Supporting information for the article: **From an Al_4-Cluster to Al^+ Complexes: Lessons on Metalloidal Clustering**

Philipp Dabringhaus, Julie Willrett, Ingo Krossing

Contents

S-1 Supporting literature searches

S-1.1 Bond lengths of $[(AlL)_4]$ compounds and selected larger Al clusters

S-Table 1: Summary of Al–Al bond lengths reported for literature known compounds of type $[(AlL)_4]$ (L = $\{N(SiMe_3)_2\}_6$. Cp*…) and selected larger Al clusters

Compound	Al–Al bond length [Å]	Literature
$[Al_7\{N(SiMe_3)_2\}_6]^-$	2.540(7) (Al_{Cp^*}–Al_{Cp^*}) 2.737(4) (Al_{center}–Al_N))	[1]
$[Al(AlCp^*)_3]^+$	2.546(2)	this publication
$[Al_7\{N(SiMe_3)_2\}_6]^-$	2.61 (Al_N–Al_N) 2.73 (Al_{center}–Al_N)	[2]
$[(Al\{Si(SiMe_3)_3\})_4]$	2.602	[3]
$[(Al\{Si(CMe_3)_3\})_4]$	2.604(4)	[4]
$[(Al\{2,6\text{-}iPr_2C_6H_3N(SiMe_3)\})_4]$	2.619	[5]
$[(Cp^*Al)_3Al\{N(SiMe_3)_2\}]$	2.6609 (Al_{Cp^*}–Al_N) 2.7575 (Al_{Cp^*}–Al_{Cp^*})	[6]
$[(Al\{C(SiMe_3)_3\})_4]$	2.739	[7]
$[(AlCp^*)_4]$	2.770(5)	[8]

S-2 Supporting experimental data

S-1.2 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. Cp*H (Sigma Aldrich), KHMDS (Sigma Aldrich, >95%), dimethylaminopyridine (Sigma-Aldrich, >98%), TMEDA (Sigma-Aldrich, >99%) were used as received. Li[*pf*] ([*pf*]$^-$ = [Al(OR^F)$_4$]$^-$ with OR^F = C(CF$_3$)$_3$),[9] hexaphenylcarbodiphosporane (C(PPh$_3$)$_2$)[10,11] and [(AlCp*)$_4$][12] (Cp* = C$_5$Me$_5$) prepared using literature known procedures. 1,3-Difluorobenzene (fluorochem, 1,3-DFB) 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. ^{1}H, ^{7}Li, ^{13}C, ^{19}F, ^{27}Al and ^{31}P-NMR spectra were acquired either on a Bruker Biospin Avance II+ 400 MHz WB or a Bruker Avance III HD 300 MHz spectrometer. ^{1}H 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.

Electron spray ionisation (ESI): The mass-spectrometric experiments were performed with a Thermo-Fischer LTQ XL linear ion-trap mass-spectrometer equipped with an electrospray-ionization (ESI) source. Mass spectra were obtained by electrospray ionization from a millimolar solution in in 1,2-DFB. Nitrogen was used as a Sheath, Sweep, and Auxiliary Gas at flow rates to 5, 10 and 20, respectively (given in arbitrary units). The capillary temperature was set to 100°C, the Source Voltage was set to 3.5 kV and the Tube Lens Voltage was adjusted to 95 V. The identity of the ions was confirmed by comparison of the relative signal intensities with simulated isotope patterns, complemented by collision-induced dissociation (CID). In the CID experiments, helium served as collision gas. The supplied collision energy was adjusted by varying the Normalized Collision Energy (NCE) between 0 and 25.

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.

UV/VIS spectroscopy: Solution UV/VIS spectra were recorded on a Varian Cary 50 UV-Vis spectrophotometer in quartz cuvettes (thickness 1 mm) in oDFB solution. Solid-state UV/VIS spectra were recorded on a Thermo Scientific Evolution 600 UV/VIS spectrophotometer.

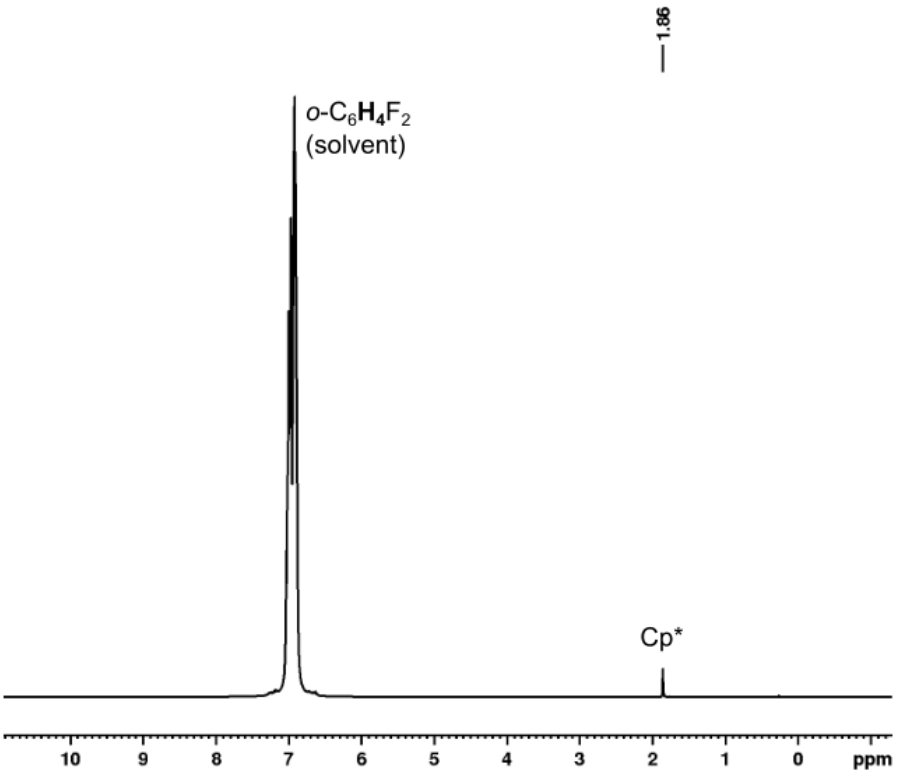
Single crystal X-ray analysis: Single crystal X-ray diffraction. Single crystal X-ray diffraction data were collected using either on a Bruker SMART APEXII QUAZAR detector with fixed-Chi D8 Goniometer, INCOATEC Mo microsource or Bruker D8 VENTURE with PHOTONIII detector, fixed-Chi D8 Goniometer and INCOATEC 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.[13] Data were collected at 100 K using monochromated Cu Kα or Mo Kα radiation (λ = 1.5418/0.71073 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.[14,15] Graphical representations have been prepared using Olex2-1.2. Finalisation of gathered data was done using final cif tool.[16]

Powder X-ray analysis: Powder diffractograms were recorded with the sample sealed with perfluoropolyalkylether oil (AB128330, abcr GmbH & Co. KG) in a 0.3 mm thick capillary (Hilgenberg GmbH, wall thickness 0.01 mm) at 100 K in the 2θ range 2.0-40.0° with a STOE STADI P powder diffractometer with Mo-$K_{\alpha1}$ radiation (λ = 0.709300 Å) equipped with a Ge-(111) monochromator and Mythen 1K detector. Data acquiring, processing and the calculation of powder diffractograms from single-crystal data were performed using STOE WinXPOW® package.

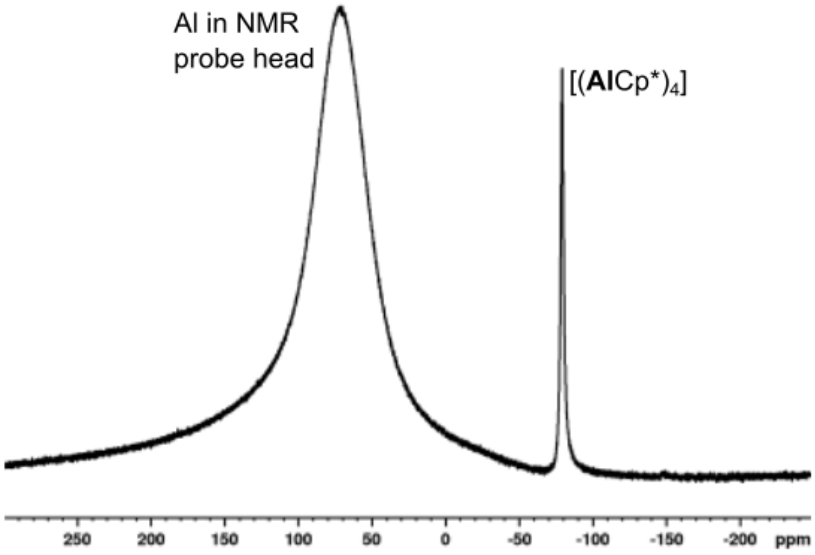
S-1.3 Additional analytical data for $[(AlCp^*)_4]$

$[(AlCp^*)_4]$ was prepared according to a literature procedure reported by Fischer.[12]

NMR spectra of $[(AlCp^*)_4]$ ($Cp^* = C_5Me_5$) in 1,2-Difluorobenzene:

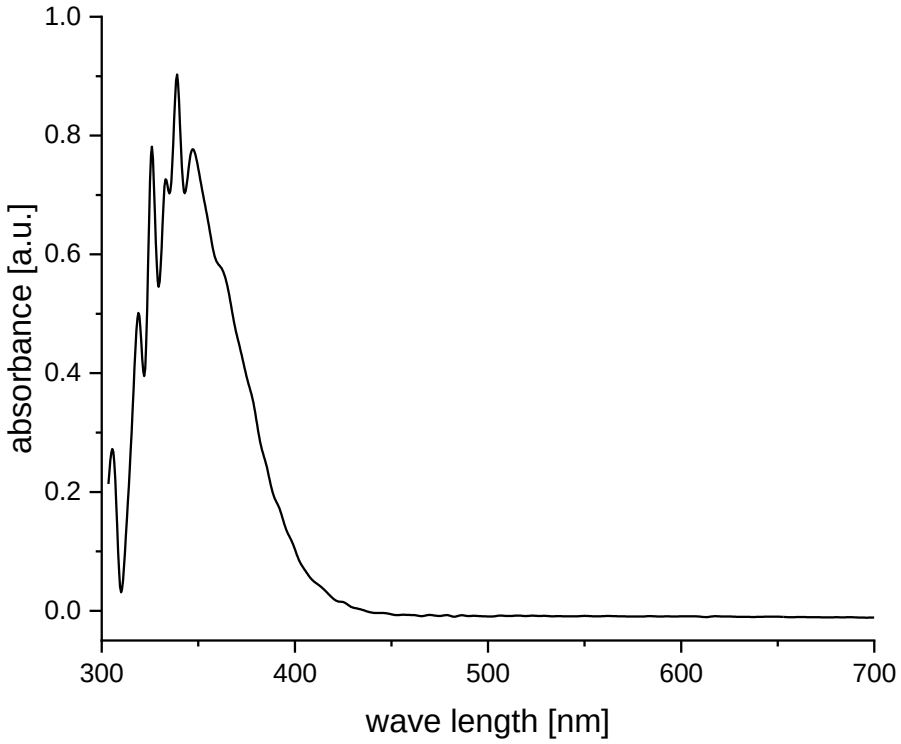


S-Figure 1: ^1H NMR spectrum (300.2 MHz, 1,2-DFB, 300K) of $[(AlCp^*)_4]$. The intense multiplet between δ = 6.6-7.2 ppm originates from the proton resonance of 1,2-difluorobenzene.



S-Figure 2: ^{27}Al NMR spectrum (78.2 MHz, 1,2-DFB, 300K) of $[(AlCp^*)_4]$. The broad signal at δ = 66 ppm originates from the resonance of aluminium in the probe head.

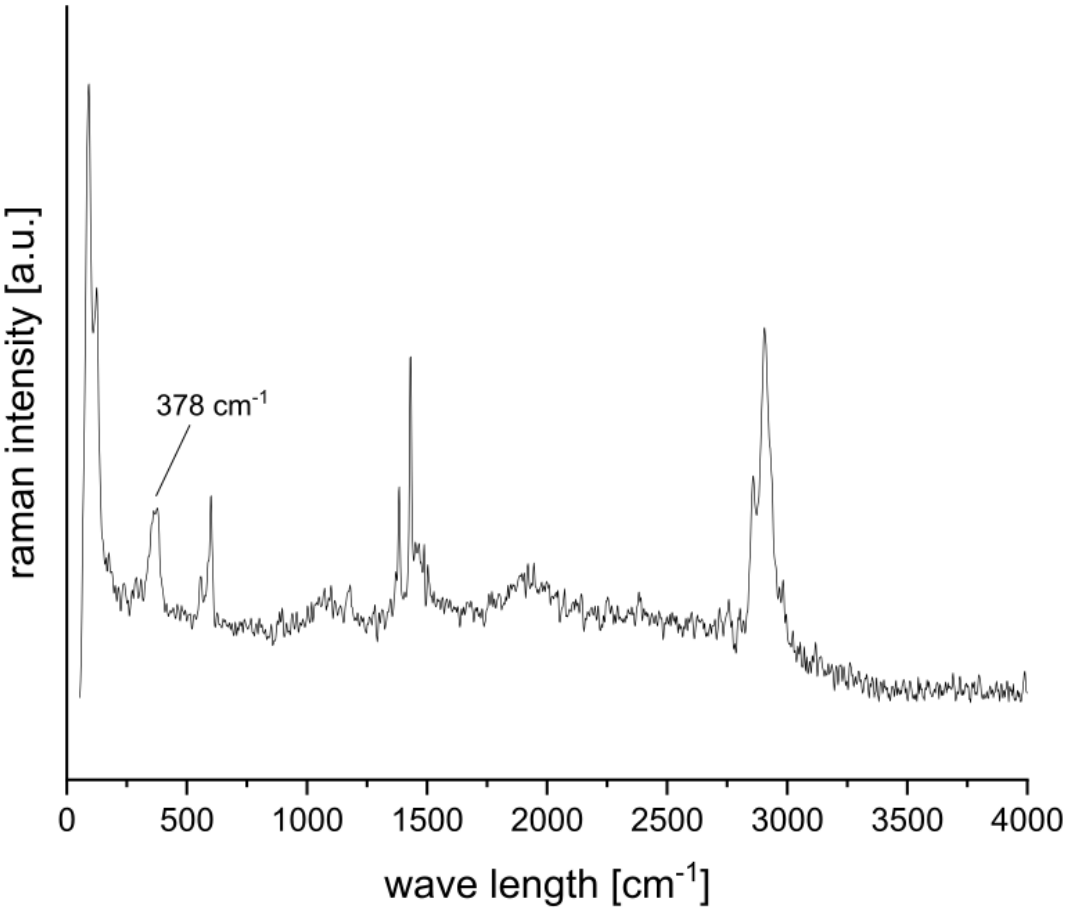
UV/VIS spectrum of [(AlCp*)$_4$] in 1,2-Difluorobenzene



S-Figure 3: Room-temperature UV/VIS spectrum of [(AlCp*)$_4$] dissolved in 1,2-DFB (0.5 mg/mL). The fine structure of the broad UV/VIS band originates from the excitation in various excited vibrational states.

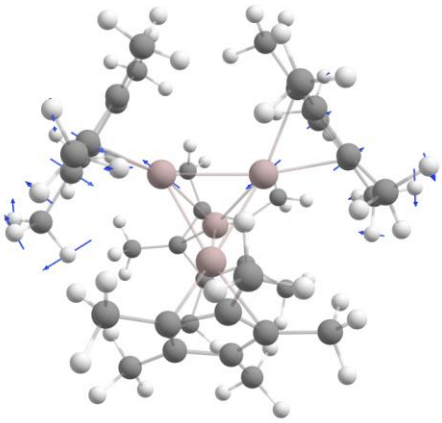
Raman spectrum of [(AlCp*)$_4$]

In the Raman spectrum of [(AlCp*)$_4$], the broad band at 378 cm^{-1} can be assigned to the iconic breathing vibration of the Al_4 tetrahedron.[8] The molecular vibration was calculated on bp86-d3bj/def2-svp-level of DFT and is visualized in S-Table 2. Similar vibrational modes can be observed in the Raman spectra of other reported Al_4 clusters.[3,4,6] Prominent signals near 2900 cm^{-1} can be assigned to C–H stretching vibrations(ν(C–H)). Raman bands near 1400 cm^{-1} and 600 cm^{-1} are attributable to breathing vibrations of the C_5Me_5 ligands as well as deformational modes of the CH_3 groups.[17,18]



S-Figure 4: Raman spectrum of $[(AlCp^*)_4]$.

S-Table 2: Observed and calculated (bp86-d3bj/def2-svp) Raman frequencies as well as visualization of the breathing mode of the Al_4 fragment in $[(AlCp^*)_4]$

Raman (Exp.) $\tilde{\nu}$ **[cm^{-1}]**	**Calc.** $\tilde{\nu}$ **[cm^{-1}]**	**Scaled displacement vectors for the vibrational modes**
378	376	

(Threshold for visualization: 0.13)

S-1.4 Experimental data for [Al(AlCp*)$_3$][*pf*] **1**

First procedure: Synthesis of impure [Al(AlCp*)$_3$][*pf*]

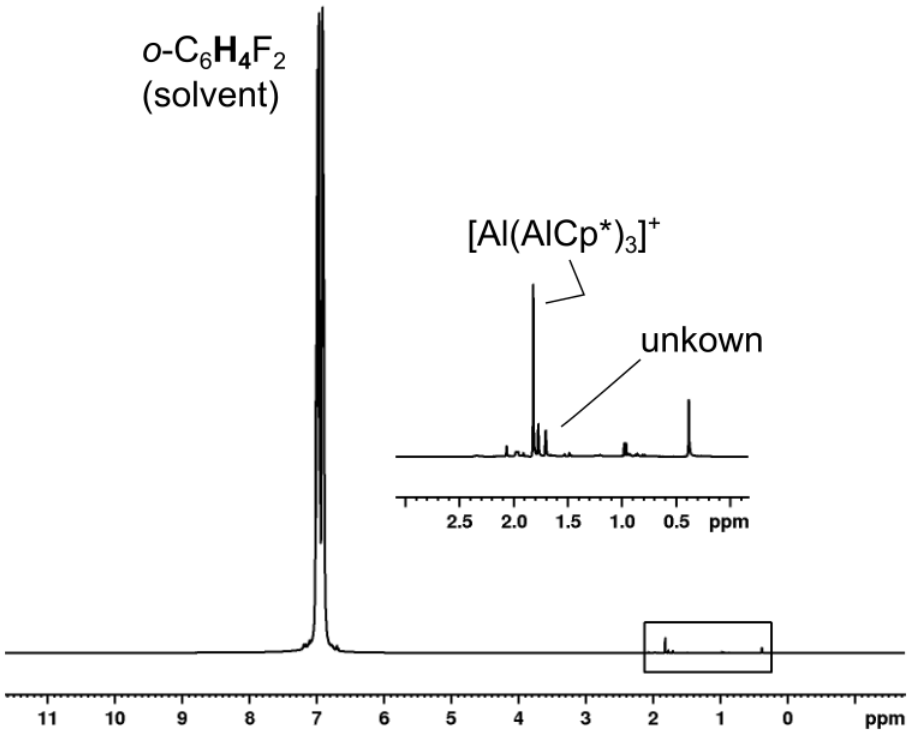
[(AlCp*)$_4$] (10 mg, 15 μmol) and Li [*pf*] (15 mg, 15 μmol, 1.0 equiv.) were weighed into a Schlenk flask. Pre-cooled 1,2-difluorobenzene (1,2-DFB; 1 mL) was added at –30°C and the reaction mixture was stirred for one hour. Then the red solution was layered with *n*-heptane (6 mL). The title compound (14 mg, 9.2 μmol) was isolated as purple crystals, strongly contaminated with a light-yellow powder. Single-crystal X-ray Diffraction identified the purple crystals to be the title compound [Al(AlCp*)$_3$][*pf*].

^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 298 K): δ = 2.06 (s, unknown compound), 1.97 (br.s, 30H, [AlCp*$_2$]$^+$), 1.91 (s, unknown compound), 1.82 (s, 45 H, [Al(AlCp*)$_3$]$^+$), 1.77 (s, unknown compound), 1.70 (unkown compound), 1.53 (s, unknown compound), 1.48 (s, unknown compound) ppm.

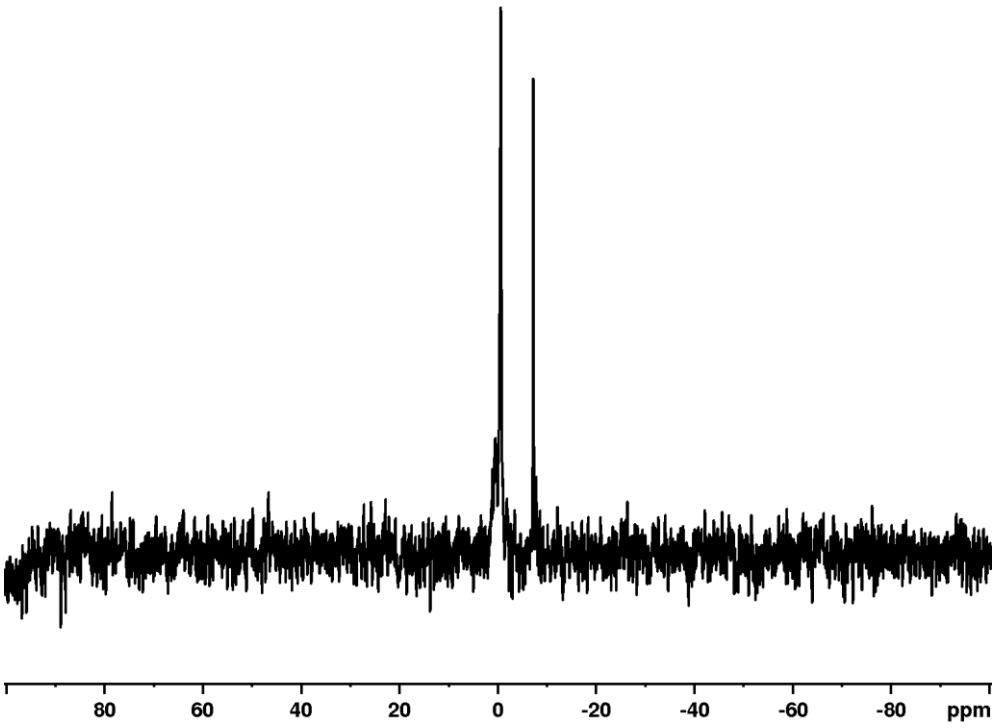
^{7}Li NMR spectrum (155.52 MHz, 1,2-DFB, 298 K): δ = 0.56 (br. s, unknown compound), –0.57 (s, unknown compound), –7.19 (s, unknown compound) ppm.

^{19}F NMR spectrum (282.45 MHz, 1,2-DFB, 298 K): δ = –75.3 (s, 36 F, [Al(OC$_4$F$_9$)$_4$]$^-$) ppm.

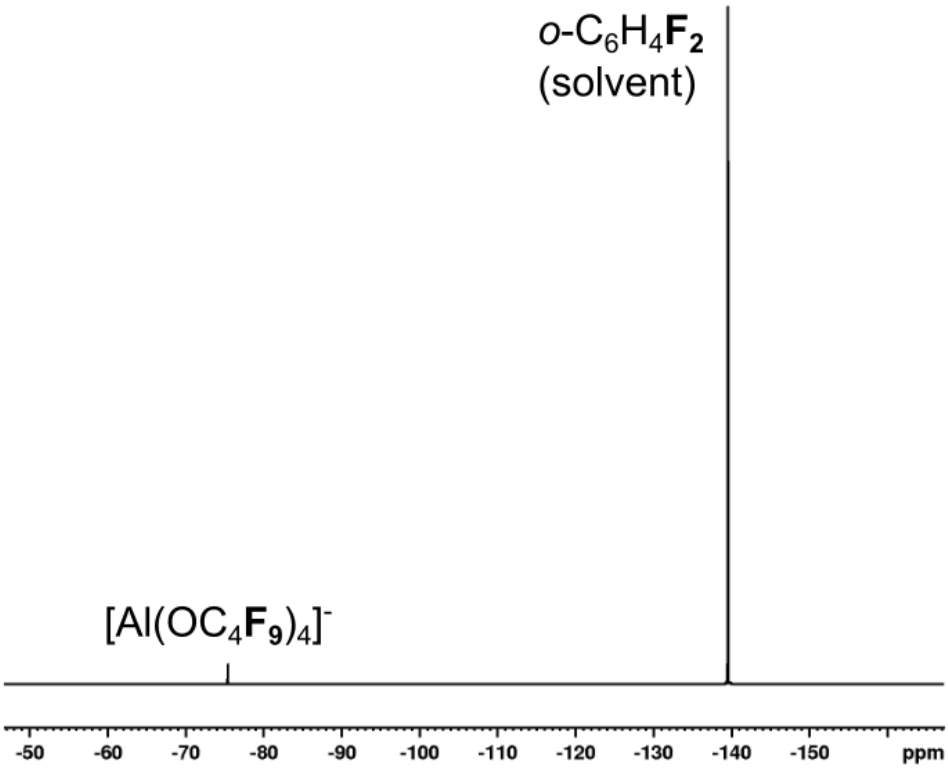
^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 298 K): δ = 35.0 (s, [Al(OC$_4$F$_9$)$_4$]$^-$), –114.6 (br. s, [AlCp*$_2$]$^+$) ppm.



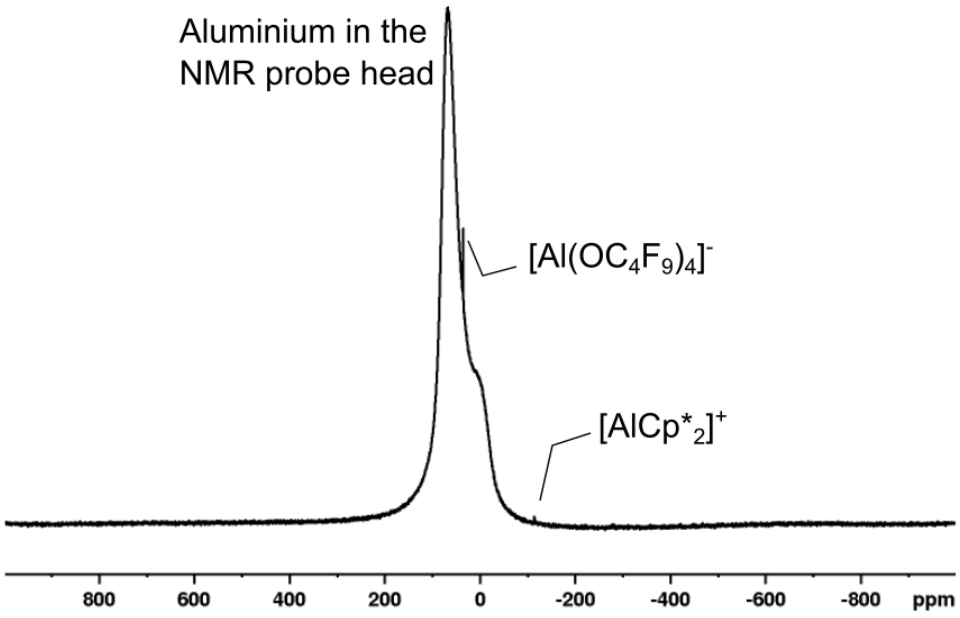
S-Figure 5: ^{1}H NMR spectrum (400.18 MHz, 1,2-DFB, 300K) of the product form the first synthesis of **1**.



S-Figure 6: ^{7}Li NMR spectrum (155.52 MHz, 1,2-DFB, 300K) of the product form the first synthesis of **1**.



S-Figure 7: ^{19}F NMR spectrum (376.54 MHz, 1,2-DFB, 300K) of the product form the first synthesis of **1**.



S-Figure 8: ^{27}Al NMR spectrum (104.27MHz, 1,2-DFB, 300K) of the product form the first synthesis of **1**.

Optimized Procedure to pure $[Al(AlCp^*)_3]^+[pf]^-$

$[(AlCp^*)_4]$ (1.28 g, 7.92 mmol) and Li[*pf*] (1.93 mg, 1.98 mmol, 0.25 eq.) were weighted into a Schlenk flask. 1,2-DFB (15 mL) was added at −40°C to yield a dark purple solution. The reaction mixture was stirred for 3 h at −40°C and then warmed up to room temperature. The solvent was evaporated under reduced pressure and 1,3-DFB (12 mL) was added. The resulting reaction mixture was stirred for 15 min and precipitation of a white solid was observed. The mixture was filter-canulated and the deep purple solution was allowed to crystallize in freezer at –40°C. The title compound (967 mg, 0.653 mmol, 33 %) was isolated as dark purple crystals.

^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 298 K): δ = 1.82 (s, 45 H, $[Al(AlCp^*)_3]^+$) ppm.

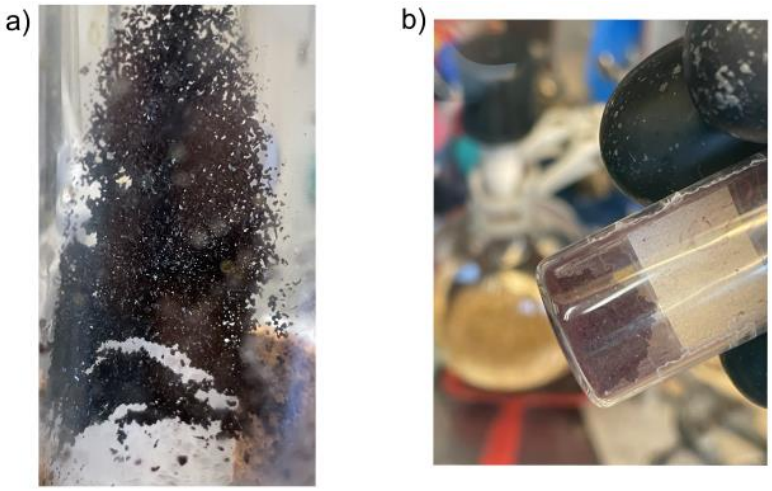
^{13}C NMR spectrum (75.48 MHz, 1,2-DFB, 298 K): δ = 115.8 (s, $\mathbf{C_5}(CH_3)_5$), 8.6 (s, $C_5(\mathbf{C}H_3)_5$)) ppm.

^{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, $[Al(OC_4F_9)_4]^-$), −41.0 (br. s, $[Al(\mathbf{Al}Cp^*)_3]^+$), −274.3 (br. s, $[\mathbf{Al}(AlCp^*)_3]^+$) ppm.

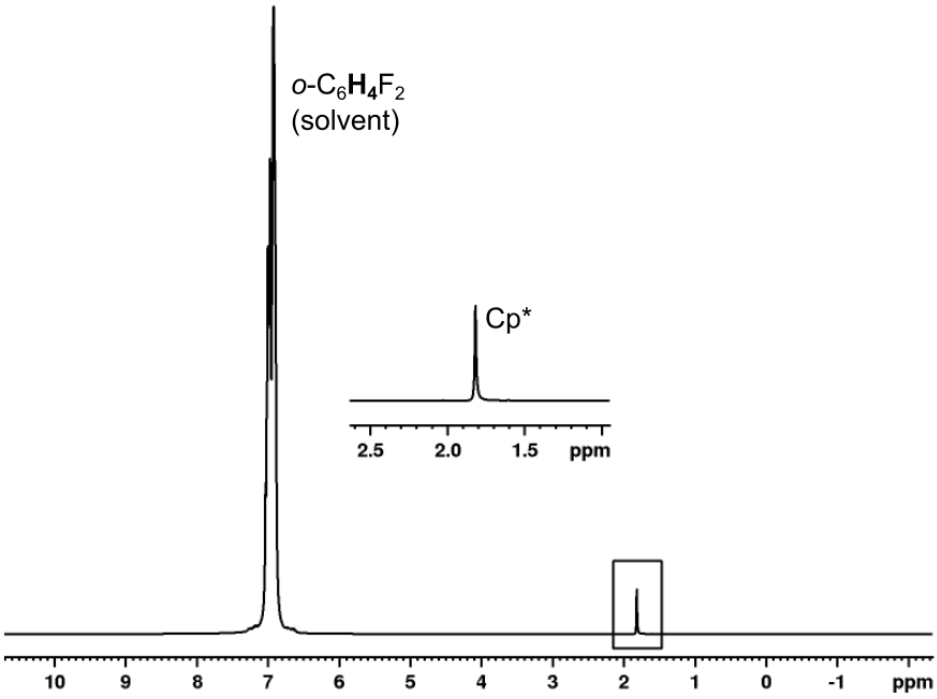
FTIR spectrum (ZnSe-ATR): $\tilde{\nu}$ = 2927 (vw), 2866 (vw), 1480 (vw), 1455 (vw), 1418 (vw), 1390 (vw), 1352 (vw), 1298 (w), 1275 (s), 1241 (m), 1211 (vs), 1161 (w), 971 (vs), 831 (vw), 798 (vw), 756 (vw), 726 (vs), 585 (vw), 560 (vw) cm^{-1}.

Raman spectrum (1000 scans): $\tilde{\nu}$ = 2927 (vw), 1420 (vw), 1393 (vw), 593 (vw), 473 (w), 396 (vw), 307 (vs), 283 (w), 210 (w), 183 (vs), 160 (m), 83 (s) cm^{-1}.

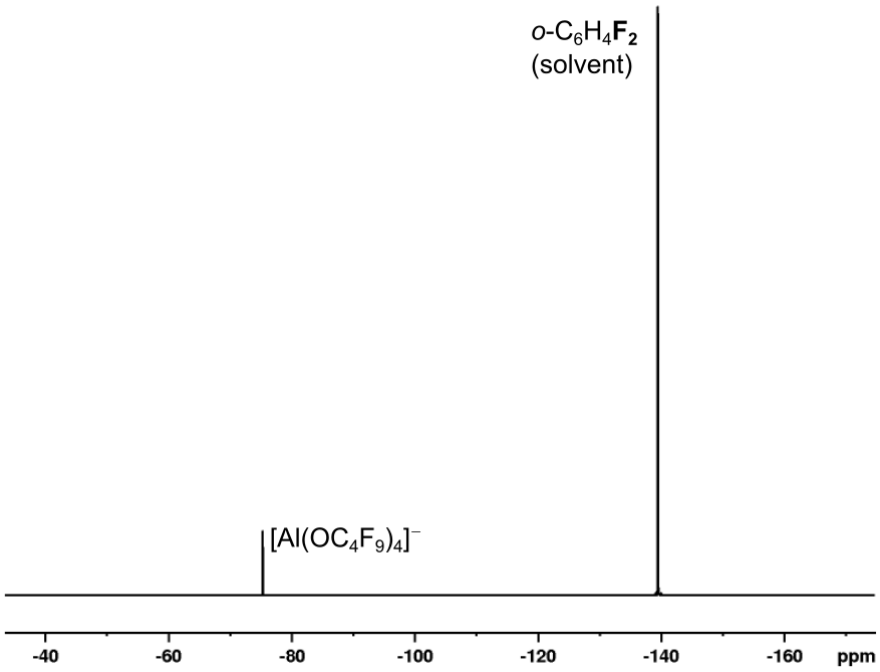


S-Figure 9: Dark-violet crystals of **1** (a) and isolated crystalline powder of **1** (b).

