES	YES
94	a	1364.28	0.03450	YES	YES
95	a	1368.12	0.98803	YES	YES
96	a	1374.06	1.07023	YES	YES
97	a	1374.65	1.44983	YES	YES
98	a	1385.04	0.57413	YES	YES

99	a	1387.70	0.14043	YES	YES
100	a	1398.26	12.22196	YES	YES
101	a	1398.95	12.85225	YES	YES
102	a	1402.93	1.25707	YES	YES
103	a	1405.16	0.35251	YES	YES
104	a	1405.56	6.63083	YES	YES
105	a	1408.51	3.15164	YES	YES
106	a	1408.68	14.27465	YES	YES
107	a	1410.90	52.15769	YES	YES
108	a	1416.79	2.02594	YES	YES
109	a	1420.32	5.19817	YES	YES
110	a	1429.10	3.55252	YES	YES
111	a	1434.01	2.13235	YES	YES
112	a	1438.49	8.28710	YES	YES
113	a	1446.14	0.59183	YES	YES
114	a	1446.62	1.28231	YES	YES
115	a	1475.21	14.59145	YES	YES
116	a	1482.93	9.71270	YES	YES
117	a	2968.98	19.49111	YES	YES
118	a	2969.55	9.43452	YES	YES
119	a	2970.02	9.08793	YES	YES
120	a	2970.20	11.88844	YES	YES
121	a	2970.89	8.11956	YES	YES
122	a	3042.77	5.01986	YES	YES
123	a	3043.38	4.66428	YES	YES
124	a	3045.15	2.80279	YES	YES
125	a	3046.02	1.18874	YES	YES
126	a	3047.32	1.44018	YES	YES
127	a	3069.86	2.15566	YES	YES
128	a	3070.33	0.45503	YES	YES
129	a	3070.65	13.60112	YES	YES
130	a	3070.99	6.92553	YES	YES
131	a	3073.24	7.13344	YES	YES
132	a	3142.11	0.26245	YES	YES
133	a	3142.44	0.69303	YES	YES
134	a	3153.38	2.44521	YES	YES
135	a	3162.26	1.49078	YES	YES
136	a	3164.73	0.35806	YES	YES
137	a	3167.24	1.16612	YES	YES
138	a	3168.96	0.12044	YES	YES
139	a	3177.63	4.69697	YES	YES
140	a	3179.33	4.92097	YES	YES
141	a	3188.99	0.17572	YES	YES

$end

[Cp(AlCp)(AlCp*)]$^{+}$ - bridging Cp*



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

Al	-0.1490952	-1.8307252	0.1911612
Al	-0.2302522	0.6013715	-0.1395434
C	1.2030027	-3.4620560	-0.5564173
C	2.0970542	-2.5456606	0.0812585
C	-0.0021079	2.7329186	0.3190932
C	1.0097142	2.0760642	1.0977418
C	1.9391549	1.4746608	0.2007267
C	1.7346132	-2.4475803	1.4513080
C	0.6118127	-3.3059215	1.6821605
C	0.2927374	-3.9539651	0.4399344
C	0.3043529	2.5143030	-1.0684232
C	-2.1912993	-1.8576141	-1.0841004
C	1.5041837	1.7278785	-1.1313920
C	-2.4976550	0.3831108	-0.5269971
C	-2.4952343	-1.7751845	0.3472131
C	-2.1952492	-0.5343413	-1.6099149
C	-2.6824071	-0.3980122	0.6755834
C	-2.0402946	-0.1701713	-3.0564605
C	-2.1891596	-3.1074926	-1.9265998
C	-2.9254640	-2.9195650	1.2328772
C	-3.1079433	0.1293359	2.0123643
C	-3.0534529	1.7775217	-0.7226154
H	2.8918635	-1.9799651	-0.4192995
H	1.2269398	-3.7674124	-1.6095744
H	2.2022726	-1.7964837	2.1996178
H	0.1098420	-3.4752180	2.6424795
H	-0.4754899	-4.7205577	0.2902801
H	1.0551633	2.0504568	2.1933789
H	2.8054777	0.8675925	0.4882923
H	1.9941154	1.3846743	-2.0507728
H	-0.2498245	2.9161066	-1.9248115

H	-0.8340388	3.3291191	0.7109627
H	-1.4397038	-3.0646228	-2.7414446
H	-3.1814024	-3.2431622	-2.4069602
H	-1.9951921	-4.0205606	-1.3342122
H	-2.5440644	-3.8963711	0.8830493
H	-4.0335353	-2.9925034	1.2397161
H	-2.6039866	-2.7849645	2.2842994
H	-2.8003078	1.1821996	2.1660424
H	-2.6921385	-0.4702783	2.8455598
H	-4.2147929	0.0998946	2.1151469
H	-2.5641833	2.3232456	-1.5513502
H	-2.9728033	2.3967876	0.1905909
H	-4.1326581	1.7094587	-0.9735790
H	-1.3256407	-0.8367832	-3.5776968
H	-1.6934899	0.8726664	-3.1935478
H	-3.0113030	-0.2566944	-3.5910958

SCF energy GEOOPT = -1261.347320866 H

ZPE = 997.8 kJ/mol

FREEH energy = 1064.73 kJ/mol

FREEH entropy = 0.72470 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
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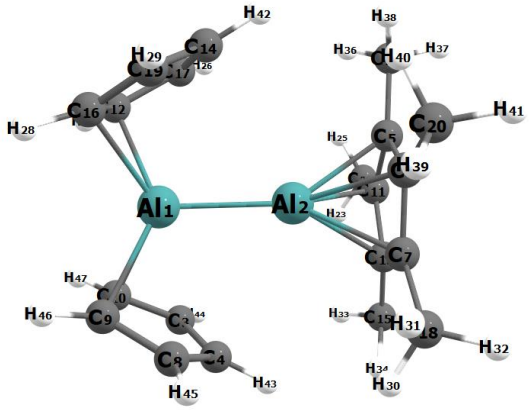
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	13.93	0.04844	YES	YES
8	a	25.58	0.00624	YES	YES
9	a	30.42	0.03878	YES	YES
10	a	59.35	0.12626	YES	YES
11	a	69.11	0.32940	YES	YES
12	a	86.49	0.27789	YES	YES
13	a	93.29	0.10655	YES	YES
14	a	106.57	3.21648	YES	YES
15	a	118.24	0.55066	YES	YES
16	a	121.04	0.27870	YES	YES
17	a	134.96	0.17931	YES	YES
18	a	140.53	0.79319	YES	YES
19	a	141.86	0.04748	YES	YES
20	a	150.52	0.16443	YES	YES
21	a	159.29	1.07871	YES	YES
22	a	187.89	0.57829	YES	YES
23	a	195.24	1.16914	YES	YES
24	a	197.12	0.09080	YES	YES
25	a	214.81	5.02590	YES	YES
26	a	219.59	14.60970	YES	YES
27	a	242.94	0.15736	YES	YES
28	a	249.58	0.13911	YES	YES
29	a	262.10	0.20638	YES	YES
30	a	265.43	0.28307	YES	YES
31	a	268.21	0.01445	YES	YES
32	a	271.19	1.39831	YES	YES
33	a	277.68	0.24847	YES	YES
34	a	341.85	116.10436	YES	YES
35	a	351.29	22.66825	YES	YES
36	a	358.10	13.50027	YES	YES
37	a	418.30	135.45376	YES	YES
38	a	532.57	0.08996	YES	YES
39	a	536.47	4.85667	YES	YES
40	a	540.35	0.03900	YES	YES
41	a	550.49	52.17631	YES	YES
42	a	582.30	0.23144	YES	YES
43	a	584.31	0.86322	YES	YES
44	a	586.25	0.29513	YES	YES
45	a	589.16	1.87133	YES	YES
46	a	590.67	3.73216	YES	YES
47	a	592.03	0.62688	YES	YES
48	a	606.31	13.03948	YES	YES
49	a	790.16	4.68778	YES	YES
50	a	796.30	39.02008	YES	YES
51	a	801.73	12.16428	YES	YES
52	a	803.78	7.80653	YES	YES
53	a	805.40	0.14971	YES	YES
54	a	808.47	0.53793	YES	YES
55	a	815.27	309.80080	YES	YES
56	a	822.78	237.12946	YES	YES
57	a	826.91	0.82733	YES	YES
58	a	827.52	2.05633	YES	YES
59	a	833.82	0.59256	YES	YES
60	a	833.99	0.29782	YES	YES
61	a	880.75	0.67238	YES	YES
62	a	882.84	0.62149	YES	YES
63	a	898.49	2.56385	YES	YES
64	a	899.83	2.25503	YES	YES
65	a	921.34	0.25013	YES	YES
66	a	924.74	0.04059	YES	YES
67	a	976.66	10.19891	YES	YES
68	a	985.08	18.71568	YES	YES
69	a	987.08	7.35878	YES	YES
70	a	988.03	2.53023	YES	YES
71	a	992.23	2.74373	YES	YES

72	a	997.13	22.54177	YES	YES
73	a	998.24	0.86856	YES	YES
74	a	999.02	13.68685	YES	YES
75	a	1000.09	19.72227	YES	YES
76	a	1040.23	0.38395	YES	YES
77	a	1042.87	1.12670	YES	YES
78	a	1043.94	0.46801	YES	YES
79	a	1046.97	1.36002	YES	YES
80	a	1049.82	0.14759	YES	YES
81	a	1050.22	0.13400	YES	YES
82	a	1075.45	0.00429	YES	YES
83	a	1118.86	13.75989	YES	YES
84	a	1120.19	10.25263	YES	YES
85	a	1152.98	0.34036	YES	YES
86	a	1153.67	0.15039	YES	YES
87	a	1230.47	0.03203	YES	YES
88	a	1231.49	0.00083	YES	YES
89	a	1340.34	0.20032	YES	YES
90	a	1341.51	0.11129	YES	YES
91	a	1348.30	10.70823	YES	YES
92	a	1350.20	4.40254	YES	YES
93	a	1350.61	2.13401	YES	YES
94	a	1362.53	0.52279	YES	YES
95	a	1365.01	0.15925	YES	YES
96	a	1367.47	6.66345	YES	YES
97	a	1368.65	0.35914	YES	YES
98	a	1369.17	0.52151	YES	YES
99	a	1380.80	0.66259	YES	YES
100	a	1385.93	13.21145	YES	YES
101	a	1398.17	5.91935	YES	YES
102	a	1399.62	0.94833	YES	YES
103	a	1405.11	2.50680	YES	YES
104	a	1408.20	0.33573	YES	YES
105	a	1408.94	4.58497	YES	YES
106	a	1410.80	2.92554	YES	YES
107	a	1414.43	49.38037	YES	YES
108	a	1422.28	11.16115	YES	YES
109	a	1423.21	2.95397	YES	YES
110	a	1425.34	5.70236	YES	YES
111	a	1427.67	1.19736	YES	YES
112	a	1429.75	1.18072	YES	YES
113	a	1444.39	4.20248	YES	YES
114	a	1448.80	10.34207	YES	YES
115	a	1459.59	3.02149	YES	YES
116	a	1487.75	24.28987	YES	YES
117	a	2957.96	13.71635	YES	YES
118	a	2958.62	11.60066	YES	YES
119	a	2967.26	10.39171	YES	YES
120	a	2969.08	14.38456	YES	YES
121	a	2973.43	12.76643	YES	YES
122	a	3032.24	3.50812	YES	YES
123	a	3032.62	2.89283	YES	YES
124	a	3039.18	2.82898	YES	YES
125	a	3041.51	4.14123	YES	YES
126	a	3048.64	6.46561	YES	YES
127	a	3065.16	3.39454	YES	YES
128	a	3065.69	8.14892	YES	YES
129	a	3078.00	5.07753	YES	YES
130	a	3079.24	5.83515	YES	YES
131	a	3079.50	9.44920	YES	YES
132	a	3165.28	0.13231	YES	YES
133	a	3166.41	0.27617	YES	YES
134	a	3168.82	0.08489	YES	YES
135	a	3168.98	0.20439	YES	YES
136	a	3178.33	4.17128	YES	YES
137	a	3179.07	4.61762	YES	YES
138	a	3181.66	1.40809	YES	YES
139	a	3182.22	2.53973	YES	YES
140	a	3190.08	0.77232	YES	YES
141	a	3190.30	0.16637	YES	YES

$end

TS_I



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

Al	-2.2691635	0.1431954	-0.4294334
Al	0.1345299	-0.0155308	0.0347801
C	-2.0301766	2.7025049	0.4067864
C	-1.0741569	2.8899322	-0.6222942
C	1.7580851	-1.2669582	0.7967661
C	2.0252456	-0.8928715	-0.5744968
C	2.1224329	0.5557881	-0.6321080
C	-1.6007507	2.3796440	-1.8359877
C	-2.9101544	1.8687107	-1.5813332

C	-3.1845466	2.0705451	-0.1577750
C	1.6640353	-0.0544949	1.5820717
C	-3.4119181	-1.5056595	0.4685495
C	1.9117270	1.0693814	0.7026024
C	-1.5505205	-2.7468089	-0.1077507
C	2.0257023	2.4994409	1.1421863
C	-3.3552451	-1.6052622	-0.9896670
C	-2.2886349	-2.2203953	0.9834049
C	2.4586984	1.3646985	-1.8514279
C	-2.1888622	-2.3717357	-1.3157709
C	2.2471503	-1.8355427	-1.7220784
C	1.4693563	0.0188931	3.0689321
C	1.6954884	-2.6610463	1.3471277
H	0.9797161	0.9621357	3.3771498
H	2.4511443	-0.0249750	3.5857479
H	0.8618981	-0.8239143	3.4500556
H	-2.0452817	-2.3292954	2.0483325
H	-4.2604676	-1.1210158	1.0511556
H	-4.1658218	-1.3341334	-1.6811085
H	-1.8601864	-2.6211342	-2.3328090
H	2.0250782	2.3815726	-1.8071970
H	2.0979719	0.8826910	-2.7799035
H	3.5586185	1.4784640	-1.9470306
H	1.2168169	2.7945579	1.8386726
H	2.0145410	3.1972178	0.2849467
H	2.9870611	2.6542351	1.6747940
H	0.8894387	-2.7847872	2.0962020
H	2.6516979	-2.9081896	1.8539262
H	1.5470513	-3.4140977	0.5514063
H	1.9682286	-1.3800899	-2.6912173
H	1.6677485	-2.7714130	-1.6082756
H	3.3189220	-2.1165034	-1.7880083
H	-0.6381115	-3.3495820	-0.0311177
H	-0.0905323	3.3579114	-0.4994604
H	-1.9184592	2.9858572	1.4613496
H	-1.0966778	2.3679724	-2.8108784
H	-3.6466569	1.5658699	-2.3385951
H	-4.1657901	1.9617346	0.3258916