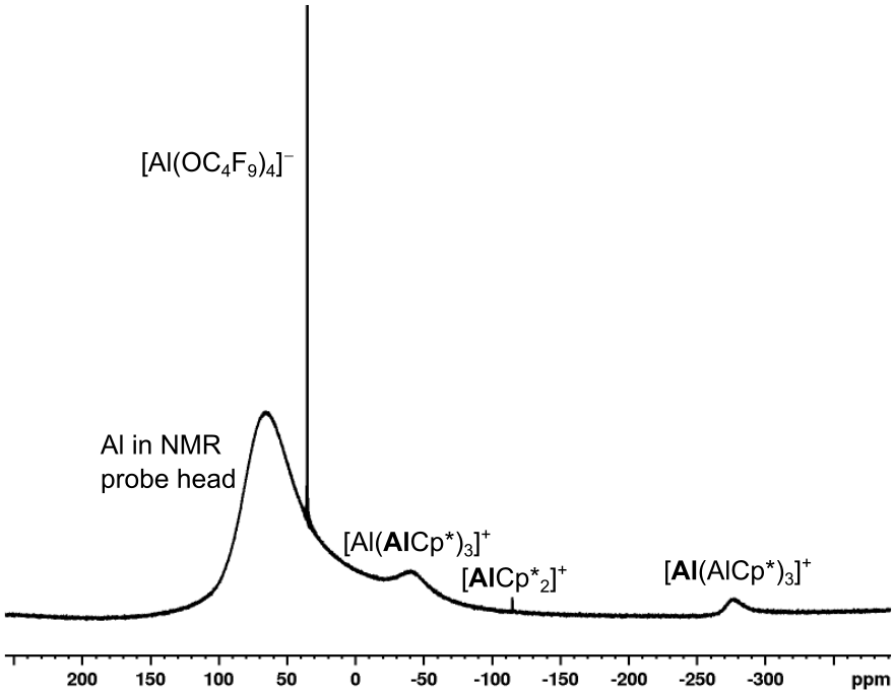
NMR spectra of [Al(AlCp*)$_3$][*pf*] 1



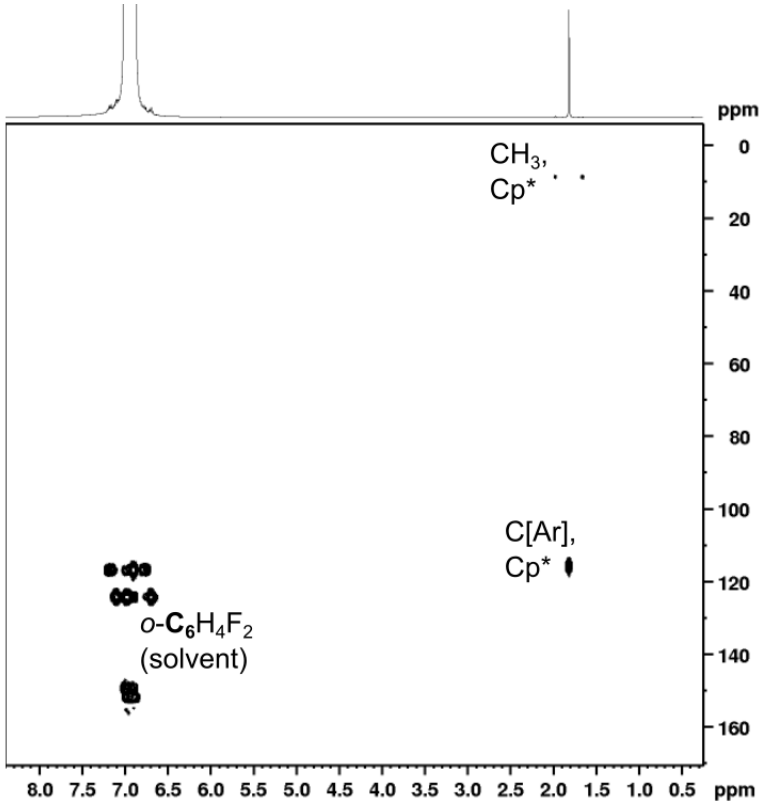
S-Figure 10: ^{1}H NMR spectrum (300.2 MHz, 1,2-DFB, 300K) of [Al(AlCp*)$_3$][*pf*] **1**. The intense multiplet between δ = 6.6-7.2 ppm originates from the proton resonance of 1,2-difluorobenzene.



S-Figure 11: ^{19}F NMR spectrum (282.5 MHz, 1,2-DFB, 300K) of [Al(AlCp*)$_3$][*pf*] **1**. The intense signal at δ = –139.6 ppm originates from the ^{19}F NMR resonance of 1,2-difluorobenzene.



S-Figure 12: ^{27}Al NMR spectrum (78.2 MHz, 1,2-DFB, 300K) of [Al(AlCp*)$_3$][*pf*] **1**. Upon comparison with the literature, the sharp singlet at δ = –114 ppm is assigned to [AlCp*$_2$][*pf*] as decomposition product of **1**.[19] The broad signal at δ = 66 ppm originates from the resonance of aluminium in the probe head.



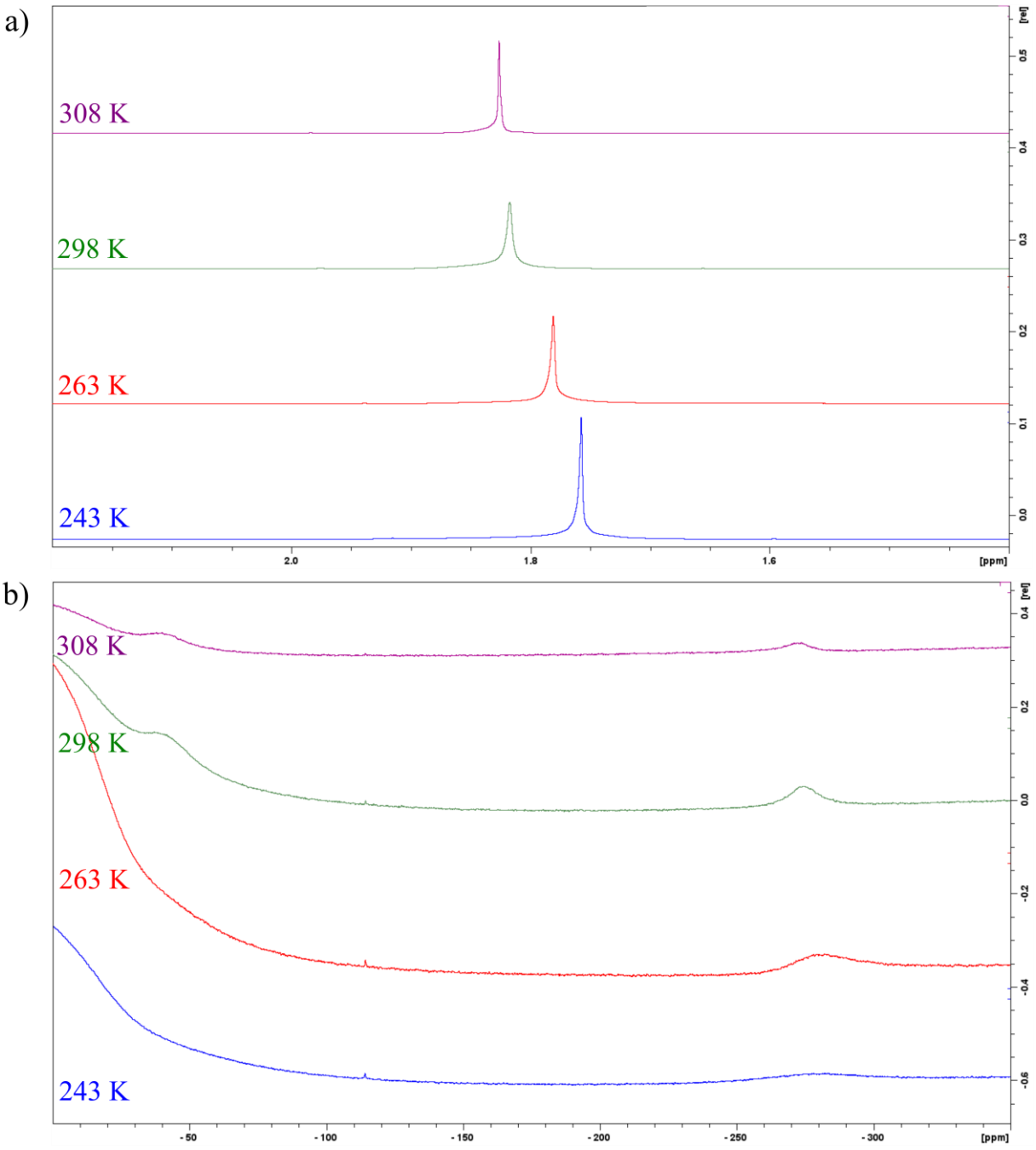
S-Figure 13: ^{1}H-^{13}C HMBC spectrum (400.2 MHz, 100.6 MHz, 1,2-DFB, 300K) of [Al(AlCp*)$_3$][*pf*] **1**.

Low-temperature NMR studies on [Al(AlCp*)$_3$][*pf*] 1

^{27}Al is a nucleus with a spin quantum number of 5/2 and a quadrupolar moment of Q = 0.149 10^{-28} m^2. Hence, ^{27}Al NMR spectra experiences significant line-broadening due to quadrupole relaxation. Notably, the quadrupolar relaxation of a single quadrupolar nucleus with a spin I and quadrupolar momentum Q is described by

$$\boldsymbol{T_1^{-1} = \frac{3\pi^2}{10}\frac{(2I+3)}{I^2(2I-1)}\left(\frac{eQ}{h}\right)^2 V_{zz}^2\left(1+\frac{1}{3}\eta^2\right)\tau_c.} \quad (1)$$

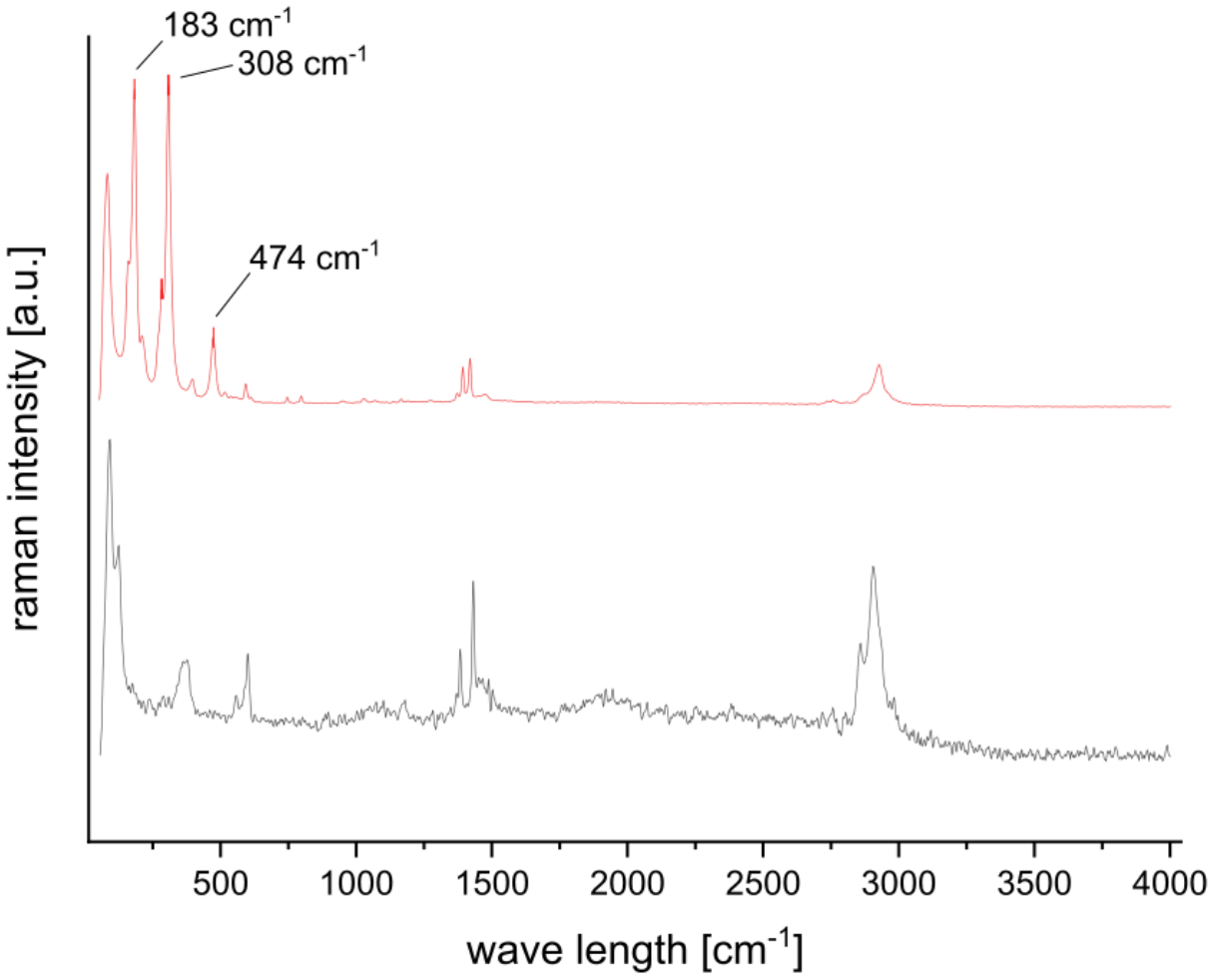
Here, V_{zz} represents the largest tensor component of the electric field gradient at the nucleus, e the charge of the electron, η the asymmetry parameter of the electric field gradient and τ_c the isotropic tumbling correlation time. Importantly, the latter parameter t_c is temperature-dependent and decreases with increasing temperature. Hence, linewidths of quadrupolar nuclei become narrower upon an increase in the probe temperature. This effect was also observed in the low-temperature NMR analysis of solutions of **1** in 1,2-DFB as displayed in S-Figure 14.[20]



S-Figure 14: a) ^{1}H NMR spectra (400.2 MHz, 1,3-DFB) of a concentrated solution (75 mg/mL) of [Al(AlCp*)$_3$][*pf*] **1** in 1,3-DFB at various temperatures; b) ^{27}Al NMR spectra (499.5 MHz, 1,3-DFB) of a concentrated solution (75 mg/mL) of [Al(AlCp*)$_3$][*pf*] **1** in 1,3-DFB at various temperatures.

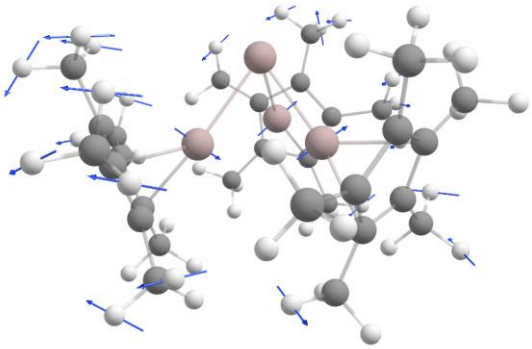
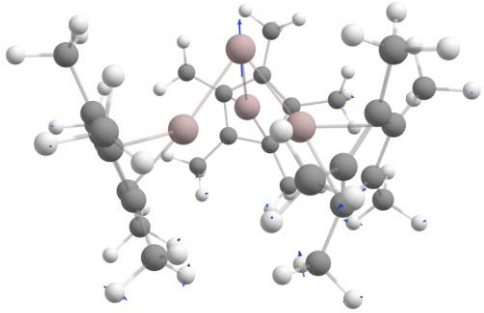
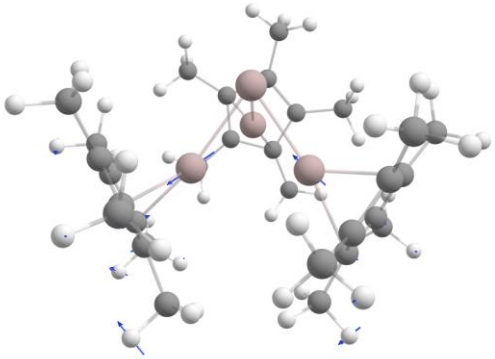
Raman spectrum of [Al(AlCp*)$_3$][*pf*] 1

In analogy to the Raman spectrum of [(AlCp*)$_4$], characteristic breathing modes of the Al_4 tetrahedron in [Al(AlCp*)$_3$][*pf*] **1** are observed in the experimental Raman spectrum. The observed broad Raman signals at $\nu_{exp.}$ = 183, 308, 474 cm^{-1} can be assigned to specific computed vibrations at $\nu_{exp.}$ = 187, 303, 474 cm^{-1} (bp86-d3bj/def2-svp; S-Table 3). Prominent signals near 2900 cm^{-1} can be assigned to C–H stretching vibrations(ν(C–H)). Raman bands near 1400 cm^{-1} and 600 cm^{-1} are attributable to breathing vibrations of the C_5Me_5 ligands as well as deformational modes of the CH_3 groups.[17,18]



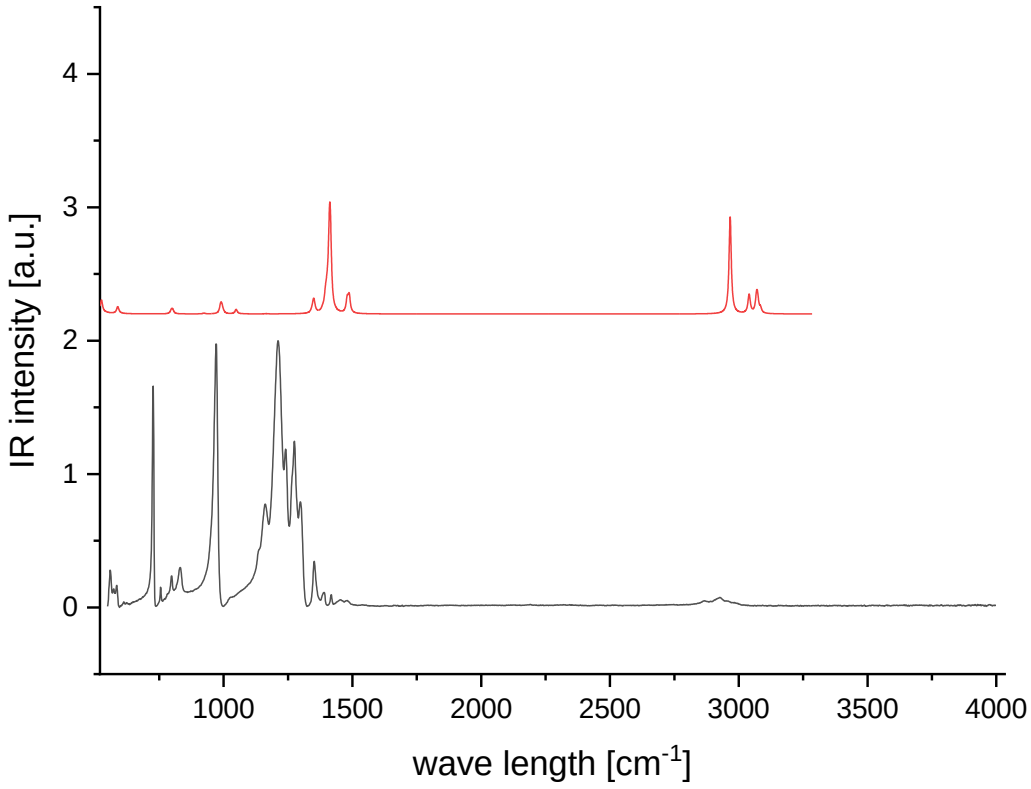
S-Figure 15: Comparison of the experimental Raman spectra of [Al(AlCp*)$_3$]$^+$[*pf*]$^-$ (red) and [(AlCp*)$_4$] (black).

S-Table 3: Observed and calculated (bp86-d3bj/def2-svp) Raman frequencies as well as visualization of the breathing mode of the Al_4 fragment in $[Al(AlCp^*)_3][pf]$ **1**

Raman (Exp.) $\tilde{\nu}$ **[cm^{-1}]**	**Calc.** $\tilde{\nu}$ **[cm^{-1}]**	**Scaled displacement vectors for the vibrational modes**
183	187	 (Threshold for visualization: 0.13)
308	303	 (Threshold for visualization: 0.13)
474	474	 (Threshold for visualization: 0.13)

IR spectrum of [Al(AlCp*)$_3$][*pf*] 1

The IR spectrum mainly shows the IR bands of free [*pf*]$^-$ ([*pf*]$^-$ = [Al(OR^F)$_4$]$^-$; R^F = C(CF$_3$)$_3$) according to the published IR spectrum of [NR$_4$][Al(OR^F)$_4$] (R = alkyl).[21] Prominent signals near 2900 cm^{-1} can be assigned to C–H stretching vibrations(ν(C–H)). The major, characteristic IR bands of the [*pf*]$^-$ anion found in the experimental spectrum of **1** are summarized in S-Table 4.

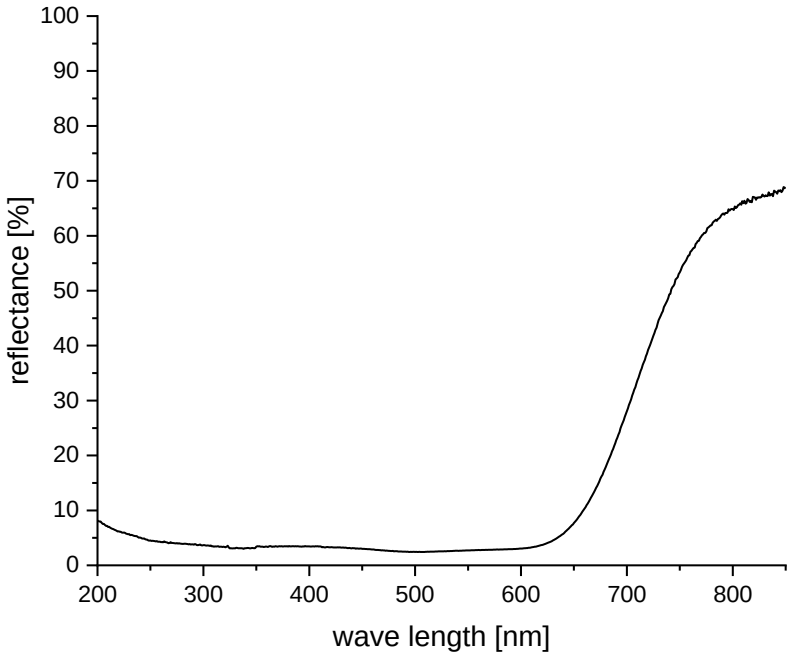


S-Figure 16: Experimental IR spectrum of [Al(AlCp*)$_3$]$^+$[*pf*]$^-$ and computed IR spectrum (red) for the cation [Al(AlCp*)$_3$]$^+$ (bp86-d3bj/def2-svp).

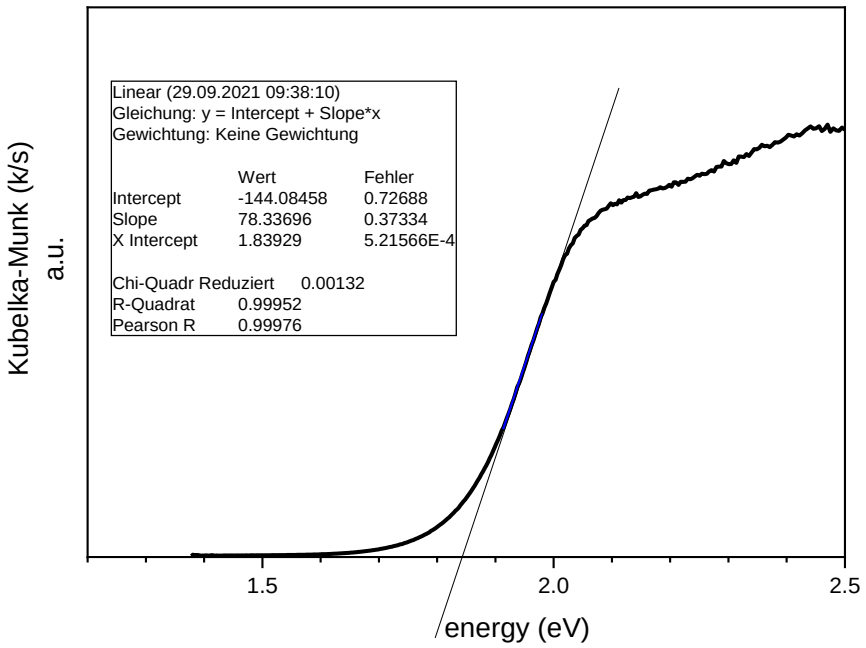
S-Table 4: Characteristic IR bands of the free [*pf*]$^-$ anion observed in the experimental IR spectrum of [Al(AlCp*)$_3$]$^+$[*pf*]$^-$

IR (Exp.) $\tilde{\nu}$ [cm^{-1}]	**Assignment[21]**
726	C–C, C–O
798	
831	Al–O, C–C
971, 1161, 1211, 1241,1275, 1298, 1352	C–C, C–F

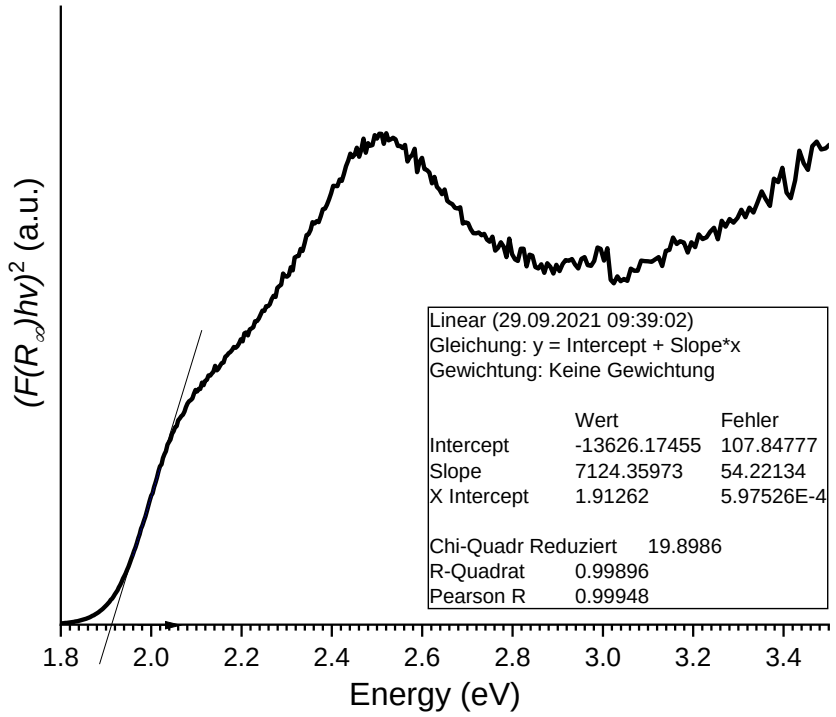
Solid-state UVVIS spectrum of [Al(AlCp*)$_3$][*pf*] 1



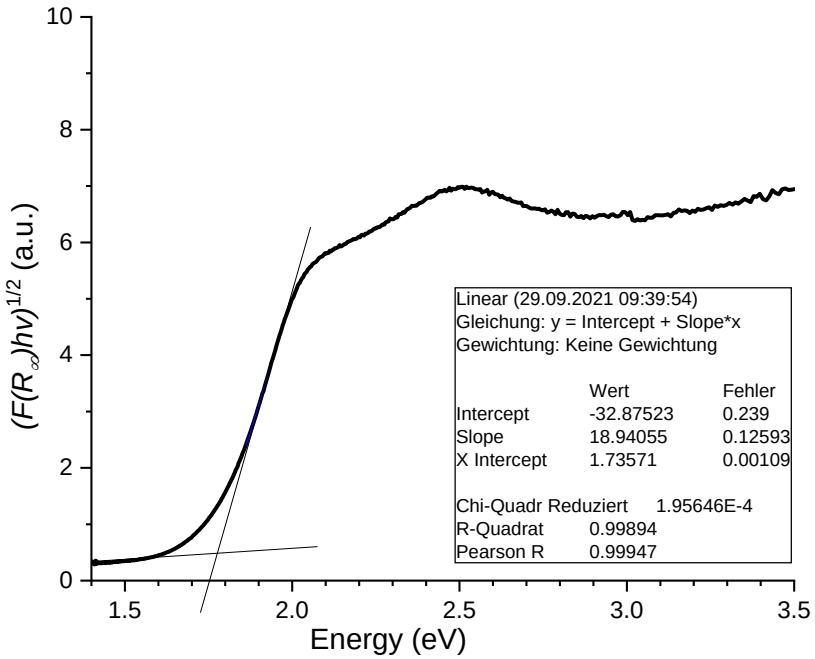
S-Figure 17: Solid state UVVIS spectrum of **1**.



S-Figure 18: Kubelka-Munk-plot for **1.**



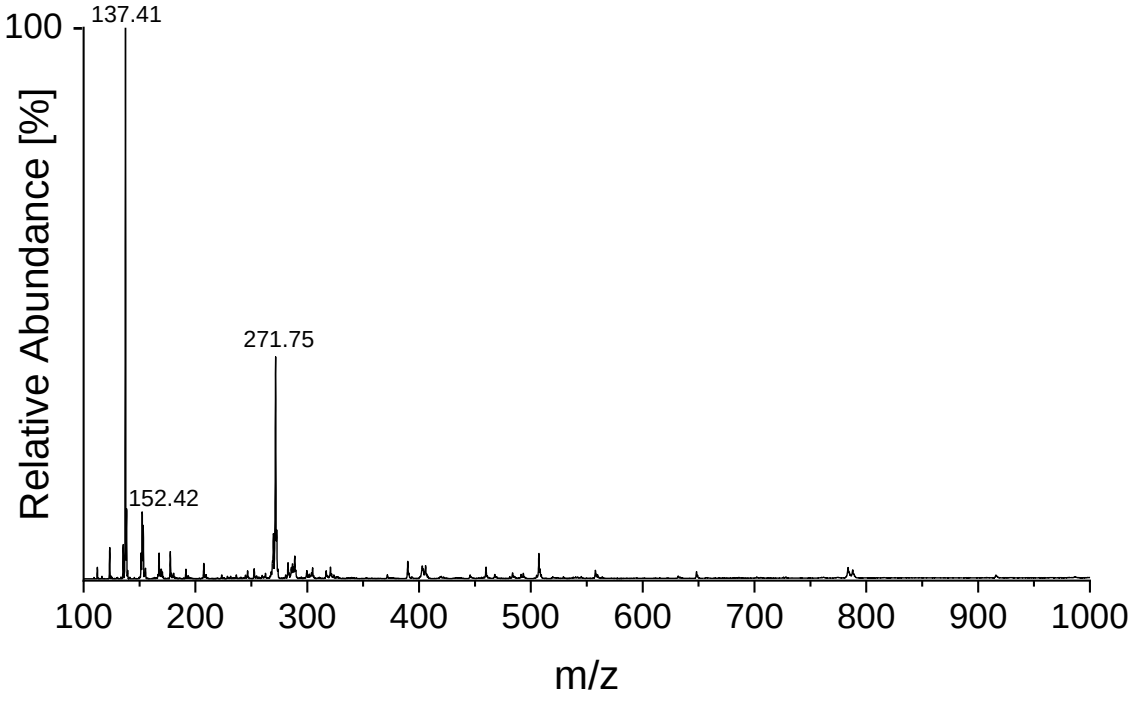
S-Figure 19: Tauc-Plot of **1** for a direct band gap.



S-Figure 20: Tauc-Plot of **1** for an indirect band-gap.

Mass spectrum of [Al(AlCp*)$_3$][*pf*] 1

As ^{27}Al is a 100% nucleus, there is unfortunately no characteristic isotope pattern helping to identify the observed signals. Nevertheless, a mass spectrum of **1** was collected. Here, no signal matching the calculated value for **1** of m/z = 513.28 could be observed. The main signal at m/z = 137.41 can be attributed to $[Cp^*H_2]^+$ (m/z_{calc} = 137.13). The second most intensive signal could potentially represent $[Cp^*_2H]^+$ (m/z_{calc} 271.24). Charge-induced collision onto the latter signal revealed a fragmentation into $[Cp^*H_2]^+$.



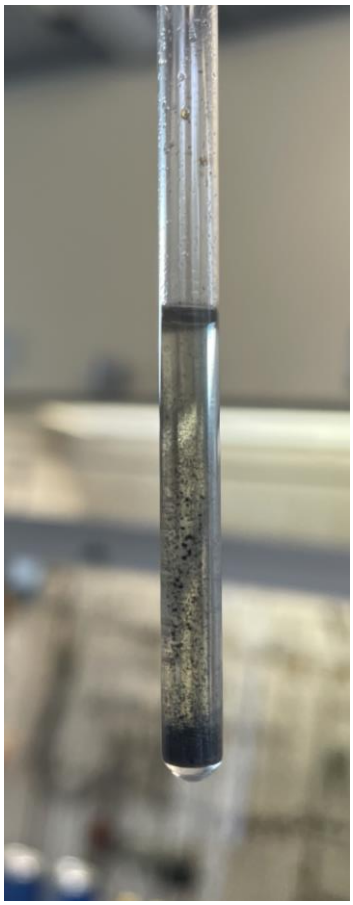
S-Figure 21: Full mass spectrum (ITMS+p-ESI, ESI voltage = 3.97 V, T_{cap} = 119.97 °C, sprayed from 1,2-DFB solution) of [Al(AlCp*)$_3$][*pf*] **1**.

S-1.5 Decomposition of [Al(AlCp*)$_3$][*pf*] **1**

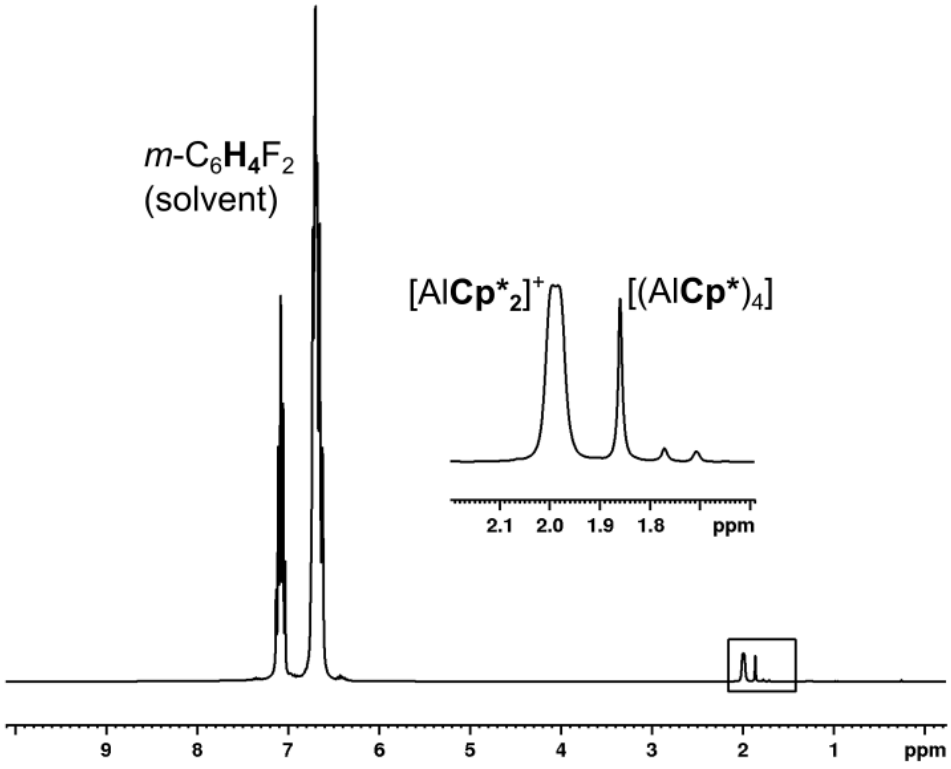
NMR spectra of the decomposition products

1.) Decomposition products of a purple solution of **1** in 1,3-DFB (125 mg/mL) after 12 h

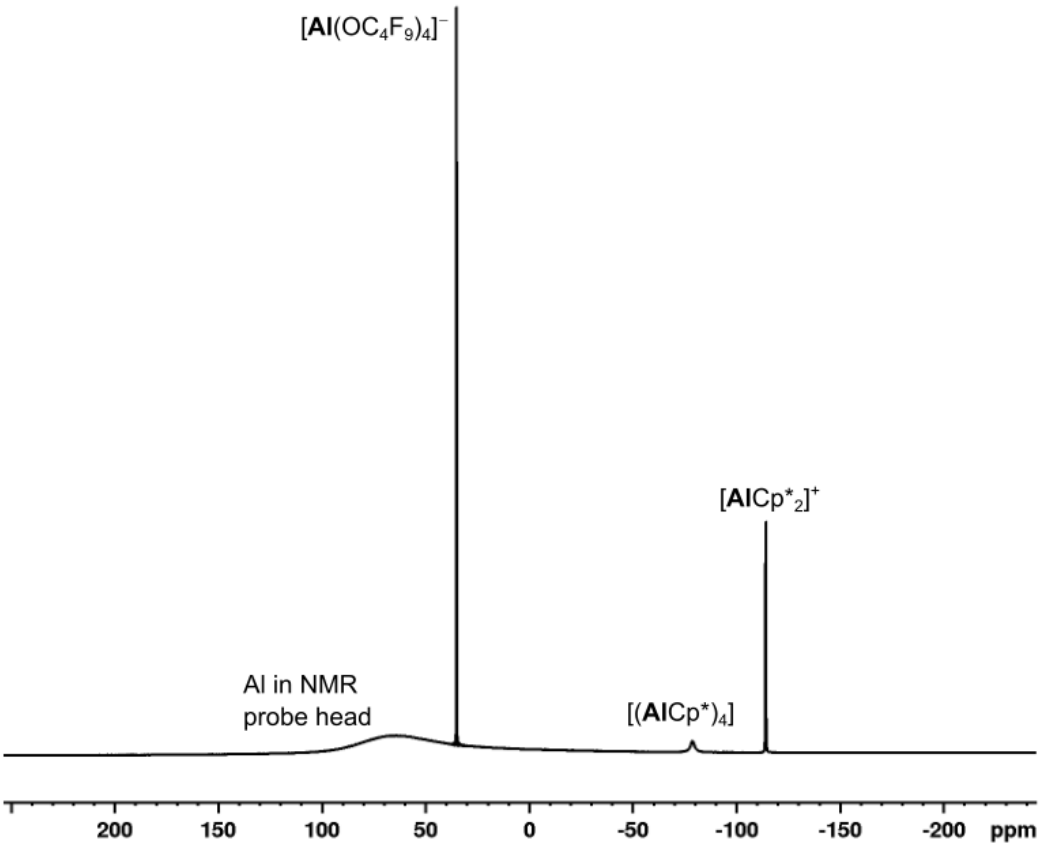
To investigate the nature of the decomposition products of **1**, a solution of **1** (125 mg/mL) in 1,3 DFB was prepared in a Young-NMR tube. After standing over night at room temperature, the violet colour of the solution had faded and a metallic precipitate had formed. The solution was separated from the metallic precipitation and was analyzed by NMR spectroscopy.



S-Figure 22: Solution of [Al(AlCp*)$_3$][*pf*] **1** in 1,3-DFB (125 mg/mL) after 12 h at room temperature.



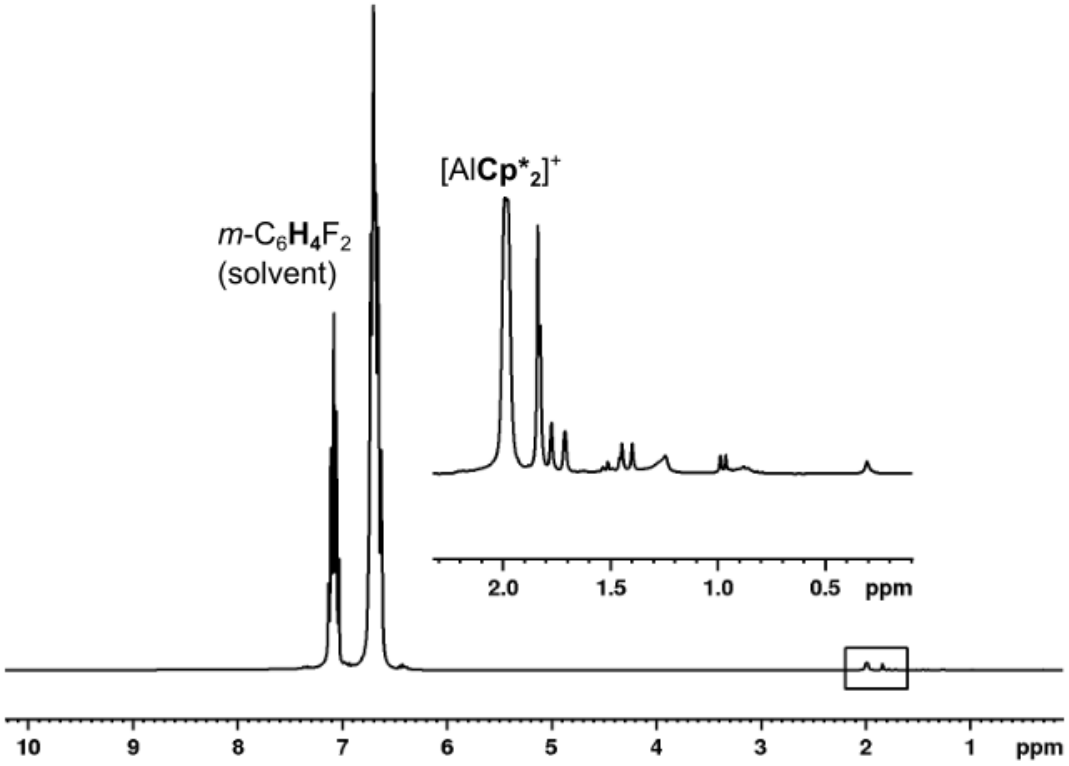
S-Figure 23: ^{1}H NMR spectrum (300.2 MHz, 1,3-DFB, 300K) of **1** (125 mg/mL) after 12 h.



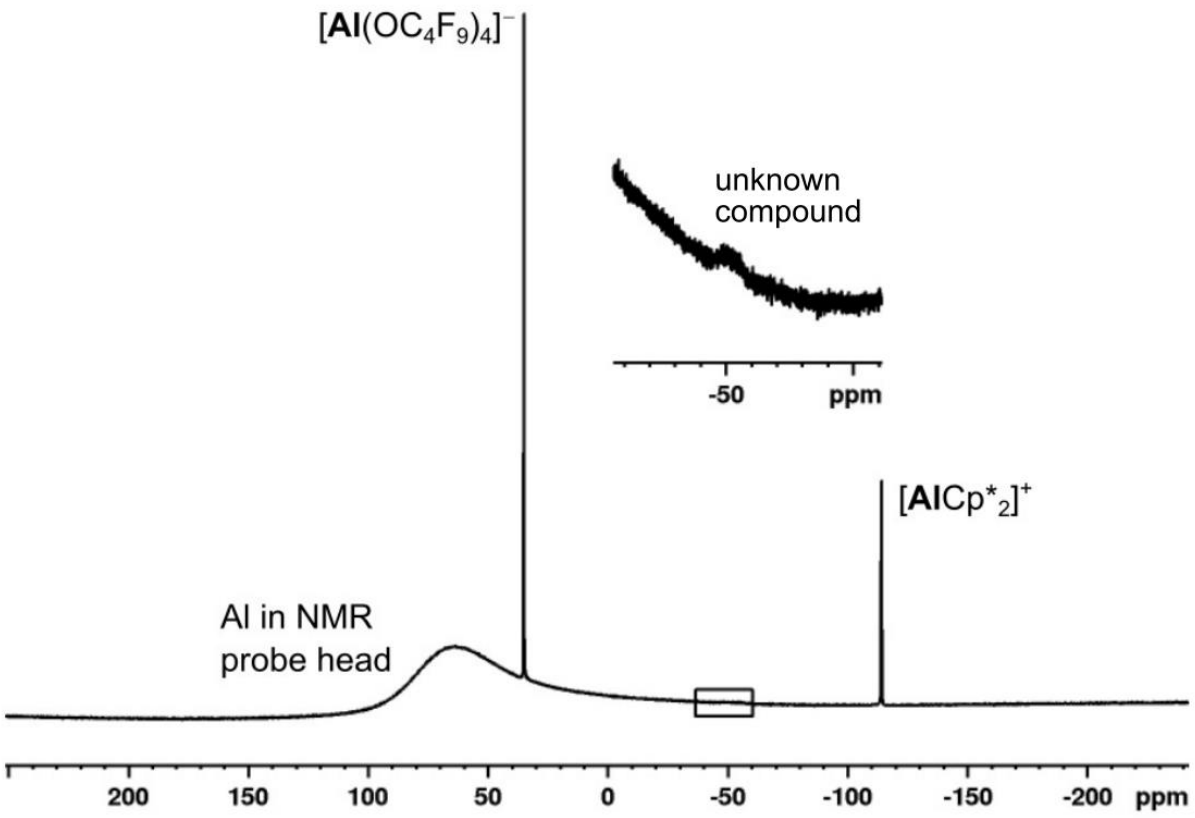
S-Figure 24: ^{27}Al NMR spectrum (78.2 MHz, 1,3-DFB, 300K) of **1** (125 mg/mL) after 12 h.

2.) Decomposition products of a red solution of 1 in 1,3-DFB (50 mg/mL) after 2d

To investigate the nature of the decomposition products of [Al(AlCp*)$_3$][*pf*] **1**, a solution of **1** (50 mg/mL) in 1,3 DFB was prepared in the glovebox. The reaction mixture was stirred over night at room temperature until the orange color of the solution had faded. The slightly yellow solution was separated from the metallic precipitation and was analyzed by NMR spectroscopy. Crystallization of the reaction mixture yielded yellow crystals of [(AlCp*)$_4$–Cp*–(AlCp*)$_4$]$^+$[*pf*]$^-$ **2** next to unidentifiable colorless crystals (see next section).



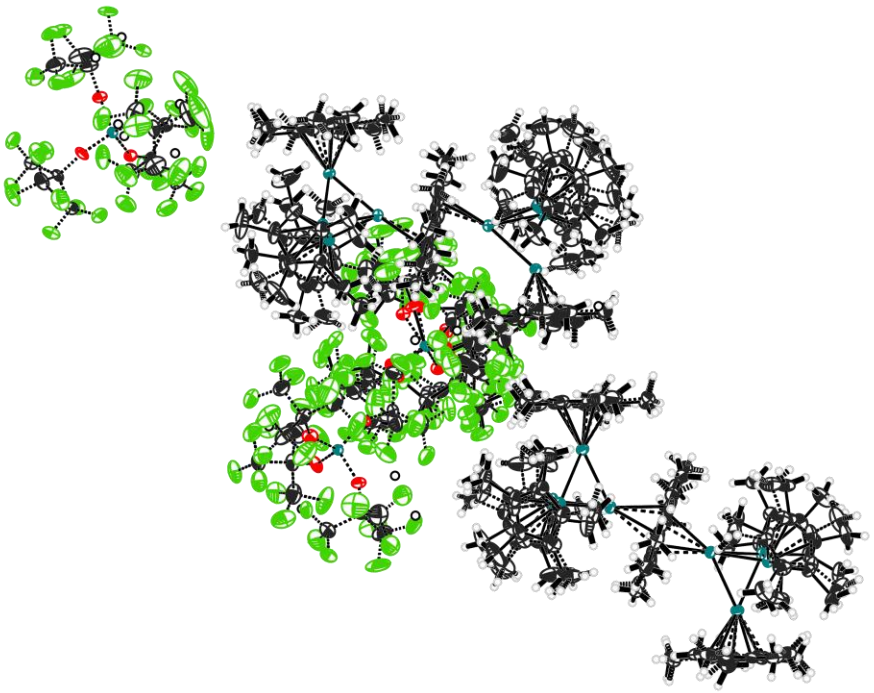
S-Figure 25: ^{1}H NMR spectrum (300.2 MHz, 1,3-DFB, 300K) of **1** (50 mg/mL) after 2 d.



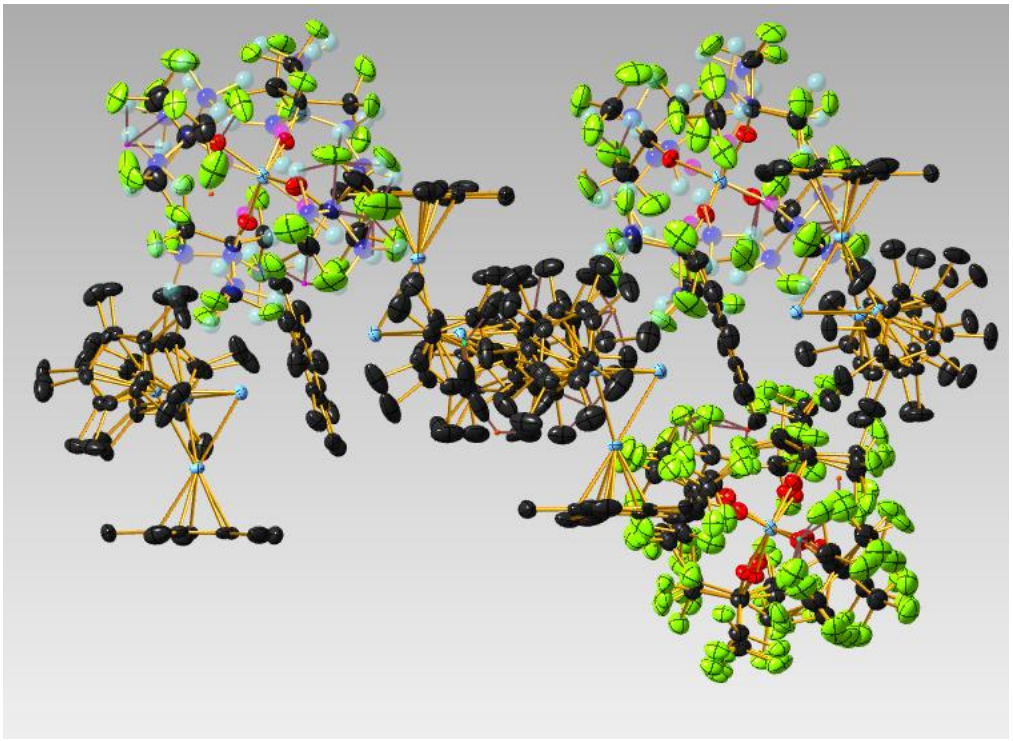
S-Figure 26: ^{27}Al NMR spectrum (78.2 MHz, 1,3-DFB, 300K) of **1** (50 mg/mL) after 2 d.

Molecular structure of [(AlCp*)$_3$Al–Cp*–Al(AlCp*)$_3$] 2

The crystal structure of [(AlCp*)$_3$Al–Cp*–Al(AlCp*)$_3$][*pf*] (**2**) most probably suffers from a superstructure, which can be approximated as a commensurate case. The structure could be solved and refined based on a monoclinic supercell (*a* = 43.08 Å, *b* = 34.02 Å, *c* = 26.75 Å, β = 97.26°). The Cp* units in the cations as well as the OR^F-groups of the [*pf*]$^-$ anions are significantly disordered (S-Figure 27), while it cannot be excluded that the disorder is a result of the treatment of the superstructure. Moreover, two of the three [*pf*]$^-$ anions in the asymmetric unit are located on special positions as illustrated in S-Figure 28. Yet, the final model converged to acceptable values for R_1 = 0.07 ($I \geq 2\sigma(I)$]), wR_2 = 0.23 (all data) and *GooF* = 1.019. Due to the need for extensive restraining of the cations and anions, bond lengths will not be discussed.



S-Figure 27: Asymmetric unit of the molecular structure of $[(AlCp^*)_3Al–Cp^*–Al(AlCp^*)_3]$ 2. Ellipsoids are shown at 50 % probability.



S-Figure 28: Asymmetric unit of the molecular structure of $[(AlCp^*)_3Al–Cp^*–Al(AlCp^*)_3][pf]$ **2** with "ghost atoms" of the $[pf]^-$ anions on special positions (picture taken from ShelXle[14]). Hydrogen atoms are omitted for clarity. Ellipsoids are shown at 50 % probability.

S-1.6 Experimental data for [(tmeda)Al(AlCp*)$_3$][*pf*] **3**

Procedure

[Al(AlCp*)$_3$]$^+$[*pf*]$^-$ **1** (25 mg, 17 μmol) was dissolved in 1,2-DFB (0.5 mL). TMEDA was added at room temperature (0.02 mL, 0.02 mg, 0.1 μmol, 8 eq). The reaction was stirred for 5 min at room temperature. Subsequently, *n*-pentane was diffused onto the solution at –30°C. The title compound (24 mg, 15 mmol, 89 %) was isolated as yellow crystals.

^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 298 K): δ = 2.66 (s, 4 H, –CH_2–), 2.66 (s, 12 H, N–CH_3), 1.86 (s, 45 H, Cp*) ppm.

^{13}C NMR spectrum (75.48 MHz, 1,2-DFB, 298 K): δ = 114.8 (s, **C_5**(CH_3)$_5$), 54.4 (s, –CH_2–), 44.3 (s, N–CH_3), 10.1 (s, C_5(**C**H_3)$_5$) 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.

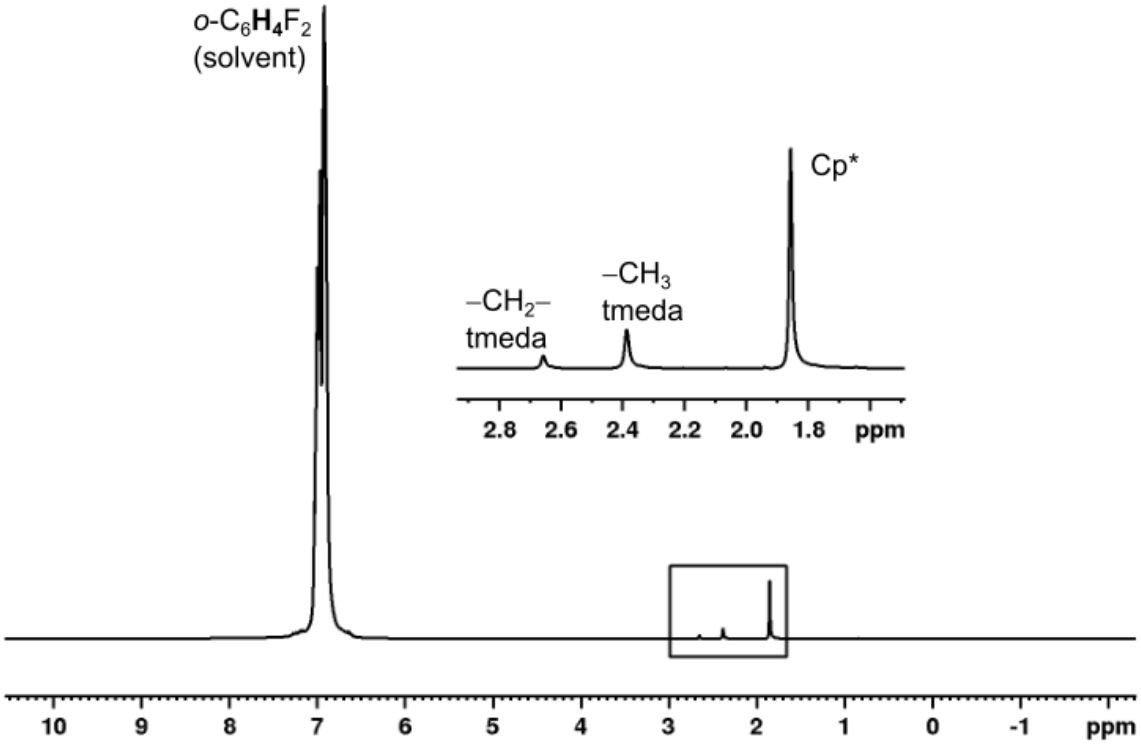
^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 298 K): δ = 47.6 (br. s, [(tmeda)**Al**(AlCp*)$_3$]$^+$), 35.0 (s, [Al(OC_4F_9)$_4$]$^-$), –64.8 (br. s, [(tmeda)Al(**Al**Cp*)$_3$]$^+$) ppm.

FTIR spectrum (ZnSe-ATR): $\tilde{\nu}$ = 2977 (vw), 2913 (vw), 2865 (vw), 2783 (vw), 1465 (vw), 1439 (vw), 1352 (vw), 1298 (m), 1275 (s), 1239 (s), 1212 (vs), 1164 (w), 1046 (vw), 1020 (vw), 972 (vs), 831 (vw), 788 (vw), 756 (vw), 727 (vs), 592 (vw), 560 (vw) cm^{-1}.

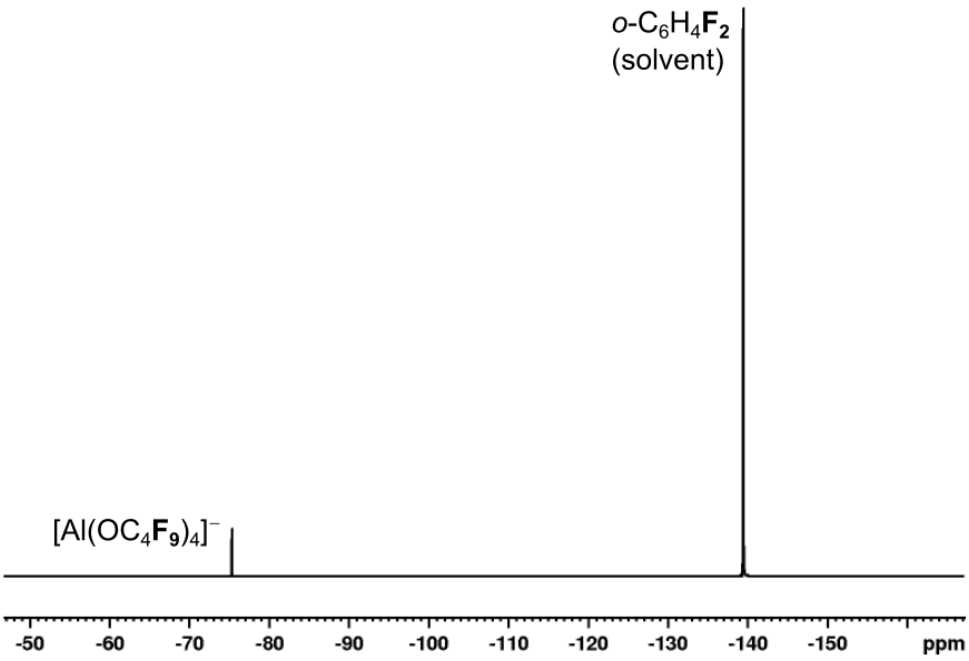
Raman spectrum (5000 scans): $\tilde{\nu}$ = 2912 (m), 2819 (vw), 1466 (w), 1428 (m), 1388 (w), 1087 (w), 797 (w), 746 (vw), 597 (w), 555 (w), 401 (w), 381 (w), 319 (w), 287 (w), 164 (w), 124 (vs) cm^{-1}.

S-Figure 29: Yellow crystals of [(tmeda)Al(AlCp*)$_3$][*pf*] **3**.

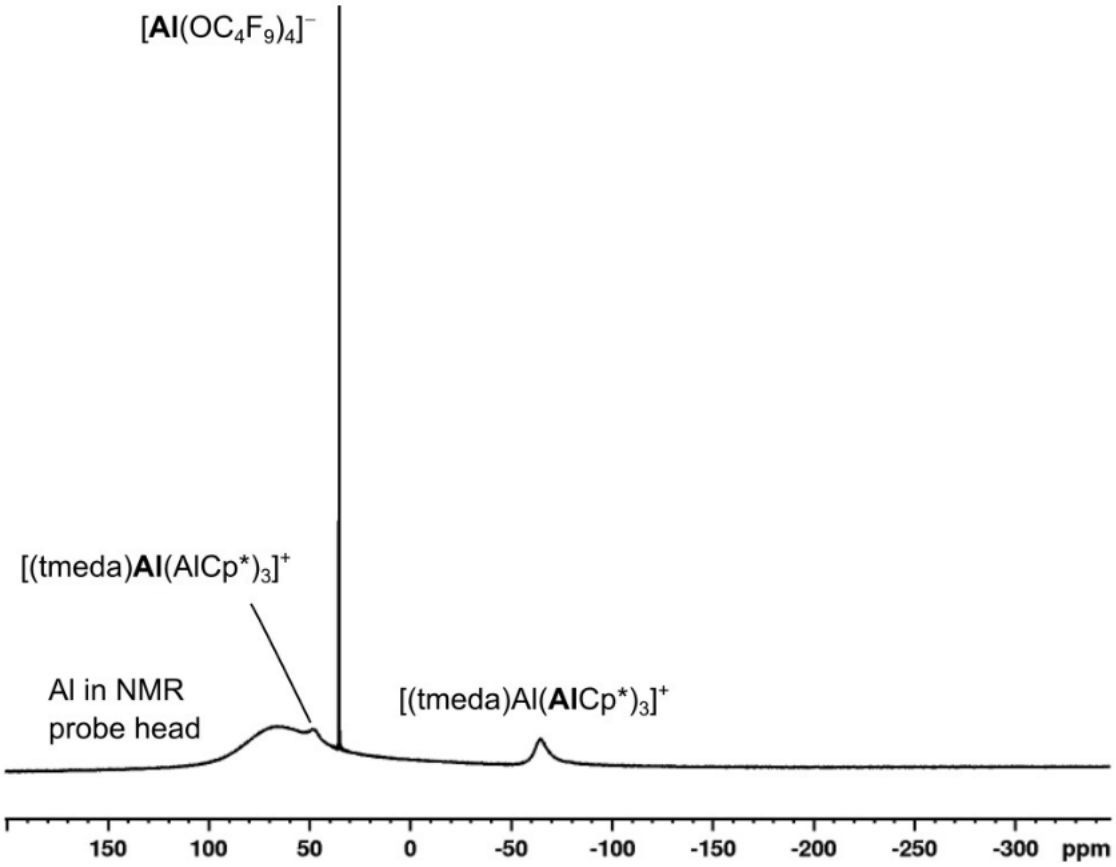
NMR spectra of [(tmeda)Al(AlCp*)$_3$][*pf*] 3



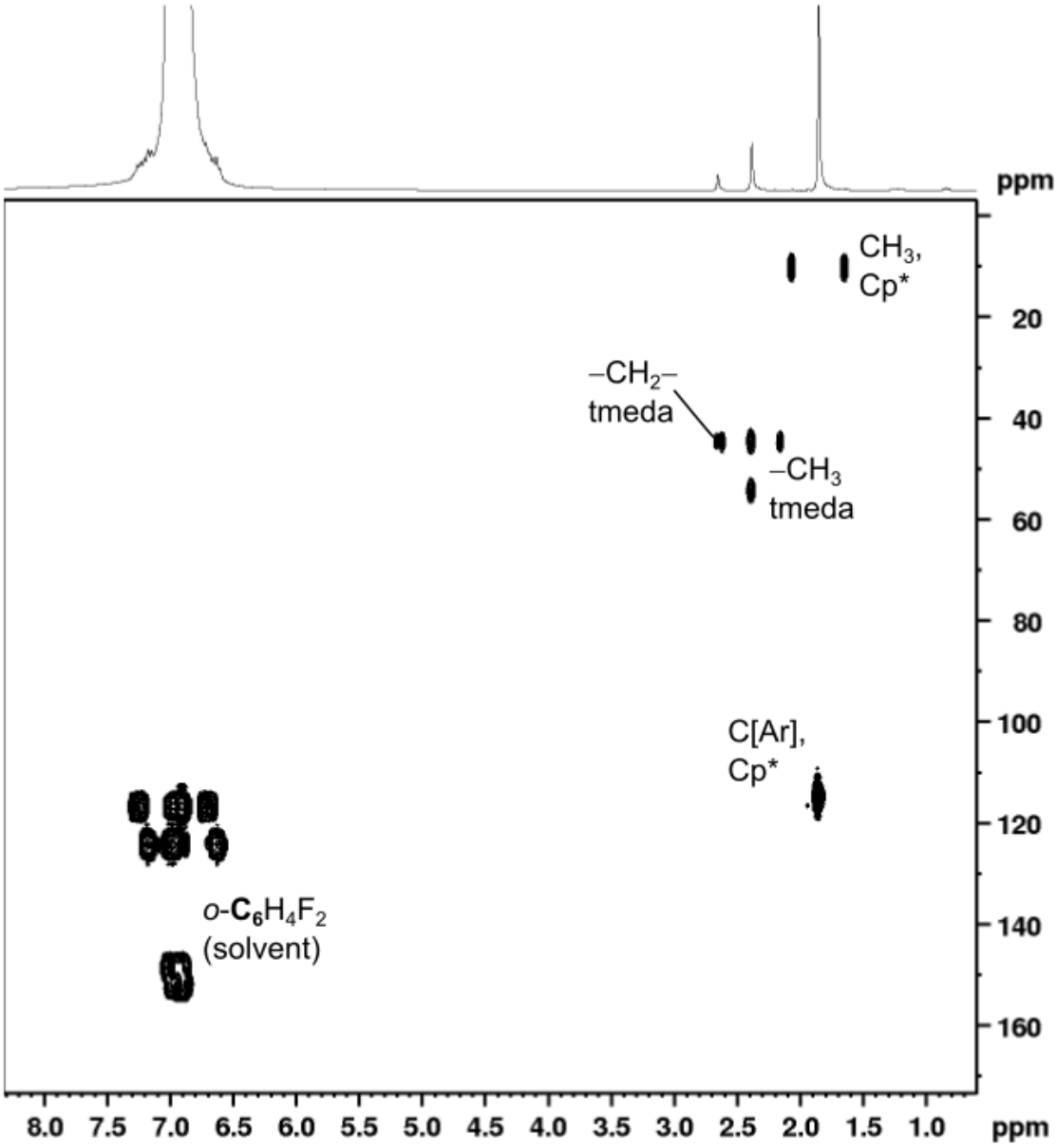
S-Figure 30: ^{1}H NMR spectrum (300.2 MHz, 1,2-DFB, 300K) of [(tmeda)Al(AlCp*)$_3$][*pf*] **3**. The intense multiplet between δ = 6.6-7.2 ppm originates from the proton resonance of 1,2-difluorobenzene.



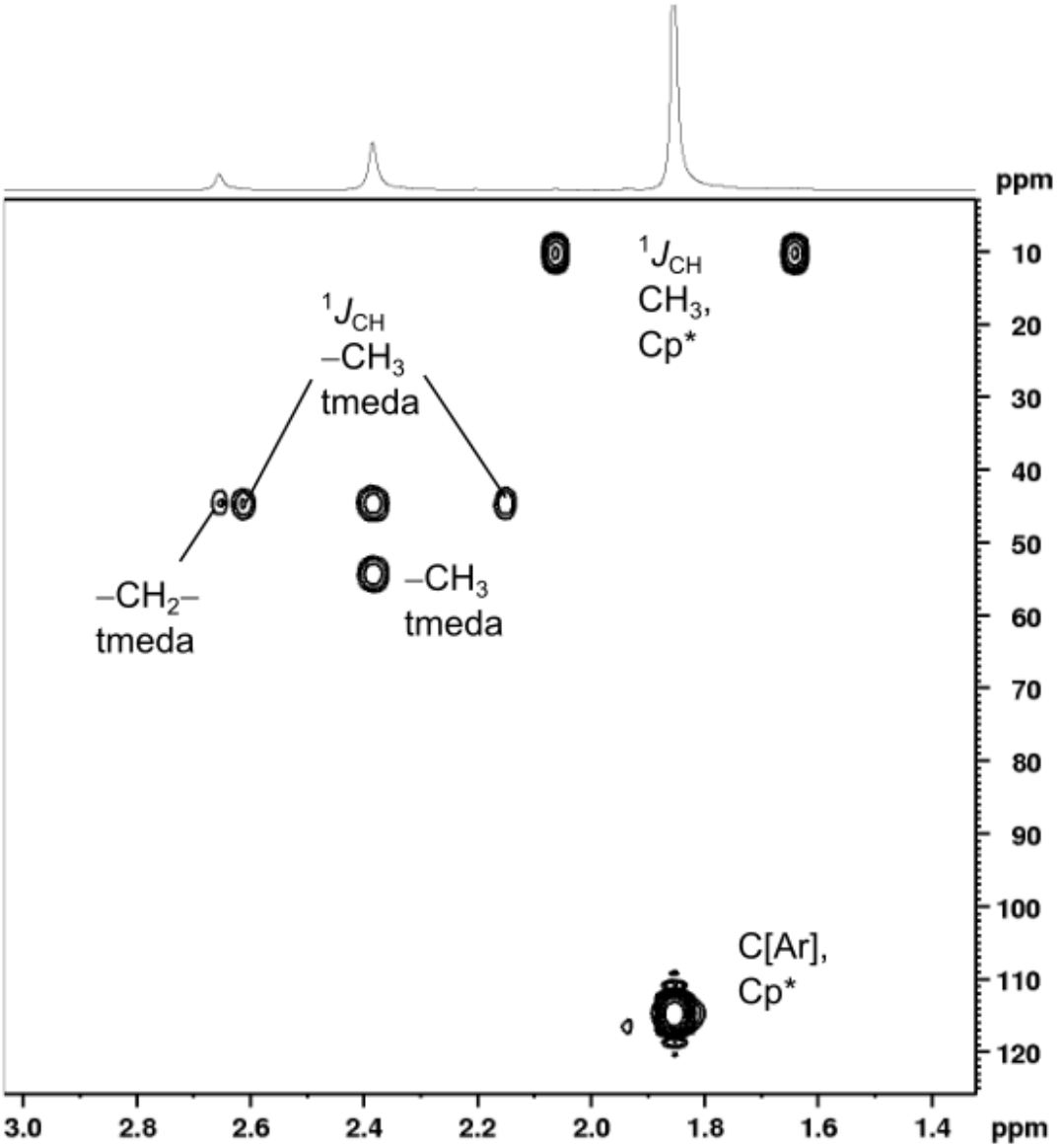
S-Figure 31: ^{19}F NMR spectrum (282.5 MHz, 1,2-DFB, 300K) of [(tmeda)Al(AlCp*)$_3$][*pf*] **3**. The intense signal at δ = –139.6 ppm originates from the ^{19}F NMR resonance of 1,2-difluorobenzene.



S-Figure 32: ^{27}Al NMR spectrum (78.2 MHz, 1,2-DFB, 300K) of [(tmeda)Al(AlCp*)$_3$][*pf*] **3**.