SCF energy GEOOPT = -1261.345558472 H

ZPE = 996.3 kJ/mol

FREEH energy = 1061.43 kJ/mol

FREEH entropy = 0.71765 kJ/mol/K

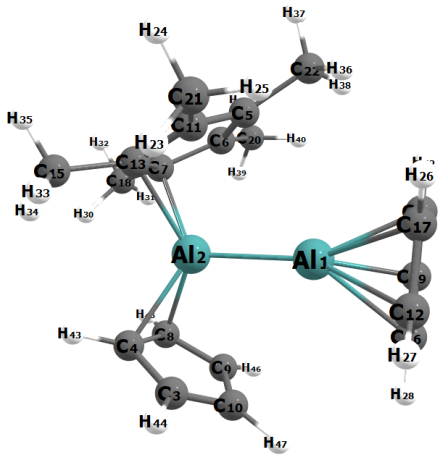
$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1	a	-53.02	0.00000	YES YES
2		-0.00	0.00000	- -
3		-0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7		0.00	0.00000	- -
8	a	10.98	0.01623	YES YES
9	a	23.81	0.17306	YES YES
10	a	25.38	0.04099	YES YES
11	a	56.70	0.98183	YES YES
12	a	81.57	0.49405	YES YES
13	a	91.62	4.91924	YES YES
14	a	96.62	0.89621	YES YES
15	a	108.45	0.18192	YES YES
16	a	113.60	0.01680	YES YES
17	a	119.00	0.23663	YES YES
18	a	139.18	0.02719	YES YES
19	a	145.09	0.68743	YES YES
20	a	149.17	0.20251	YES YES
21	a	161.55	1.81416	YES YES
22	a	162.32	1.70679	YES YES
23	a	165.54	1.05827	YES YES
24	a	178.86	0.38468	YES YES
25	a	199.00	0.32812	YES YES
26	a	203.33	0.50780	YES YES
27	a	214.68	6.39273	YES YES
28	a	226.29	1.05536	YES YES
29	a	265.22	7.00197	YES YES
30	a	265.69	2.90133	YES YES
31	a	276.55	0.14688	YES YES
32	a	287.30	1.17184	YES YES
33	a	289.57	1.78692	YES YES
34	a	402.70	74.80342	YES YES
35	a	405.26	0.82058	YES YES
36	a	408.48	3.23228	YES YES
37	a	470.85	84.21351	YES YES
38	a	542.48	0.04145	YES YES
39	a	544.15	0.10132	YES YES
40	a	545.31	0.01459	YES YES
41	a	560.07	0.14460	YES YES
42	a	583.03	72.66633	YES YES
43	a	586.42	1.06780	YES YES
44	a	587.17	1.58017	YES YES
45	a	598.41	13.06182	YES YES
46	a	602.50	22.75631	YES YES
47	a	610.28	0.57127	YES YES
48	a	610.71	0.14326	YES YES
49	a	744.46	2.33380	YES YES

50	a	761.35	110.66405	YES	YES
51	a	764.86	76.60184	YES	YES
52	a	768.70	3.20271	YES	YES
53	a	789.74	303.10702	YES	YES
54	a	794.24	0.00463	YES	YES
55	a	796.42	2.78550	YES	YES
56	a	810.03	8.07868	YES	YES
57	a	820.69	0.38590	YES	YES
58	a	821.32	0.73088	YES	YES
59	a	822.52	1.32841	YES	YES
60	a	822.83	1.18651	YES	YES
61	a	851.77	0.15200	YES	YES
62	a	866.75	16.16717	YES	YES
63	a	896.02	2.70114	YES	YES
64	a	899.27	1.07336	YES	YES
65	a	917.40	0.14241	YES	YES
66	a	926.42	1.12244	YES	YES
67	a	977.06	16.76469	YES	YES
68	a	983.02	19.48822	YES	YES
69	a	991.98	13.63538	YES	YES
70	a	992.68	12.81586	YES	YES
71	a	996.90	0.26528	YES	YES
72	a	997.38	0.21643	YES	YES
73	a	999.08	15.55827	YES	YES
74	a	999.76	1.76812	YES	YES
75	a	1001.06	1.36957	YES	YES
76	a	1041.12	0.57094	YES	YES
77	a	1044.54	0.32776	YES	YES
78	a	1045.21	3.73666	YES	YES
79	a	1046.50	2.55980	YES	YES
80	a	1048.48	1.64893	YES	YES
81	a	1049.91	2.24525	YES	YES
82	a	1073.95	0.56202	YES	YES
83	a	1120.25	15.28801	YES	YES
84	a	1122.98	3.60254	YES	YES
85	a	1160.08	0.07721	YES	YES
86	a	1161.53	0.05921	YES	YES
87	a	1226.20	0.00079	YES	YES
88	a	1226.86	0.12505	YES	YES
89	a	1341.90	0.92247	YES	YES
90	a	1343.13	0.52287	YES	YES
91	a	1344.06	2.59628	YES	YES
92	a	1348.60	0.37695	YES	YES
93	a	1351.66	11.66288	YES	YES
94	a	1352.27	11.67014	YES	YES
95	a	1356.13	1.01926	YES	YES
96	a	1358.85	0.16030	YES	YES
97	a	1376.11	0.48104	YES	YES
98	a	1381.63	0.84285	YES	YES
99	a	1388.44	0.06111	YES	YES
100	a	1395.41	10.86690	YES	YES
101	a	1396.62	9.01972	YES	YES
102	a	1402.22	2.14250	YES	YES
103	a	1404.11	0.10530	YES	YES
104	a	1408.07	55.36613	YES	YES
105	a	1409.15	19.10456	YES	YES
106	a	1410.16	1.99216	YES	YES
107	a	1411.60	4.62734	YES	YES
108	a	1428.44	11.01373	YES	YES
109	a	1430.32	8.42722	YES	YES
110	a	1432.00	1.62185	YES	YES
111	a	1437.76	1.54900	YES	YES
112	a	1438.35	2.88761	YES	YES
113	a	1442.42	0.11362	YES	YES
114	a	1444.91	1.94876	YES	YES
115	a	1467.46	17.41654	YES	YES
116	a	1476.20	15.08796	YES	YES
117	a	2972.41	9.39514	YES	YES
118	a	2973.79	7.36567	YES	YES
119	a	2974.55	11.70788	YES	YES
120	a	2974.67	1.08111	YES	YES
121	a	2974.94	8.37563	YES	YES
122	a	3048.22	3.42447	YES	YES
123	a	3048.57	3.68958	YES	YES
124	a	3051.00	0.46370	YES	YES
125	a	3052.54	2.26922	YES	YES
126	a	3053.40	0.87597	YES	YES
127	a	3078.34	3.06199	YES	YES
128	a	3078.94	2.70870	YES	YES
129	a	3079.60	6.43564	YES	YES
130	a	3083.06	4.03422	YES	YES
131	a	3084.08	4.48361	YES	YES
132	a	3139.25	1.17063	YES	YES
133	a	3140.75	3.36403	YES	YES
134	a	3146.08	0.84891	YES	YES
135	a	3146.95	4.87471	YES	YES
136	a	3157.66	0.57045	YES	YES
137	a	3158.94	3.86576	YES	YES
138	a	3159.65	0.65139	YES	YES
139	a	3160.34	1.34038	YES	YES
140	a	3176.19	1.04062	YES	YES
141	a	3176.65	0.78847	YES	YES

$end

TS$_{II}$



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

Al	-1.5123299	0.5808615	-0.6504448
Al	0.9137269	0.6315927	-0.3253075
C	0.8086538	3.2841637	-0.7584473
C	1.9737763	2.4517597	-0.7060983
C	-0.2617559	-1.7360650	1.0708447
C	0.7069800	-1.9982023	0.0524397
C	1.8594855	-1.1624078	0.2899426
C	1.9932021	1.6596984	-1.9351658
C	0.8472850	2.0369339	-2.6981348
C	0.1339284	3.0292321	-1.9779526
C	0.2445428	-0.7160797	1.9342236
C	-3.3727273	1.7404052	-0.3701360
C	1.5607911	-0.3437108	1.4853405
C	-3.4031044	-0.5362535	-0.8232167
C	2.5782662	0.4214934	2.2950396
C	-3.1596312	1.5661230	-1.7747494
C	-3.5264583	0.4386589	0.2200076
C	3.2340549	-1.3634015	-0.3015617
C	-3.1663291	0.1612552	-2.0559441
C	0.5890720	-3.0113893	-1.0467367
C	-0.4394227	-0.1554759	3.1452865
C	-1.5317518	-2.5117622	1.2843647
H	-0.1835016	0.9094996	3.3114692
H	-0.1361282	-0.7047496	4.0630071
H	-1.5424222	-0.2363166	3.0784791
H	-3.7123600	0.2315122	1.2808341
H	-3.4136047	2.6980905	0.1633481
H	-2.9989701	2.3657028	-2.5068403
H	-3.0278025	-0.3009490	-3.0412142
H	3.8566232	-0.4482832	-0.2529030
H	3.1878861	-1.6828328	-1.3606630
H	3.7805615	-2.1523782	0.2575040
H	2.1286297	1.2837472	2.8252208
H	3.4114803	0.8051384	1.6749683
H	3.0307377	-0.2389742	3.0651732
H	-2.3390655	-1.8995906	1.7330089
H	-1.3562092	-3.3562629	1.9848111
H	-1.9128487	-2.9601071	0.3461575
H	1.1857192	-2.7299964	-1.9361742
H	-0.4599861	-3.1554628	-1.3732003
H	0.9588948	-4.0047141	-0.7118850
H	-3.4741350	-1.6226381	-0.7016342
H	2.8037189	2.5475147	0.0078555
H	0.5063899	3.9977920	0.0187387
H	2.8296977	1.0382949	-2.2830684
H	0.5739181	1.6179710	-3.6752200
H	-0.7830437	3.5302181	-2.3125787

SCF energy GEOOPT = -1261.337491536 H

ZPE = 996.1 kJ/mol

FREEH energy = 1061.33 kJ/mol

FREEH entropy = 0.72346 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1	a	-78.62	0.00000	YES YES
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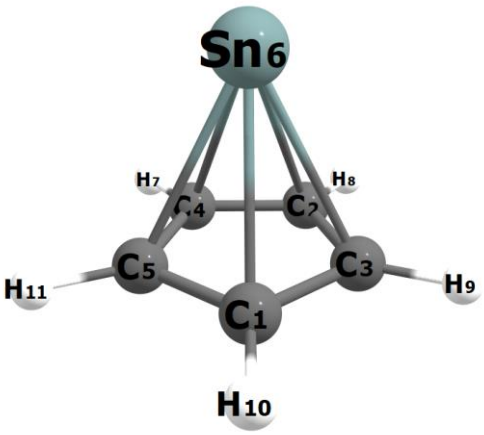
3		-0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7		0.00	0.00000	- -
8	a	7.80	0.03735	YES YES
9	a	20.92	0.00673	YES YES
10	a	24.53	0.02122	YES YES
11	a	53.56	0.41624	YES YES
12	a	83.70	0.00564	YES YES
13	a	88.66	2.10875	YES YES
14	a	94.49	1.66171	YES YES
15	a	95.18	3.87684	YES YES
16	a	100.34	1.07477	YES YES
17	a	109.40	1.46742	YES YES
18	a	124.70	0.17419	YES YES
19	a	140.81	3.14237	YES YES
20	a	156.39	2.08953	YES YES
21	a	164.43	3.27225	YES YES
22	a	172.23	0.81641	YES YES
23	a	173.84	0.14411	YES YES

24	a	185.24	0.51532	YES	YES
25	a	186.59	0.17346	YES	YES
26	a	210.89	1.96873	YES	YES
27	a	240.78	6.36039	YES	YES
28	a	264.97	0.70530	YES	YES
29	a	270.55	0.87164	YES	YES
30	a	277.09	1.63010	YES	YES
31	a	279.29	3.06028	YES	YES
32	a	283.28	1.54447	YES	YES
33	a	299.55	0.26849	YES	YES
34	a	333.53	56.52185	YES	YES
35	a	366.36	1.04684	YES	YES
36	a	397.83	29.29292	YES	YES
37	a	500.34	123.46774	YES	YES
38	a	533.57	0.71189	YES	YES
39	a	538.34	0.39215	YES	YES
40	a	545.44	0.06521	YES	YES
41	a	555.35	23.99026	YES	YES
42	a	566.68	1.77027	YES	YES
43	a	591.35	0.19793	YES	YES
44	a	592.40	0.80257	YES	YES
45	a	593.96	12.01922	YES	YES
46	a	595.12	3.43775	YES	YES
47	a	600.47	16.56537	YES	YES
48	a	632.77	12.75471	YES	YES
49	a	753.72	1.64132	YES	YES
50	a	764.35	103.33769	YES	YES
51	a	790.03	89.26055	YES	YES
52	a	795.32	94.40888	YES	YES
53	a	798.60	3.42658	YES	YES
54	a	811.52	7.36349	YES	YES
55	a	819.26	4.77418	YES	YES
56	a	821.57	1.18561	YES	YES
57	a	822.32	16.33039	YES	YES
58	a	829.34	255.63090	YES	YES
59	a	833.84	11.78840	YES	YES
60	a	834.89	0.67982	YES	YES
61	a	856.66	7.09828	YES	YES
62	a	893.94	1.43798	YES	YES
63	a	895.92	0.53964	YES	YES
64	a	906.25	4.49524	YES	YES
65	a	917.12	2.48440	YES	YES
66	a	928.34	0.25127	YES	YES
67	a	977.94	17.19519	YES	YES
68	a	980.51	18.21173	YES	YES
69	a	982.36	11.94745	YES	YES
70	a	992.45	1.12268	YES	YES
71	a	997.25	6.10353	YES	YES
72	a	997.34	1.38073	YES	YES
73	a	998.61	17.23285	YES	YES
74	a	999.05	14.42009	YES	YES
75	a	1001.06	20.17970	YES	YES
76	a	1042.90	2.90419	YES	YES
77	a	1043.38	1.13304	YES	YES
78	a	1044.04	0.94870	YES	YES
79	a	1045.41	0.32915	YES	YES
80	a	1047.50	1.57168	YES	YES
81	a	1049.04	0.12529	YES	YES
82	a	1076.20	0.03507	YES	YES
83	a	1115.06	12.33087	YES	YES
84	a	1121.86	10.41284	YES	YES
85	a	1154.95	0.17193	YES	YES
86	a	1158.70	0.80287	YES	YES
87	a	1227.10	0.04645	YES	YES
88	a	1230.48	0.01466	YES	YES
89	a	1333.31	0.10405	YES	YES
90	a	1344.47	1.35230	YES	YES
91	a	1347.03	2.08175	YES	YES
92	a	1347.81	0.83701	YES	YES
93	a	1349.87	9.06418	YES	YES
94	a	1353.07	11.22265	YES	YES
95	a	1360.56	0.49013	YES	YES
96	a	1362.20	0.02465	YES	YES
97	a	1364.97	1.47387	YES	YES
98	a	1365.90	1.64198	YES	YES
99	a	1381.73	6.37721	YES	YES
100	a	1396.09	10.98662	YES	YES
101	a	1400.50	7.21511	YES	YES
102	a	1402.37	1.97589	YES	YES
103	a	1406.33	8.38091	YES	YES
104	a	1408.69	18.62288	YES	YES
105	a	1409.24	4.72486	YES	YES
106	a	1410.89	0.70061	YES	YES
107	a	1415.81	24.26784	YES	YES
108	a	1416.54	8.09310	YES	YES
109	a	1420.35	3.12641	YES	YES
110	a	1425.95	10.58185	YES	YES
111	a	1431.22	8.04814	YES	YES
112	a	1438.14	2.72002	YES	YES
113	a	1440.34	0.44160	YES	YES
114	a	1447.19	5.89029	YES	YES
115	a	1484.46	26.01828	YES	YES
116	a	1487.09	4.85038	YES	YES
117	a	2958.68	17.99913	YES	YES
118	a	2960.02	14.39752	YES	YES
119	a	2961.51	21.89747	YES	YES