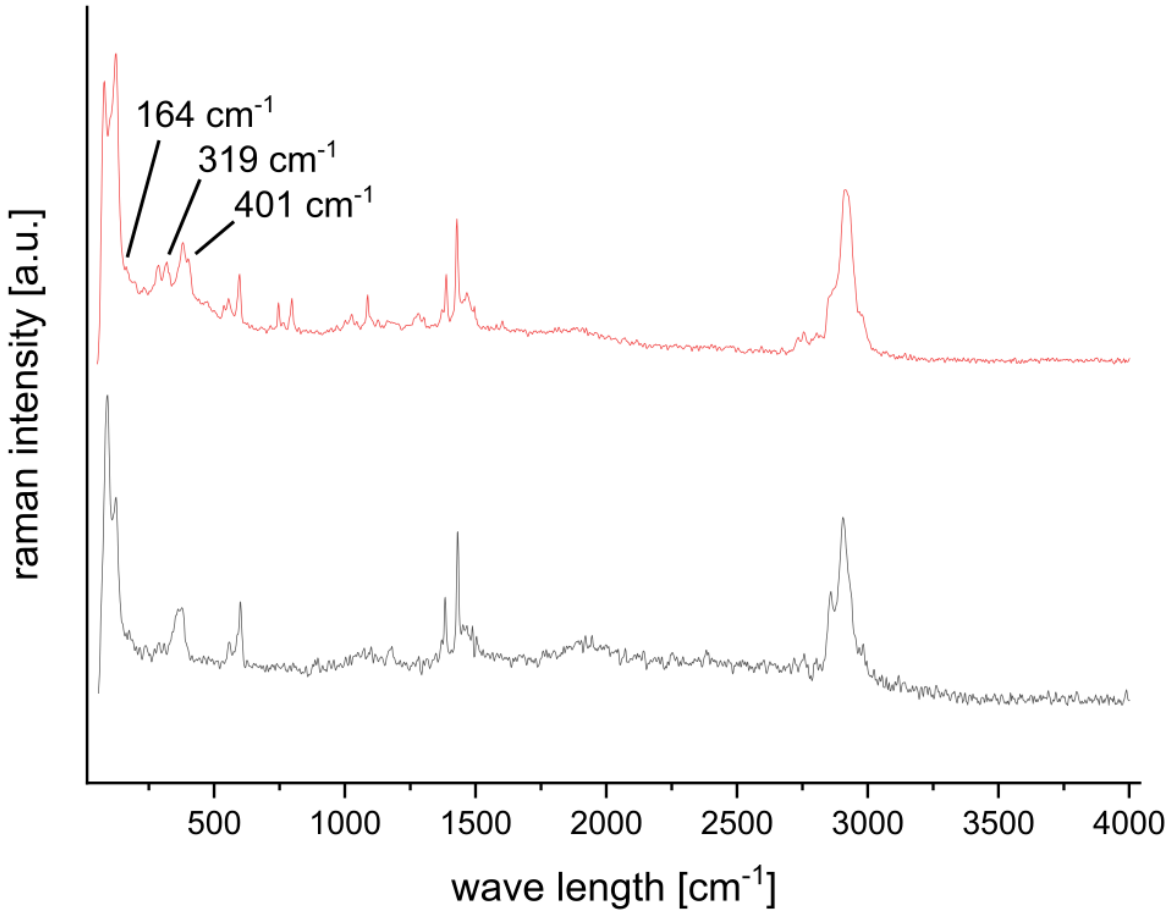
S-Figure 33: ^{1}H-^{13}C HMBC spectrum (300.2 MHz, 75.5 MHz, 1,2-DFB, 300K) of [(tmeda)Al(AlCp*)$_3$][*pf*] **3**.



S-Figure 34: Zoom on ^{1}H-^{13}C HMBC spectrum (300.2 MHz, 75.5 MHz, 1,2-DFB, 300K) of [(tmeda)Al(AlCp*)$_3$][*pf*] **3**.

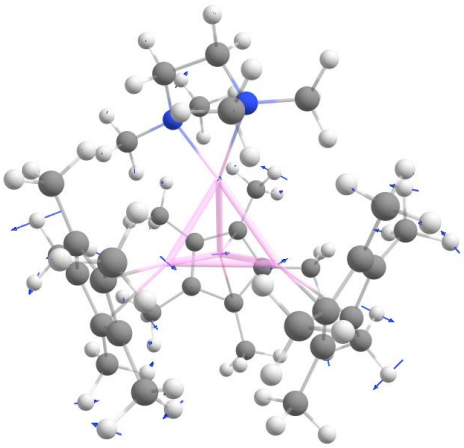
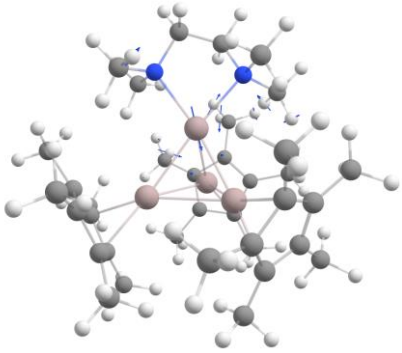
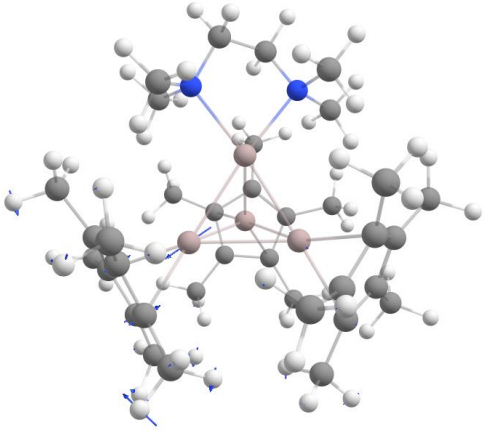
Raman spectrum of [(tmeda)Al(AlCp*)$_3$][*pf*] 3

In analogy to the experimental Raman spectrum of [(AlCp*)$_4$], characteristic breathing modes of Al_4 clusters for **3** are observed at $\nu_{exp.}$ = 164, 318, 403 cm^{-1} ($\nu_{comp.}$ = 166, 323, 405 cm^{-1}; bp86-d3bj/def2-svp). Prominent signals near 2900 cm^{-1} can be assigned to C–H stretching vibrations(ν(C–H)). Raman bands near 1400 cm^{-1} and 600 cm^{-1} are attributable to breathing vibrations of the C_5Me_5 ligands as well as deformational modes of the CH_3 groups.[17,18] Raman bands at 197 cm^{-1} as well as at 797 cm^{-1} and 746 cm^{-1} correspond to deformational modes of the tmeda-ligand.



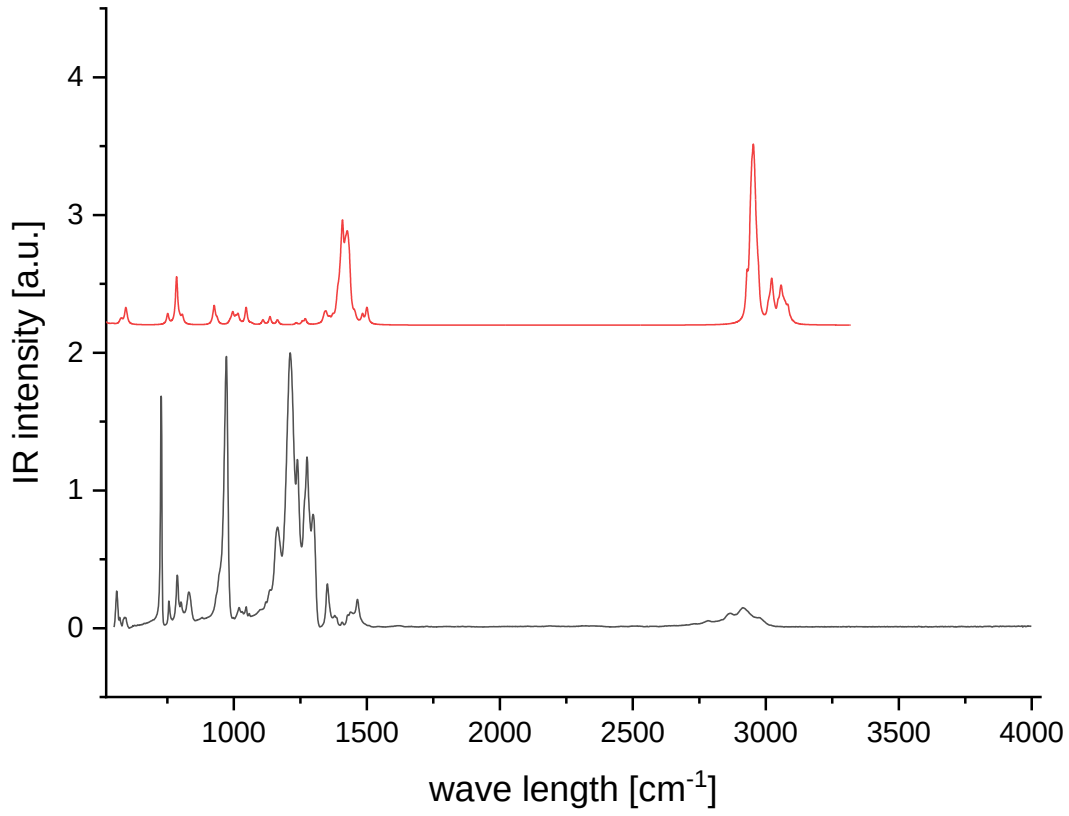
S-Figure 35: Comparison of the experimental Raman spectra of [(tmeda)Al(AlCp*)$_3$]$^+$[*pf*]$^-$ (red) and [(AlCp*)$_4$] (black).

S-Table 5: Observed and calculated (bp86-d3bj/def2-svp) Raman frequencies as well as visualization of the breathing mode of the Al_4 fragment in [(tmeda)Al($AlCp^*)_3$][*pf*] **3**

Raman (Exp.) $\tilde{\nu}$ [cm^{-1}]	**Calc. $\tilde{\nu}$ [cm^{-1}]**	**Scaled displacement vectors for the vibrational modes**
164	166	 (Threshold for visualization: 0.001; due to small scaled vectors, the Al_4 tetrahedron is displayed as thin sticks)
319	323	 (Threshold for visualization: 0.13)
401	405	 (Threshold for visualization: 0.13)

IR spectrum of [(tmeda)Al(AlCp*)$_3$][*pf*] 3

The IR spectrum mainly shows the IR bands of free [*pf*]$^-$ according to the published IR spectrum of [NR$_4$][Al(OR^F)$_4$] (R = alkyl).[21] Prominent signals near 2900 cm^{-1} can be assigned to C–H stretching vibrations(ν(C–H)). The major, characteristic bonds of the [*pf*]$^-$ anion found in the experimental spectrum of **3** are summarized in S-Table 6.



S-Figure 36: Experimental IR spectrum of [(tmeda)Al(AlCp*)$_3$]$^+$[*pf*]$^-$ and computed IR spectrum (red) for [(tmeda)Al(AlCp*)$_3$]$^+$ (bp86-d3bj/def2-svp).

S-Table 6: Charateristic IR bands of the free [*pf*]$^-$ anion observed in the experimental IR spectrum of [(tmeda)Al(AlCp*)$_3$]$^+$[*pf*]$^-$

IR (Exp.) $\tilde{\nu}$ [cm^{-1}]	**Assignment[21]**
727	C–C, C–O
798	
831	Al–O, C–C
972, 1164, 1212, 1239,1275, 1298, 1352	C–C, C–F

S-1.7 Experimental data for [(cdp)Al(AlCp*)$_3$][*pf*] **4**

Procedure

[Al(AlCp*)$_3$]$^+$[*pf*]$^-$ **1** (25 mg, 17 μmol) was dissolved in 1,2-DFB (0.4 mL) and C(PPh$_3$)$_2$ (9 mg, 0.02 μmol, 1 eq.) suspended in 1,2-DFB (0.1 mL). The solution of **1** was added to the suspension of CDP at room temperature to yield an orange solution. Subsequently, *n*-pentane were diffused onto the solution at –30°C. The title compound (15 mg, 7.4 μmol, 44 %) was isolated as orange crystals.

^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 298 K): δ = 7.62 (m$_c$, 12 H, [(C{P**Ph$_3$**}$_2$)Al(AlCp*)$_3$]$^+$), 7.41 (m$_c$, 6 H, [(C{P**Ph$_3$**}$_2$)Al(AlCp*)$_3$]$^+$), 1.67 (s, 45 H, Cp*) ppm. (remaining proton signals of the cdp ligand are covered up by the solvent signals)

^{13}C NMR spectrum (75.48 MHz, 1,2-DFB, 298 K): δ = 127.7-134.6 ([(C{P**Ph$_3$**}$_2$)Al(AlCp*)$_3$]$^+$), 114.4 (s, **C$_5$**(CH$_3$)$_5$), 9.9 (s, C$_5$(**C**H$_3$)$_5$) ppm.

^{19}F NMR spectrum (282.45 MHz, 1,2-DFB, 298 K): δ = –75.3 (s, 36 F, [Al(OC$_4$F$_9$)$_4$]$^-$) ppm.

^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 298 K): δ = 35.0 (s, [Al(OC$_4$F$_9$)$_4$]$^-$), –59.2 (br. s, [(cdp)Al(**Al**Cp*)$_3$]$^+$) ppm.

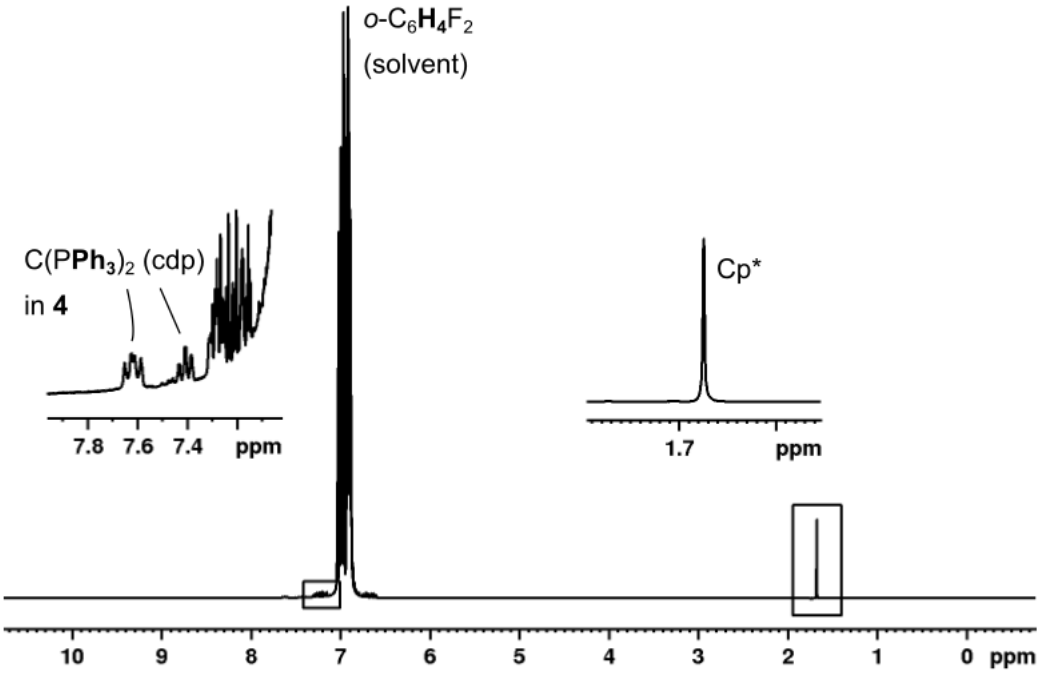
^{31}P NMR spectrum (78.22 MHz, 1,2-DFB, 298 K): δ = 20.2 (s, 2 P, [(C{**P**Ph$_3$}$_2$)Al(AlCp*)$_3$]$^+$) ppm.

FTIR spectrum (ZnSe-ATR): $\tilde{\nu}$ = 3067 (vw), 2912 (vw), 2863 (vw), 1482 (vw), 1438 (vw), 1351 (vw), 1298 (w), 1275 (s), 1239 (s), 1215 (vs), 1165 (w), 1097 (w), 1039 (vw), 1016 (vw), 996 (vw), 972 (vs), 831 (vw), 801 (w), 743 (w), 727 (vs), 708 (w), 690 (m), 560 (vw) cm^{-1}.

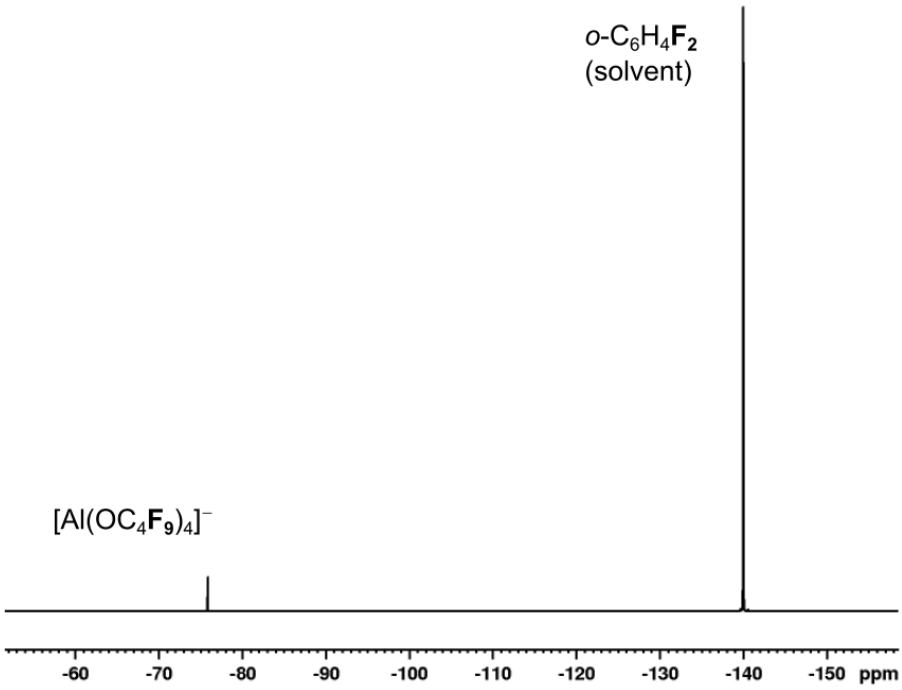
Raman spectrum (1000 scans): $\tilde{\nu}$ = 3065 (vw), 2919 (w), 2864 (vw), 1589 (w), 1496 (vw), 1430 (w), 1387 (vw), 1162 (vw), 1099 (vw), 1030 (vw), 1003 (w), 807 (vw), 745 (vw), 680 (vw), 665 (vw), 618 (vw), 594 (vw), 559 (vw), 482 (vw), 449 (vw), 436 (vw), 404 (vw), 392 (vw), 332 (vw), 319 (vw), 265 (vw), 234 (vw), 166 (w), 82 (vs) cm^{-1}.

S-Figure 37: Picture of orange crystals of [(cdp)Al(AlCp)$_3$][*pf*] grown from layering a solution of [(cdp)Al(AlCp)$_3$][*pf*] in 1,2-DFB with *n*-pentane at –30°C.

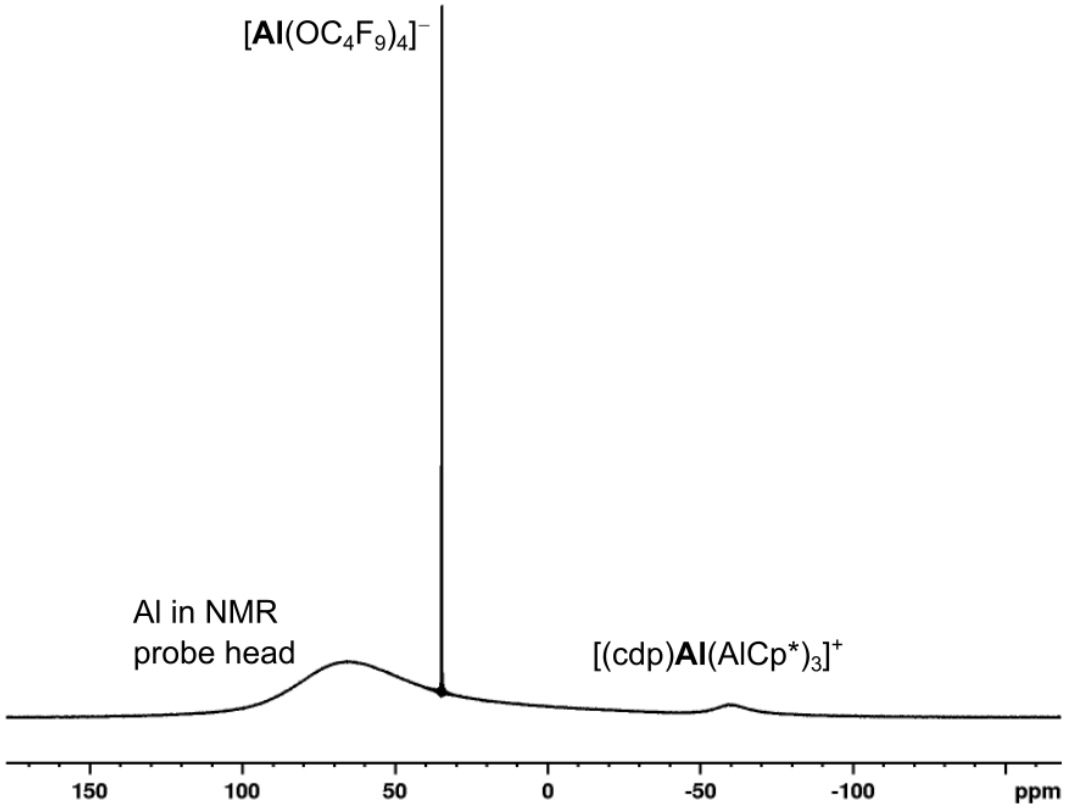
NMR spectra of [(cdp)Al(AlCp*)$_3$][*pf*] 4



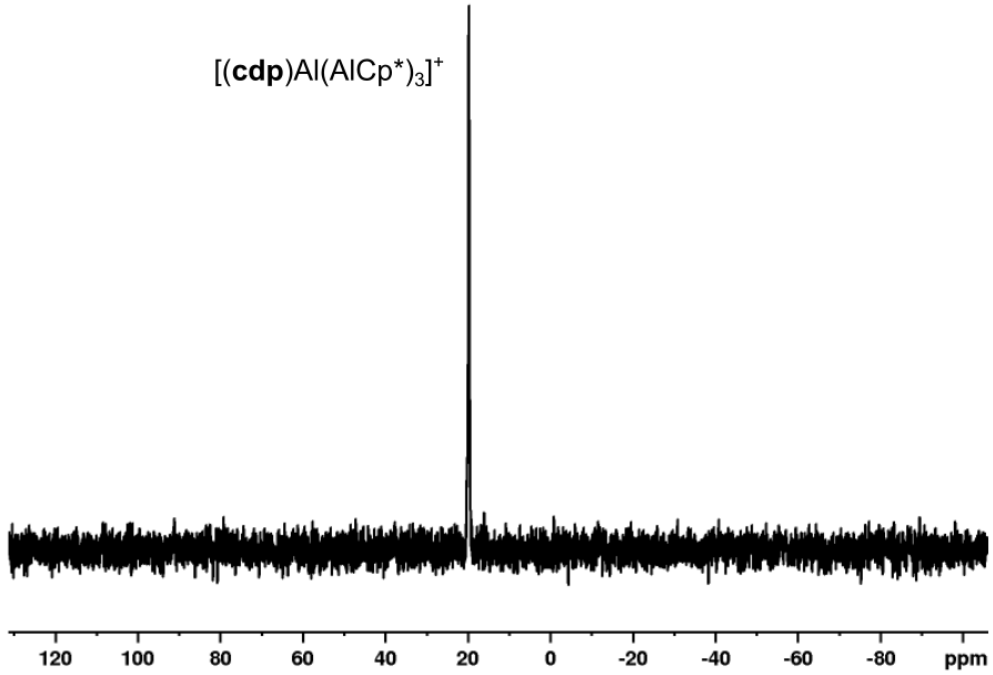
S-Figure 38: ^{1}H NMR spectrum (300.2 MHz, 1,2-DFB, 300K) of [(cdp)Al(AlCp*)$_3$][*pf*] **4**.



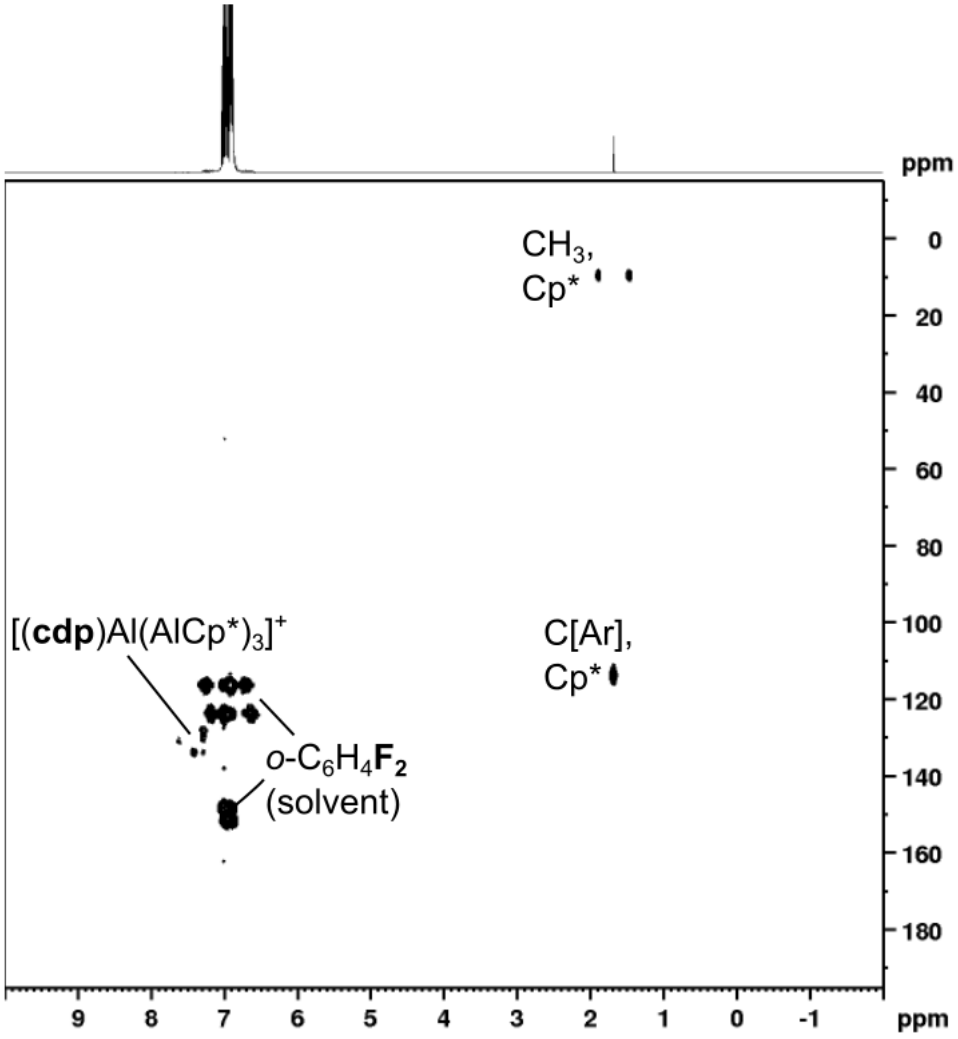
S-Figure 39: ^{19}F NMR spectrum (282.5 MHz, 1,2-DFB, 300K) of [(cdp)Al(AlCp*)$_3$][*pf*] **4**.



S-Figure 40: ^{27}Al NMR spectrum (78.2 MHz, 1,2-DFB, 300K) of [(cdp)Al(AlCp*)$_3$][*pf*] **4**.



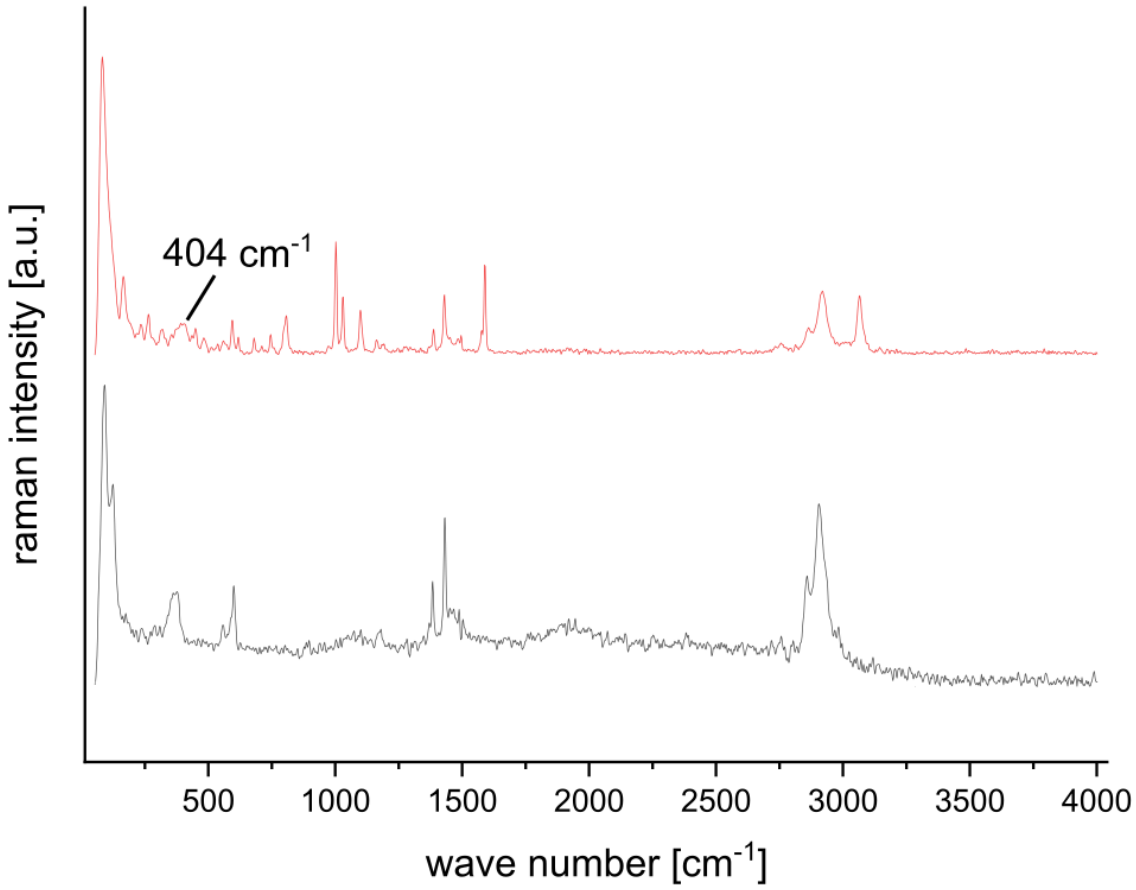
S-Figure 41: ^{31}P NMR spectrum (121.5 MHz, 1,2-DFB, 300K) of [(cdp)Al(AlCp*)$_3$][*pf*] **4**.



S-Figure 42: ^{1}H-^{13}C HMBC spectrum (300.2 MHz, 75.5 MHz, 1,2-DFB, 300K) of [(cdp)Al(AlCp*)$_3$][*pf*] **4**.

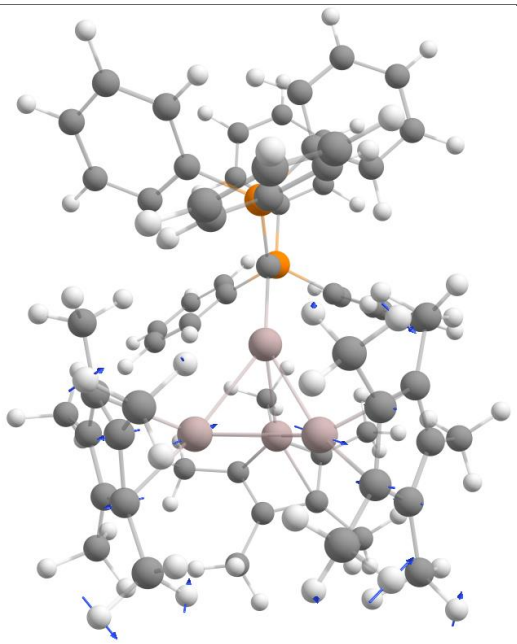
Raman spectrum of [(cdp)Al(AlCp*)$_3$][*pf*] 4

In analogy the raman spectra of the other Al_4 complexes, the prominent signals near 2900 cm^{-1} can be assigned to C–H stretching vibrations(ν(C–H)). Raman bands near 1400 cm^{-1} and 600 cm^{-1} are attributable to breathing vibrations of the C_5Me_5 ligands as well as deformational modes of the CH_3 groups.[17,18] Additionally, C–H stretching vibration ((ν(C–H)) of the phenyl-groups of the cdp ligand show a singlet at 3065 cm^{-1}. Moreover, the intense raman bands at 1577 cm^{-1} as well as between 1100 and 1000 cm^{-1} are attributable to deformational modes of the phenyl-groups at the carbodiphosphorane in **4**. Unfortunately, deformational modes in the backbone of the carbodiphosphorane ligands generate various raman bands below 500 cm^{-1} and possibly cover breathing modes of the Al_4 tetrahedron. Hence, only one breathing mode of Al_4 clusters for **4** is observed as broad signal at $\nu_{exp.}$ = 404 cm^{-1} ($\nu_{comp.}$ = 408 cm^{-1}; bp86-d3bj/def2-svp).



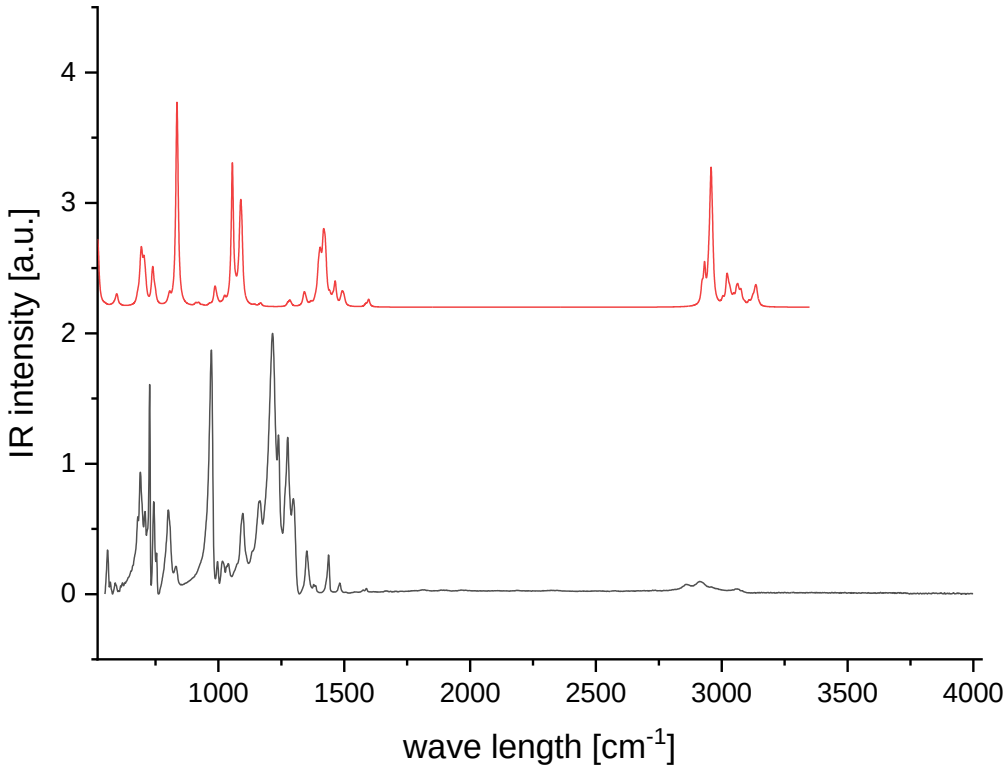
S-Figure 43: Comparison of the experimental Raman spectra of [(cdp)Al(AlCp*)$_3$]$^+$[*pf*]$^-$ (red) and [(AlCp*)$_4$] (black).

S-Table 7: Observed and calculated (bp86-d3bj/def2-svp) Raman frequencies as well as visualization of the breathing mode of the Al_4 fragment in $[(cdp)Al(AlCp^*)_3]^+$

Raman (Exp.) $\tilde{\nu}$ **[cm^{-1}]**	**Calc.** $\tilde{\nu}$ **[cm^{-1}]**	**Scaled displacement vectors for the vibrational modes**
404	408	 (Threshold for visualization: 0.13)

IR spectrum of [(cdp)Al(AlCp*)$_3$][*pf*] 3

The IR spectrum mainly shows the IR bands of free [*pf*]$^-$ according to the published IR spectrum of [NR$_4$][Al(OR^F)$_4$] (R = alkyl).[21] Prominent signals near 2900 cm^{-1} can be assigned to C–H stretching vibrations(ν(C–H)). The major, characteristic bonds of the [*pf*]$^-$ anion found in the experimental spectrum of **4** are summarized in S-Table 6. IR bands near 690 cm^{-1} are attributable to deformational vibrations of the phenyl-groups of the coordinated cdp-ligand. Moreover, the P–C-stretching modes of cdp are observed at 1097 cm^{-1}.



S-Figure 44: Experimental IR spectrum of [(cdp)Al(AlCp*)$_3$]$^+$[*pf*]$^-$ and computed IR spectrum (red) for [(cdp)Al(AlCp*)$_3$]$^+$ (bp86-d3bj/def2-svp).

S-Table 8: Charateristic IR bands of the free [*pf*]$^-$ anion observed in the experimental IR spectrum of [(cdp)Al(AlCp*)$_3$]$^+$[*pf*]$^-$

IR (Exp.) $\tilde{\nu}$ [cm^{-1}]	**Assignment[21]**
727	C–C, C–O
801	
831	Al–O, C–C
972, 1165, 1215, 1239,1275, 1298, 1351	C–C, C–F

S-1.8 Experimental data for $[(dmap)_3Al(AlCp^*)_3][pf]$ **5**

Procedure

$[Al(AlCp^*)_3]^+[pf]^-$ **1** (50 mg, 34 mmol) and dimethylaminopyridine (12 mg, 0.10 mmol, 3 eq) were dissolved in 1,2-DFB (1 mL). The solution was shaken and then vacced after 10s. The obtained orange powder was washed with toluene (3 × 1 mL) and dried under vacuum. The title compound (28 mg, 15 μmol, 45 %) was isolated as orange powder. Since **5** decomposes in solution, bulk purity was verified by powder X-ray diffraction and vibrational spectroscopy. scXRD-quality crystals of **5** could be grown by layering a solution of **5** in 1,2-DFB with *n*-heptane at –30°C.

^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 298 K): δ = 8.16 (br. s, unknown impurity), 2.92 (br. s, 18 H, -N(CH_3)$_2$, dmap) 1.87 (s, 45 H, $[(dmap)_3Al(AlCp^*)_3]^+$), 1.86 (s, 60 H, $[(AlCp^*)_4]$) 1.77 (br. s, unknown impurity) ppm.

^{19}F NMR spectrum (282.45 MHz, 1,2-DFB, 298 K): δ = –75.4 (s, 36 F, $[Al(OC_4F_9)_4]^-$) ppm.

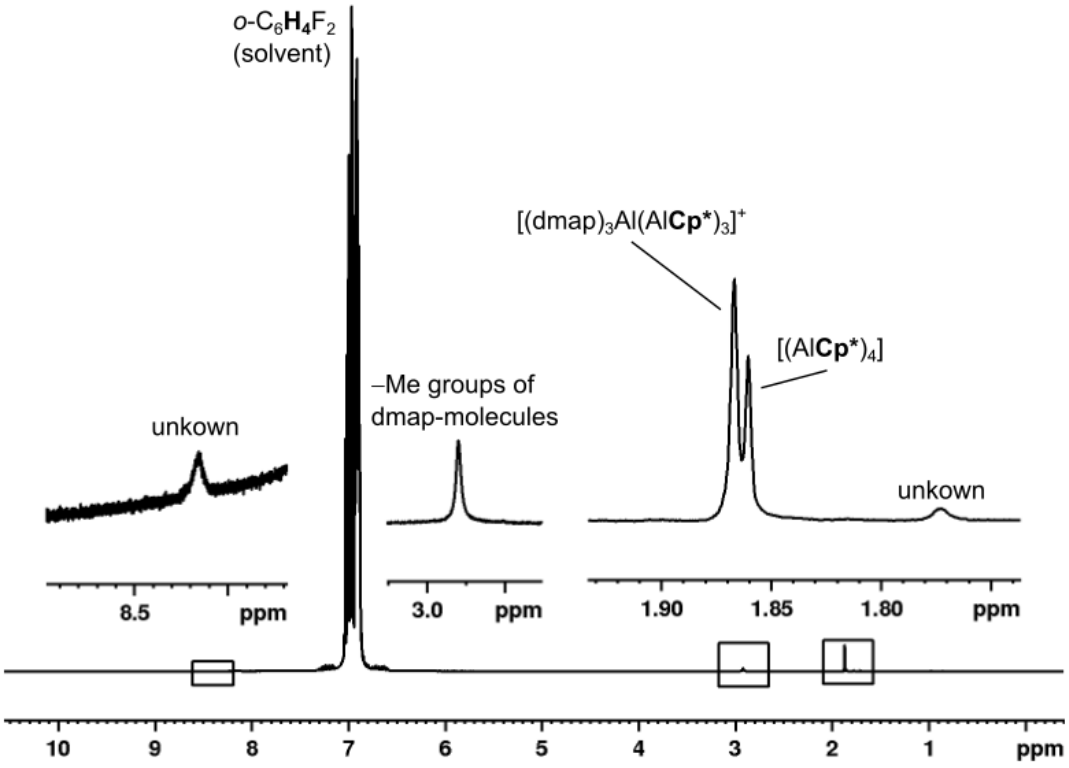
^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 298 K): δ = 35.0 (s, $[Al(OC_4F_9)_4]^-$), –79.1 (br. s, $[(\mathbf{Al}Cp^*)_4]$), –83.3 (br. s, $[(dmap)_3Al(\mathbf{Al}Cp^*)_3]^+$) ppm.

FTIR spectrum (ZnSe-ATR): $\tilde{\nu}$ = 2904 (vw), 2860 (vw), 1627 (m), 1549 (w), 1447 (vw), 1397 (vw), 1351 (vw), 1298 (w), 1275 (m), 1239 (s), 1213 (vs), 1165 (w), 1119 (vw), 1064 (vw), 1011 (w), 971 (vs), 812 (w), 764 (vw), 727 (s), 559 (vw) cm^{-1}.

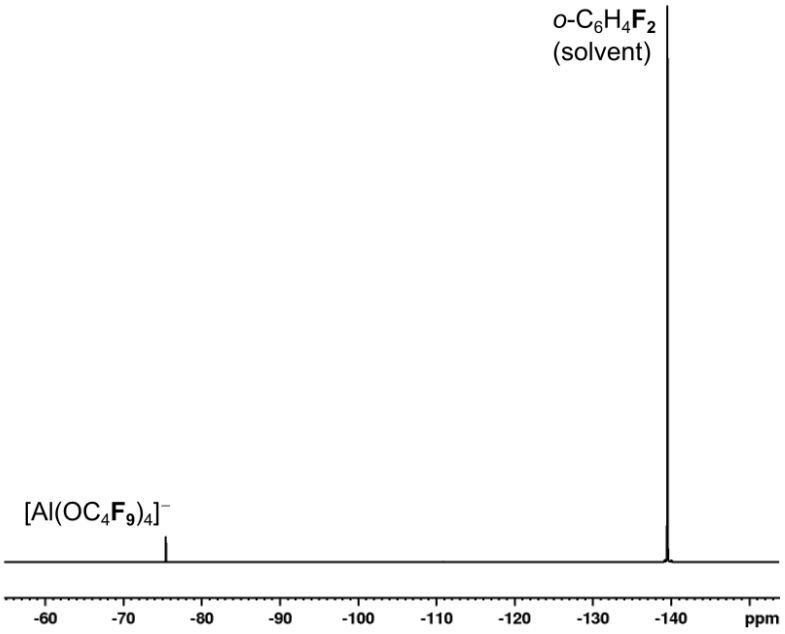
Raman spectrum (1000 scans): $\tilde{\nu}$ = 2908 (m), 1431 (w), 1063 (w), 2860 (w), 1633 (vw), 1548 (w), 1466 (vw), 1454 (w), 1383 (w), 1363 (vw), 1300 (vw), 1277 (vw), 1013 (vw), 950 (w), 797 (vw), 765 (w), 597 (w), 560 (vw), 370 (w), 331 (w), 286 (vw), 236 (vw), 118 (s), 88 (vs) cm^{-1}.

S-Figure 45: Crystals of $[(dmap)_3Al(AlCp^*)_3][pf]$ **5** grown from layering of a 1,2-DFB solution with *n*-pentane at room temperature.

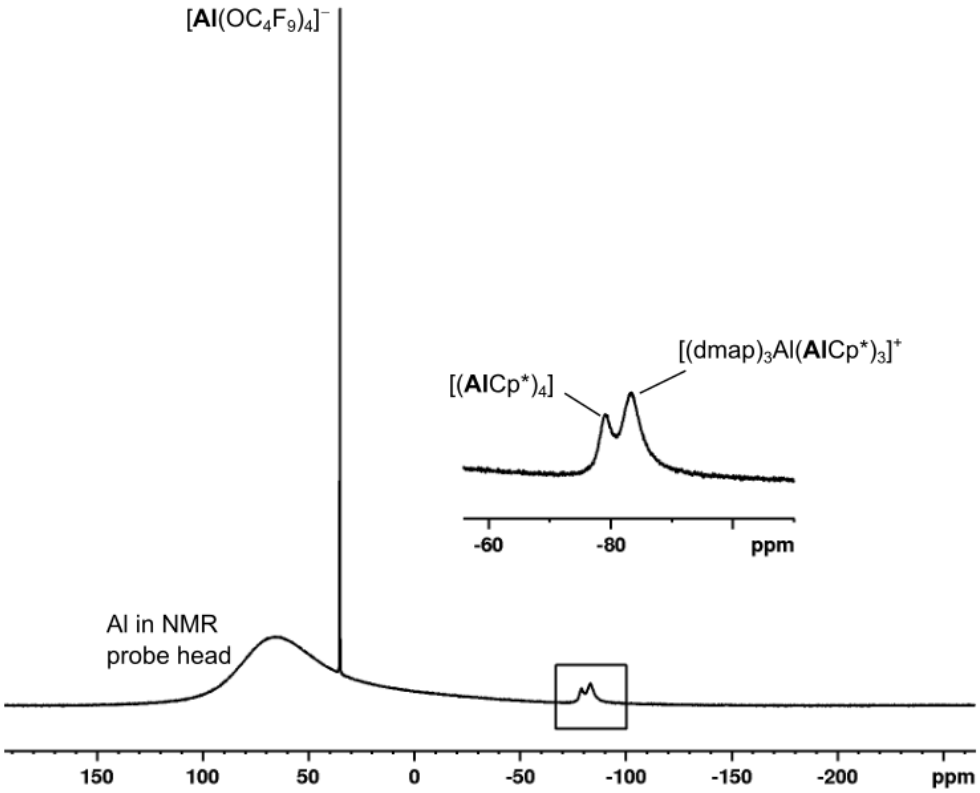
NMR spectra of [(dmap)$_3$Al(AlCp*)$_3$][*pf*] 5



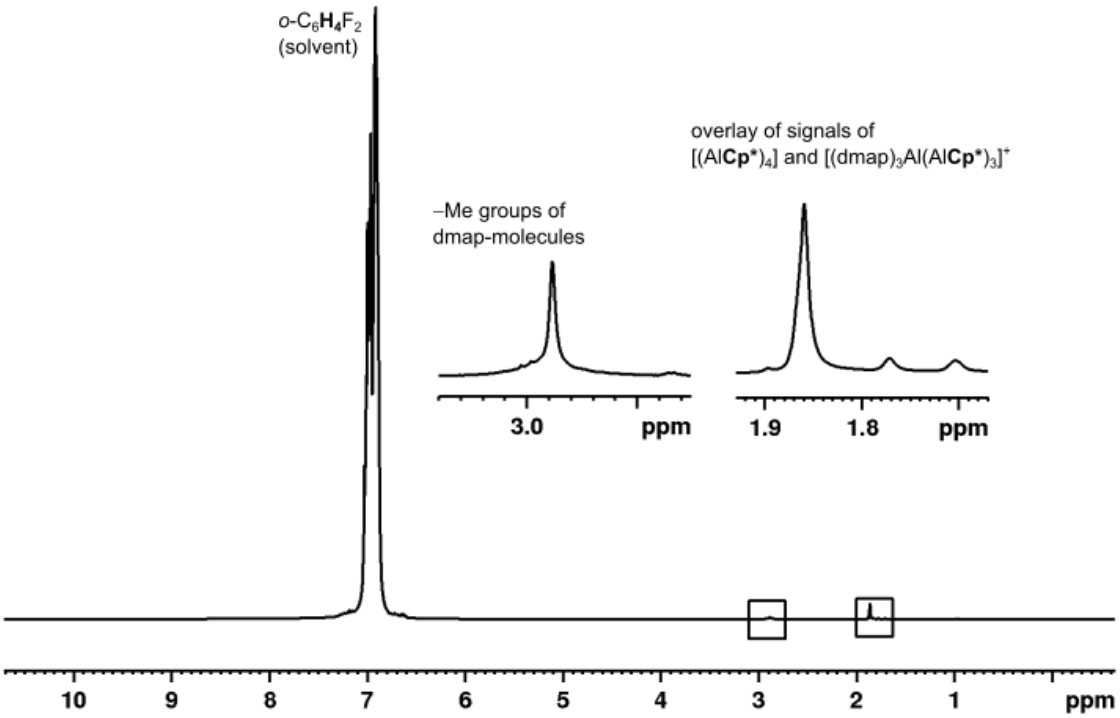
S-Figure 46: ^{1}H NMR spectrum (300.2 MHz, 1,2-DFB, 300K) of **5** after a few minutes.



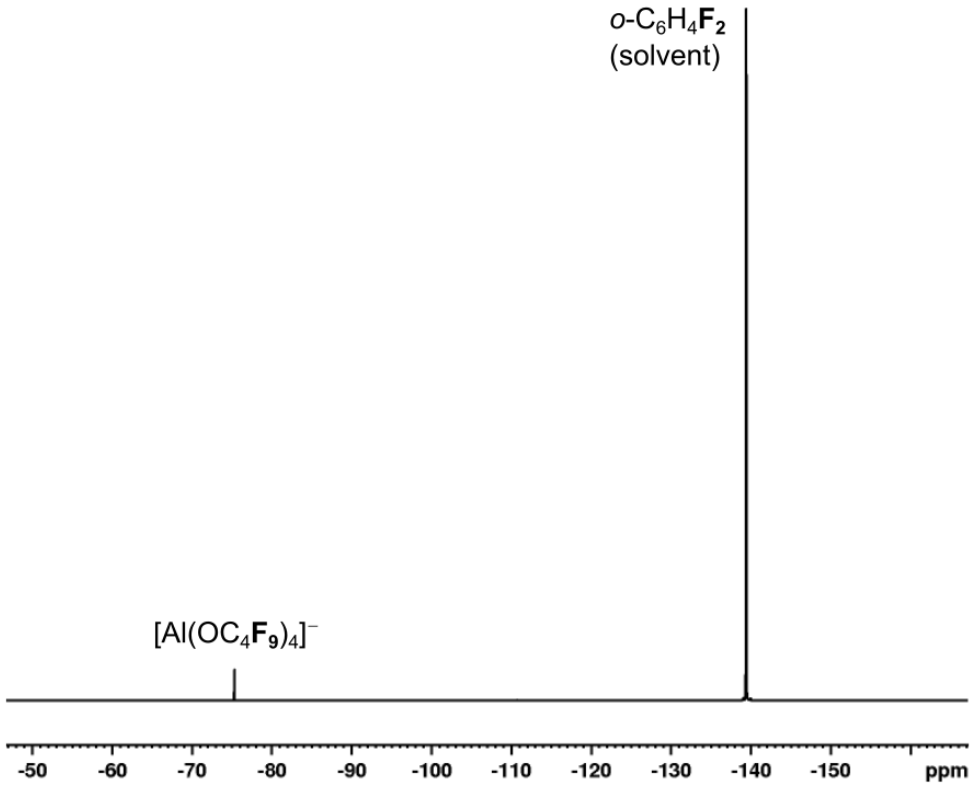
S-Figure 47: ^{19}F NMR spectrum (282.5 MHz, 1,2-DFB, 300K) of **5** after a few minutes.



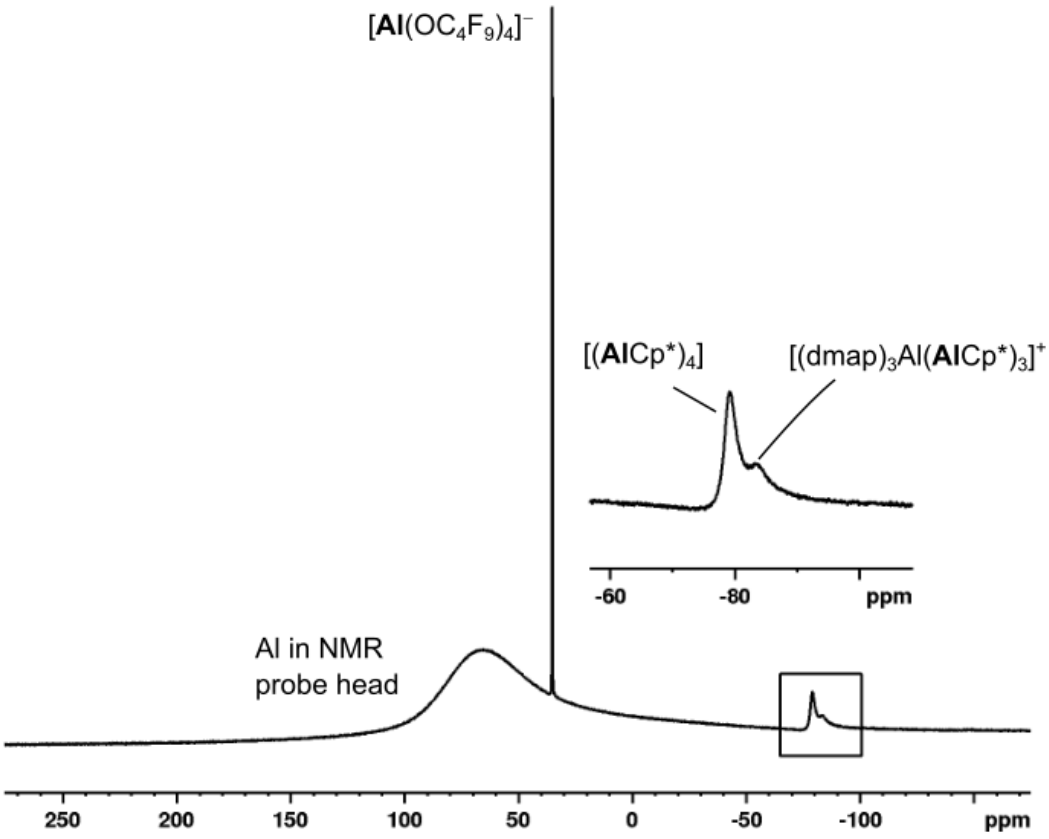
S-Figure 48: ^{27}Al NMR spectrum (78.2 MHz, 1,2-DFB, 300K) of **5** after a few minutes.



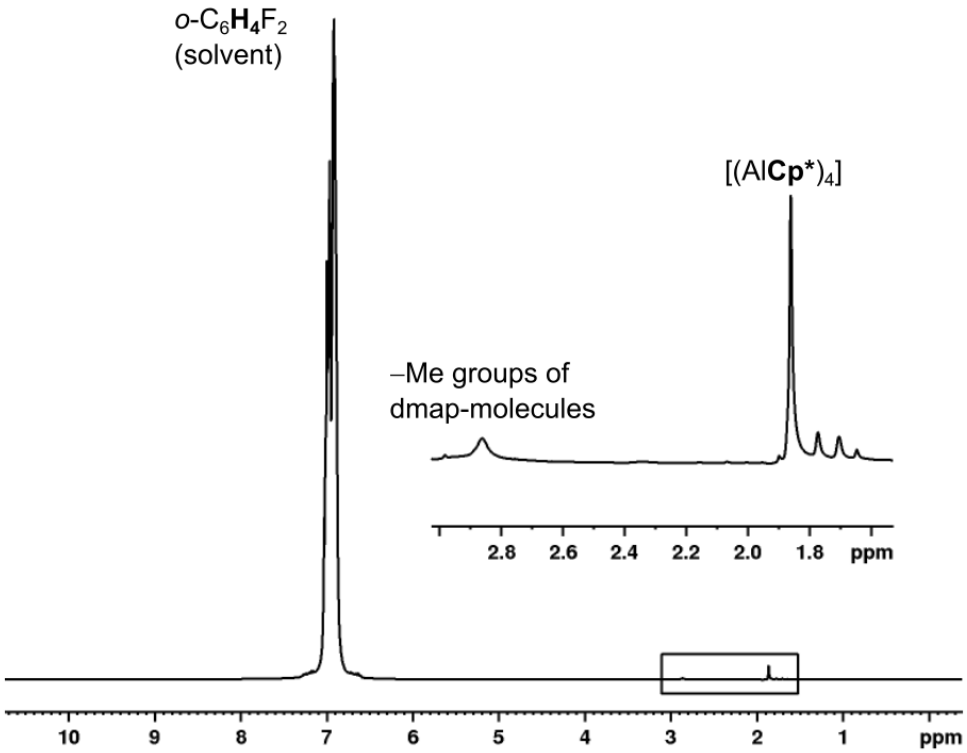
S-Figure 49: ^{1}H NMR spectrum (300.2 MHz, 1,2-DFB, 300K) of **5** after 6 days.



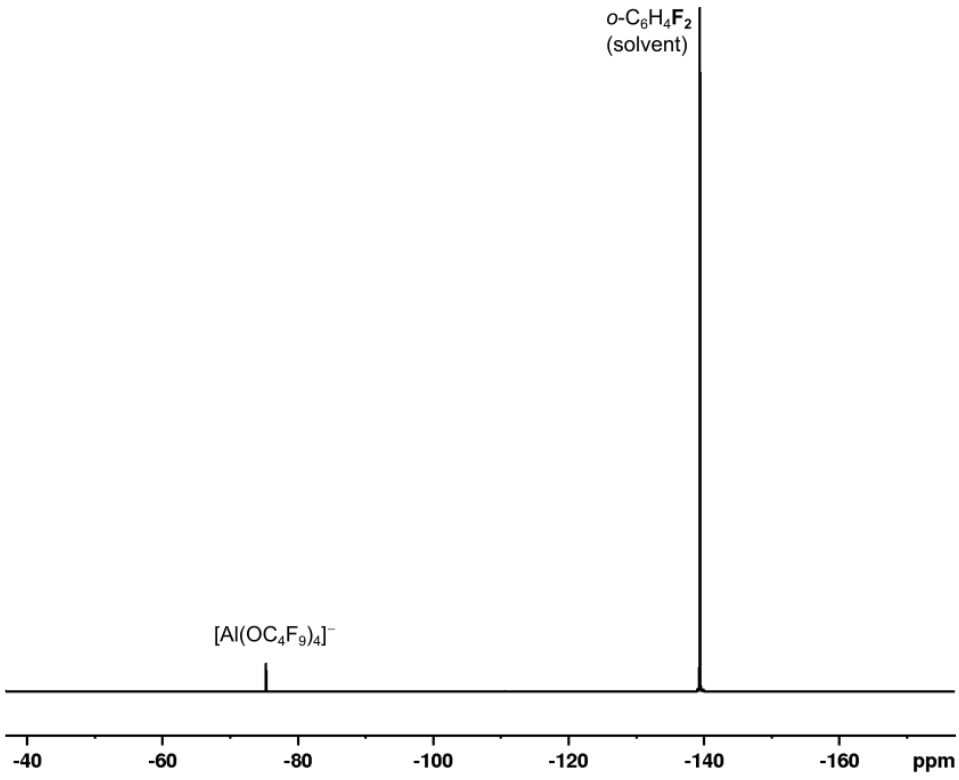
S-Figure 50: ^{19}F NMR spectrum (282.5 MHz, 1,2-DFB, 300K) of **5** after 6 days.



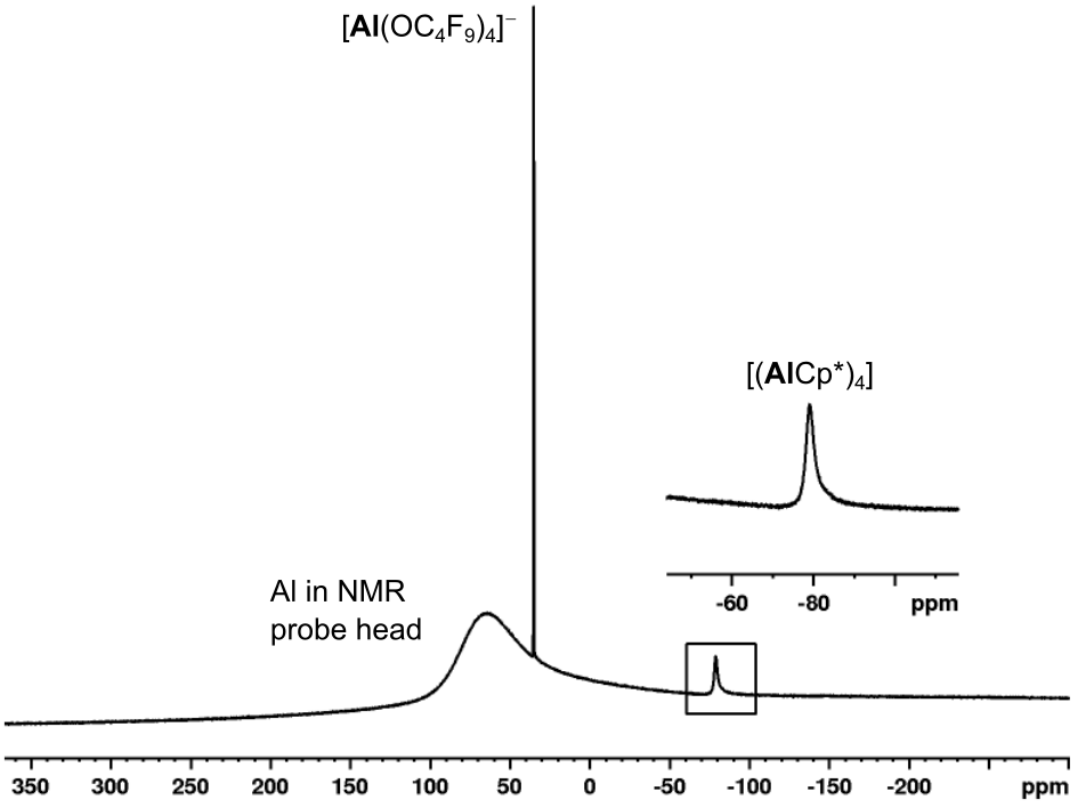
S-Figure 51: ^{27}Al NMR spectrum (78.2 MHz, 1,2-DFB, 300K) of **5** after 6 days.



S-Figure 52: ^{1}H NMR spectrum (300.2 MHz, 1,2-DFB, 300K) of **5** after 2 weeks.



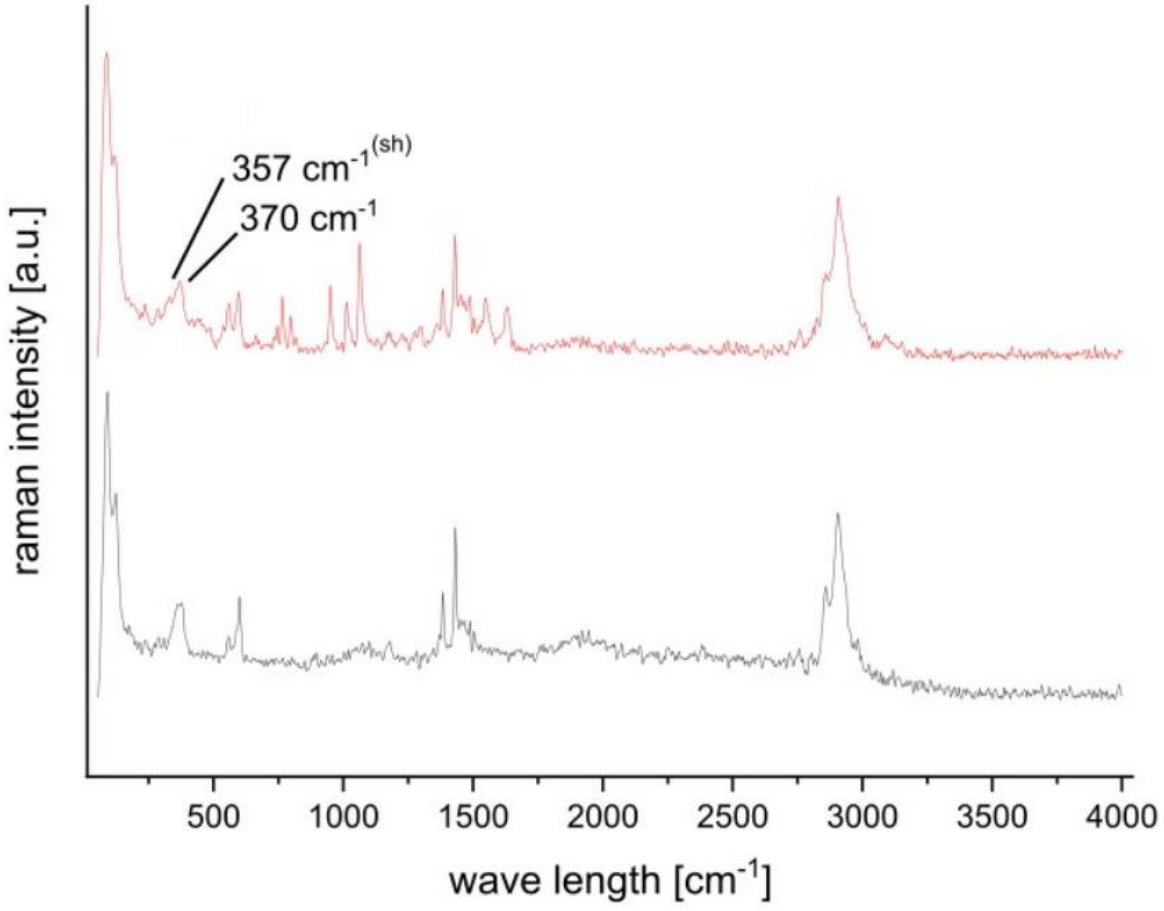
S-Figure 53: ^{19}F NMR spectrum (282.5 MHz, 1,2-DFB, 300K) of **5** after 2 weeks.



S-Figure 54: ^{27}Al NMR spectrum (78.2 MHz, 1,2-DFB, 300K) of **5** after 6 days.

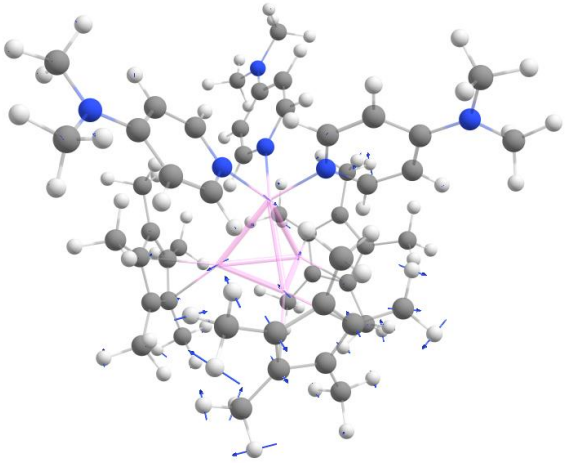
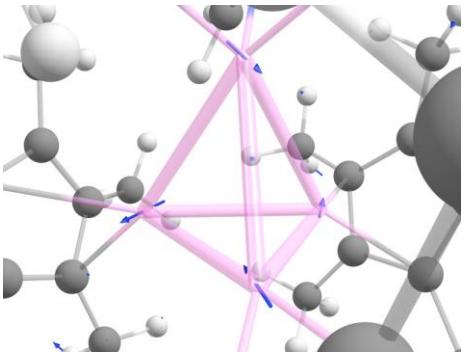
Raman spectrum of $[(dmap)_3Al(AlCp^*)_3][pf]$ 5

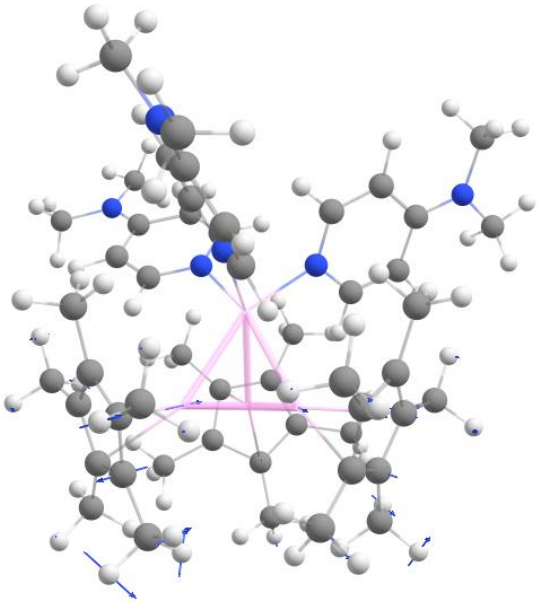
In analogy to the experimental Raman spectrum of $[(AlCp^*)_4]$, characteristic breathing modes of Al_4 clusters for **5** are observed at $\nu_{exp.}$ = 357, 370 cm^{-1} ($\nu_{comp.}$ = 356, 370 cm^{-1}; bp86-d3bj/def2-svp). Prominent signals near 2900 cm^{-1} can be assigned to C–H stretching vibrations(ν(C–H)). Raman bands near 1400 cm^{-1} and 600 cm^{-1} are attributable to breathing vibrations of the C_5Me_5 ligands as well as deformational modes of the CH_3 groups.[17,18] Moreover, Raman bands at 1633 cm^{-1} and 1535 cm^{-1} can be assigned to breathing modes of the pyridine-system in the dimethylaminopyridine ligands. The bands near 1000 cm^{-1} are attributable to deformational modes of the dimethylamino-moieties of the dmap ligands.



S-Figure 55: Comparison of the experimental Raman spectra of $[(dmap)_3Al(AlCp^*)_3]^+[pf]^-$ (red) and $[(AlCp^*)_4]$ (black).