120	a	2963.02	6.94936	YES	YES
121	a	2964.07	17.38685	YES	YES
122	a	3028.02	12.63563	YES	YES
123	a	3030.59	1.67115	YES	YES
124	a	3032.76	2.18197	YES	YES
125	a	3038.29	0.89619	YES	YES
126	a	3039.48	6.00075	YES	YES
127	a	3060.86	5.41854	YES	YES
128	a	3061.25	9.52572	YES	YES
129	a	3063.66	7.51348	YES	YES
130	a	3065.00	8.93338	YES	YES
131	a	3066.94	5.86878	YES	YES
132	a	3141.13	1.60705	YES	YES
133	a	3145.65	2.22845	YES	YES
134	a	3156.06	0.41135	YES	YES
135	a	3160.27	0.58732	YES	YES
136	a	3170.77	0.66176	YES	YES
137	a	3171.47	1.65531	YES	YES
138	a	3173.12	1.68736	YES	YES
139	a	3181.32	11.11449	YES	YES
140	a	3189.66	9.21118	YES	YES
141	a	3195.49	0.92041	YES	YES

$end

$SnCp^+$



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c5v

Cartesian coordinates in Ångström:

C	0.3779282	-1.1631433	-0.1820724
C	0.3779282	1.1631433	-0.1820724
C	1.2230013	0.0000000	-0.1820724
C	-0.9894288	0.7188621	-0.1820724
C	-0.9894288	-0.7188621	-0.1820724
Sn	0.0000000	0.0000000	2.0082368
H	-1.8773490	1.3639739	-0.2197428
H	0.7170835	2.2069561	-0.2197428
H	2.3205310	0.0000000	-0.2197428
H	0.7170835	-2.2069561	-0.2197428
H	-1.8773490	-1.3639739	-0.2197428

SCF energy GEOOPT = -407.6304541461 H

ZPE = 213.4 kJ/mol

FREEH energy = 227.31 kJ/mol

FREEH entropy = 0.30785 kJ/mol/K

$vibrational spectrum

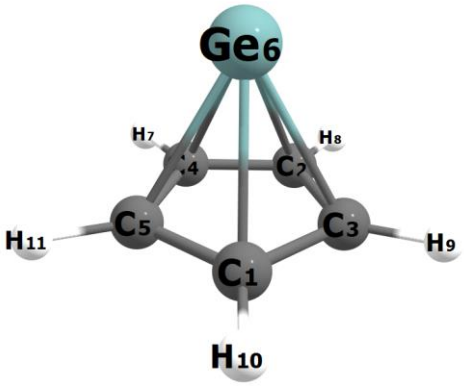
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	e1	248.88	0.59837	YES	YES
8	e1	248.88	0.59837	YES	YES
9	a1	270.78	11.60955	YES	YES
10	e2	572.26	0.00000	NO	YES
11	e2	572.26	0.00000	NO	YES
12	e2	818.60	0.00000	NO	YES
13	e2	818.60	0.00000	NO	YES
14	a1	823.81	143.28950	YES	YES
15	e1	836.25	0.02203	YES	YES
16	e1	836.25	0.02203	YES	YES
17	e2	913.02	0.00000	NO	YES
18	e2	913.02	0.00000	NO	YES
19	e1	994.05	10.92745	YES	YES
20	e1	994.05	10.92745	YES	YES
21	e2	1046.21	0.00000	NO	YES
22	e2	1046.21	0.00000	NO	YES
23	a1	1102.86	15.19297	YES	YES
24	a2	1234.53	0.00000	NO	NO
25	e2	1351.78	0.00000	NO	YES
26	e2	1351.78	0.00000	NO	YES
27	e1	1411.61	24.07434	YES	YES

28	e1	1411.61	24.07434	YES	YES
29	e2	3165.07	0.00000	NO	YES
30	e2	3165.07	0.00000	NO	YES
31	e1	3175.73	31.94414	YES	YES
32	e1	3175.73	31.94414	YES	YES
33	a1	3184.55	0.15702	YES	YES

$end

GeCp$^+$



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

C	0.3776066	-1.1620906	-0.1781900
C	0.3776080	1.1620699	-0.1781382
C	1.2219387	-0.0000136	-0.1781690
C	-0.9885314	0.7181971	-0.1781296
C	-0.9885279	-0.7182209	-0.1781619
Ge	-0.0001246	0.0001128	1.7591742
H	-1.8770533	1.3637835	-0.1737775
H	0.7169482	2.2066307	-0.1738377
H	2.3202320	-0.0000101	-0.1738604
H	0.7169441	-2.2066522	-0.1739023
H	-1.8770503	-1.3638067	-0.1738176

SCF energy GEOOPT = -2270.199503655 H

ZPE = 214.9 kJ/mol

FREEH energy = 228.37 kJ/mol

FREEH entropy = 0.31223 kJ/mol/K

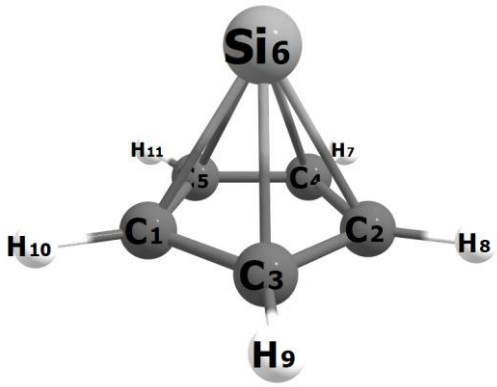
$vibrational spectrum

mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	273.25	0.21174	YES	YES
8	a	273.45	0.21200	YES	YES
9	a	323.32	10.67489	YES	YES
10	a	553.95	0.00000	YES	YES
11	a	554.01	0.00000	YES	YES
12	a	821.05	0.00000	YES	YES
13	a	821.08	0.00011	YES	YES
14	a	847.07	144.29627	YES	YES
15	a	859.58	0.24254	YES	YES
16	a	859.61	0.26766	YES	YES
17	a	924.95	0.00000	YES	YES
18	a	925.19	0.00001	YES	YES
19	a	999.06	10.96530	YES	YES
20	a	999.08	10.97687	YES	YES
21	a	1052.60	0.00002	YES	YES
22	a	1052.70	0.00002	YES	YES
23	a	1109.85	9.71355	YES	YES
24	a	1235.95	0.00000	YES	YES
25	a	1363.46	0.00000	YES	YES
26	a	1363.51	0.00000	YES	YES
27	a	1417.35	26.28315	YES	YES
28	a	1417.37	26.29235	YES	YES
29	a	3167.51	0.00000	YES	YES
30	a	3167.54	0.00026	YES	YES
31	a	3177.28	46.39544	YES	YES
32	a	3177.31	46.38954	YES	YES
33	a	3185.86	0.11816	YES	YES

$end

$SiCp^+$



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c5v

Cartesian coordinates in Ångström:

C	0.3770835	-1.1605437	-0.1788558
C	0.3770835	1.1605437	-0.1788558
C	1.2202678	0.0000000	-0.1788558
C	-0.9872174	0.7172554	-0.1788558
C	-0.9872174	-0.7172554	-0.1788558
Si	0.0000000	0.0000000	1.6382436
H	-1.8755617	1.3626753	-0.1485420
H	0.7164008	2.2048550	-0.1485420
H	2.3183217	0.0000000	-0.1485420
H	0.7164008	-2.2048550	-0.1485420
H	-1.8755617	-1.3626753	-0.1485420

SCF energy GEOOPT = -482.5780354464 H

ZPE = 216.9 kJ/mol

FREEH energy = 229.69 kJ/mol

FREEH entropy = 0.28586 kJ/mol/K

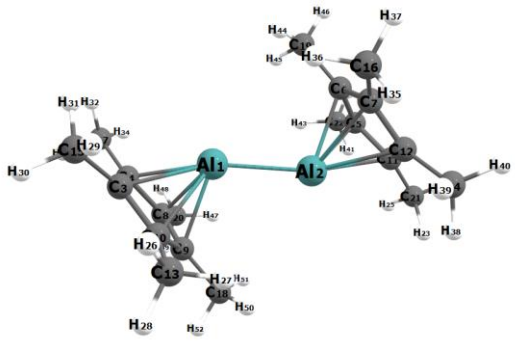
$vibrational spectrum

mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	e1	321.95	0.93417	YES	YES
8	e1	321.95	0.93417	YES	YES
9	a1	464.06	26.47177	YES	YES
10	e2	543.44	0.00000	NO	YES
11	e2	543.44	0.00000	NO	YES
12	e2	824.56	0.00000	NO	YES
13	e2	824.56	0.00000	NO	YES
14	a1	872.74	176.44838	YES	YES
15	e1	873.93	0.97384	YES	YES
16	e1	873.93	0.97384	YES	YES
17	e2	931.62	0.00000	NO	YES
18	e2	931.62	0.00000	NO	YES
19	e1	1003.31	11.06099	YES	YES
20	e1	1003.31	11.06099	YES	YES
21	e2	1056.91	0.00000	NO	YES
22	e2	1056.91	0.00000	NO	YES
23	a1	1118.38	7.84302	YES	YES
24	a2	1235.50	0.00000	NO	NO
25	e2	1370.93	0.00000	NO	YES
26	e2	1370.93	0.00000	NO	YES
27	e1	1422.06	27.34817	YES	YES
28	e1	1422.06	27.34817	YES	YES
29	e2	3167.36	0.00000	NO	YES
30	e2	3167.36	0.00000	NO	YES
31	e1	3176.46	56.44893	YES	YES
32	e1	3176.46	56.44893	YES	YES
33	a1	3184.94	0.08062	YES	YES

$end

[Cp*Al–AlCp*] (triplett)



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

Al	1.0691058	-0.1871613	-0.6166546
Al	-1.0675354	0.1021636	0.6261745
C	3.1672617	-1.0906263	-0.9022764
C	3.1763270	0.2518614	-1.4447097
C	-2.9271975	1.1897522	-0.1862018
C	-2.7173492	-0.0305098	-0.9198488
C	-2.8758886	-1.1360052	-0.0086467
C	2.9131377	1.1663534	-0.3677952
C	2.7114283	0.3949271	0.8304699
C	2.8866894	-0.9978093	0.5035673
C	-3.1786996	0.8445619	1.1859327
C	-3.1549404	-0.5990342	1.2943593
C	2.7687340	-2.1365566	1.4742314
C	-3.4092758	-1.3901616	2.5443766
C	3.4376087	-2.3501847	-1.6727939
C	-2.7480324	-2.5861218	-0.3743180
C	3.4710650	0.6167108	-2.8712006
C	2.4094812	0.9534578	2.1908014
C	-2.4233873	-0.1289807	-2.3887038
C	2.8021038	2.6601369	-0.4545999
C	-3.4756817	1.8009132	2.3048419
C	-2.8316059	2.5682869	-0.7707374
H	-3.1120651	1.4184080	3.2792345
H	-4.5688773	1.9735488	2.4083369
H	-2.9996431	2.7871298	2.1386192
H	2.7147529	-3.1105609	0.9514593
H	1.8511294	-2.0461202	2.0933555
H	3.6395185	-2.1726507	2.1631215
H	2.8932830	-3.2157114	-1.2457975
H	4.5199212	-2.6034933	-1.6678826
H	3.1286706	-2.2560732	-2.7327837
H	3.1174924	-0.1623309	-3.5755244
H	4.5631776	0.7383417	-3.0390401
H	2.9843409	1.5688770	-3.1600523
H	-2.6661946	-3.2250742	0.5256681
H	-1.8417111	-2.7693973	-0.9890613
H	-3.6278456	-2.9357780	-0.9557555
H	-3.1091138	-0.8294742	3.4516876
H	-2.8474796	-2.3453021	2.5453497
H	-4.4870582	-1.6390604	2.6540065
H	-2.9007635	3.3481621	0.0113993
H	-3.6449521	2.7546034	-1.5035326
H	-1.8637245	2.7143639	-1.2986688
H	-1.8820355	-1.0644687	-2.6314043
H	-1.7944694	0.7163912	-2.7329336
H	-3.3584122	-0.1183376	-2.9903251
H	1.8319968	3.0153388	-0.0430341
H	2.8643477	3.0131931	-1.5016286
H	3.6124689	3.1599927	0.1169436
H	1.8714471	0.2176594	2.8203636
H	1.7742152	1.8593766	2.1241304
H	3.3408620	1.2355111	2.7286030

SCF energy GEOOPT = -1264.501898721 H

ZPE = 1126. kJ/mol

FREEH energy = 1207.22 kJ/mol

FREEH entropy = 0.86233 kJ/mol/K

$vibrational spectrum

mode symmetry wave number IR intensity selection rules

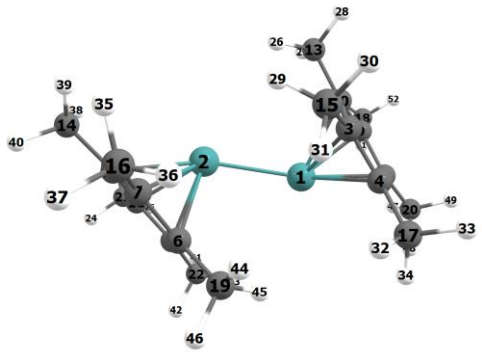
#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		-0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	7.96	0.00065	YES	YES
8	a	20.77	0.08171	YES	YES
9	a	26.05	0.23840	YES	YES
10	a	28.61	0.44256	YES	YES
11	a	52.00	0.36782	YES	YES
12	a	61.94	0.22109	YES	YES
13	a	65.07	0.50769	YES	YES
14	a	65.91	0.19693	YES	YES
15	a	69.61	0.13210	YES	YES
16	a	70.86	0.04844	YES	YES
17	a	73.70	0.10611	YES	YES
18	a	84.84	0.57230	YES	YES
19	a	90.36	0.04461	YES	YES
20	a	95.40	0.11402	YES	YES