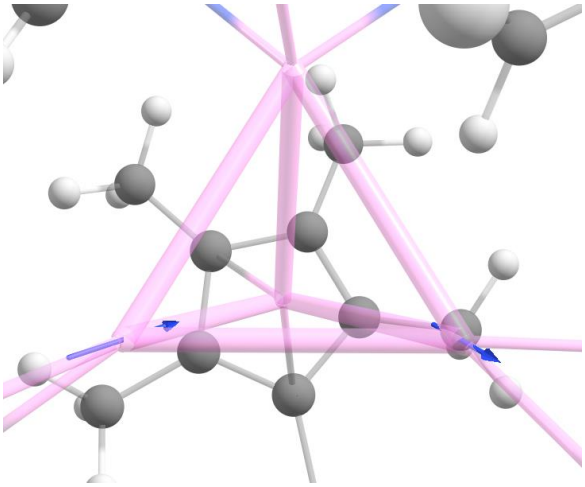
S-Table 9: Observed and calculated (bp86-d3bj/def2-svp) Raman frequencies as well as visualization of the breathing mode of the Al_4 fragment in $[(dmap)_3(AlCp^*)_3][pf]$ **5**

Raman (Exp.) $\tilde{\nu}$ [cm^{-1}]	**Calc. $\tilde{\nu}$ [cm^{-1}]**	**Scaled displacement vectors for the vibrational modes**
357	356	 (threshold for visualization: 0.001; due to small scaled vectors, the Al_4 tetrahedron is displayed as thin sticks) **Zoom:** 



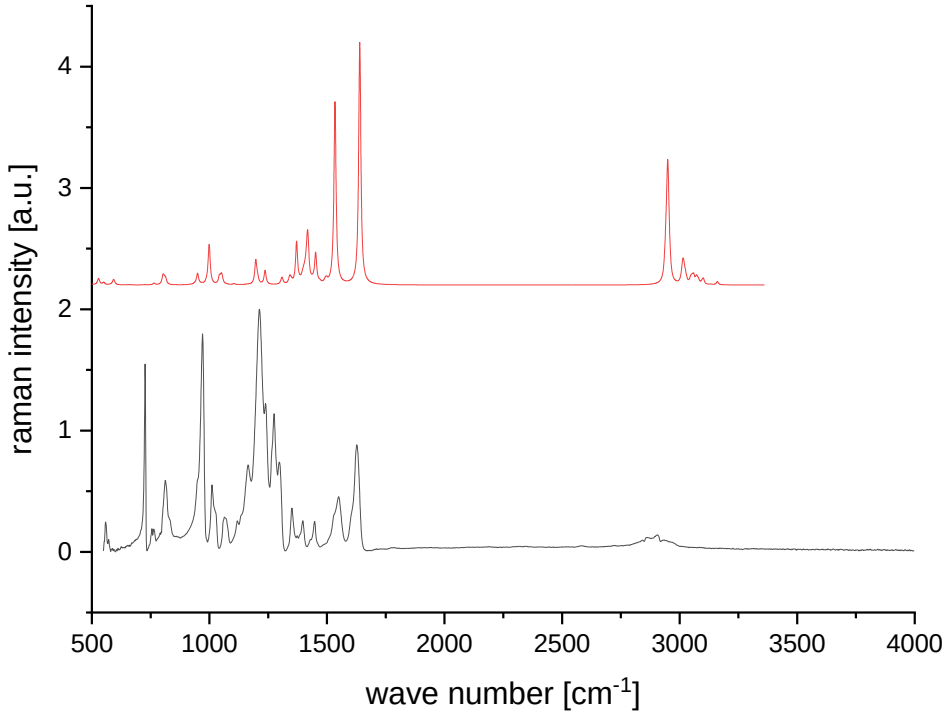
370 370 (threshold for visualization: 0.001; due to small scaled vectors, the Al_4 tetrahedron is displayed as thin sticks)

Zoom:



IR spectrum of $[(dmap)_3Al(AlCp^*)_3][pf]$ 5

The IR spectrum shows the IR bands of free $[pf]^-$ according to the published IR spectrum of $[NR_4][Al(OR^F)_4]$ (R = alkyl)[21] as well as IR bands characteristic to the dimethylaminopyridine-ligand (dmap). Prominent signals near 2900 cm^{-1} can be assigned to C–H stretching vibrations(ν(C–H)). The major, characteristic bands of the $[pf]^-$ anion and the dmap-ligand in the experimental spectrum of **1** are summarized in S-Table 6.



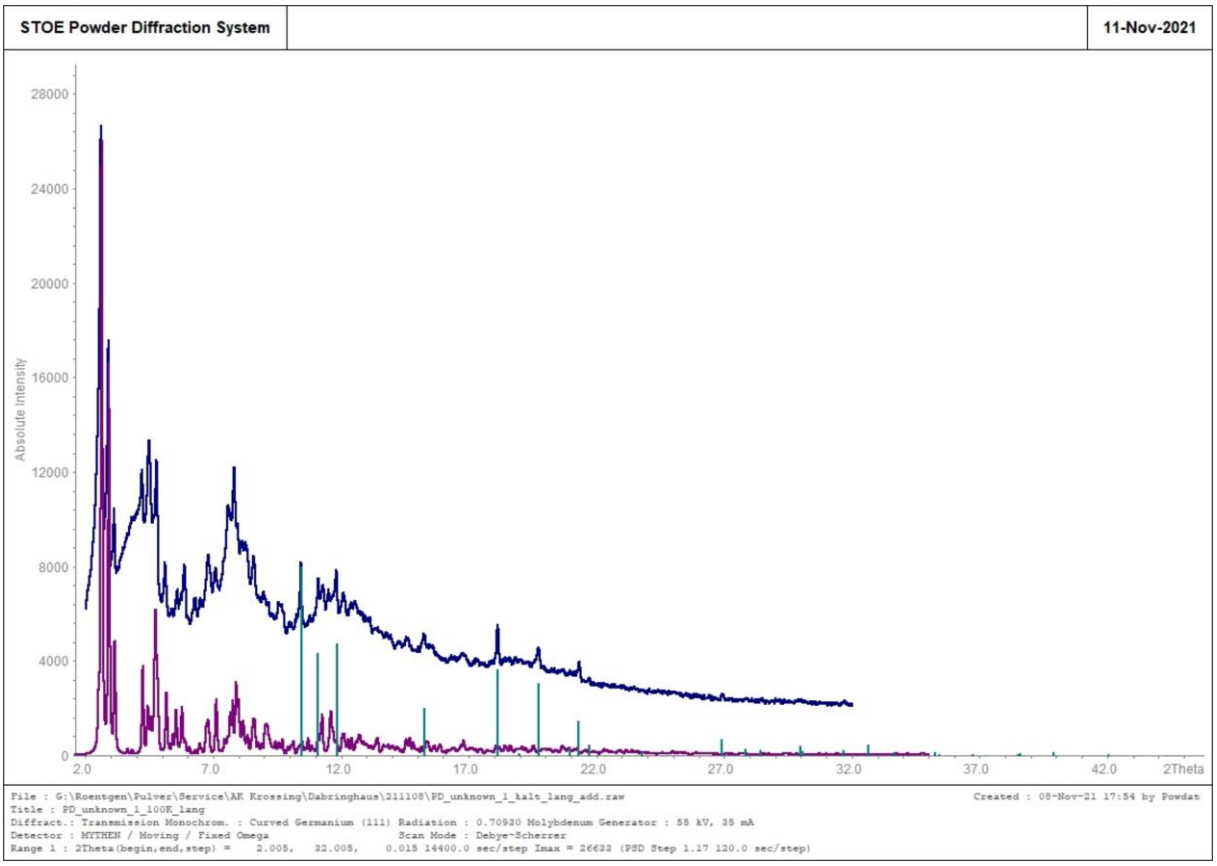
S-Figure 56: Experimental IR spectrum of $[(dmap)_3Al(AlCp^*)_3]^+[pf]^-$ and computed IR spectrum (red) for $[(dmap)_3Al(AlCp^*)_3]^+$ (bp86-d3bj/def2-svp).

S-Table 10: Characteristic IR bands of the free $[pf]^-$ anion as well as of the dimethylaminopyridine ligand are observed in the experimental IR spectrum of $[Al(AlCp^*)_3]^+[pf]^-$

IR (Exp.) $\tilde{\nu}$ [cm^{-1}]	**Assignment[21]**
727	C–C, C–O
831	Al–O, C–C
971, 1165, 1213, 1239,1275, 1297, 1351	C–C, C–F
1397, 1351	C–H
1447	C–C (Cp*)
1549,1627	C–C, C–NMe_2 (dmap)

Powder X-Ray diffraction of [(dmap)$_3$Al(AlCp*)$_3$][*pf*] 5

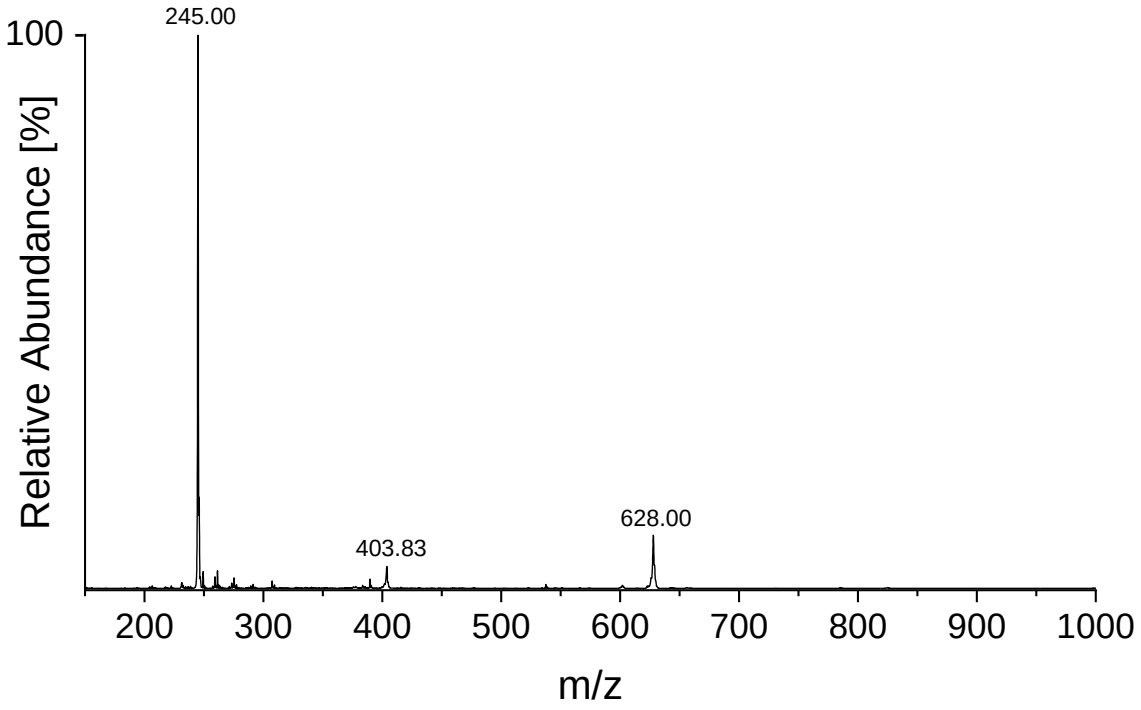
The bulk purity of [(dmap)$_3$Al(AlCp*)$_3$][*pf*] **5** was verified by pwdXRD.



S-Figure 57: Experimental spectrum of [(dmap)$_3$Al(AlCp*)$_3$][*pf*] **5** and simulated spectrum for **5.** The reflexes marked with green lines are assigned to ice crystals formed on the capillary during the measurement.

Mass spectrum of [(dmap)$_3$Al(AlCp*)$_3$][*pf*] 5

In the mass spectrum, no signal matching the calculated value for **1** of m/z = 879.53 could be observed. The main signal of the mass spectrum of **5** at m/z = 245.00 can be attributed to $[dmap_2H]^+$ (m/z_{calc} = 245.18). In a charge induced decomposition experiment, the decomposition of $[dmap_2H]^+$ to $[dmapH]^+$ (m/z_{exp} = 123.17, m/z_{calc} = 123.09) could be observed. The signal at m/z = 403.83 and m/z = 628.00 could no be assigned.

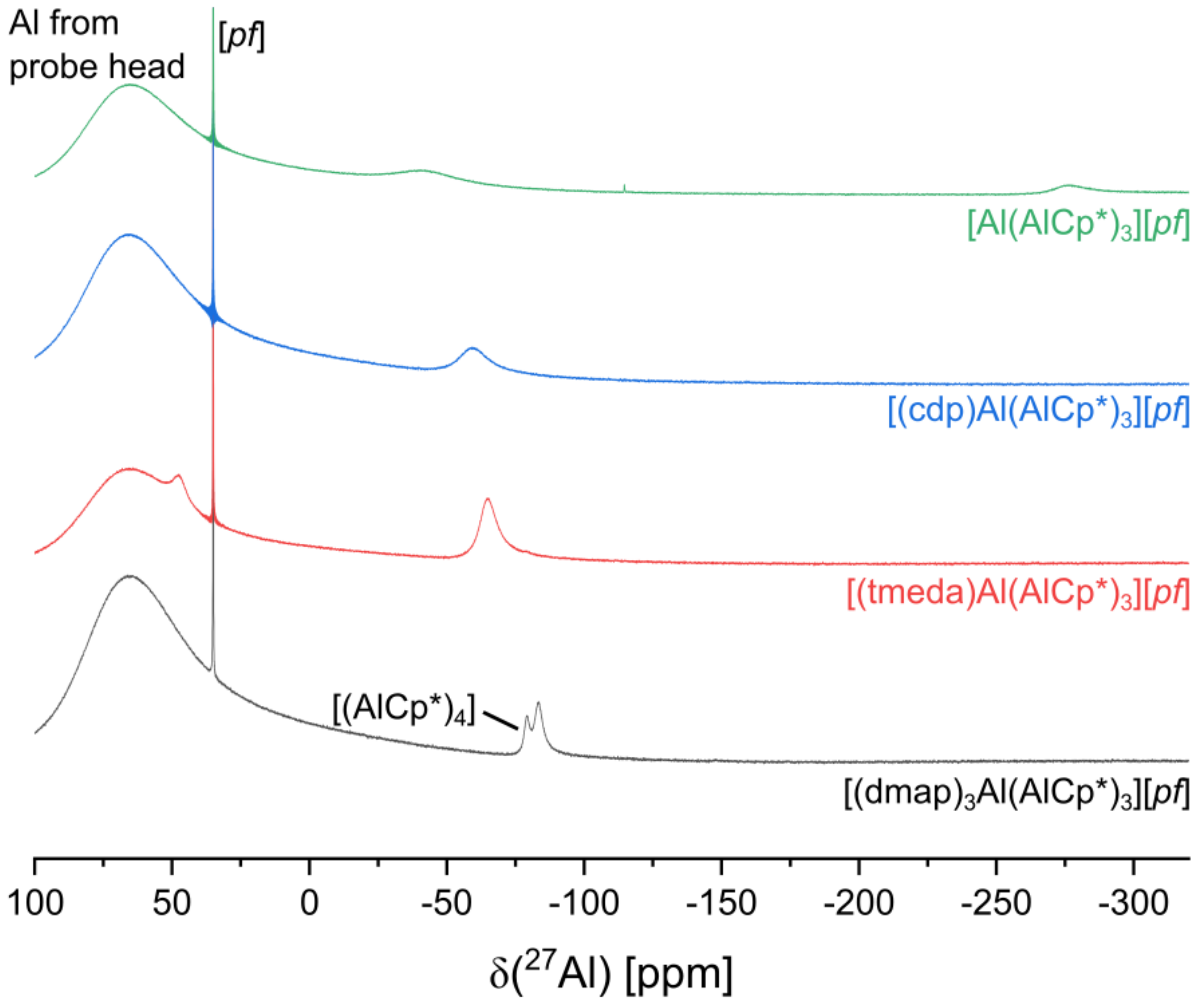


S-Figure 58: Full mass spectrum (ITMS+p-ESI, ESI voltage = 3.97 V, T_{cap} = 120.03 °C, sprayed from 1,2-DFB solution) of **5**.

S-1.9 Comparison of the isolated Al_4 complexes: NMR and Raman

NMR spectra of the Al_4 complexes

Upon comparison of the ^{27}Al NMR signals of Cp*-coordinated aluminium atoms in the isolated complexes, a clear trend is observed. Here, coordination of the unique Al atom results in an high-field shift of the Al_{Cp^*} signal compared to [Al(AlCp*)$_3$][*pf*] (δ_{27Al} = –41 ppm). The high field shift increases with the number of donor-atoms at the unique Al atom from δ_{27Al} = –59 ppm in [(cdp)Al(AlCp*)$_3$][*pf*] via δ_{27Al} = –65 ppm in [(tmeda)Al(AlCp*)$_3$][*pf*] to δ_{27Al} = –83 ppm in [(dmap)$_3$Al(AlCp*)$_3$][*pf*]. The ^{27}Al resonances assigned to the AlCp* in [(dmap)$_3$Al(AlCp*)$_3$][*pf*] are observed at higher field compared to [(AlCp*)$_4$].

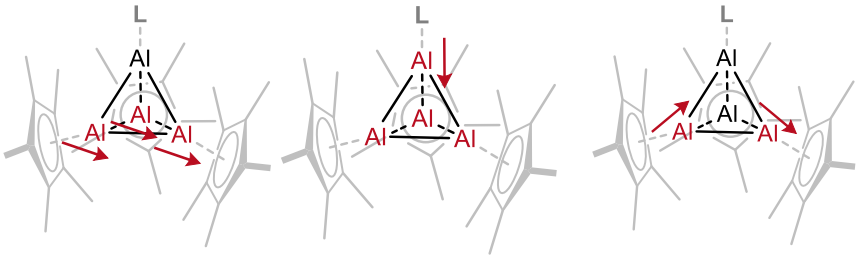


S-Figure 59: Comparison of the ^{27}Al NMR spectra (78.2 MHz, 1,2-DFB, 300K) of the Al_4 complexes presented in this publication.

Raman: comparison of breathing vibrations of the isolated Al_4 complexes

The trend of the observed and calculated Raman bands of the breathing modes of the isolated Al_4 complexes is in-line with trends observed for the respective bond lengths and NMR signals (S-Table 11). Here, the shift of the characteristic breathing mode $\tilde{\nu}_3(Al_4)$ correlates with the bond strength of the Al–Al bond between the unique aluminium atom and the AlCp* moieties. Hence, in $[Al(AlCp^*)_3]^+$, the corresponding Raman band is significantly shifted to higher wave lengths compared to the starting material $[(AlCp^*)_4]$. However, coordination of the unique atom results in a significant shift to lower wave lengths to such an extent, that $\tilde{\nu}_3(Al_4)$ of $[(dmap)_3Al(AlCp^*)_3]^+[pf]^-$ is observed at lower wave lengths compared to $[(AlCp^*)_4]$.

S-Table 11: Comparison of the breathing vibrations of the isolated Al_4 complexes

	$\tilde{\nu}_1(Al_4$, exp.) ($\tilde{\nu}_1(Al_4$, calc.)) in cm^{-1}	**$\tilde{\nu}_2(Al_4$, exp.) ($\tilde{\nu}_2(Al_4$, calc.)) in cm^{-1}**	**$\tilde{\nu}_3(Al_4$, exp.) ($\tilde{\nu}_3(Al_4$, calc.)) in cm^{-1}**
Displacement vectors of the breathing mode (for scaled vectors see corresponding sections)			
$[(AlCp^*)_4]$	–	–	378 (378)
$[Al(AlCp^*)_3]^+[pf]^-$	183 (187)	308 (303)	474 (474)
$[(tmeda)Al(AlCp^*)_3]^+$ $[pf]^-$	164 (166)	319 (323)	405 (401)
$[(cdp)Al(AlCp^*)_3]^+$ $[pf]^-$	–	–	404 (408)
$[(dmap)_3Al(AlCp^*)_3]^+$ $[pf]^-$	–	357 (356)	370 (370)

S-3 Supporting quantum-chemical calculations

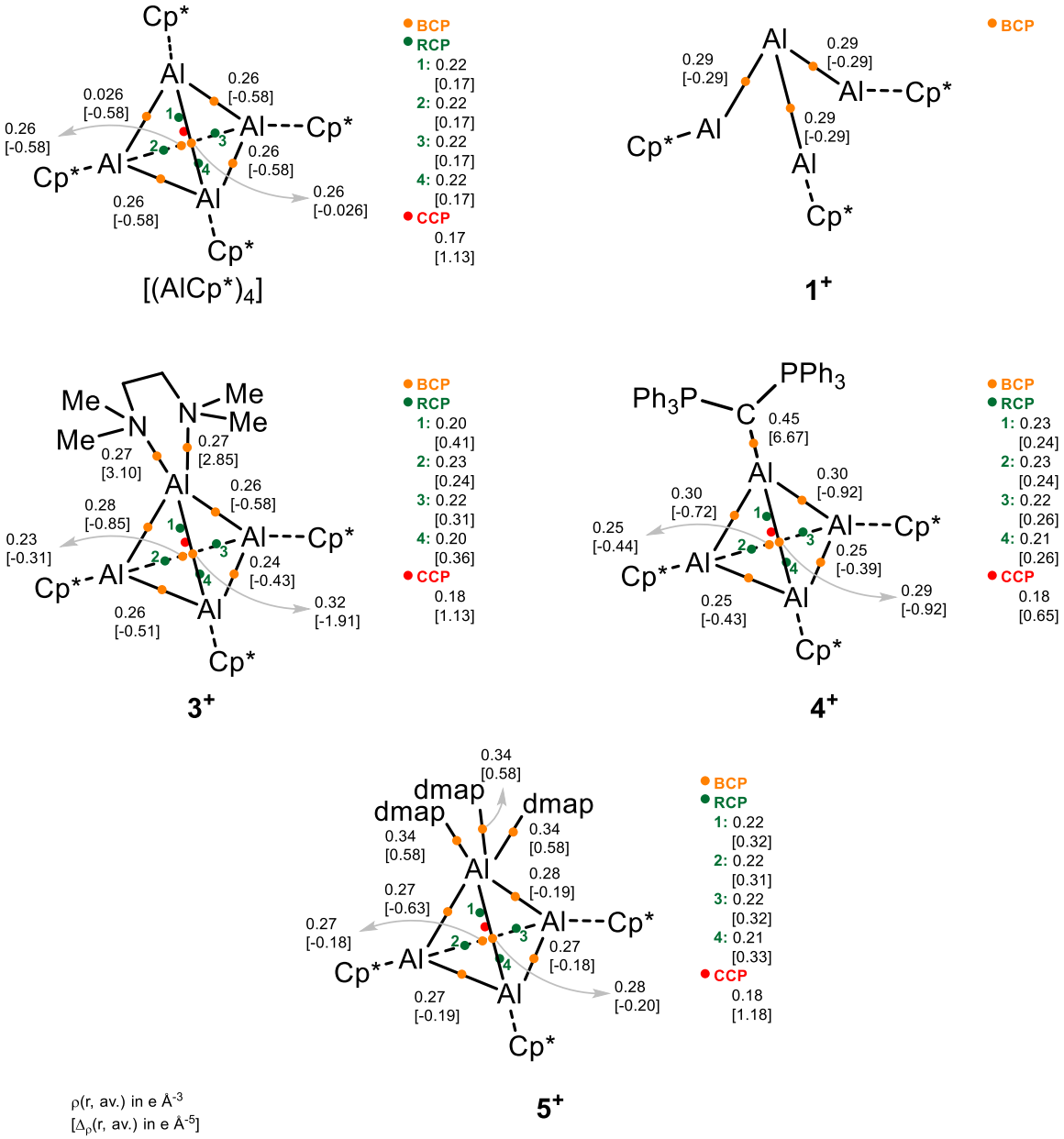
Computational details

Geometry optimizations were performed with the TURBOMOLE software[22,23] (v7.2 oder v7.5) using DFT functionals bp86[24,25] with the def2-svp[26] basis set, the resolution-of-identity (RI) approximation,[27–29] dispersion correction (d3bj),[30,31] 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.[32] 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 $10 cm^{-1}$. UV/VIS spectra were computed using the *escf* module[33] (20 excited states, singlet, with thermal smearing of occ. Numbers ($fermi)) starting from scXRD or bp96-d3bj/def2-svp structures.

Gibbs free energies of solvation were calculated with the COSMO-RS model[34,35] at the bp86-d3/def2-tzvpd//bp86-d3/def2-tzvp[36] level of theory using the CosmoThermX[37] software (v C39_1501). Single-point calculations with the pbe0[38,39]-d3bj/def2-tzvpp method were performed based on bp86-d3bj/def2-svp structures using TURBOMOLE.

QTAIM calculations were performed with the MultiWFN program package[40] on bp86-d3bj/def2-svp structures. EDA-NOCV analysis[41] of the compounds was performed as implemented in the ADF program package (2019.304).[42] All EDA-NOCV calculations were formed on BP86-D3BJ/TZ2P//BP86-D3BJ/def2-SVP level of DFT (numerical quality verygood, nosym).

Quantum Theory of Atoms in Molecules



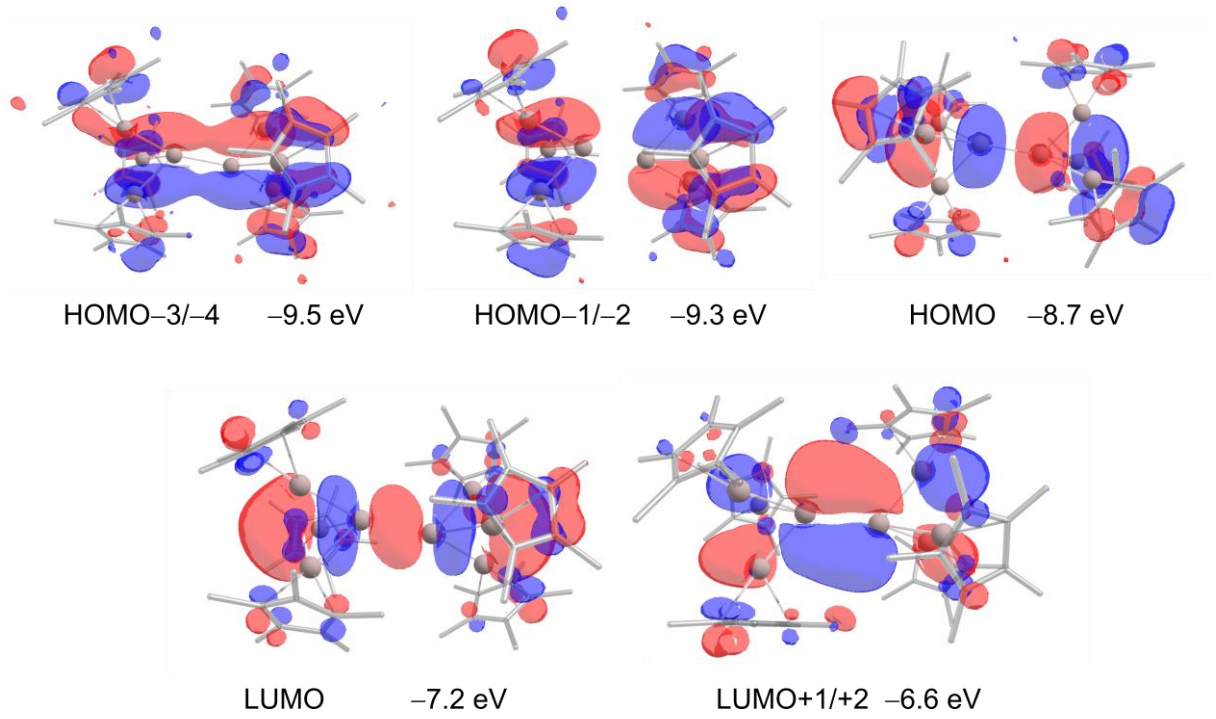
S-Figure 60: Computed electron densities ρ(r) and Laplacian of the electron density Δ_ρ(r) at the critical points (BCP: bond critical point; RCP: ring critical point, CCP: cubic critical point) of the Al_4 compounds [$(AlCp^*)_4$], **1**$^+$, **3**$^+$, **4**$^+$ and **5**$^+$.

S-Table 12: Average values for the electron densities ρ(r) and the Laplacian of the electron density Δ_ρ(r) at critical points in cations **1**$^+$ - **5**$^+$

ρ(r, av.) in e Å^{-3} [Δ_ρ(r, av.) in e Å^{-5}]	[(AlCp*)$_4$]	**1**$^+$ no L	**3**$^+$ L = tmeda	**4**$^+$ L = cdp	**5**$^+$ L = (dmap)$_3$
BCPs LAl–AlCp*	-	0.29	0.29	0.30	0.28
		[–0.29]	[–0.87]	[–0.85]	[–0.68]
BCPs Cp*Al–AlCp*	0.26	-	0.24	0.25	0.27
	[–0.56]		[–0.68]	[–0.43]	[–0.65]
BCPs L–Al	-	-	0.27	0.45	0.33
			[2.97]	[6.67]	[0.56]
RCPs LAl–AlCp*–AlCp*	-	-	0.22	0.23	0.22
			[0.34]	[0.27]	[0.34]
RCPs AlCp*–AlCp*–AlCp*	0.22	-	0.20	0.21	0.21
	[0.17]		[0.36]	[0.11]	[0.34]
CCP	0.17	-	0.18	0.18	0.18
	[1.14]		[0.14]	[1.13]	[1.18]

Kohn-Sham orbitals for $[Al_2(AlCp^*)_6]^{2+}$

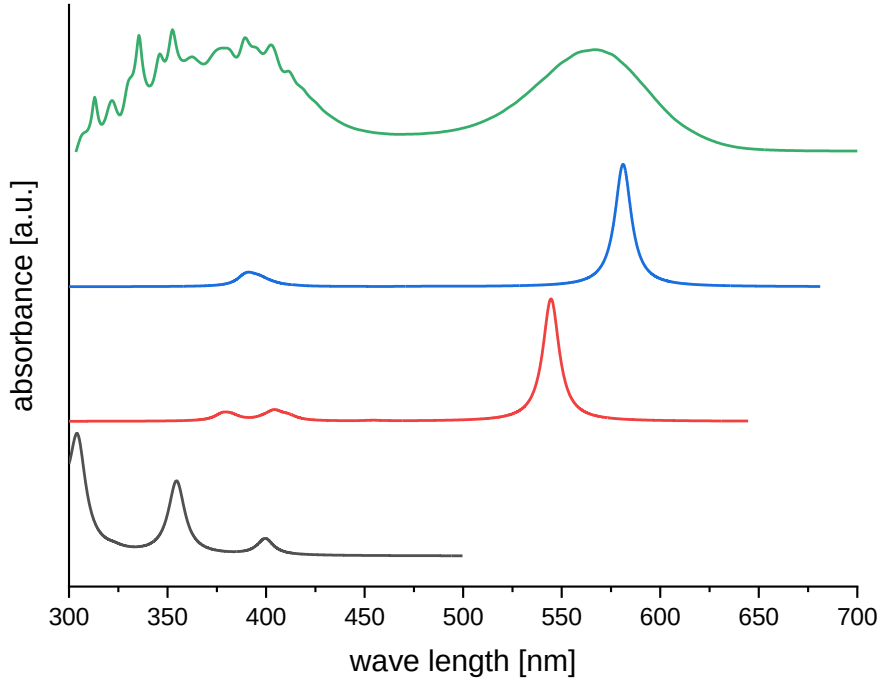
As indicated by the HOMO–3/–4, the bonding between the $[Al(AlCp^*)_3]^+$ fragments represents a π-bonding interaction.



S-Figure 61: Kohn-Sham orbitals (isovalue 0.02) of $[Al_2(AlCp^*)_6]^{2+}$ calculated at bp86-d3bj/def2-svp-level of DFT.

TDDFT: Computed UV/VIS spectrum

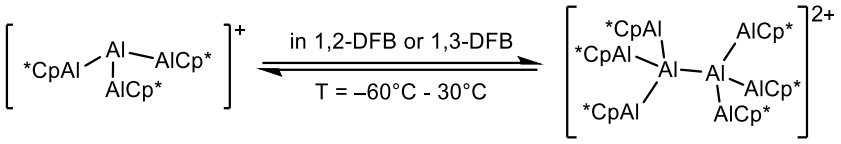
To understand the experimental UV/VIS spectra, TDDFT calculations on the monomeric and dimeric structures of $[Al(AlCp^*)_3]^+$ were performed. Since the molecular structures in the crystal are expected to represent a meaningful representation of the solution structure of the dimeric $[Al_8Cp^*_6]^{2+}$, both dimeric complexes found in the molecular structure were chosen as starting geometry for the calculations. The computed spectrum for the dimeric structure with the $(CpAl^*)_3Al–Al(AlCp^*)_3$ bond length of 2.838(2) Å shows a major UV/VIS band at 581 nm. This most intense UV/VIS band is shifted to 544 nm for the molecular structure with the longer $(CpAl^*)_3Al–Al(AlCp^*)_3$ distance of 3.005(2) Å. TDDFT calculations show that the respective prominent absorptions originate from a HOMO-LUMO excitation. Hence, as shown by the Kohn-Sham orbitals (S-Figure 61) of the dimer, the absorptions represent a metal-centred electronic transition. Here, shorter $(CpAl^*)_3Al–Al(AlCp^*)_3$ bond lengths result in a narrower HOMO-LUMO gap and the absorption band is shifted to higher wave lengths. Hence, with the experimental UVVIS band observable at 564 nm, the solution structure of the dimer is expected to possess a $(CpAl^*)_3Al–Al(AlCp^*)_3$ distance between 2.838(2) Å and 3.005(2) Å on average. In contrast, the computed UV/VIS spectrum of the monomer does not show a band between 500 and 600 nm.



S-Figure 62: Comparison of the experimental spectrum of $[Al(AlCp^*)_3]^+[pf]^-$ **1** (green) at –30° with the computed UV/VIS spectra of the two dimeric $[Al_8Cp^*_6]^{2+}$ (with short Al–Al distance in blue; with longer Al–Al distance in red) cation taken from the scXRD experiment as well as of the gas-phase optimized monomeric $[Al(AlCp^*)_3]^+$ (black). UVVIS spectra computed with TDDFT at bp86-d3bj/def2-svp.