21	a	96.20	0.19717	YES	YES	62	a	802.34	2.28234	YES	YES
22	a	99.22	0.03968	YES	YES	63	a	919.30	0.23678	YES	YES
23	a	147.54	0.05226	YES	YES	64	a	919.76	0.07039	YES	YES
24	a	150.01	0.01109	YES	YES	65	a	931.00	2.32602	YES	YES
25	a	154.39	0.09559	YES	YES	66	a	931.58	0.80961	YES	YES
26	a	157.01	0.03695	YES	YES	67	a	989.69	12.31723	YES	YES
27	a	158.04	0.01043	YES	YES	68	a	990.47	4.15725	YES	YES
28	a	159.74	0.05495	YES	YES	69	a	993.46	5.89839	YES	YES
29	a	166.12	0.93114	YES	YES	70	a	994.12	3.35869	YES	YES
30	a	190.11	5.20078	YES	YES	71	a	999.33	0.20791	YES	YES
31	a	191.52	0.50123	YES	YES	72	a	999.37	0.59214	YES	YES
32	a	260.37	0.38413	YES	YES	73	a	1000.44	1.29239	YES	YES
33	a	260.85	0.09203	YES	YES	74	a	1001.45	0.69257	YES	YES
34	a	269.59	0.00903	YES	YES	75	a	1006.78	0.50027	YES	YES
35	a	274.56	0.72859	YES	YES	76	a	1007.53	0.55003	YES	YES
36	a	279.23	0.09907	YES	YES	77	a	1046.35	1.86904	YES	YES
37	a	280.17	0.30536	YES	YES	78	a	1046.88	0.11885	YES	YES
38	a	284.11	0.80682	YES	YES	79	a	1047.21	1.08297	YES	YES
39	a	284.74	0.05676	YES	YES	80	a	1047.62	0.61590	YES	YES
40	a	291.39	0.00671	YES	YES	81	a	1073.10	1.33412	YES	YES
41	a	322.33	0.21374	YES	YES	82	a	1073.49	1.44524	YES	YES
42	a	336.36	62.58471	YES	YES	83	a	1162.65	1.52382	YES	YES
43	a	337.81	8.90273	YES	YES	84	a	1164.08	0.07026	YES	YES
44	a	362.45	0.04642	YES	YES	85	a	1165.66	0.11336	YES	YES
45	a	401.18	526.68140	YES	YES	86	a	1167.09	0.03781	YES	YES
46	a	498.51	0.00247	YES	YES	87	a	1336.19	7.03027	YES	YES
47	a	543.97	0.04307	YES	YES	88	a	1337.09	5.55949	YES	YES
48	a	544.21	0.02757	YES	YES	89	a	1339.58	2.18381	YES	YES
49	a	545.80	0.07324	YES	YES	90	a	1340.44	1.80709	YES	YES
50	a	546.20	0.05875	YES	YES	91	a	1343.02	9.08158	YES	YES
51	a	546.55	0.03705	YES	YES	92	a	1344.08	5.54914	YES	YES
52	a	547.10	0.04871	YES	YES	93	a	1344.40	3.70255	YES	YES
53	a	568.17	0.78039	YES	YES	94	a	1344.60	4.37372	YES	YES
54	a	576.78	2.05719	YES	YES	95	a	1348.85	5.46025	YES	YES
55	a	587.49	7.60980	YES	YES	96	a	1348.97	1.23431	YES	YES
56	a	588.75	0.04339	YES	YES	97	a	1381.50	1.76632	YES	YES
57	a	600.20	1.16029	YES	YES	98	a	1382.47	0.14659	YES	YES
58	a	603.68	0.33560	YES	YES	99	a	1386.34	2.86701	YES	YES
59	a	797.43	1.74276	YES	YES	100	a	1386.76	1.26716	YES	YES
60	a	798.01	3.47097	YES	YES	101	a	1395.03	3.26954	YES	YES
61	a	800.97	6.50657	YES	YES	102	a	1395.38	6.45288	YES	YES

103	a	1395.56	1.68456	YES	YES
104	a	1396.62	5.65813	YES	YES
105	a	1399.38	9.52272	YES	YES
106	a	1399.93	0.82886	YES	YES
107	a	1401.14	1.00948	YES	YES
108	a	1401.93	1.72214	YES	YES
109	a	1403.80	11.40734	YES	YES
110	a	1404.69	3.30127	YES	YES
111	a	1408.89	0.99096	YES	YES
112	a	1409.37	0.59270	YES	YES
113	a	1409.71	3.06075	YES	YES
114	a	1410.24	1.29050	YES	YES
115	a	1412.16	108.97916	YES	YES
116	a	1413.43	0.07562	YES	YES
117	a	1434.01	5.30411	YES	YES
118	a	1434.56	0.05071	YES	YES
119	a	1439.91	0.35123	YES	YES
120	a	1440.30	0.09297	YES	YES
121	a	1449.53	0.52324	YES	YES
122	a	1449.90	0.01822	YES	YES
123	a	1480.44	13.96242	YES	YES
124	a	1481.18	0.79463	YES	YES
125	a	1492.15	10.54768	YES	YES
126	a	1492.23	4.07037	YES	YES
127	a	2940.15	28.52099	YES	YES
128	a	2941.31	95.60398	YES	YES
129	a	2948.28	39.13192	YES	YES
130	a	2948.75	38.33664	YES	YES
131	a	2949.28	47.00944	YES	YES
132	a	2949.56	31.15926	YES	YES
133	a	2952.48	38.48170	YES	YES
134	a	2952.60	54.72008	YES	YES
135	a	2953.62	123.40079	YES	YES
136	a	2954.10	8.91372	YES	YES
137	a	3011.18	6.38851	YES	YES
138	a	3011.87	2.40394	YES	YES
139	a	3018.12	12.81083	YES	YES
140	a	3018.86	6.89247	YES	YES
141	a	3025.39	3.19779	YES	YES
142	a	3025.62	2.55775	YES	YES
143	a	3026.46	13.92913	YES	YES
144	a	3026.56	9.41989	YES	YES
145	a	3027.93	2.55791	YES	YES
146	a	3028.21	3.73601	YES	YES
147	a	3055.43	4.13438	YES	YES
148	a	3055.60	1.33834	YES	YES
149	a	3055.98	4.34143	YES	YES
150	a	3056.00	21.83543	YES	YES
151	a	3058.10	9.30214	YES	YES
152	a	3058.35	9.33110	YES	YES
153	a	3059.36	8.76773	YES	YES
154	a	3060.14	3.73739	YES	YES
155	a	3060.23	10.57508	YES	YES
156	a	3060.56	12.52293	YES	YES

$end

[Cp*Al–AlCp*]$^{+}$



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

Al	-1.2353425	0.6341738	0.5055133
Al	1.2201524	0.6847484	-0.4589418
C	-2.1344459	-0.8699174	-0.8863905
C	-2.6754383	-1.0572090	0.4414097
C	2.4758730	0.4072894	1.3668364
C	2.1520080	-0.8888471	0.8298535
C	2.6977967	-0.9742728	-0.5064076
C	-3.3747889	0.1533135	0.8115340
C	-3.2436505	1.0957186	-0.2840582
C	-2.4877811	0.4519089	-1.3346333
C	3.2174006	1.1370509	0.3633771
C	3.3698851	0.2736810	-0.7929457
C	-2.1478938	1.0396963	-2.6725567

C	4.1569501	0.5897149	-2.0299009
C	-1.3685604	-1.8856368	-1.6830621
C	2.6684868	-2.1792222	-1.4011051
C	-2.6175291	-2.3186877	1.2529429
C	-3.8947811	2.4467898	-0.3579737
C	1.4091774	-1.9725273	1.5555823
C	-4.1667009	0.3676729	2.0670815
C	3.8379908	2.4943497	0.5292473
C	2.1225952	0.8955981	2.7408990
H	3.9078502	3.0394344	-0.4312930
H	4.8699261	2.3961120	0.9270387
H	3.2716360	3.1264092	1.2392088
H	-1.1438770	0.7229545	-3.0195642
H	-2.1657455	2.1457915	-2.6551463
H	-2.8786127	0.7092601	-3.4402884
H	-0.5776716	-1.4158002	-2.3021622
H	-2.0425962	-2.4292896	-2.3777309
H	-0.8901979	-2.6431417	-1.0332976
H	-1.7194166	-2.9211668	1.0193491
H	-3.5029917	-2.9540174	1.0404894
H	-2.6161619	-2.1133583	2.3405799
H	2.6624036	-1.9011581	-2.4723844
H	1.7842954	-2.8164745	-1.2101739
H	3.5681886	-2.8071970	-1.2306222
H	4.1526451	1.6721695	-2.2602628
H	3.7715775	0.0505025	-2.9162210
H	5.2171740	0.2869407	-1.8969791
H	2.1163553	2.0004881	2.7986379
H	2.8600233	0.5297870	3.4858539
H	1.1256098	0.5342266	3.0636734
H	0.9544253	-2.6993804	0.8558572
H	0.6031119	-1.5636788	2.1979730
H	2.0939139	-2.5413490	2.2189161
H	-4.1872871	1.4322233	2.3689677
H	-3.7672835	-0.2201523	2.9154892
H	-5.2198002	0.0497216	1.9145092
H	-3.3441542	3.1377300	-1.0240808
H	-3.9749913	2.9243656	0.6371062
H	-4.9250019	2.3523776	-0.7611373

SCF energy GEOOPT = -1264.366730848 H

ZPE = 1133. kJ/mol

FREEH energy = 1211.60 kJ/mol

FREEH entropy = 0.81647 kJ/mol/K

$vibrational spectrum

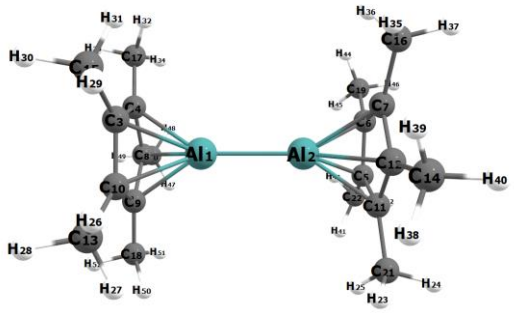
# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		-0.00	0.00000	- -
2		-0.00	0.00000	- -
3		-0.00	0.00000	- -
4		-0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	6.87	0.00207	YES YES
8	a	25.02	0.00213	YES YES
9	a	34.29	0.01468	YES YES
10	a	39.38	0.02333	YES YES
11	a	64.57	0.00653	YES YES
12	a	84.83	0.29877	YES YES
13	a	87.08	0.06862	YES YES
14	a	94.36	0.10585	YES YES
15	a	95.52	0.06533	YES YES
16	a	106.41	0.09000	YES YES
17	a	107.71	0.03435	YES YES
18	a	116.47	0.20652	YES YES
19	a	119.68	0.17918	YES YES
20	a	121.72	0.17622	YES YES
21	a	126.72	0.17104	YES YES
22	a	128.53	0.12631	YES YES
23	a	148.38	0.00698	YES YES
24	a	150.36	0.00463	YES YES
25	a	153.14	0.00944	YES YES
26	a	155.25	0.03458	YES YES
27	a	187.24	5.58765	YES YES
28	a	190.64	0.97885	YES YES
29	a	193.39	0.14061	YES YES
30	a	200.70	0.54075	YES YES
31	a	203.88	0.16031	YES YES
32	a	262.98	0.22265	YES YES
33	a	272.48	0.02345	YES YES
34	a	273.67	0.04491	YES YES

35	a	274.07	0.00990	YES	YES	76	a	999.05	1.17808	YES	YES
36	a	277.32	0.02375	YES	YES	77	a	1047.20	2.11837	YES	YES
37	a	280.81	0.91742	YES	YES	78	a	1047.53	1.63602	YES	YES
38	a	284.91	0.48266	YES	YES	79	a	1047.90	2.87313	YES	YES
39	a	286.02	0.49916	YES	YES	80	a	1048.55	2.46352	YES	YES
40	a	297.40	0.91967	YES	YES	81	a	1073.87	0.05126	YES	YES
41	a	383.27	10.06191	YES	YES	82	a	1074.54	0.00896	YES	YES
42	a	392.22	0.39972	YES	YES	83	a	1157.76	0.79919	YES	YES
43	a	392.77	0.75042	YES	YES	84	a	1158.83	0.33351	YES	YES
44	a	399.28	0.00688	YES	YES	85	a	1160.55	1.02923	YES	YES
45	a	456.41	350.58840	YES	YES	86	a	1161.49	0.01629	YES	YES
46	a	509.87	8.40422	YES	YES	87	a	1338.20	0.63292	YES	YES
47	a	542.54	0.00794	YES	YES	88	a	1338.65	1.73470	YES	YES
48	a	542.64	0.03188	YES	YES	89	a	1342.13	0.03454	YES	YES
49	a	543.27	0.11301	YES	YES	90	a	1343.04	0.02736	YES	YES
50	a	543.64	0.06362	YES	YES	91	a	1346.91	5.03068	YES	YES
51	a	543.86	0.01766	YES	YES	92	a	1349.11	5.14963	YES	YES
52	a	545.16	0.00648	YES	YES	93	a	1350.00	14.08087	YES	YES
53	a	585.25	12.58991	YES	YES	94	a	1351.00	10.17222	YES	YES
54	a	586.96	2.01000	YES	YES	95	a	1353.68	4.77642	YES	YES
55	a	587.66	0.01481	YES	YES	96	a	1354.36	4.64215	YES	YES
56	a	588.37	0.12824	YES	YES	97	a	1380.05	0.13887	YES	YES
57	a	605.84	0.02560	YES	YES	98	a	1382.04	1.06458	YES	YES
58	a	607.83	0.83048	YES	YES	99	a	1384.58	0.30295	YES	YES
59	a	794.53	4.17266	YES	YES	100	a	1386.07	0.00950	YES	YES
60	a	794.64	1.05695	YES	YES	101	a	1392.85	7.66319	YES	YES
61	a	797.73	6.44083	YES	YES	102	a	1393.75	1.75226	YES	YES
62	a	798.49	3.55715	YES	YES	103	a	1396.50	21.45687	YES	YES
63	a	919.23	0.17321	YES	YES	104	a	1396.87	5.92722	YES	YES
64	a	920.34	0.07920	YES	YES	105	a	1399.41	3.98788	YES	YES
65	a	923.09	0.59331	YES	YES	106	a	1399.92	1.32708	YES	YES
66	a	923.71	0.06075	YES	YES	107	a	1402.69	0.30100	YES	YES
67	a	987.72	12.31680	YES	YES	108	a	1403.00	0.10545	YES	YES
68	a	988.41	2.06168	YES	YES	109	a	1404.40	2.67975	YES	YES
69	a	991.25	5.60900	YES	YES	110	a	1405.18	10.34594	YES	YES
70	a	992.31	13.36039	YES	YES	111	a	1406.14	37.80591	YES	YES
71	a	994.37	0.10690	YES	YES	112	a	1408.27	1.68611	YES	YES
72	a	994.61	0.21302	YES	YES	113	a	1408.66	57.83303	YES	YES
73	a	997.40	0.88335	YES	YES	114	a	1409.20	64.23816	YES	YES
74	a	997.61	0.05240	YES	YES	115	a	1409.93	0.70527	YES	YES
75	a	998.70	0.96829	YES	YES	116	a	1410.84	14.48306	YES	YES