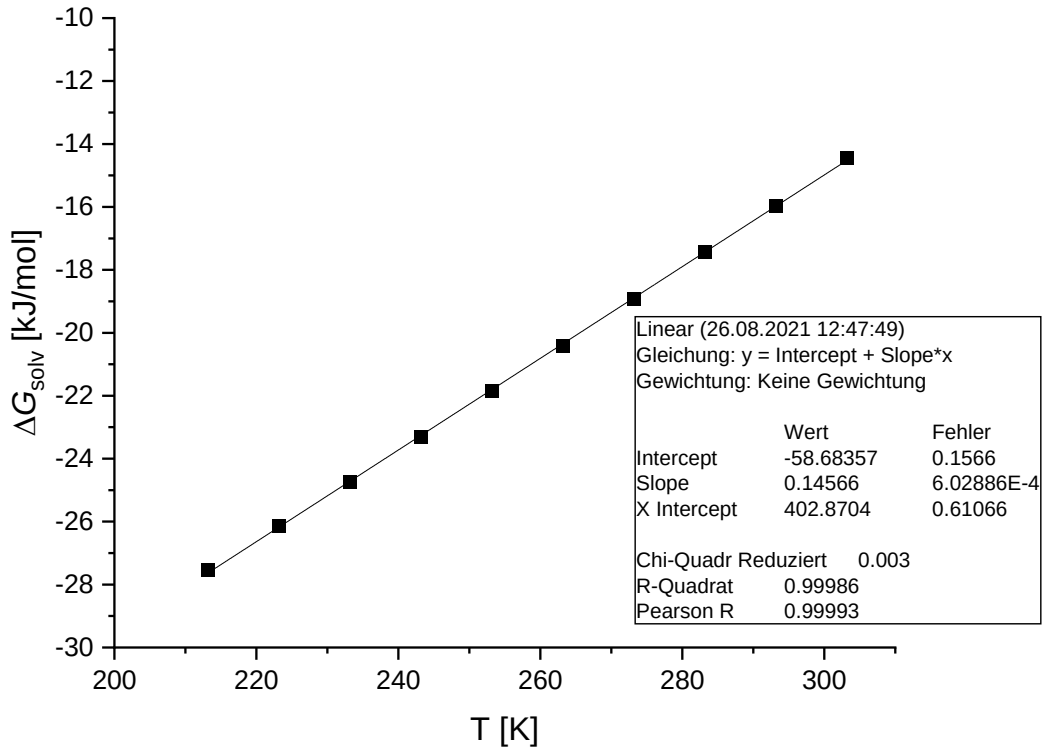
Thermodynamics

1.) Dimerization of $[Al(AlCp^*)_3]^+$ in 1,2-DFB and 1,3-DFB

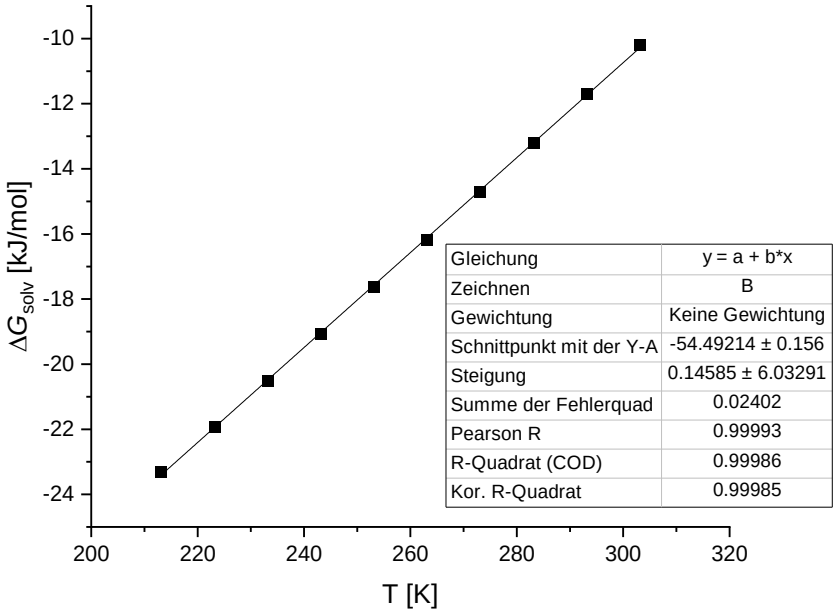


S-Scheme 1: Reaction equation for the dimerization of **1**.

To estimate the values of the enthalpic and entropic contribution to the solvated free reaction enthalpy for the dimerization of $\mathbf{1}^+$ according to S-Scheme 1, the temperature dependency of the computed values of ΔG_{solv} between –60°C and +30°C was analyzed. Linear regression yielded values for ΔH_{solv} and ΔS_{solv}.



S-Figure 63: Plot of the temperature dependence of the free enthalpy ΔG_{solv} for the dimerization of **1** in 1,2-DFB. Thermodynamics calculated on bp86-d3bj/def2-svp level of the DFT. Free enthalpy of solvation determined with COSMO-RS mole as implemented in Turbomole.



S-Figure 64: Plot of the temperature dependence of the free enthalpy ΔG_{solv} for the dimerization of **1** in 1,3-DFB. Thermodynamics calculated on bp86-d3bj/def2-svp level of the DFT. Free enthalpy of solvation determined with COSMO-RS mole as implemented in Turbomole.

S-Table 13: Obtained values for ΔH_{solv} and ΔS_{solv} in 1,2-DFB and 1,3-DFB.

Solvent	ΔH_{solv} [kJmol^{-1}]	ΔS_{solv} [KJmol^{-1}K^{-1}]
in 1,2-DFB	–59	0.16
in 1,3-DFB	–55	0.15

2.) Breakup of the clusters 3-5

[(AlCp*)$_4$] L = Cp*
3 L = tmeda (x = 1)
4 L = C(PPh$_3$)$_2$ (x = 1)
5 L = dmap (x = 3)

S-Scheme 2: Breakup of the reported Al$_4$ clusters into a monomeric Al compound and [(AlCp*)$_3$].

S-Table 14: Computed thermodynamics for the breakup of the cationic Al$_4$ complexes **3**, **4** and **5** in comparison to [(AlCp*)$_4$] according to S-Scheme 2. All values calculated on bp86-d3bj/def2-svp level of dft. Solvation effects computed with cosmos-rs module as implemented in Turbomole

	ΔH_{gas} [kJmol^{-1}]	ΔG_{gas} [kJmol^{-1}]	ΔG_{solv} [kJmol^{-1}]
[(AlCp*)$_4$]	188	117	150
[(tmeda)Al(AlCp*)]$^+$ 3$^+$	303	229	237
[(cdp)Al(AlCp*)]$^+$ 4$^+$	320	227	245
[(dmap)$_3$Al(AlCp*)]$^+$ 5$^+$	296	215	229

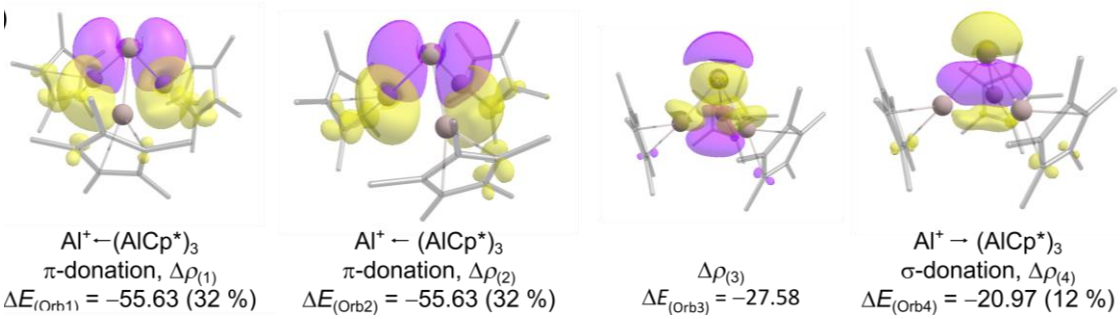
EDA-NOCV analysis

EDA-NOCV analysis of the compounds was performed as implemented in the ADF program package. All EDA-NOCV calculations were formed on BP86-D3BJ/TZ2P//BP86-D3BJ/def2-SVP level of DFT.

1.) EDA-NOCV analysis of $[Al(AlCp^*)_3]^+[pf]^-$ 1

S-Table 15: Results of the EDA-NOCV analysis for the interaction of an Al^+ atom with the $(AlCp^*)_3$ fragment in **1**$^+$

Energy terms	Orbital interaction	value in kcal/mol
ΔE_{int}		**−133.85**
ΔE_{Pauli}		134.91
ΔE_{elstat}		−85.07
ΔE_{Orb}		−173.65
$\Delta E_{Orb(1)}$	$(AlCp^*)_3$ → Al^+ (p_y) π-donation	−55.63
$\Delta E_{Orb(2)}$	$(AlCp^*)_3$ → Al^+ (p_x) π-donation	−55.62
$\Delta E_{Orb(3)}$	$(AlCp^*)_3$ ← Al^+ (s) σ-back donation	−27.59
$\Delta E_{Orb(4)}$	$(AlCp^*)_3$ ← Al^+ (s) σ-back donation	−20.98
ΔE_{Rest}		−13.82
ΔE_{Disp}		−10.04

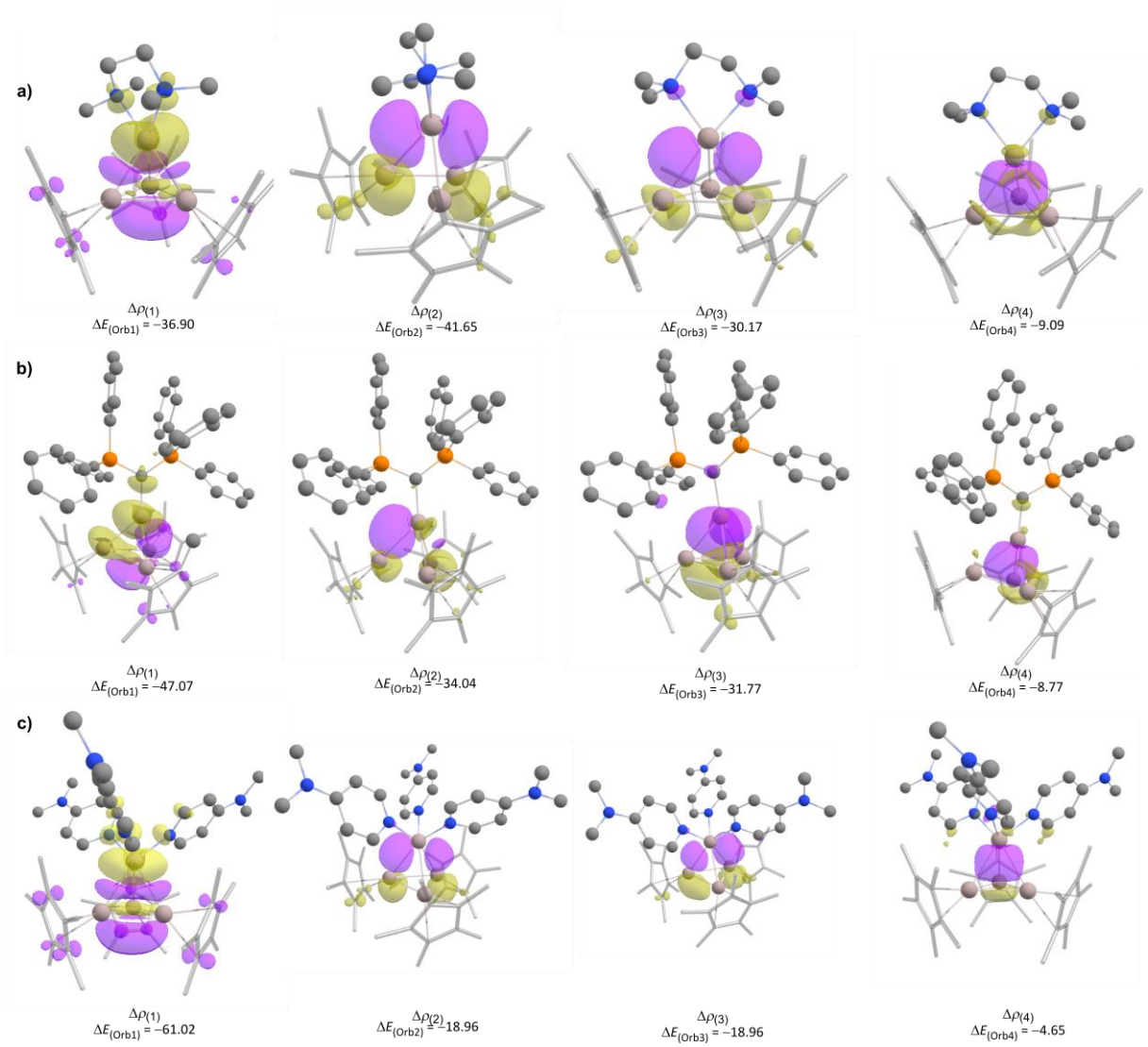


S-Figure 65: Plots of deformation densities $\Delta\rho_{(1)-(4)}$) of the pairwise orbital interaction in **1**$^+$ (isovalue 0.001) associated with energy terms $\Delta E_{Orb(1)-Orb(4)}$ (values in kcal/mol). Charge flows from yellow to purple.

2.) EDA-NOCV analysis of the clusters $[(tmeda)Al(AlCp^*)_3]^+$ **3**$^+$, $[(cdp)Al(AlCp^*)_3]^+$ **4**$^+$ and $[(dmap)_3Al(AlCp^*)_3]^+$ **5**$^+$

S-Table 16: Results of the EDA-NOCV analysis for the interaction of the $[LAl]^+$ fragment with the $(AlCp^*)_3$ fragment in **3⁺**, **4⁺** and **5⁺**

		3⁺	**4⁺**	**5⁺**
Energy terms	**Orbital interaction**	**value in kcal/mol**	**value in kcal/mol**	**value in kcal/mol**
ΔE_{int}		-86.37	-93.98	-83.33
ΔE_{Pauli}		185.02	221.99	230.98
ΔE_{elstat}		-112.17	-132.74	-148.79
ΔE_{Orb}		-132.51	-136.95	-117.59
$\Delta E_{Orb(1)}$	$(AlCp^*)_3 \leftarrow Al^+$ (*s*) σ-back donation	-36.90	-47.07	-61.02
$\Delta E_{Orb(2)}$	$(AlCp^*)_3 \rightarrow Al^+$ (p_y) π-donation	-41.65	-34.04	-18.94
$\Delta E_{Orb(3)}$	$(AlCp^*)_3 \rightarrow Al^+$ (p_x) π-donation	-30.17	-31.77	-18.96
$\Delta E_{Orb(4)}$		-9.09	-8.77	-4.65
ΔE_{Rest}		-14.9	-15.28	-14.02
ΔE_{Disp}		-26.72	-46.28	-47.94



S-Figure 66: Plots of deformation densities $\Delta\rho_{(1)-(4)}$ of the pairwise orbital interaction in **5**$^{+}$ (isovalue 0.001, 0.005 for $\Delta\rho_{(4)}$ (for all)) associated with energy terms $\Delta E_{Orb(1)-Orb(4)}$ (values in kcal/mol). Charge flows from yellow to purple.

Thermodynamic data of computed molecules

S-Table 17: Thermodynamic data for computed molecules

Compound	E(SCF) [Eh]	FreeH Energy [Eh]	FreeH entropy at 298 K [Eh]	COSMO-RS (in 1,2-DFB) [kcalmol^{-1}]
[(AlCp*)$_3$]	-1896.860947	1814.37	1.13047	-13.26904913
AlCp*	-632.2715013	600.57	0.481	-28.85999308
[(AlCp*)$_4$]	-2529.207598	2426.51	1.37152	-75.71320721
[Al(AlCp*)$_3$]$^+$	-2139.13126	1830.26	1.17714	-159.7644243
[Al$_2$(AlCp*)$_6$]$^{2+}$	-4278.249196	3667.69	2.13374	-437.70867179
[(tmeda)Al(AlCp*)$_3$]$^+$	-2486.722864	2434.57	1.31814	-198.99947387
[(cdp)Al(AlCp*)$_3$]$^+$	-4248.991054	3349.17	1.76131	-224.03256783
[(dmap)$_3$Al(AlCp*)$_3$]$^+$	-3285.384189	3161.12	1.73098	-229.04943639
[(tmeda)Al]$^+$	-589.7423101	606.6	0.43614	-178.04916218
[(cdp)Al]$^+$	-2352.00404	1521.02	0.94172	-192.93454461
[(dmap)$_3$Al]$^+$	-1388.407796	1336.78	0.87197	-201.62332306

Optimized structures

$[Al(AlCp^*)_3]^+$

Method: (RI-)BP86(D3BJ)/def2-SVP
Symmetry: c1

Cartesian coordinates in Ångström:

Al	-2.8635069	2.5468949	12.0595352
Al	-0.5897840	2.7517469	13.9577223
Al	-0.7284887	4.5602276	11.6071869
C	-4.6371707	2.1801515	10.7244520
C	1.0085655	3.3780389	15.3994051
C	-4.3414712	0.9647212	11.4377320
C	-0.2816109	3.7854740	15.8997966
C	-4.9627523	3.1962565	11.6933938
C	-0.2578054	1.4521033	15.7641432
C	-4.4910058	1.2214000	12.8470685
C	-4.2943347	0.2091802	13.9371088
C	-4.8700725	2.6035027	13.0114569
C	2.1564451	4.2757550	15.0416308
C	-0.7136971	5.1799184	16.2475101
C	-5.4631636	4.5793735	11.4014617
C	-2.4171230	2.5525172	16.7758223
C	1.0184709	1.9405666	15.3103069
C	2.1641528	1.1009240	14.8277896
C	-5.2298148	3.2925218	14.2951579
C	-4.6222002	2.3481182	9.2335246
C	-0.6635019	0.0103640	15.8549550
C	-1.0652436	2.5892084	16.1278971
C	-3.9463267	-0.3454883	10.8233316
C	0.7999860	6.1112556	11.0406719
C	0.1092815	5.6920295	9.8487336
C	-1.2857045	6.0179334	9.9979366
C	-1.4649102	6.6321426	11.2908657
C	-0.1694732	6.6918089	11.9353164
C	0.1180708	7.3812857	13.2356016
C	-2.7306897	7.2226130	11.8397113
C	-2.3488304	5.7670324	8.9693394
C	0.7312296	5.0301082	8.6547396
C	2.2729611	5.9788421	11.2938260
H	-3.3934710	-0.4135205	13.7649434
H	-5.1621564	-0.4799230	13.9988224
H	-4.1881148	0.6919486	14.9267462
H	2.6468860	3.9630579	14.0979218
H	2.9325650	4.2610226	15.8348339
H	1.8300892	5.3258833	14.9216118
H	-0.1019064	5.9392498	15.7277255
H	-0.6073241	5.3612241	17.3378413
H	-1.7751942	5.3651984	15.9887052
H	-5.0742197	4.9656009	10.4400199
H	-5.1882232	5.2969103	12.1978967
H	-6.5712861	4.5824042	11.3275423
H	-2.9901749	1.6510974	16.4860735
H	-3.0233641	3.4430134	16.5223562
H	-2.3157997	2.5303450	17.8815776
H	2.7705807	1.6309658	14.0676205
H	1.8162168	0.1507629	14.3782856
H	2.8431472	0.8392050	15.6666502
H	-4.8679408	4.3396293	14.3228052

```
H    -4.8107272    2.7674791   15.1724895
H    -6.3320535    3.3246544   14.4258103
H    -5.5780469    2.0022601    8.7869845
H    -3.8098912    1.7608185    8.7613859
H    -4.4864390    3.4065966    8.9410140
H    -0.2466724   -0.5876861   15.0205126
H    -1.7634763   -0.1084182   15.8379930
H    -0.2968989   -0.4449229   16.7988878
H    -4.8399843   -0.9737355   10.6237269
H    -3.2784895   -0.9265674   11.4888064
H    -3.4214208   -0.2049873    9.8586168
H     1.0172609    6.9693343   13.7324041
H    -0.7308022    7.3068091   13.9416247
H     0.3083554    8.4623416   13.0664584
H    -3.6254332    6.8044548   11.3441885
H    -2.7496856    8.3215832   11.6818324
H    -2.8346682    7.0482521   12.9291712
H    -2.2434036    4.7676944    8.5014793
H    -2.2958769    6.5181511    8.1539577
H    -3.3624560    5.8304340    9.4077851
H     0.0224289    4.3462914    8.1482593
H     1.6273955    4.4416038    8.9315152
H     1.0515603    5.7855000    7.9064801
H     2.6815415    5.0428726   10.8642764
H     2.5054166    5.9826477   12.3756366
H     2.8306977    6.8211891   10.8333236
Al   -0.4241621    2.0272262   11.5155696

SCF energy GEOOPT =  -2139.131259733 H
ZPE =   1705. kJ/mol
FREEH energy =  1830.26 kJ/mol
FREEH entropy =   1.17714 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              7.90         0.00235       YES     YES
     8        a             16.47         0.01406       YES     YES
     9        a             18.42         0.00623       YES     YES
    10        a             28.52         0.00538       YES     YES
    11        a             35.07         0.00943       YES     YES
    12        a             36.97         0.01140       YES     YES
    13        a             47.34         0.03009       YES     YES
    14        a             50.27         0.11342       YES     YES
    15        a             52.17         0.12120       YES     YES
    16        a             62.19         0.40618       YES     YES
    17        a             66.34         0.04987       YES     YES
    18        a             70.91         0.04951       YES     YES
    19        a             78.45         0.10242       YES     YES
    20        a             80.70         0.10614       YES     YES
    21        a             82.21         0.47980       YES     YES
    22        a             85.32         0.18460       YES     YES
    23        a             86.63         0.22203       YES     YES
    24        a             88.30         0.11094       YES     YES
    25        a             92.72         0.03842       YES     YES
```

26	a	94.38	0.08462	YES	YES
27	a	99.32	0.06393	YES	YES
28	a	100.51	0.29696	YES	YES
29	a	104.90	0.36349	YES	YES
30	a	108.62	0.16123	YES	YES
31	a	135.04	0.05569	YES	YES
32	a	136.83	0.11071	YES	YES
33	a	138.53	0.05654	YES	YES
34	a	146.22	0.90158	YES	YES
35	a	147.70	0.92724	YES	YES
36	a	152.00	0.13748	YES	YES
37	a	155.01	0.07438	YES	YES
38	a	156.29	0.03977	YES	YES
39	a	159.00	0.02747	YES	YES
40	a	172.14	0.01989	YES	YES
41	a	173.67	0.04714	YES	YES
42	a	177.35	0.05491	YES	YES
43	a	187.59	1.11366	YES	YES
44	a	188.13	1.14223	YES	YES
45	a	193.25	0.01117	YES	YES
46	a	215.78	0.25953	YES	YES
47	a	229.91	0.79282	YES	YES
48	a	230.09	0.74550	YES	YES
49	a	268.09	3.94530	YES	YES
50	a	269.25	3.62140	YES	YES
51	a	271.48	0.35420	YES	YES
52	a	271.85	0.48660	YES	YES
53	a	272.41	0.45618	YES	YES
54	a	273.80	0.12140	YES	YES
55	a	275.31	1.20055	YES	YES
56	a	275.63	1.50985	YES	YES
57	a	277.68	1.94071	YES	YES
58	a	283.82	1.37584	YES	YES
59	a	284.53	2.04202	YES	YES
60	a	286.57	2.28754	YES	YES
61	a	294.81	8.28486	YES	YES
62	a	295.45	8.82684	YES	YES
63	a	303.54	7.08603	YES	YES
64	a	377.62	12.56271	YES	YES
65	a	378.28	10.51329	YES	YES
66	a	378.75	3.16830	YES	YES
67	a	387.97	0.95792	YES	YES
68	a	393.44	1.78115	YES	YES
69	a	394.44	1.86658	YES	YES
70	a	473.68	345.58471	YES	YES
71	a	474.06	345.84660	YES	YES
72	a	525.84	29.73893	YES	YES
73	a	543.53	0.05823	YES	YES
74	a	543.83	0.03501	YES	YES
75	a	544.19	0.01963	YES	YES
76	a	544.40	0.09645	YES	YES
77	a	544.59	0.08088	YES	YES
78	a	544.94	0.13741	YES	YES
79	a	546.09	0.04644	YES	YES
80	a	546.58	0.05724	YES	YES
81	a	546.77	0.03701	YES	YES
82	a	588.11	5.42234	YES	YES
83	a	588.34	6.92335	YES	YES
84	a	588.98	1.05345	YES	YES
85	a	590.68	2.17345	YES	YES
86	a	591.12	1.91116	YES	YES

87	a	591.98	0.82910	YES	YES
88	a	605.01	0.17992	YES	YES
89	a	605.64	0.15589	YES	YES
90	a	605.81	0.15616	YES	YES
91	a	796.74	2.81982	YES	YES
92	a	797.11	2.66516	YES	YES
93	a	797.52	2.76765	YES	YES
94	a	801.14	3.58619	YES	YES
95	a	802.35	3.90102	YES	YES
96	a	802.97	2.33964	YES	YES
97	a	922.00	0.25607	YES	YES
98	a	923.04	0.74343	YES	YES
99	a	924.19	0.66595	YES	YES
100	a	925.69	0.06978	YES	YES
101	a	926.84	0.03532	YES	YES
102	a	927.37	0.11191	YES	YES
103	a	987.80	5.51040	YES	YES
104	a	988.47	3.09118	YES	YES
105	a	988.71	12.58992	YES	YES
106	a	992.45	5.04681	YES	YES
107	a	993.53	5.40256	YES	YES
108	a	993.88	4.99990	YES	YES
109	a	995.57	0.08643	YES	YES
110	a	996.58	0.47362	YES	YES
111	a	996.72	0.55639	YES	YES
112	a	997.70	0.44189	YES	YES
113	a	998.73	0.25572	YES	YES
114	a	999.35	0.23691	YES	YES
115	a	1000.96	0.13687	YES	YES
116	a	1001.73	0.04340	YES	YES
117	a	1002.02	0.62421	YES	YES
118	a	1047.88	4.77585	YES	YES
119	a	1048.75	3.18129	YES	YES
120	a	1049.36	3.44892	YES	YES
121	a	1050.34	0.11579	YES	YES
122	a	1050.43	0.18885	YES	YES
123	a	1051.02	0.06361	YES	YES
124	a	1074.39	0.08408	YES	YES
125	a	1074.78	0.09812	YES	YES
126	a	1077.07	0.03622	YES	YES
127	a	1163.47	0.06449	YES	YES
128	a	1163.72	0.01529	YES	YES
129	a	1164.28	0.00993	YES	YES
130	a	1165.16	0.06302	YES	YES
131	a	1165.58	0.26366	YES	YES
132	a	1165.75	0.24711	YES	YES
133	a	1338.87	0.26488	YES	YES
134	a	1340.11	0.60780	YES	YES
135	a	1340.66	0.16723	YES	YES
136	a	1341.17	0.42126	YES	YES
137	a	1342.12	0.87990	YES	YES
138	a	1342.64	0.89168	YES	YES
139	a	1345.27	0.95660	YES	YES
140	a	1346.48	4.18631	YES	YES
141	a	1346.96	4.00431	YES	YES
142	a	1348.96	8.20995	YES	YES
143	a	1349.35	0.30886	YES	YES
144	a	1350.61	19.75960	YES	YES
145	a	1352.09	0.96737	YES	YES
146	a	1352.90	0.88646	YES	YES
147	a	1354.63	3.05940	YES	YES

148	a	1383.52	1.85795	YES	YES
149	a	1383.87	0.68653	YES	YES
150	a	1384.09	2.39912	YES	YES
151	a	1388.27	0.27235	YES	YES
152	a	1388.32	0.62440	YES	YES
153	a	1388.87	0.57260	YES	YES
154	a	1394.47	16.72912	YES	YES
155	a	1395.69	4.88029	YES	YES
156	a	1395.88	2.99501	YES	YES
157	a	1397.27	2.94183	YES	YES
158	a	1397.60	1.99151	YES	YES
159	a	1398.11	2.13889	YES	YES
160	a	1398.31	4.67297	YES	YES
161	a	1400.87	11.27337	YES	YES
162	a	1401.55	11.87375	YES	YES
163	a	1402.22	0.23695	YES	YES
164	a	1402.46	1.43830	YES	YES
165	a	1403.10	2.43511	YES	YES
166	a	1405.49	1.85070	YES	YES
167	a	1405.82	6.44130	YES	YES
168	a	1406.35	0.25675	YES	YES
169	a	1407.54	7.57368	YES	YES
170	a	1409.46	22.45433	YES	YES
171	a	1409.91	17.77399	YES	YES
172	a	1411.18	62.61749	YES	YES
173	a	1411.32	51.96844	YES	YES
174	a	1412.58	5.79230	YES	YES
175	a	1414.32	73.02461	YES	YES
176	a	1414.52	59.57268	YES	YES
177	a	1416.33	23.88748	YES	YES
178	a	1434.59	0.36017	YES	YES
179	a	1435.12	0.54595	YES	YES
180	a	1436.08	0.40546	YES	YES
181	a	1444.42	0.04526	YES	YES
182	a	1446.37	0.11049	YES	YES
183	a	1446.66	0.19119	YES	YES
184	a	1449.20	0.03713	YES	YES
185	a	1449.41	0.07549	YES	YES
186	a	1450.25	0.21699	YES	YES
187	a	1479.59	18.12282	YES	YES
188	a	1480.06	14.21134	YES	YES
189	a	1480.20	2.15621	YES	YES
190	a	1487.16	3.76695	YES	YES
191	a	1487.50	20.26103	YES	YES
192	a	1487.75	19.12958	YES	YES
193	a	2965.76	31.31782	YES	YES
194	a	2965.89	22.59165	YES	YES
195	a	2966.07	43.93425	YES	YES
196	a	2966.26	14.19815	YES	YES
197	a	2966.39	29.68291	YES	YES
198	a	2966.48	7.33832	YES	YES
199	a	2966.54	2.96153	YES	YES
200	a	2966.61	8.27083	YES	YES
201	a	2966.83	7.50535	YES	YES
202	a	2967.16	25.57504	YES	YES
203	a	2967.21	17.17706	YES	YES
204	a	2967.32	18.20564	YES	YES
205	a	2967.54	2.25752	YES	YES
206	a	2967.61	11.99947	YES	YES
207	a	2967.78	12.10346	YES	YES
208	a	3038.48	4.77388	YES	YES

209	a	3038.55	3.56854	YES	YES
210	a	3038.63	3.23433	YES	YES
211	a	3039.46	5.08852	YES	YES
212	a	3039.51	6.13036	YES	YES
213	a	3039.94	5.35191	YES	YES
214	a	3041.17	3.68274	YES	YES
215	a	3041.26	5.29934	YES	YES
216	a	3041.29	4.52070	YES	YES
217	a	3041.66	2.40670	YES	YES
218	a	3041.73	2.72818	YES	YES
219	a	3041.89	3.96248	YES	YES
220	a	3042.99	0.22547	YES	YES
221	a	3043.18	0.31098	YES	YES
222	a	3043.31	0.05978	YES	YES
223	a	3067.98	3.94420	YES	YES
224	a	3068.13	4.85164	YES	YES
225	a	3068.24	6.07932	YES	YES
226	a	3068.45	4.13647	YES	YES
227	a	3068.64	4.05821	YES	YES
228	a	3069.52	4.72155	YES	YES
229	a	3070.43	7.54172	YES	YES
230	a	3070.44	4.24640	YES	YES
231	a	3070.49	5.55792	YES	YES
232	a	3073.26	7.89015	YES	YES
233	a	3073.46	8.12452	YES	YES
234	a	3073.65	9.73403	YES	YES
235	a	3084.03	2.55024	YES	YES
236	a	3084.15	4.89489	YES	YES
237	a	3085.02	4.23471	YES	YES

$end

$[Al_2(AlCp^*)_6]^{2+}$

Method: (RI-)BP86(D3BJ)/def2-SVP
Symmetry: c1

Cartesian coordinates in Ångström:

Al	-0.97214	-2.55349	12.73629
Al	-2.12396	-1.04784	11.05960
Al	-1.61060	0.27318	13.17010
Al	0.34721	-0.50845	11.14033
C	-2.07108	-4.48576	13.15004
C	-0.56291	-3.55419	14.66792
C	-1.96224	-3.72173	14.36598
C	0.19477	-4.21410	13.62451
C	-3.20068	1.09172	14.54883
C	-0.74232	-4.79206	12.68999
C	-1.84096	2.50060	13.27882
C	0.02201	-2.89784	15.88312
C	-1.06632	2.03442	14.40163
C	-3.12560	-3.20992	15.16182
C	-1.91088	1.15490	15.18897
C	-3.15046	1.90904	13.36674
C	-3.36917	-4.84952	12.48764
C	2.07344	-1.38099	10.02058
C	-4.26833	2.10592	12.38581
C	0.31643	2.46781	14.78974
C	-1.53845	0.56972	16.51900
C	-0.37024	-5.60847	11.48711

C	1.38313	-0.47312	9.14177
C	1.68243	-4.40362	13.61250
C	1.44065	0.84554	9.71669
C	2.55871	-0.62369	11.15007
C	2.16812	0.75823	10.95794
C	-1.38259	3.42091	12.18589
C	-4.40201	0.32955	15.02243
C	0.85752	2.08666	9.10775
C	2.57821	1.90355	11.83416
C	0.71360	-0.83030	7.84889
C	3.40680	-1.13858	12.27518
C	2.26604	-2.85048	9.78686
Al	-5.72592	0.57904	8.23319
Al	-4.57329	-0.92796	9.90787
Al	-5.08669	-2.24819	7.79690
Al	-7.04424	-1.46754	9.82911
C	-4.62674	2.51089	7.81867
C	-6.13248	1.57739	6.29964
C	-4.73367	1.74560	6.60339
C	-6.89187	2.23823	7.34123
C	-3.49754	-3.06853	6.41829
C	-5.95623	2.81731	8.27659
C	-4.85650	-4.47575	7.69097
C	-6.71552	0.91928	5.08449
C	-5.63181	-4.01111	6.56801
C	-3.56906	1.23272	5.81007
C	-4.78778	-3.13258	5.77904
C	-3.54705	-3.88433	7.60149
C	-3.32969	2.87583	8.48247
C	-8.77252	-0.59287	10.94379
C	-2.42869	-4.08013	8.58207
C	-7.01468	-4.44516	6.18108
C	-5.16091	-2.54930	4.44836
C	-6.32985	3.63522	9.47797
C	-8.08340	-1.49868	11.82571
C	-8.37956	2.42756	7.35050
C	-8.13970	-2.81859	11.25350
C	-9.25587	-1.35267	9.81520
C	-8.86527	-2.73404	10.01090
C	-5.31410	-5.39446	8.78558
C	-2.29637	-2.30769	5.94223
C	-7.55760	-4.05865	11.86561
C	-9.27401	-3.88152	9.13691
C	-7.41657	-1.13806	13.11902
C	-10.10189	-0.84021	8.68744
C	-8.96565	0.87706	11.17425
H	-6.01661	0.18726	4.63997
H	-6.94404	1.67389	4.30298
H	-7.66091	0.38906	5.31286
H	-8.91006	1.57793	6.87986
H	-8.65642	3.33986	6.78101
H	-8.77393	2.55715	8.37667
H	-3.88423	0.47516	5.06844
H	-2.80017	0.76940	6.46106
H	-3.07688	2.05531	5.25028
H	-2.76885	1.97605	8.81936
H	-3.49343	3.51902	9.36679
H	-2.67055	3.43347	7.78643
H	-7.19779	3.20725	10.01703
H	-6.60792	4.66759	9.17959
H	-5.49453	3.71220	10.19797