117	a	1431.47	6.95716	YES	YES
118	a	1432.71	4.83158	YES	YES
119	a	1442.27	0.68867	YES	YES
120	a	1442.60	0.53176	YES	YES
121	a	1444.54	1.49371	YES	YES
122	a	1445.82	0.00498	YES	YES
123	a	1472.42	22.76239	YES	YES
124	a	1473.20	30.00995	YES	YES
125	a	1475.52	25.42575	YES	YES
126	a	1476.75	14.37323	YES	YES
127	a	2962.79	9.93847	YES	YES
128	a	2963.55	9.92634	YES	YES
129	a	2966.28	10.48128	YES	YES
130	a	2966.72	8.81023	YES	YES
131	a	2970.18	25.03418	YES	YES
132	a	2970.23	0.15022	YES	YES
133	a	2971.41	9.53513	YES	YES
134	a	2971.53	14.37083	YES	YES
135	a	2972.44	10.10889	YES	YES
136	a	2972.52	10.65480	YES	YES
137	a	3035.71	4.32826	YES	YES
138	a	3036.18	4.45226	YES	YES
139	a	3040.15	1.71668	YES	YES
140	a	3040.75	1.38502	YES	YES
141	a	3047.55	4.26179	YES	YES
142	a	3047.60	1.52816	YES	YES
143	a	3048.83	1.87713	YES	YES
144	a	3048.91	2.18307	YES	YES
145	a	3050.76	1.17583	YES	YES
146	a	3050.85	1.69589	YES	YES
147	a	3063.78	6.47645	YES	YES
148	a	3064.97	6.90835	YES	YES
149	a	3071.19	3.71663	YES	YES
150	a	3071.47	3.94208	YES	YES
151	a	3076.38	3.32323	YES	YES
152	a	3076.48	5.55729	YES	YES
153	a	3077.41	4.91554	YES	YES
154	a	3077.61	5.33033	YES	YES
155	a	3078.69	4.29733	YES	YES
156	a	3078.72	4.86241	YES	YES

$end

$[Cp^*Al–AlCp^*]^{2+}$



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

Al	1.2420081	-0.0047796	-0.0043553
Al	-1.2419793	-0.0049043	-0.0035707
C	2.9802839	-1.2233722	-0.2090947
C	2.9794123	-0.1807404	-1.2287547
C	-2.9749704	1.2382566	0.0135104
C	-2.9774193	0.3957559	-1.1767724
C	-2.9791238	-0.9966555	-0.7433134
C	2.9749991	1.1111248	-0.5522385
C	2.9732869	0.8669365	0.8854433
C	2.9764159	-0.5758389	1.0975391
C	-2.9752381	0.3666098	1.1825939
C	-2.9777699	-1.0146686	0.7149023
C	3.1048929	-1.2687626	2.4213888
C	-3.1078378	-2.2339978	1.5783365
C	3.1140911	-2.6960622	-0.4589922
C	-3.1107999	-2.1943364	-1.6363084
C	3.1121626	-0.3976982	-2.7067191
C	3.0975442	1.9119429	1.9539686
C	-3.1068160	0.8753438	-2.5918565
C	3.1017208	2.4502132	-1.2155523
C	-3.1020902	0.8111410	2.6093397
C	-3.1016404	2.7325558	0.0320803
H	-2.6510393	0.0903480	3.3164435
H	-4.1780991	0.8941206	2.8710048
H	-2.6487277	1.8049413	2.7822957
H	2.6547236	-2.2788018	2.4129185
H	2.6515010	-0.6880326	3.2461798
H	4.1812087	-1.3937636	2.6644939

H	2.6623105	-3.3025481	0.3478828
H	4.1914301	-2.9620018	-0.5020045
H	2.6658865	-3.0018584	-1.4226116
H	2.6651073	-1.3549886	-3.0333057
H	4.1893121	-0.4331682	-2.9745567
H	2.6585937	0.4217297	-3.2947321
H	-2.6599393	-3.1014782	-1.1927233
H	-2.6601377	-2.0281538	-2.6324738
H	-4.1877002	-2.4117450	-1.7982658
H	-2.6558883	-2.0922055	2.5776936
H	-2.6572507	-3.1297554	1.1119620
H	-4.1844493	-2.4557234	1.7363301
H	-2.6488048	3.1820129	0.9353711
H	-4.1776254	3.0072562	0.0359825
H	-2.6496475	3.2043062	-0.8602036
H	-2.6566312	0.1724144	-3.3172363
H	-2.6541352	1.8733097	-2.7409382
H	-4.1832811	0.9642662	-2.8496526
H	2.6474567	3.2613383	-0.6165346
H	2.6513574	2.4636574	-2.2254544
H	4.1777127	2.6973445	-1.3353112
H	2.6446841	1.5914702	2.9106411
H	2.6444839	2.8753865	1.6548441
H	4.1730832	2.1052968	2.1515084

SCF energy GEOOPT = -1264.054636406 H

ZPE = 1137. kJ/mol

FREEH energy = 1213.64 kJ/mol

FREEH entropy = 0.80315 kJ/mol/K

$vibrational spectrum

mode symmetry wave number IR intensity selection rules

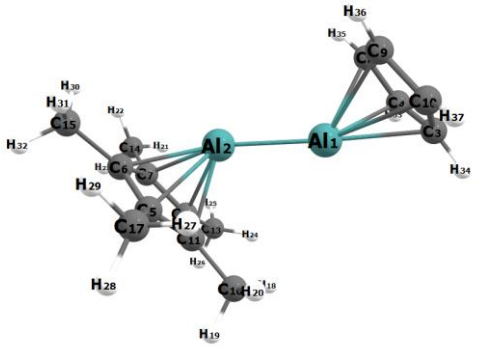
#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		-0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	2.66	0.00052	YES	YES
8	a	19.60	0.65683	YES	YES
9	a	22.86	0.67476	YES	YES
10	a	57.72	0.00107	YES	YES
11	a	58.55	0.00056	YES	YES
12	a	100.86	0.00010	YES	YES
13	a	129.06	0.00734	YES	YES
14	a	129.64	0.00623	YES	YES
15	a	130.00	0.00855	YES	YES
16	a	131.28	0.00147	YES	YES
17	a	136.75	0.41396	YES	YES
18	a	137.31	0.38246	YES	YES
19	a	137.73	0.23720	YES	YES
20	a	138.86	0.30583	YES	YES
21	a	139.15	0.30310	YES	YES
22	a	140.01	0.11317	YES	YES
23	a	148.02	0.00131	YES	YES
24	a	148.57	0.00083	YES	YES
25	a	148.75	0.00590	YES	YES
26	a	149.09	0.00435	YES	YES
27	a	192.16	11.59547	YES	YES
28	a	220.50	0.24711	YES	YES
29	a	220.72	0.24566	YES	YES
30	a	225.17	0.00153	YES	YES
31	a	225.36	0.00025	YES	YES
32	a	258.43	0.00016	YES	YES
33	a	271.88	0.00058	YES	YES
34	a	271.91	0.00260	YES	YES
35	a	272.05	0.00074	YES	YES
36	a	273.67	0.00013	YES	YES
37	a	291.76	2.05476	YES	YES
38	a	292.39	2.06528	YES	YES
39	a	294.37	0.07839	YES	YES
40	a	294.87	0.02513	YES	YES
41	a	422.74	3.03638	YES	YES
42	a	422.93	3.04148	YES	YES
43	a	426.24	0.00587	YES	YES
44	a	426.42	0.01630	YES	YES
45	a	531.25	241.53076	YES	YES
46	a	540.27	0.00955	YES	YES
47	a	540.32	0.00890	YES	YES
48	a	540.41	0.00909	YES	YES
49	a	540.54	0.00004	YES	YES

50	a	540.68	0.00009	YES	YES	91	a	1351.70	6.93117	YES	YES
51	a	540.78	0.00383	YES	YES	92	a	1352.12	8.08880	YES	YES
52	a	581.22	7.55830	YES	YES	93	a	1352.90	26.32302	YES	YES
53	a	582.74	0.00292	YES	YES	94	a	1353.34	26.55369	YES	YES
54	a	611.89	0.00006	YES	YES	95	a	1354.29	11.09285	YES	YES
55	a	611.95	0.00007	YES	YES	96	a	1355.89	0.21588	YES	YES
56	a	612.36	0.00008	YES	YES	97	a	1373.58	0.00249	YES	YES
57	a	612.41	0.00017	YES	YES	98	a	1373.70	0.00454	YES	YES
58	a	632.13	0.00075	YES	YES	99	a	1374.18	0.02134	YES	YES
59	a	787.31	4.62636	YES	YES	100	a	1374.20	0.01701	YES	YES
60	a	787.45	4.56756	YES	YES	101	a	1383.78	7.54550	YES	YES
61	a	788.54	0.06079	YES	YES	102	a	1383.89	7.16896	YES	YES
62	a	788.69	0.08047	YES	YES	103	a	1385.05	0.04408	YES	YES
63	a	913.06	0.00013	YES	YES	104	a	1385.20	0.15240	YES	YES
64	a	913.27	0.00093	YES	YES	105	a	1388.00	260.74345	YES	YES
65	a	913.84	0.00099	YES	YES	106	a	1392.89	0.00414	YES	YES
66	a	914.16	0.00107	YES	YES	107	a	1398.72	0.00774	YES	YES
67	a	986.58	33.46638	YES	YES	108	a	1398.92	0.00006	YES	YES
68	a	986.64	31.66205	YES	YES	109	a	1402.13	0.00203	YES	YES
69	a	987.04	0.62098	YES	YES	110	a	1402.31	0.00941	YES	YES
70	a	987.23	4.58250	YES	YES	111	a	1403.37	0.00063	YES	YES
71	a	988.31	0.36236	YES	YES	112	a	1403.53	0.00751	YES	YES
72	a	988.47	0.68466	YES	YES	113	a	1408.05	0.02499	YES	YES
73	a	988.51	0.26607	YES	YES	114	a	1408.18	0.35907	YES	YES
74	a	988.54	0.52811	YES	YES	115	a	1408.71	7.18140	YES	YES
75	a	995.21	2.62476	YES	YES	116	a	1408.90	6.82249	YES	YES
76	a	995.97	0.03348	YES	YES	117	a	1425.82	45.05748	YES	YES
77	a	1047.37	4.78585	YES	YES	118	a	1426.51	4.06814	YES	YES
78	a	1047.49	4.43287	YES	YES	119	a	1434.20	0.00429	YES	YES
79	a	1047.76	5.19560	YES	YES	120	a	1434.36	0.00053	YES	YES
80	a	1047.90	4.94280	YES	YES	121	a	1434.80	0.00270	YES	YES
81	a	1072.97	0.00056	YES	YES	122	a	1434.97	0.03394	YES	YES
82	a	1073.02	0.00103	YES	YES	123	a	1448.54	88.64245	YES	YES
83	a	1147.00	0.00000	YES	YES	124	a	1448.70	88.80472	YES	YES
84	a	1147.19	0.00012	YES	YES	125	a	1450.56	0.14044	YES	YES
85	a	1148.98	0.00011	YES	YES	126	a	1450.73	0.39439	YES	YES
86	a	1149.19	0.00005	YES	YES	127	a	2978.53	3.48671	YES	YES
87	a	1336.04	0.00776	YES	YES	128	a	2978.58	2.90422	YES	YES
88	a	1336.61	0.00464	YES	YES	129	a	2978.73	0.26388	YES	YES
89	a	1336.87	0.02118	YES	YES	130	a	2978.84	0.35350	YES	YES
90	a	1337.39	0.01944	YES	YES	131	a	2978.89	0.10296	YES	YES

132	a	2978.92	0.44252	YES	YES
133	a	2979.02	0.08749	YES	YES
134	a	2979.08	0.12886	YES	YES
135	a	2979.10	0.07065	YES	YES
136	a	2979.17	0.03939	YES	YES
137	a	3058.97	7.32482	YES	YES
138	a	3058.99	6.03852	YES	YES
139	a	3059.06	5.31134	YES	YES
140	a	3059.12	4.33262	YES	YES
141	a	3059.22	5.84382	YES	YES
142	a	3059.25	7.23843	YES	YES
143	a	3060.13	0.06518	YES	YES
144	a	3060.18	0.02284	YES	YES
145	a	3060.22	0.10645	YES	YES
146	a	3060.37	0.02315	YES	YES
147	a	3091.42	0.33306	YES	YES
148	a	3091.62	0.01990	YES	YES
149	a	3091.74	0.11051	YES	YES
150	a	3091.78	0.22567	YES	YES
151	a	3091.98	0.07740	YES	YES
152	a	3092.07	0.26878	YES	YES
153	a	3092.07	2.59696	YES	YES
154	a	3092.15	3.17002	YES	YES
155	a	3092.41	2.93657	YES	YES
156	a	3092.48	3.25741	YES	YES

$end

[CpAl–AlCp*]



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

Al	-1.9593209	0.1581011	-0.1667917
Al	0.4085075	-0.1774485	0.5167769
C	-4.3093218	0.1630444	-0.7814852
C	-4.0231497	-1.0280832	-0.0527345
C	2.1255682	1.1840532	-0.1727059
C	2.6355276	0.3156780	0.8516832
C	2.5287773	-1.0478966	0.3750900
C	-3.5443553	-0.6511262	1.2421303
C	-3.5618430	0.7826960	1.3181373
C	-4.0396784	1.2827983	0.0675486
C	1.6785851	0.3641928	-1.2694141
C	1.9454174	-1.0133813	-0.9380735
C	1.6508903	-2.1923124	-1.8186830
C	2.9875679	-2.2743557	1.1089988
C	3.2269699	0.7400854	2.1648961
C	1.0829368	0.8665888	-2.5526978
C	2.0163698	2.6795615	-0.1185298
H	0.4067289	0.1162810	-3.0081026
H	1.8721398	1.1004276	-3.2999884
H	0.4931950	1.7905798	-2.3907776
H	2.3744587	-3.1601537	0.8495883
H	2.9289008	-2.1411331	2.2072976
H	4.0436762	-2.5195618	0.8640950
H	0.6599704	-2.0946391	-2.3082120
H	1.6394290	-3.1371851	-1.2421702
H	2.4138132	-2.2974663	-2.6197273
H	0.9800929	3.0161819	-0.3388695
H	2.6902399	3.1606821	-0.8585758
H	2.2835788	3.0710797	0.8813540
H	3.0617219	-0.0197150	2.9542256
H	2.7877519	1.6913218	2.5241127
H	4.3248359	0.8921445	2.0814498
H	-4.0928191	-2.0529542	-0.4358895
H	-4.6564384	0.2136704	-1.8207405
H	-3.2335027	-1.3345796	2.0414770
H	-3.2582562	1.3849192	2.1826997
H	-4.1350559	2.3401082	-0.2067724

SCF energy GEOOPT = -1068.022822710 H

ZPE = 776.1 kJ/mol

FREEH energy = 833.94 kJ/mol

FREEH entropy = 0.69932 kJ/mol/K

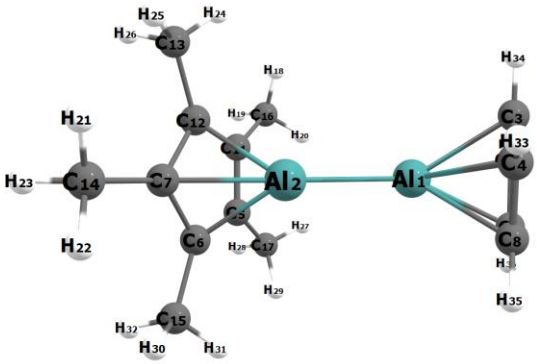
$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	1.81	0.00367	YES	YES
8	a	22.65	0.05299	YES	YES
9	a	31.14	0.98344	YES	YES
10	a	39.20	0.36191	YES	YES
11	a	67.31	0.34335	YES	YES
12	a	69.80	0.23845	YES	YES
13	a	75.75	0.33805	YES	YES
14	a	81.69	0.91710	YES	YES
15	a	94.47	0.07734	YES	YES
16	a	95.19	0.02301	YES	YES
17	a	107.69	6.39176	YES	YES
18	a	120.04	1.04386	YES	YES
19	a	147.74	0.06438	YES	YES
20	a	155.73	0.08005	YES	YES
21	a	157.43	0.01298	YES	YES
22	a	167.06	36.66154	YES	YES
23	a	190.03	4.70336	YES	YES
24	a	256.65	0.09447	YES	YES
25	a	263.24	0.24634	YES	YES
26	a	278.47	0.11516	YES	YES
27	a	279.81	1.58540	YES	YES
28	a	283.95	0.52035	YES	YES
29	a	326.35	5.15022	YES	YES
30	a	350.89	62.40172	YES	YES
31	a	376.44	328.01103	YES	YES
32	a	488.84	29.41056	YES	YES
33	a	543.86	0.02966	YES	YES
34	a	545.41	0.13652	YES	YES
35	a	546.48	0.04794	YES	YES
36	a	561.70	2.53618	YES	YES
37	a	572.06	0.78247	YES	YES
38	a	580.50	0.27660	YES	YES
39	a	587.90	4.64896	YES	YES
40	a	601.55	0.72637	YES	YES
41	a	764.31	6.67269	YES	YES
42	a	774.87	31.58877	YES	YES
43	a	792.05	280.12686	YES	YES
44	a	797.19	2.65158	YES	YES
45	a	800.98	3.70030	YES	YES
46	a	822.68	0.39010	YES	YES
47	a	826.91	0.18567	YES	YES
48	a	865.05	1.03663	YES	YES
49	a	871.70	0.63648	YES	YES
50	a	919.57	0.11231	YES	YES
51	a	930.17	1.08522	YES	YES
52	a	990.34	9.25008	YES	YES
53	a	992.64	6.13626	YES	YES
54	a	995.04	9.88179	YES	YES
55	a	997.21	9.52685	YES	YES
56	a	999.48	0.22830	YES	YES
57	a	999.88	1.69136	YES	YES
58	a	1005.93	0.36124	YES	YES
59	a	1042.05	0.45765	YES	YES
60	a	1042.41	0.05575	YES	YES
61	a	1046.75	0.59408	YES	YES
62	a	1047.39	1.44745	YES	YES
63	a	1073.42	0.99063	YES	YES
64	a	1117.00	10.38423	YES	YES
65	a	1163.04	0.41857	YES	YES
66	a	1166.13	0.15318	YES	YES
67	a	1231.39	0.00136	YES	YES
68	a	1337.54	4.50808	YES	YES
69	a	1339.89	2.02476	YES	YES
70	a	1343.67	6.50518	YES	YES
71	a	1344.42	5.05312	YES	YES
72	a	1348.90	3.57650	YES	YES
73	a	1363.95	1.97240	YES	YES
74	a	1365.80	0.74171	YES	YES
75	a	1382.44	0.64891	YES	YES
76	a	1386.92	1.64087	YES	YES
77	a	1395.21	3.33895	YES	YES
78	a	1396.40	6.61328	YES	YES

79	a	1399.54	4.46361	YES	YES
80	a	1401.41	1.58378	YES	YES
81	a	1404.34	7.07617	YES	YES
82	a	1408.52	0.40303	YES	YES
83	a	1410.32	1.64806	YES	YES
84	a	1412.76	51.94803	YES	YES
85	a	1420.13	8.21622	YES	YES
86	a	1424.43	5.25410	YES	YES
87	a	1433.81	2.23880	YES	YES
88	a	1440.85	0.44322	YES	YES
89	a	1449.78	0.20564	YES	YES
90	a	1479.62	8.39807	YES	YES
91	a	1491.27	8.79709	YES	YES
92	a	2944.55	56.33653	YES	YES
93	a	2951.20	25.79522	YES	YES
94	a	2951.65	52.99425	YES	YES
95	a	2953.60	42.92323	YES	YES
96	a	2955.10	59.58349	YES	YES
97	a	3014.39	4.26494	YES	YES
98	a	3023.66	9.30364	YES	YES
99	a	3027.36	0.33294	YES	YES
100	a	3027.78	11.09878	YES	YES
101	a	3029.64	4.51353	YES	YES
102	a	3056.62	1.47513	YES	YES
103	a	3056.97	14.11219	YES	YES
104	a	3059.38	6.05339	YES	YES
105	a	3059.96	12.53663	YES	YES
106	a	3062.59	9.05895	YES	YES
107	a	3159.01	0.59396	YES	YES
108	a	3162.18	0.09867	YES	YES
109	a	3174.09	0.08517	YES	YES
110	a	3176.16	0.04555	YES	YES
111	a	3185.71	0.57728	YES	YES

$end

[CpAl–AlCp*]$^{+}$



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

Al	1.5924980	5.0466472	14.7028760
Al	4.2039351	5.5248103	14.7891884
C	0.4811965	3.2760339	13.9038735
C	1.2603068	2.8520810	15.0292655
C	4.3530076	7.7383649	14.9110824
C	5.4473522	7.1337814	15.6416752
C	6.2407647	6.3669717	14.7018132
C	0.7999969	3.5638300	16.1806224
C	-0.2834105	4.4155032	15.7726939
C	-0.4867060	4.2305530	14.3684806
C	4.4593828	7.3390050	13.5313545
C	5.6189162	6.4828212	13.3972082
C	6.1608098	5.9186485	12.1158445
C	7.5252539	5.6552167	15.0062815
C	5.7792223	7.3597372	17.0882092
C	3.5466394	7.7727105	12.4217384
C	3.3115853	8.6584188	15.4783710
H	3.5397581	7.0502565	11.5834887
H	3.8740504	8.7503711	12.0098405
H	2.5030225	7.9015626	12.7712525
H	7.6895086	4.7891976	14.3372894
H	7.5620696	5.2926671	16.0511180
H	8.3850224	6.3443875	14.8676638
H	5.3643053	5.7433813	11.3679911
H	6.6963710	4.9635948	12.2754940
H	6.8844540	6.6291848	11.6638244
H	2.3311634	8.5322156	14.9775631
H	3.6126884	9.7179436	15.3393405
H	3.1644961	8.4999582	16.5636995

H	6.2947734	6.4897938	17.5375309
H	4.8781551	7.5734833	17.6937564
H	6.4578523	8.2325629	17.1906783
H	2.0813336	2.1248706	15.0065824
H	0.5824800	2.9113100	12.8739861
H	1.1925218	3.4657876	17.2004343
H	-0.8577863	5.0846573	16.4254375
H	-1.2351712	4.7424193	13.7510203

SCF energy GEOOPT = -1067.878177878 H

ZPE = 782.9 kJ/mol

FREEH energy = 838.04 kJ/mol

FREEH entropy = 0.66509 kJ/mol/K

$vibrational spectrum

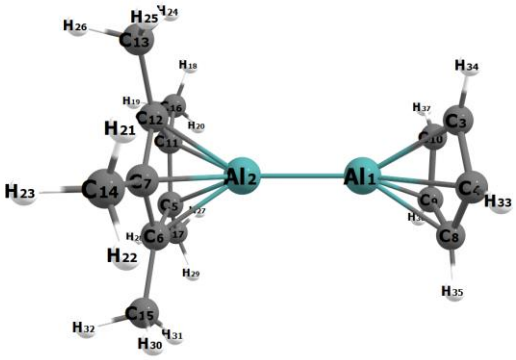
mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		-0.00	0.00000	-	-
2		-0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	7.02	0.00042	YES	YES
8	a	15.49	0.00879	YES	YES
9	a	20.18	0.13093	YES	YES
10	a	32.77	0.03889	YES	YES
11	a	77.58	0.23289	YES	YES
12	a	95.74	0.13531	YES	YES
13	a	104.51	0.13003	YES	YES
14	a	113.48	0.12568	YES	YES
15	a	123.61	0.27521	YES	YES
16	a	126.90	0.17372	YES	YES
17	a	129.88	0.26699	YES	YES
18	a	149.35	0.00841	YES	YES
19	a	150.87	0.00349	YES	YES
20	a	191.18	3.74685	YES	YES
21	a	201.78	0.02789	YES	YES
22	a	236.32	1.56302	YES	YES
23	a	273.23	0.00539	YES	YES
24	a	273.81	1.42700	YES	YES
25	a	274.86	5.39917	YES	YES
26	a	284.69	0.52632	YES	YES
27	a	286.20	0.39184	YES	YES
28	a	287.63	0.41729	YES	YES
29	a	391.56	8.56566	YES	YES
30	a	396.03	0.02883	YES	YES
31	a	435.81	248.64739	YES	YES
32	a	505.90	43.75330	YES	YES
33	a	542.59	0.00210	YES	YES
34	a	543.03	0.01396	YES	YES
35	a	543.28	0.00823	YES	YES
36	a	569.47	0.81369	YES	YES
37	a	584.51	1.13347	YES	YES
38	a	586.60	6.57191	YES	YES
39	a	589.75	0.88240	YES	YES
40	a	608.84	0.47712	YES	YES
41	a	793.35	2.62175	YES	YES
42	a	796.17	6.69516	YES	YES
43	a	814.25	13.79245	YES	YES
44	a	819.64	1.02323	YES	YES
45	a	827.24	271.51343	YES	YES
46	a	830.25	2.20195	YES	YES
47	a	830.93	8.36963	YES	YES
48	a	896.61	0.16167	YES	YES
49	a	900.64	0.40132	YES	YES
50	a	919.98	0.01430	YES	YES
51	a	920.60	0.13951	YES	YES
52	a	989.28	9.96779	YES	YES
53	a	991.94	10.85321	YES	YES
54	a	994.66	0.19916	YES	YES
55	a	995.85	13.40430	YES	YES
56	a	996.93	0.05599	YES	YES
57	a	998.83	0.31066	YES	YES
58	a	999.93	9.59449	YES	YES
59	a	1046.27	0.16163	YES	YES
60	a	1047.42	1.85173	YES	YES
61	a	1047.68	0.73133	YES	YES
62	a	1048.02	2.22085	YES	YES
63	a	1073.91	0.03985	YES	YES
64	a	1114.89	23.24528	YES	YES
65	a	1157.04	0.13928	YES	YES

66	a	1160.17	0.21714	YES	YES
67	a	1232.38	0.00022	YES	YES
68	a	1338.92	0.07263	YES	YES
69	a	1342.21	0.61182	YES	YES
70	a	1349.89	13.60505	YES	YES
71	a	1351.21	8.61553	YES	YES
72	a	1354.01	4.32494	YES	YES
73	a	1359.40	0.40901	YES	YES
74	a	1363.02	0.46207	YES	YES
75	a	1381.50	0.03987	YES	YES
76	a	1384.27	0.09790	YES	YES
77	a	1393.96	6.81415	YES	YES
78	a	1396.33	11.18123	YES	YES
79	a	1402.39	1.52276	YES	YES
80	a	1403.08	2.73338	YES	YES
81	a	1403.66	2.24589	YES	YES
82	a	1408.18	53.91203	YES	YES
83	a	1408.56	2.10300	YES	YES
84	a	1408.77	31.12964	YES	YES
85	a	1416.35	8.44319	YES	YES
86	a	1422.06	14.86666	YES	YES
87	a	1431.27	5.69251	YES	YES
88	a	1441.60	0.90279	YES	YES
89	a	1444.37	0.70844	YES	YES
90	a	1470.15	25.51838	YES	YES
91	a	1473.18	27.42715	YES	YES
92	a	2967.88	11.93449	YES	YES
93	a	2967.91	5.16139	YES	YES
94	a	2971.35	9.79948	YES	YES
95	a	2972.87	13.89274	YES	YES
96	a	2972.94	3.70230	YES	YES
97	a	3041.91	3.39318	YES	YES
98	a	3043.18	0.04917	YES	YES
99	a	3049.24	2.74498	YES	YES
100	a	3050.96	2.57318	YES	YES
101	a	3051.39	0.52969	YES	YES
102	a	3070.04	7.34848	YES	YES
103	a	3070.33	1.97043	YES	YES
104	a	3079.04	1.16661	YES	YES
105	a	3079.49	6.08879	YES	YES
106	a	3079.81	5.25251	YES	YES
107	a	3166.88	0.03237	YES	YES
108	a	3167.63	0.02445	YES	YES
109	a	3178.38	11.50890	YES	YES
110	a	3179.38	11.62739	YES	YES
111	a	3187.83	0.89193	YES	YES

$end

[CpAl–AlCp*]$^{2+}$



Method: (RI-)BP86(D3BJ)/def2-SVP

Symmetry: c1

Cartesian coordinates in Ångström:

Al	1.9011963	4.4132567	14.9381211
Al	3.7791198	6.0302526	14.6156790
C	0.9364050	2.6533927	14.1710007
C	1.3744969	2.4142248	15.5237940
C	4.3874859	8.0465348	14.9028103
C	5.2883420	7.1441666	15.6154125
C	5.8938227	6.2448714	14.6364278
C	0.7074840	3.3615188	16.3821839
C	-0.1427932	4.1861246	15.5599203
C	-0.0013406	3.7484871	14.1933694
C	4.4363429	7.7050820	13.4834515
C	5.3671859	6.5915409	13.3188058
C	5.8233909	6.0152243	12.0121309
C	6.9828225	5.2522658	14.9127217
C	5.6501820	7.2320420	17.0676412
C	3.7745659	8.4668064	12.3746649
C	3.6668354	9.2181711	15.4989422
H	3.5724409	7.8344293	11.4903755
H	4.4511425	9.2829432	12.0431468
H	2.8280681	8.9406632	12.6946838
H	6.9852043	4.4160477	14.1891049
H	6.9239605	4.8352160	15.9351532

H	7.9661836	5.7611449	14.8249892
H	5.0437005	6.0737227	11.2301812
H	6.1517234	4.9634707	12.1064686
H	6.6958688	6.5967869	11.6457250
H	2.7505233	9.4798370	14.9379134
H	4.3328600	10.1064661	15.4667156
H	3.3978701	9.0532461	16.5587561
H	5.9689192	6.2578925	17.4826682
H	4.8222574	7.6261830	17.6857360
H	6.5052783	7.9311179	17.1851906
H	2.0738392	1.6307786	15.8471119
H	1.2433596	2.0841089	13.2826759
H	0.8095127	3.4266345	17.4743131
H	-0.8023161	4.9898481	15.9155419
H	-0.5341207	4.1602401	13.3250420

SCF energy GEOOPT = -1067.548101629 H

ZPE = 786.6 kJ/mol

FREEH energy = 839.36 kJ/mol

FREEH entropy = 0.63166 kJ/mol/K

$vibrational spectrum

mode symmetry wave number IR intensity selection rules

#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	6.15	0.00033	YES	YES
8	a	29.11	0.70573	YES	YES
9	a	29.74	0.69854	YES	YES
10	a	91.70	0.97003	YES	YES
11	a	92.19	0.97823	YES	YES
12	a	128.04	0.03446	YES	YES
13	a	131.40	0.02067	YES	YES
14	a	134.61	0.07729	YES	YES
15	a	138.87	0.39855	YES	YES
16	a	141.52	0.40622	YES	YES
17	a	146.20	0.34064	YES	YES
18	a	147.65	0.00581	YES	YES
19	a	149.07	0.01203	YES	YES
20	a	225.48	0.11921	YES	YES
21	a	225.58	0.10927	YES	YES
22	a	234.88	7.26598	YES	YES
23	a	270.98	0.00311	YES	YES
24	a	273.78	0.00394	YES	YES
25	a	295.16	1.18429	YES	YES
26	a	296.02	1.19627	YES	YES
27	a	341.62	0.01245	YES	YES
28	a	342.05	0.01203	YES	YES
29	a	425.55	2.27793	YES	YES
30	a	425.91	2.29553	YES	YES
31	a	516.38	136.75184	YES	YES
32	a	539.53	0.00013	YES	YES
33	a	539.66	0.00163	YES	YES
34	a	539.77	0.00033	YES	YES
35	a	580.87	6.56278	YES	YES
36	a	591.52	0.00010	YES	YES
37	a	591.63	0.00015	YES	YES
38	a	610.72	0.00004	YES	YES
39	a	611.19	0.00011	YES	YES
40	a	620.76	5.79784	YES	YES
41	a	785.93	2.18548	YES	YES
42	a	786.66	2.20875	YES	YES
43	a	834.15	0.00020	YES	YES
44	a	834.37	0.00011	YES	YES
45	a	847.27	0.47739	YES	YES
46	a	847.96	0.21022	YES	YES
47	a	855.88	267.80717	YES	YES
48	a	910.13	0.00052	YES	YES
49	a	912.38	0.00162	YES	YES
50	a	918.92	0.01089	YES	YES
51	a	919.36	0.00431	YES	YES
52	a	984.75	18.29035	YES	YES
53	a	985.20	17.36898	YES	YES
54	a	985.72	4.98058	YES	YES
55	a	986.26	2.82958	YES	YES
56	a	992.55	12.78065	YES	YES
57	a	992.71	12.75200	YES	YES
58	a	993.89	1.98360	YES	YES

59	a	1045.87	0.00002	YES	YES
60	a	1045.97	0.00005	YES	YES
61	a	1047.04	5.43622	YES	YES
62	a	1047.30	5.49182	YES	YES
63	a	1072.18	0.00641	YES	YES
64	a	1098.20	38.00885	YES	YES
65	a	1144.96	0.00017	YES	YES
66	a	1145.06	0.00012	YES	YES
67	a	1227.07	0.00000	YES	YES
68	a	1334.24	0.00979	YES	YES
69	a	1335.15	0.06381	YES	YES
70	a	1338.54	0.00023	YES	YES
71	a	1338.60	0.00366	YES	YES
72	a	1351.47	18.08711	YES	YES
73	a	1352.00	16.62381	YES	YES
74	a	1354.76	6.43797	YES	YES
75	a	1371.01	0.01805	YES	YES
76	a	1371.21	0.01900	YES	YES
77	a	1380.15	2.15683	YES	YES
78	a	1380.65	2.06236	YES	YES
79	a	1385.94	131.59611	YES	YES
80	a	1396.85	0.03316	YES	YES
81	a	1401.46	15.61545	YES	YES
82	a	1401.55	12.82422	YES	YES
83	a	1401.62	8.21950	YES	YES
84	a	1402.31	0.03124	YES	YES
85	a	1407.61	1.85349	YES	YES
86	a	1408.04	1.77678	YES	YES
87	a	1425.29	27.09367	YES	YES
88	a	1431.95	0.04699	YES	YES
89	a	1432.33	0.09638	YES	YES
90	a	1444.52	50.05699	YES	YES
91	a	1445.02	50.33878	YES	YES
92	a	2978.33	6.66832	YES	YES
93	a	2978.56	0.40037	YES	YES
94	a	2978.68	0.22536	YES	YES
95	a	2978.75	0.16887	YES	YES
96	a	2978.88	0.08153	YES	YES
97	a	3059.56	7.02374	YES	YES
98	a	3059.59	7.55234	YES	YES
99	a	3059.76	7.27137	YES	YES
100	a	3060.64	0.07057	YES	YES
101	a	3060.80	0.06073	YES	YES
102	a	3093.84	0.01373	YES	YES
103	a	3093.98	0.36284	YES	YES
104	a	3094.05	0.42207	YES	YES
105	a	3094.50	1.64670	YES	YES
106	a	3094.64	1.63756	YES	YES
107	a	3161.99	0.00384	YES	YES
108	a	3162.04	0.00053	YES	YES
109	a	3170.34	59.79434	YES	YES
110	a	3170.42	59.76515	YES	YES
111	a	3178.85	6.34694	YES	YES

$end

S-3 Overview on crystal data

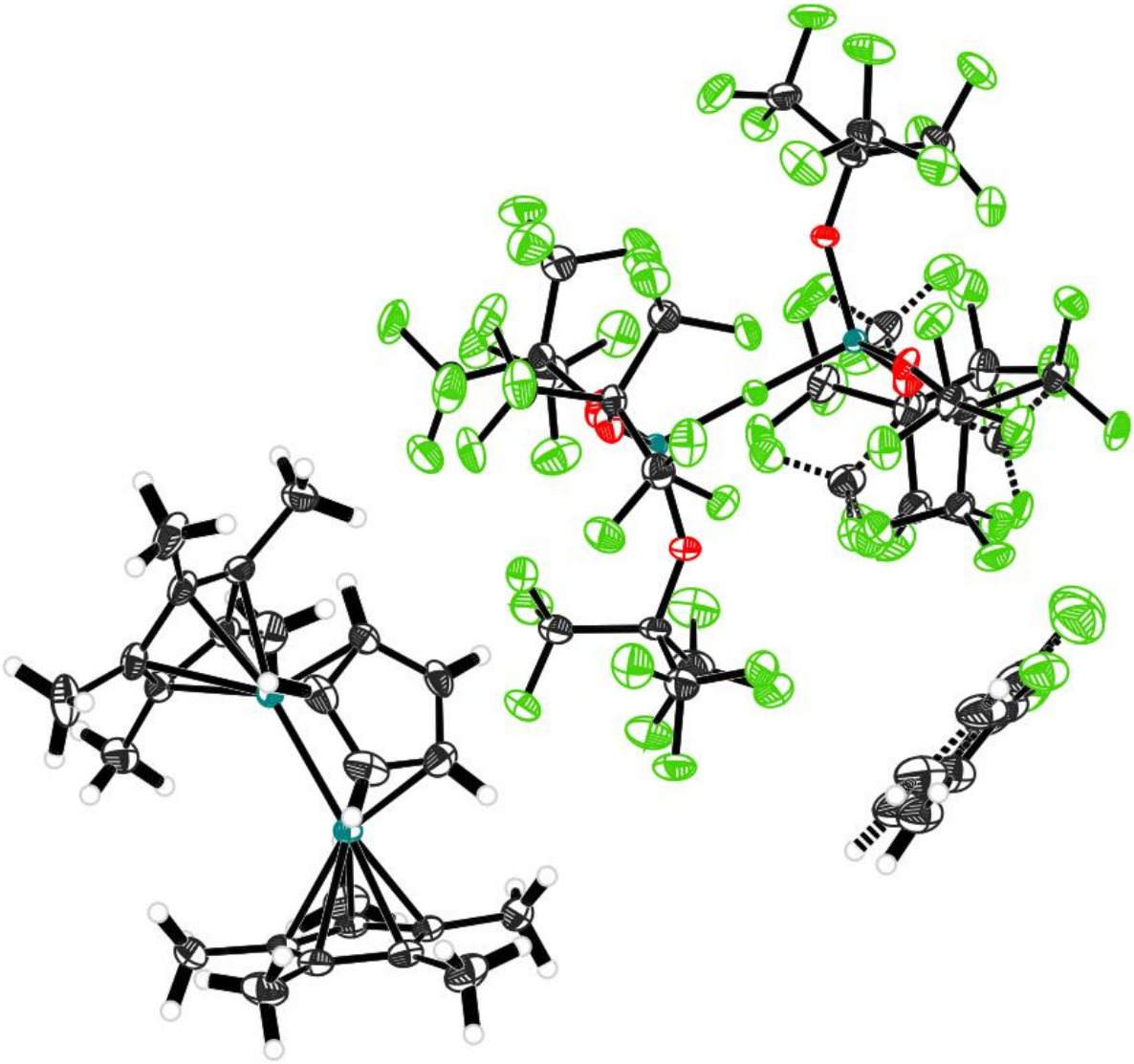
S-Table 14: Summary of crystallographic data for the molecular structures

Compound	Compound 1A	Compound 1B	Compound 3
CCDC number	2210632	2210631	2210630
Empirical formula	$C_{55}H_{39}Al_4F_{57}O_6$	$C_{43.88}H_{38}Al_3F_{36.75}O_4$	$C_{26}H_{10}Al_2F_{36}O_4$
Formula weight	1986.78	1408.45	1124.30
Temperature [K]	100(2)	100(2)	100(2)
Crystal system	triclinic	triclinic	monoclinic
Space group (number)	$P\overline{1}$ (2)	$P\overline{1}$ (2)	$C2/c$ (15)
a [Å]	13.709(5)	13.698(2)	19.578(10)
b [Å]	17.095(7)	15.496(7)	19.397(10)
c [Å]	17.529(6)	15.603(6)	19.321(11)
α [°]	113.074(10)	115.63(3)	90
β [°]	102.677(16)	111.470(13)	98.024(16)
γ [°]	96.97(2)	92.372(17)	90
Volume [Å^3]	3587(2)	2699.2(18)	7266(7)
Z	2	2	8
ρ_{calc} [gcm^{-3}]	1.839	1.733	2.056
μ [mm^{-1}]	0.262	0.240	0.302
F(000)	1964	1406	4384
Crystal size [mm^3]	0.222×0.219×0.198	0.198×0.187×0.082	0.252×0.233×0.100
Crystal colour	colourless	colourless	colourless
Crystal shape	block	block	block
Radiation	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)
2Θ range [°]	2.64 to 55.20 (0.77 Å)	3.00 to 59.28 (0.72 Å)	2.97 to 61.32 (0.70 Å)
Index ranges	−17 ≤ h ≤ 17 −22 ≤ k ≤ 22 −22 ≤ l ≤ 22	−19 ≤ h ≤ 17 −21 ≤ k ≤ 21 −21 ≤ l ≤ 21	−27 ≤ h ≤ 28 −27 ≤ k ≤ 27 −27 ≤ l ≤ 27
Reflections collected	90757	81381	97744
Independent reflections	16611 R_{int} = 0.0344	15180 R_{int} = 0.0285	11190 R_{int} = 0.0510
	R_{sigma} = 0.0286	R_{sigma} = 0.0203	R_{sigma} = 0.0294
Completeness to Θ = 25.242°	100.0 %	100.0 %	100.0 %
Data / Restraints / Parameters	16611/9454/1312	15180/12752/1494	11190/4712/740
Goodness-of-fit on F^2	1.027	1.048	1.029
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0421	R_1 = 0.0418	R_1 = 0.0346
	wR_2 = 0.0985	wR_2 = 0.1080	wR_2 = 0.0723
Final *R* indexes [all data]	R_1 = 0.0607	R_1 = 0.0579	R_1 = 0.0534
	wR_2 = 0.1078	wR_2 = 0.1222	wR_2 = 0.0799
Largest peak/hole [eÅ^{-3}]	0.59/-0.36	0.48/-0.51	0.44/-0.29

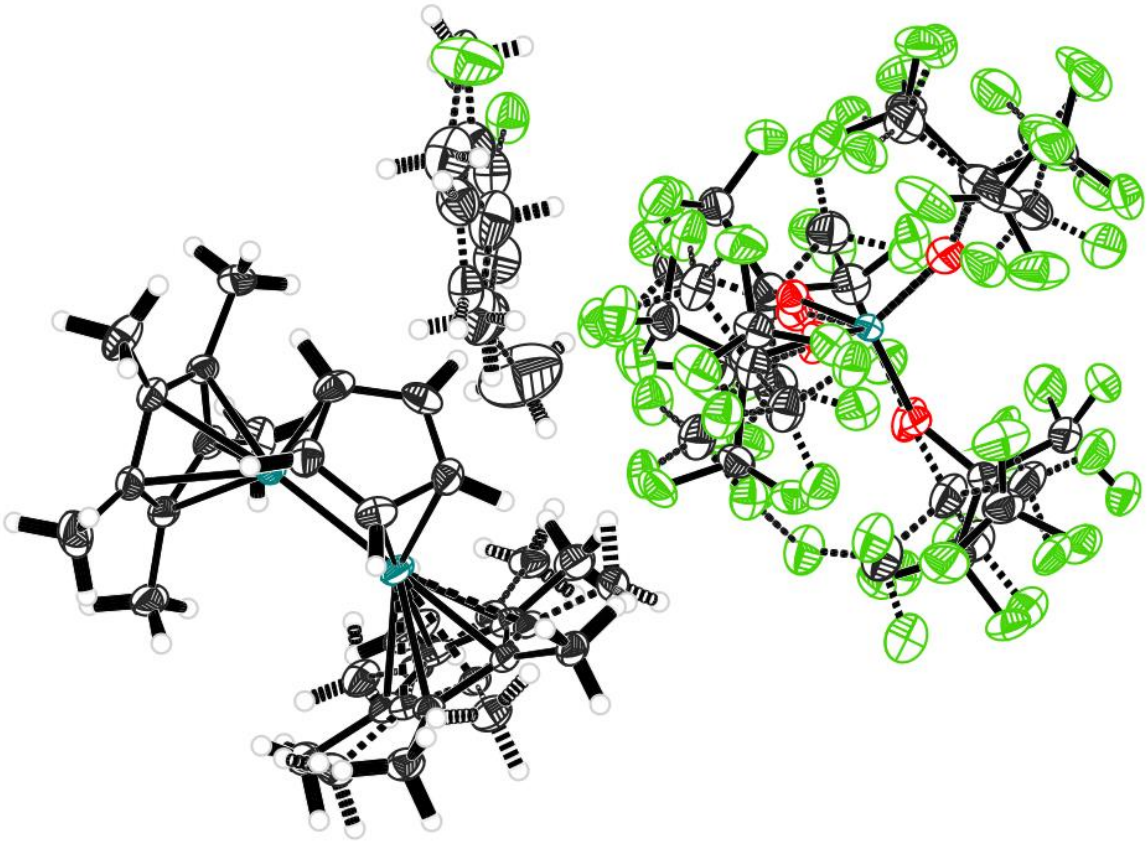
S-Table 15: Summary of crystallographic data for the molecular structures

Compound	Compound 4	[Al(Cp)(Cp*)][Al(OR^F)$_4$]
CCDC number	2210633	2214274
Empirical formula	$C_{36}H_{25}Al_3F_{36}O_4$	$C_{27.67}H_{17.33}Al_2F_{36.67}O_4$
Formula weight	1286.43	1164.37
Temperature [K]	100(2)	100(2)
Crystal system	orthorhombic	triclinic
Space group (number)	$P2_12_12_1$ (19)	$P\bar{1}$ (2)
a [Å]	20.350(2)	14.183(10)
b [Å]	22.947(3)	15.753(10)
c [Å]	40.507(4)	16.525(8)
α [°]	90	62.461(15)
β [°]	90	69.749(7)
γ [°]	90	70.422(11)
Volume [Å^3]	18915(4)	3002(3)
Z	16	3
ρ_{calc} [gcm^{-3}]	1.807	1.932
μ [mm^{-1}]	0.262	0.280
F(000)	10175	1714
Crystal size [mm^3]	0.272×0.196×0.158	0.326×0.246×0.160
Crystal colour	colourless	colourless
Crystal shape	block	block
Radiation	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)
2Θ range [°]	2.67 to 60.33 (0.71 Å)	2.86 to 61.15 (0.70 Å)
Index ranges	−28 ≤ h ≤ 27 −30 ≤ k ≤ 32 −55 ≤ l ≤ 54	−20 ≤ h ≤ 20 −22 ≤ k ≤ 22 −23 ≤ l ≤ 23
Reflections collected	482475	135405
Independent reflections	54386 R_{int} = 0.0392	18396 R_{int} = 0.0772
	R_{sigma} = 0.0269	R_{sigma} = 0.0397
Completeness to Θ = 25.242°	99.8 %	100.0 %
Data / Restraints / Parameters	54386/220340/5952	18396/16881/1540
Goodness-of-fit on F^2	1.045	1.056
Final *R* indexes [*I*≥2σ(*I*)]	R_1 = 0.0488	R_1 = 0.0474
	wR_2 = 0.1127	wR_2 = 0.1136
Final *R* indexes [all data]	R_1 = 0.0625	R_1 = 0.0671
	wR_2 = 0.1207	wR_2 = 0.1285
Largest peak/hole [eÅ^{-3}]	0.69/-0.40	0.64/-0.40

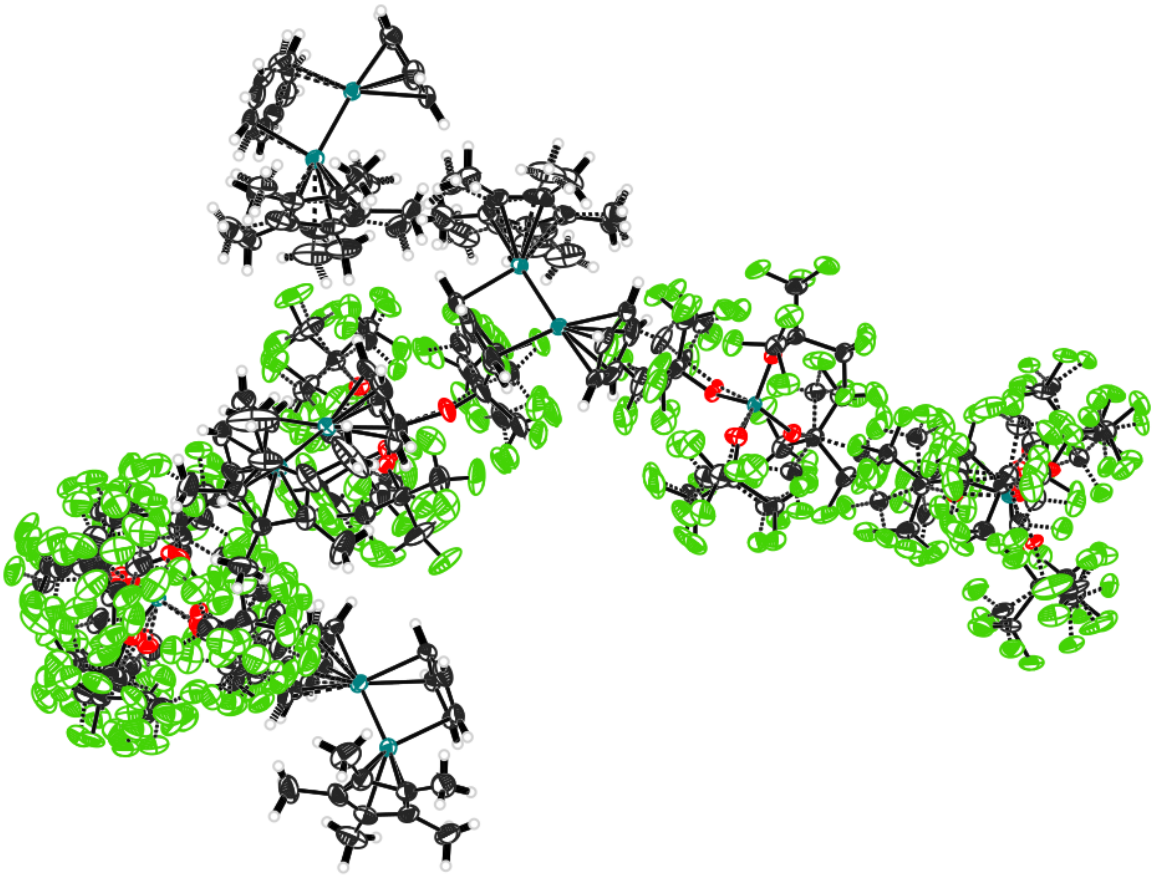
S-3.1 Asymetric units of the crystal structures



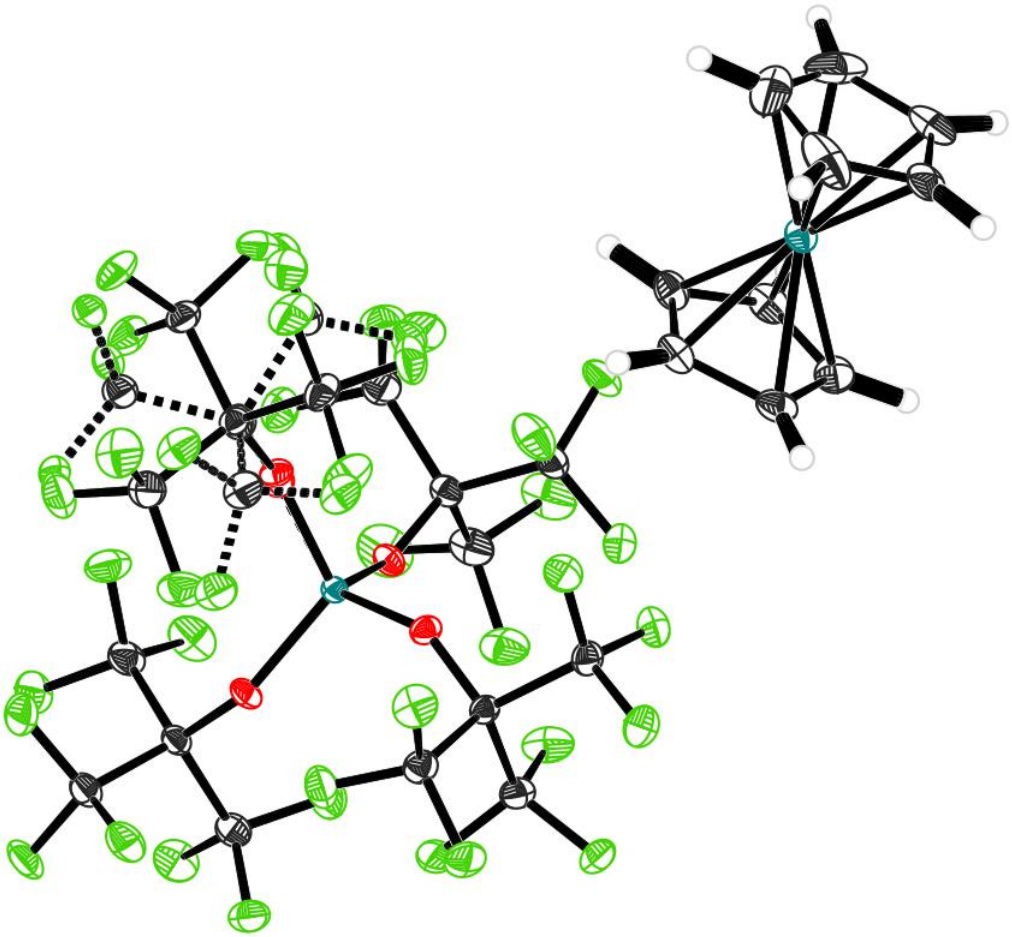
S-Figure 61: Asymmetric unit of the molecular structure of compound **1A**. Thermal displacement of the ellipsoids was set at 50 % probability.



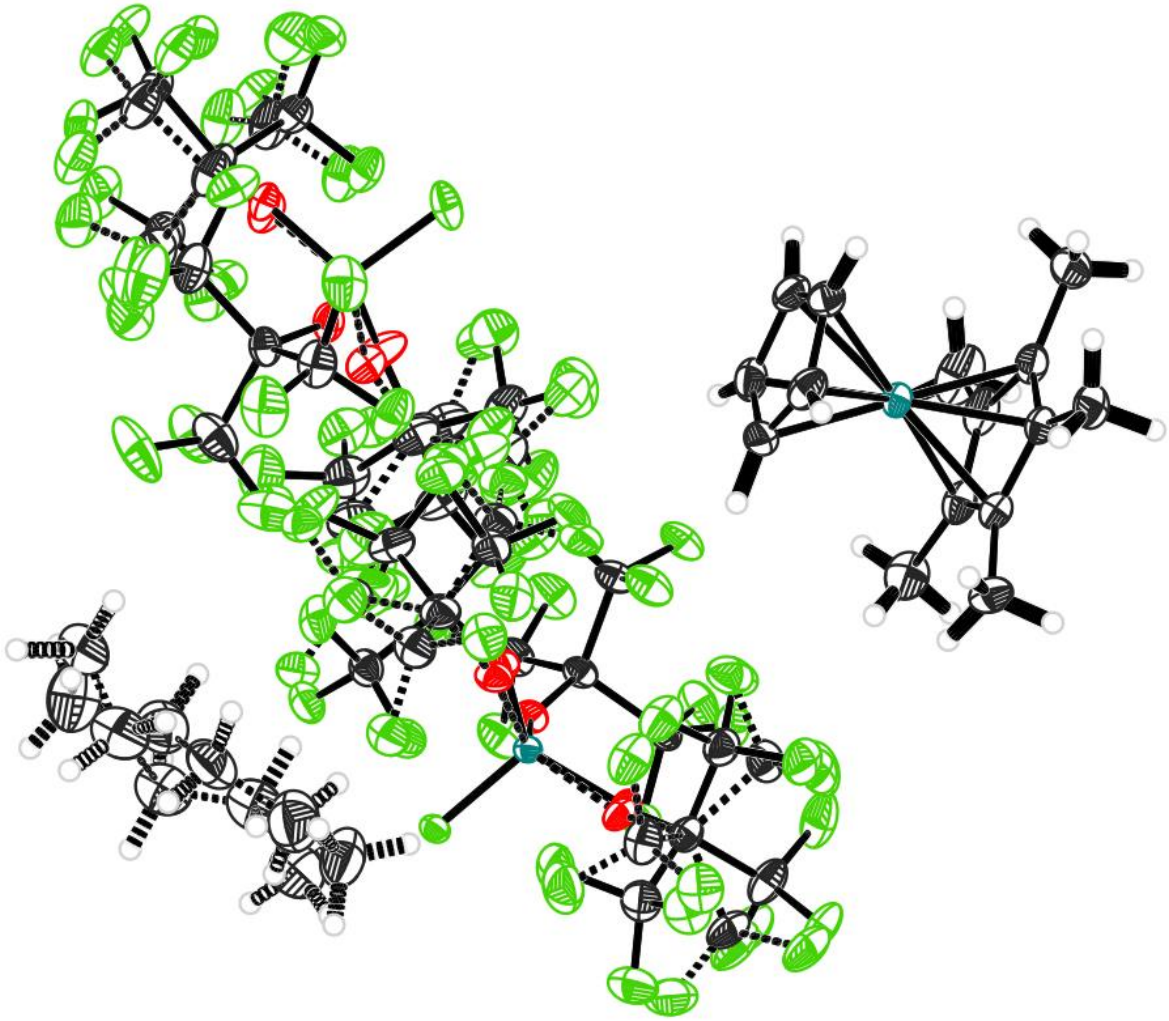
S-Figure 62: Asymmetric unit of the molecular structure of compound **1B**. Thermal displacement of the ellipsoids was set at 50 % probability.



S-Figure 63: Asymmetric unit of the molecular structure of compound **4**. Thermal displacement of the ellipsoids was set at 50 % probability.



S-Figure 64: Asymmetric unit of the molecular structure of compound **3**. Thermal displacement of the ellipsoids was set at 50 % probability.



S-Figure 65: Asymmetric unit of the molecular structure of compound $[Al(Cp)(Cp^*)][Al(OR^F)_4]$. Thermal displacement of the ellipsoids was set at 50 % probability.

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