H	-7.40586	-4.85619	11.11430
H	-8.23019	-4.46715	12.64870
H	-6.57916	-3.85830	12.34677
H	-6.50036	-1.73926	13.28619
H	-8.09156	-1.32271	13.98108
H	-7.13372	-0.06835	13.14847
H	-9.16683	1.41409	10.22801
H	-8.07620	1.34169	11.64471
H	-9.82906	1.06379	11.84621
H	-9.87140	-1.34906	7.73089
H	-9.96680	0.24649	8.53474
H	-11.17855	-1.01134	8.89770
H	-9.33219	-3.59206	8.07057
H	-10.27930	-4.25074	9.43016
H	-8.57719	-4.73681	9.22540
H	-2.54864	-1.61087	5.12241
H	-1.51896	-3.00036	5.55813
H	-1.83471	-1.71671	6.75830
H	-6.22609	-2.25150	4.40754
H	-5.00071	-3.29523	3.64147
H	-4.54682	-1.66373	4.19637
H	-6.96886	-5.20783	5.37573
H	-7.62561	-3.60423	5.79720
H	-7.55655	-4.89711	7.03098
H	-6.40644	-5.56294	8.74506
H	-5.07293	-4.98852	9.78965
H	-4.82501	-6.38700	8.70318
H	-1.71823	-3.23006	8.56994
H	-1.84985	-4.99943	8.35042
H	-2.80669	-4.17677	9.61871
H	-3.88970	2.20526	11.34968
H	-4.84829	3.02410	12.61915
H	-4.97792	1.25507	12.39556
H	-4.86016	-0.26344	14.20578
H	-5.18181	1.02137	15.40313
H	-4.15097	-0.36567	15.84398
H	-1.62469	3.01737	11.18109
H	-0.29002	3.58790	12.22632
H	-1.87034	4.41393	12.27050
H	0.85923	2.91958	13.94032
H	0.92664	1.62652	15.17400
H	0.27037	3.23043	15.59514
H	-2.15248	-0.31638	16.76925
H	-1.69924	1.31440	17.32694
H	-0.47322	0.27208	16.55999
H	-3.20688	-5.49230	11.60275
H	-3.92986	-3.94922	12.15187
H	-4.02785	-5.40715	13.18413
H	-3.89591	-2.74647	14.51263
H	-2.80942	-2.45280	15.90349
H	-3.61636	-4.03317	15.72189
H	0.96755	-2.36808	15.65420
H	0.25090	-3.65351	16.66351
H	-0.67582	-2.16580	16.32931
H	-1.20878	-5.69032	10.77144
H	-0.08504	-6.63916	11.78451
H	0.49262	-5.17604	10.94339
H	0.43659	-1.90136	7.81462
H	1.38435	-0.63713	6.98540
H	-0.20659	-0.23328	7.68840
H	1.37633	-3.31379	9.31559

```
H          2.46720       -3.38968       10.73188
H          3.12927       -3.03606        9.11435
H          4.48304       -0.96646       12.06353
H          3.27244       -2.22571       12.42543
H          3.17772       -0.63217       13.23338
H          1.88235        2.75979       11.74728
H          3.58397        2.27215       11.54174
H          2.63592        1.61201       12.89998
H         -0.12416        1.88821        8.63233
H          1.52633        2.49354        8.32060
H          0.71183        2.88468        9.85971
H          2.07497       -4.53199       12.58547
H          1.96012       -5.31668       14.18040
H          2.21387       -3.55465       14.08327

SCF energy GEOOPT =  -4278.249196417 H
ZPE =   3414. kJ/mol
FREEH energy =  3667.69 kJ/mol
FREEH entropy =   2.13374 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              8.84         0.01808       YES     YES
     8        a             10.96         0.06505       YES     YES
     9        a             13.89         0.00006       YES     YES
    10        a             15.91         0.00092       YES     YES
    11        a             18.56         0.02804       YES     YES
    12        a             20.36         0.00090       YES     YES
    13        a             21.04         0.06139       YES     YES
    14        a             21.25         0.00068       YES     YES
    15        a             24.26         0.19340       YES     YES
    16        a             24.31         0.01740       YES     YES
    17        a             29.29         0.08581       YES     YES
    18        a             32.86         0.00096       YES     YES
    19        a             35.08         0.90537       YES     YES
    20        a             37.86         0.00005       YES     YES
    21        a             38.10         0.05416       YES     YES
    22        a             43.00         0.00007       YES     YES
    23        a             45.53         0.01180       YES     YES
    24        a             48.89         0.00013       YES     YES
    25        a             52.82         0.80113       YES     YES
    26        a             56.08         0.00338       YES     YES
    27        a             57.23         2.28724       YES     YES
    28        a             58.95         0.00846       YES     YES
    29        a             60.19         0.30545       YES     YES
    30        a             65.66         0.00740       YES     YES
    31        a             70.53        21.87994       YES     YES
    32        a             72.33         0.09582       YES     YES
    33        a             72.77         1.05357       YES     YES
    34        a             74.40         0.01544       YES     YES
    35        a             76.59         0.00161       YES     YES
    36        a             78.23         0.90748       YES     YES
    37        a             82.65         0.55083       YES     YES
    38        a             86.18         0.03550       YES     YES
```

39	a	88.09	0.03930	YES	YES
40	a	88.68	0.11355	YES	YES
41	a	89.47	1.35447	YES	YES
42	a	89.95	0.29440	YES	YES
43	a	93.90	0.74206	YES	YES
44	a	94.57	0.18096	YES	YES
45	a	96.39	0.18400	YES	YES
46	a	99.30	0.06810	YES	YES
47	a	102.39	0.15521	YES	YES
48	a	102.58	0.29860	YES	YES
49	a	103.03	0.51453	YES	YES
50	a	104.52	0.00441	YES	YES
51	a	110.04	1.66475	YES	YES
52	a	111.38	0.10141	YES	YES
53	a	114.16	0.01680	YES	YES
54	a	115.33	0.13828	YES	YES
55	a	119.98	0.65639	YES	YES
56	a	121.57	0.49055	YES	YES
57	a	124.76	2.00500	YES	YES
58	a	125.69	0.00424	YES	YES
59	a	130.17	0.89043	YES	YES
60	a	131.83	0.68804	YES	YES
61	a	132.83	0.12336	YES	YES
62	a	134.29	0.03080	YES	YES
63	a	145.72	0.06125	YES	YES
64	a	146.25	0.00124	YES	YES
65	a	148.38	0.00103	YES	YES
66	a	148.65	0.60519	YES	YES
67	a	148.91	0.02500	YES	YES
68	a	151.45	2.45726	YES	YES
69	a	152.18	2.71273	YES	YES
70	a	153.05	0.00780	YES	YES
71	a	154.26	1.58309	YES	YES
72	a	154.57	0.01079	YES	YES
73	a	156.07	0.00168	YES	YES
74	a	156.99	0.26427	YES	YES
75	a	162.02	0.00422	YES	YES
76	a	162.41	0.15848	YES	YES
77	a	163.52	0.57301	YES	YES
78	a	163.96	0.00171	YES	YES
79	a	171.35	0.74892	YES	YES
80	a	172.57	0.00004	YES	YES
81	a	174.68	0.16441	YES	YES
82	a	174.93	0.02522	YES	YES
83	a	179.08	2.16379	YES	YES
84	a	188.07	2.07410	YES	YES
85	a	188.38	0.06437	YES	YES
86	a	189.85	1.55624	YES	YES
87	a	190.05	0.18282	YES	YES
88	a	193.71	5.07664	YES	YES
89	a	193.92	0.55980	YES	YES
90	a	203.51	0.00001	YES	YES
91	a	211.06	69.47801	YES	YES
92	a	217.02	0.00167	YES	YES
93	a	225.98	0.00041	YES	YES
94	a	228.04	3.49605	YES	YES
95	a	229.74	1.62878	YES	YES
96	a	231.72	0.00053	YES	YES
97	a	261.89	0.00537	YES	YES
98	a	262.35	1.02703	YES	YES
99	a	263.36	0.00576	YES	YES

100	a	264.52	0.84629	YES	YES
101	a	267.23	0.00994	YES	YES
102	a	268.20	10.56499	YES	YES
103	a	269.03	0.06044	YES	YES
104	a	269.27	4.71990	YES	YES
105	a	270.04	1.54028	YES	YES
106	a	270.15	1.44672	YES	YES
107	a	273.65	0.10337	YES	YES
108	a	274.26	9.49082	YES	YES
109	a	276.09	0.01490	YES	YES
110	a	276.75	7.59571	YES	YES
111	a	278.46	7.16871	YES	YES
112	a	278.46	0.08056	YES	YES
113	a	280.15	20.66675	YES	YES
114	a	280.59	0.11210	YES	YES
115	a	285.20	0.00145	YES	YES
116	a	285.90	2.92681	YES	YES
117	a	286.60	0.01568	YES	YES
118	a	287.36	5.55360	YES	YES
119	a	289.14	0.00851	YES	YES
120	a	289.62	1.80581	YES	YES
121	a	290.88	240.48982	YES	YES
122	a	292.41	0.00250	YES	YES
123	a	293.37	0.02543	YES	YES
124	a	298.34	20.60576	YES	YES
125	a	304.59	109.78223	YES	YES
126	a	365.14	0.00004	YES	YES
127	a	373.07	0.11668	YES	YES
128	a	374.07	19.40889	YES	YES
129	a	376.29	15.60800	YES	YES
130	a	376.55	0.03659	YES	YES
131	a	379.32	8.73841	YES	YES
132	a	379.43	6.14799	YES	YES
133	a	388.16	10.32668	YES	YES
134	a	388.77	0.02967	YES	YES
135	a	390.95	0.00105	YES	YES
136	a	391.51	6.66000	YES	YES
137	a	396.16	0.00013	YES	YES
138	a	396.64	1.74486	YES	YES
139	a	470.73	0.03904	YES	YES
140	a	474.07	501.68740	YES	YES
141	a	475.57	0.11728	YES	YES
142	a	479.60	556.90057	YES	YES
143	a	515.73	515.96729	YES	YES
144	a	539.83	0.00020	YES	YES
145	a	542.47	0.00146	YES	YES
146	a	542.61	0.15480	YES	YES
147	a	543.60	0.00516	YES	YES
148	a	543.72	0.12881	YES	YES
149	a	544.00	0.81710	YES	YES
150	a	544.21	0.00101	YES	YES
151	a	544.79	0.00023	YES	YES
152	a	544.86	0.10446	YES	YES
153	a	545.10	0.08491	YES	YES
154	a	545.45	0.00004	YES	YES
155	a	545.83	0.00038	YES	YES
156	a	545.92	0.16188	YES	YES
157	a	546.84	0.11378	YES	YES
158	a	547.20	0.00029	YES	YES
159	a	547.27	0.00146	YES	YES
160	a	547.40	0.34141	YES	YES

161	a	548.81	0.00096	YES	YES
162	a	549.00	0.06650	YES	YES
163	a	587.33	5.74510	YES	YES
164	a	587.44	1.54085	YES	YES
165	a	587.57	0.04994	YES	YES
166	a	587.77	6.96512	YES	YES
167	a	588.99	0.03246	YES	YES
168	a	589.10	16.16436	YES	YES
169	a	590.34	0.13350	YES	YES
170	a	590.46	9.33214	YES	YES
171	a	591.15	0.17106	YES	YES
172	a	591.34	1.76508	YES	YES
173	a	591.72	10.86192	YES	YES
174	a	593.00	0.00011	YES	YES
175	a	603.71	2.06773	YES	YES
176	a	604.04	0.05077	YES	YES
177	a	604.17	0.19799	YES	YES
178	a	604.40	0.00727	YES	YES
179	a	605.09	0.36607	YES	YES
180	a	605.18	0.25329	YES	YES
181	a	795.06	4.81528	YES	YES
182	a	795.22	0.05664	YES	YES
183	a	795.88	0.03118	YES	YES
184	a	796.01	4.84329	YES	YES
185	a	797.86	4.31691	YES	YES
186	a	797.97	0.42382	YES	YES
187	a	801.23	11.59966	YES	YES
188	a	801.33	0.10701	YES	YES
189	a	802.88	2.99483	YES	YES
190	a	802.93	5.00116	YES	YES
191	a	804.23	2.19187	YES	YES
192	a	804.36	15.10785	YES	YES
193	a	921.43	0.10617	YES	YES
194	a	921.53	4.07776	YES	YES
195	a	922.81	2.04509	YES	YES
196	a	922.95	0.07855	YES	YES
197	a	923.11	2.17370	YES	YES
198	a	923.49	0.00282	YES	YES
199	a	924.52	0.00578	YES	YES
200	a	924.86	1.13230	YES	YES
201	a	926.02	0.85690	YES	YES
202	a	926.09	2.23112	YES	YES
203	a	927.39	1.57053	YES	YES
204	a	927.56	1.40069	YES	YES
205	a	986.97	0.28244	YES	YES
206	a	987.04	6.81342	YES	YES
207	a	988.77	8.65198	YES	YES
208	a	988.87	2.10569	YES	YES
209	a	989.19	0.84749	YES	YES
210	a	989.20	4.15618	YES	YES
211	a	990.95	6.32766	YES	YES
212	a	991.08	0.00215	YES	YES
213	a	993.02	0.06842	YES	YES
214	a	993.15	4.82812	YES	YES
215	a	993.83	3.35402	YES	YES
216	a	993.91	0.11800	YES	YES
217	a	994.17	0.86847	YES	YES
218	a	994.24	0.00306	YES	YES
219	a	994.58	0.18120	YES	YES
220	a	994.75	3.37441	YES	YES
221	a	996.84	0.96775	YES	YES

222	a	996.94	0.02352	YES	YES
223	a	997.33	0.16592	YES	YES
224	a	997.39	0.86875	YES	YES
225	a	997.74	2.52317	YES	YES
226	a	998.14	0.01521	YES	YES
227	a	998.61	0.00445	YES	YES
228	a	998.89	0.27291	YES	YES
229	a	1000.07	0.00583	YES	YES
230	a	1000.22	0.44667	YES	YES
231	a	1006.67	0.11943	YES	YES
232	a	1006.81	0.03405	YES	YES
233	a	1009.70	0.03221	YES	YES
234	a	1009.71	0.12717	YES	YES
235	a	1047.09	2.44517	YES	YES
236	a	1047.48	0.02111	YES	YES
237	a	1047.98	0.00101	YES	YES
238	a	1048.48	1.85747	YES	YES
239	a	1048.72	4.58572	YES	YES
240	a	1048.83	0.01055	YES	YES
241	a	1049.14	1.25697	YES	YES
242	a	1049.34	0.01264	YES	YES
243	a	1050.76	0.03978	YES	YES
244	a	1050.92	1.61210	YES	YES
245	a	1051.25	1.00508	YES	YES
246	a	1051.28	0.33719	YES	YES
247	a	1073.10	0.65093	YES	YES
248	a	1073.30	0.02446	YES	YES
249	a	1074.11	0.00086	YES	YES
250	a	1074.55	0.18779	YES	YES
251	a	1076.38	0.09597	YES	YES
252	a	1076.59	0.00005	YES	YES
253	a	1161.97	10.96495	YES	YES
254	a	1162.17	0.01133	YES	YES
255	a	1163.00	6.03710	YES	YES
256	a	1163.47	0.00065	YES	YES
257	a	1163.65	2.39725	YES	YES
258	a	1163.88	0.00088	YES	YES
259	a	1164.14	0.01250	YES	YES
260	a	1164.17	3.13327	YES	YES
261	a	1164.74	0.02942	YES	YES
262	a	1164.87	1.11724	YES	YES
263	a	1164.98	0.00455	YES	YES
264	a	1165.39	0.13353	YES	YES
265	a	1335.84	6.61716	YES	YES
266	a	1336.14	0.23547	YES	YES
267	a	1337.37	4.69316	YES	YES
268	a	1337.72	0.03716	YES	YES
269	a	1338.70	0.00433	YES	YES
270	a	1339.33	9.94596	YES	YES
271	a	1339.70	5.09331	YES	YES
272	a	1340.02	0.03619	YES	YES
273	a	1340.93	0.02637	YES	YES
274	a	1341.26	2.30978	YES	YES
275	a	1341.77	0.04901	YES	YES
276	a	1341.83	0.27586	YES	YES
277	a	1343.03	0.49889	YES	YES
278	a	1343.11	6.95900	YES	YES
279	a	1343.63	0.29796	YES	YES
280	a	1343.69	4.18650	YES	YES
281	a	1344.69	0.06363	YES	YES
282	a	1344.83	8.66255	YES	YES

283	a	1346.45	9.90112	YES	YES
284	a	1347.16	0.04886	YES	YES
285	a	1347.97	0.30064	YES	YES
286	a	1348.12	10.09679	YES	YES
287	a	1349.01	1.73715	YES	YES
288	a	1349.09	10.69059	YES	YES
289	a	1351.52	0.03473	YES	YES
290	a	1351.77	4.11829	YES	YES
291	a	1352.34	0.01436	YES	YES
292	a	1352.51	0.06899	YES	YES
293	a	1354.62	0.26743	YES	YES
294	a	1354.71	0.19016	YES	YES
295	a	1381.38	0.05847	YES	YES
296	a	1381.74	13.19208	YES	YES
297	a	1382.53	6.09403	YES	YES
298	a	1383.10	0.00902	YES	YES
299	a	1383.97	0.00706	YES	YES
300	a	1384.38	1.48644	YES	YES
301	a	1386.42	0.00206	YES	YES
302	a	1387.10	6.97553	YES	YES
303	a	1387.73	7.46616	YES	YES
304	a	1388.42	0.01174	YES	YES
305	a	1389.67	0.01582	YES	YES
306	a	1390.07	1.45109	YES	YES
307	a	1392.74	7.06354	YES	YES
308	a	1393.13	0.05544	YES	YES
309	a	1394.77	10.83301	YES	YES
310	a	1394.89	0.42479	YES	YES
311	a	1395.40	0.00548	YES	YES
312	a	1395.54	1.10327	YES	YES
313	a	1396.03	1.42878	YES	YES
314	a	1396.23	0.01018	YES	YES
315	a	1396.83	5.14378	YES	YES
316	a	1397.21	13.54729	YES	YES
317	a	1397.29	0.31665	YES	YES
318	a	1398.33	25.23466	YES	YES
319	a	1398.53	0.01237	YES	YES
320	a	1398.92	0.30651	YES	YES
321	a	1399.36	0.08597	YES	YES
322	a	1400.23	18.35338	YES	YES
323	a	1400.65	6.88980	YES	YES
324	a	1400.84	0.20189	YES	YES
325	a	1401.70	2.82937	YES	YES
326	a	1401.92	0.02770	YES	YES
327	a	1402.23	0.00937	YES	YES
328	a	1402.61	2.05873	YES	YES
329	a	1403.56	32.69135	YES	YES
330	a	1403.60	0.27051	YES	YES
331	a	1404.27	6.01880	YES	YES
332	a	1404.70	0.01377	YES	YES
333	a	1405.21	0.04970	YES	YES
334	a	1405.53	15.42113	YES	YES
335	a	1406.12	0.02341	YES	YES
336	a	1406.15	0.01755	YES	YES
337	a	1407.16	15.03095	YES	YES
338	a	1407.48	45.44349	YES	YES
339	a	1408.27	15.68510	YES	YES
340	a	1408.55	0.41596	YES	YES
341	a	1410.04	16.33821	YES	YES
342	a	1410.16	0.94900	YES	YES
343	a	1410.70	126.14277	YES	YES

344	a	1411.18	0.28681	YES	YES
345	a	1412.26	0.27285	YES	YES
346	a	1412.74	60.32776	YES	YES
347	a	1413.06	83.85541	YES	YES
348	a	1413.47	0.89167	YES	YES
349	a	1413.97	110.15121	YES	YES
350	a	1414.29	0.65108	YES	YES
351	a	1415.87	163.89494	YES	YES
352	a	1416.57	2.21313	YES	YES
353	a	1416.79	5.08413	YES	YES
354	a	1416.90	43.15057	YES	YES
355	a	1430.27	0.00634	YES	YES
356	a	1430.43	1.44553	YES	YES
357	a	1431.30	14.47468	YES	YES
358	a	1431.50	0.02065	YES	YES
359	a	1434.68	17.24402	YES	YES
360	a	1434.94	0.35296	YES	YES
361	a	1442.36	10.03521	YES	YES
362	a	1442.80	0.00009	YES	YES
363	a	1444.50	0.28656	YES	YES
364	a	1444.57	0.82169	YES	YES
365	a	1445.78	0.02870	YES	YES
366	a	1445.96	1.32652	YES	YES
367	a	1447.49	0.48707	YES	YES
368	a	1447.70	0.02033	YES	YES
369	a	1448.84	0.00076	YES	YES
370	a	1449.00	4.21242	YES	YES
371	a	1450.04	0.00074	YES	YES
372	a	1450.34	0.42550	YES	YES
373	a	1475.69	0.10291	YES	YES
374	a	1475.91	33.73966	YES	YES
375	a	1478.75	3.94653	YES	YES
376	a	1478.91	45.96502	YES	YES
377	a	1479.38	0.20011	YES	YES
378	a	1479.52	10.26233	YES	YES
379	a	1486.03	13.47411	YES	YES
380	a	1486.14	6.30310	YES	YES
381	a	1488.87	25.13626	YES	YES
382	a	1489.18	0.00454	YES	YES
383	a	1489.46	0.04437	YES	YES
384	a	1490.00	29.11003	YES	YES
385	a	2943.05	0.35021	YES	YES
386	a	2943.14	22.09649	YES	YES
387	a	2956.61	0.93452	YES	YES
388	a	2956.75	18.06028	YES	YES
389	a	2961.73	8.69272	YES	YES
390	a	2961.86	12.33091	YES	YES
391	a	2963.06	7.65111	YES	YES
392	a	2963.10	6.52151	YES	YES
393	a	2963.18	2.74725	YES	YES
394	a	2963.21	24.98654	YES	YES
395	a	2965.49	13.50683	YES	YES
396	a	2965.62	15.88468	YES	YES
397	a	2966.41	19.43022	YES	YES
398	a	2966.47	11.56683	YES	YES
399	a	2967.98	20.02768	YES	YES
400	a	2968.07	14.91850	YES	YES
401	a	2968.37	19.69394	YES	YES
402	a	2968.43	12.43685	YES	YES
403	a	2969.40	19.33957	YES	YES
404	a	2969.51	13.80155	YES	YES

405	a	2969.85	12.90493	YES	YES
406	a	2969.94	12.68498	YES	YES
407	a	2970.03	20.01664	YES	YES
408	a	2970.15	13.58380	YES	YES
409	a	2971.11	11.17485	YES	YES
410	a	2971.17	11.57822	YES	YES
411	a	2971.32	25.77834	YES	YES
412	a	2971.44	16.03060	YES	YES
413	a	2971.79	19.08777	YES	YES
414	a	2971.81	4.54934	YES	YES
415	a	3023.18	11.49390	YES	YES
416	a	3023.19	0.55060	YES	YES
417	a	3033.88	3.96865	YES	YES
418	a	3033.95	15.45399	YES	YES
419	a	3034.86	6.60345	YES	YES
420	a	3035.12	5.54611	YES	YES
421	a	3035.83	4.03179	YES	YES
422	a	3035.90	7.02088	YES	YES
423	a	3036.18	0.22383	YES	YES
424	a	3036.20	1.86406	YES	YES
425	a	3037.95	0.36206	YES	YES
426	a	3038.16	0.32152	YES	YES
427	a	3040.94	2.05945	YES	YES
428	a	3040.97	1.79619	YES	YES
429	a	3042.16	1.99027	YES	YES
430	a	3042.36	1.50901	YES	YES
431	a	3042.47	4.91025	YES	YES
432	a	3042.54	6.06326	YES	YES
433	a	3042.59	6.85695	YES	YES
434	a	3042.67	7.05498	YES	YES
435	a	3043.74	4.56516	YES	YES
436	a	3043.89	4.53576	YES	YES
437	a	3044.10	1.39094	YES	YES
438	a	3044.15	1.45017	YES	YES
439	a	3045.00	0.76996	YES	YES
440	a	3045.10	0.80944	YES	YES
441	a	3045.21	1.62071	YES	YES
442	a	3045.30	1.57896	YES	YES
443	a	3045.72	0.95378	YES	YES
444	a	3045.87	0.94664	YES	YES
445	a	3056.91	2.15513	YES	YES
446	a	3056.99	2.74353	YES	YES
447	a	3063.68	4.14048	YES	YES
448	a	3063.81	4.38499	YES	YES
449	a	3066.99	3.73536	YES	YES
450	a	3067.13	3.75816	YES	YES
451	a	3069.33	4.81103	YES	YES
452	a	3069.39	5.87958	YES	YES
453	a	3070.05	3.56547	YES	YES
454	a	3070.14	4.63714	YES	YES
455	a	3072.01	4.24631	YES	YES
456	a	3072.11	4.46196	YES	YES
457	a	3073.20	6.37275	YES	YES
458	a	3073.27	6.79078	YES	YES
459	a	3073.88	0.52933	YES	YES
460	a	3073.95	0.56628	YES	YES
461	a	3074.07	7.31941	YES	YES
462	a	3074.15	12.10485	YES	YES
463	a	3075.17	5.83481	YES	YES
464	a	3075.35	5.82806	YES	YES
465	a	3079.98	3.20007	YES	YES

```
   466        a            3080.01         3.47325       YES     YES
   467        a            3081.29         3.62481       YES     YES
   468        a            3081.43         3.69952       YES     YES
   469        a            3082.25         3.38028       YES     YES
   470        a            3082.30         3.40353       YES     YES
   471        a            3082.98         2.03125       YES     YES
   472        a            3082.98         6.99948       YES     YES
   473        a            3089.03         3.50733       YES     YES
   474        a            3089.27         3.52578       YES     YES
$end
```

[(tmeda)Al(AlCp*)$_3$]$^+$

```
Method: (RI-)BP86(D3BJ)/def2-SVP
Symmetry: c1

Cartesian coordinates in Ångström:
Al   -1.3622953   -0.4635247    1.2050831
Al    1.4337922   -0.5151397    1.1028422
Al    0.0260824    1.6834206    0.2365231
C    -3.6629847   -0.8796355    1.3213067
C     3.6453904    0.0198017    1.6290627
C    -2.9744752   -2.1341470    1.3981423
C     2.8966899   -0.1287622    2.8436978
C    -3.2616839   -0.0833550    2.4514353
C     2.9049144   -2.1865786    1.7458228
C    -2.1442709   -2.1181403    2.5730372
C    -1.3223383   -3.2869124    3.0296176
C    -2.3313947   -0.8517221    3.2349273
C     4.3818226    1.2341382    1.1467902
C     2.6469575    0.8993143    3.9065246
C    -3.8482095    1.2456059    2.8248241
C     1.7527120   -2.0874412    4.1088264
C     3.6587417   -1.2522164    0.9565983
C     4.4988395   -1.5584810   -0.2489469
C    -1.6948065   -0.3976260    4.5177010
C    -4.7086263   -0.4775683    0.3233553
C     2.6999832   -3.6437771    1.4508973
C     2.4353958   -1.4900738    2.9151805
C    -3.0898298   -3.3077618    0.4714508
C     1.0506142    3.6447425   -0.4609787
C    -0.2095985    3.5785789   -1.1449378
C    -1.2583888    3.5745444   -0.1624564
C    -0.6423287    3.6469856    1.1365287
C     0.7860037    3.6979094    0.9510898
C     1.7745290    3.9283330    2.0528251
C    -1.3322402    3.7530875    2.4650345
C    -2.7371504    3.5044392   -0.4162841
C    -0.3473445    3.5512895   -2.6379141
C     2.3896165    3.7147105   -1.1342973
H    -0.4482691   -3.4715392    2.3690888
H    -1.9298195   -4.2150978    3.0299132
H    -0.9399154   -3.1404187    4.0553238
H     4.0523618    1.5513814    0.1357496
H     5.4727194    1.0375324    1.0860480
H     4.2413873    2.0935467    1.8280011
H     3.1789687    1.8447041    3.6962833
H     2.9923476    0.5350263    4.8958903
H     1.5657236    1.1380322    4.0089299
```

H	-3.9749656	1.9090130	1.9463576
H	-3.2201908	1.7801391	3.5601939
H	-4.8540022	1.1163030	3.2791600
H	1.4120481	-3.1198191	3.9151993
H	0.8790494	-1.4913788	4.4347444
H	2.4553807	-2.1296509	4.9684466
H	4.3987885	-0.7986980	-1.0498772
H	4.2681367	-2.5499934	-0.6822479
H	5.5744100	-1.5788126	0.0304138
H	-0.8637328	0.3220970	4.3461493
H	-1.2775732	-1.2519986	5.0836080
H	-2.4318466	0.1035763	5.1756903
H	-5.7294854	-0.6195066	0.7383089
H	-4.6544705	-1.0751721	-0.6071445
H	-4.6274263	0.5931267	0.0453512
H	2.7735057	-3.8599522	0.3671872
H	1.7048217	-3.9950071	1.7892980
H	3.4605327	-4.2712266	1.9623449
H	-3.3771115	-4.2246444	1.0272384
H	-2.1282333	-3.5308327	-0.0404502
H	-3.8638324	-3.1478268	-0.3032808
H	2.7951234	3.6155329	1.7657270
H	1.4971022	3.3815191	2.9737237
H	1.8214429	5.0072769	2.3138039
H	-2.4308370	3.7350777	2.3534429
H	-1.0633942	4.7005347	2.9764605
H	-1.0537160	2.9229973	3.1488501
H	-3.1714228	2.5345327	-0.0893654
H	-2.9728769	3.6261206	-1.4907253
H	-3.2789173	4.3034872	0.1289504
H	-1.4036867	3.6208861	-2.9607715
H	0.0825418	2.6249895	-3.0814556
H	0.1915105	4.4015336	-3.1043248
H	2.5264799	2.9026771	-1.8786605
H	3.2182132	3.6429501	-0.4055551
H	2.5143928	4.6749413	-1.6785108
C	2.1783944	-0.0853646	-2.9666976
C	-2.5501363	0.5679470	-2.5848839
H	-0.4736342	0.7208248	-4.0560526
Al	-0.1128400	-0.5034550	-1.1121532
N	-1.5868523	-0.5302980	-2.7966625
C	-0.8212208	-0.3325921	-4.0476266
N	1.1664017	-1.1584703	-2.8470378
H	-1.4653499	-0.4705598	-4.9459099
C	0.3673186	-1.2840687	-4.0929062
H	0.9888250	-1.0859380	-4.9932984
C	1.8087022	-2.4370398	-2.4783368
C	-2.2933934	-1.8271484	-2.7711463
H	0.0191271	-2.3314959	-4.1775682
H	2.5465846	-2.7584861	-3.2459744
H	1.0382616	-3.2225338	-2.3589427
H	2.3207050	-2.3105809	-1.5079159
H	2.9659315	-0.3591385	-3.7029497
H	2.6355197	0.0923862	-1.9746386
H	1.6938186	0.8577341	-3.2824484
H	-3.0212519	-1.9065663	-3.6092258
H	-2.8302364	-1.9195186	-1.8113145
H	-1.5805560	-2.6702512	-2.8346669
H	-3.3365144	0.5709432	-3.3714307
H	-2.0141274	1.5315876	-2.5936885
H	-3.0215991	0.4471355	-1.5934321

SCF energy GEOOPT = -2486.722863724 H
ZPE =   2282. kJ/mol
FREEH energy = 2434.57 kJ/mol
FREEH entropy =   1.31814 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules 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	19.34	0.13483	YES	YES
8	a	23.59	0.05063	YES	YES
9	a	34.50	0.15753	YES	YES
10	a	38.45	0.55530	YES	YES
11	a	40.97	0.23335	YES	YES
12	a	46.69	0.11951	YES	YES
13	a	50.81	0.37202	YES	YES
14	a	53.85	0.30379	YES	YES
15	a	60.14	0.33873	YES	YES
16	a	61.56	0.04917	YES	YES
17	a	66.35	0.42856	YES	YES
18	a	71.35	0.04658	YES	YES
19	a	76.20	0.19330	YES	YES
20	a	79.60	0.41006	YES	YES
21	a	85.23	0.72407	YES	YES
22	a	88.21	0.16600	YES	YES
23	a	89.58	0.21054	YES	YES
24	a	95.92	0.04857	YES	YES
25	a	98.67	0.32392	YES	YES
26	a	105.64	0.48810	YES	YES
27	a	106.02	0.51104	YES	YES
28	a	113.26	0.70067	YES	YES
29	a	119.49	0.73969	YES	YES
30	a	121.59	0.07230	YES	YES
31	a	130.76	0.24840	YES	YES
32	a	132.84	0.11807	YES	YES
33	a	137.79	0.14823	YES	YES
34	a	142.57	0.19984	YES	YES
35	a	142.99	0.67768	YES	YES
36	a	144.02	0.32959	YES	YES
37	a	149.93	0.66729	YES	YES
38	a	152.45	0.37589	YES	YES
39	a	155.35	0.16968	YES	YES
40	a	159.23	0.38775	YES	YES
41	a	162.76	0.63726	YES	YES
42	a	166.70	0.02982	YES	YES
43	a	171.16	0.25650	YES	YES
44	a	173.22	1.22017	YES	YES
45	a	174.23	0.54790	YES	YES
46	a	178.19	0.16815	YES	YES
47	a	179.79	1.51007	YES	YES
48	a	181.51	1.97232	YES	YES
49	a	187.96	0.98798	YES	YES
50	a	192.72	4.73297	YES	YES
51	a	195.50	3.47603	YES	YES
52	a	201.01	1.93409	YES	YES

53	a	203.39	3.01047	YES	YES
54	a	206.48	0.22800	YES	YES
55	a	220.52	1.21497	YES	YES
56	a	230.53	2.44026	YES	YES
57	a	233.37	0.33462	YES	YES
58	a	238.78	0.51042	YES	YES
59	a	241.78	0.57634	YES	YES
60	a	245.12	1.65275	YES	YES
61	a	250.73	3.32906	YES	YES
62	a	256.11	1.56070	YES	YES
63	a	258.99	1.87925	YES	YES
64	a	260.84	0.71705	YES	YES
65	a	264.59	0.94444	YES	YES
66	a	265.50	0.04442	YES	YES
67	a	269.71	1.26378	YES	YES
68	a	273.71	1.90463	YES	YES
69	a	275.36	7.95071	YES	YES
70	a	276.78	1.90150	YES	YES
71	a	279.42	1.08304	YES	YES
72	a	281.27	7.57986	YES	YES
73	a	282.83	3.15248	YES	YES
74	a	284.13	6.85763	YES	YES
75	a	287.68	1.27782	YES	YES
76	a	301.15	32.26356	YES	YES
77	a	323.09	93.14423	YES	YES
78	a	337.45	9.69812	YES	YES
79	a	344.08	15.10371	YES	YES
80	a	350.34	7.65014	YES	YES
81	a	358.49	10.98988	YES	YES
82	a	367.95	6.25976	YES	YES
83	a	372.97	22.85354	YES	YES
84	a	383.46	2.00756	YES	YES
85	a	391.33	38.29509	YES	YES
86	a	404.54	339.84779	YES	YES
87	a	413.98	22.10111	YES	YES
88	a	419.05	238.10437	YES	YES
89	a	419.95	134.79901	YES	YES
90	a	433.06	15.05213	YES	YES
91	a	448.70	22.99771	YES	YES
92	a	507.58	18.70478	YES	YES
93	a	542.75	0.46265	YES	YES
94	a	543.37	0.07909	YES	YES
95	a	543.98	0.27235	YES	YES
96	a	544.65	0.05102	YES	YES
97	a	546.05	0.02830	YES	YES
98	a	547.17	0.08522	YES	YES
99	a	547.56	0.04171	YES	YES
100	a	549.00	0.02004	YES	YES
101	a	549.04	0.00563	YES	YES
102	a	573.40	3.46339	YES	YES
103	a	576.23	2.32582	YES	YES
104	a	577.54	2.24543	YES	YES
105	a	580.43	1.02735	YES	YES
106	a	582.93	0.21971	YES	YES
107	a	585.97	0.66663	YES	YES
108	a	587.51	0.54714	YES	YES
109	a	593.10	10.90916	YES	YES
110	a	594.15	11.08099	YES	YES
111	a	597.83	5.46174	YES	YES
112	a	751.36	15.79938	YES	YES
113	a	784.75	71.91711	YES	YES

114	a	795.58	1.13627	YES	YES
115	a	796.63	2.88303	YES	YES
116	a	797.45	0.80590	YES	YES
117	a	805.25	2.79302	YES	YES
118	a	806.68	8.14006	YES	YES
119	a	808.09	0.90249	YES	YES
120	a	919.61	1.46979	YES	YES
121	a	922.53	1.46701	YES	YES
122	a	924.01	1.37304	YES	YES
123	a	926.15	23.73644	YES	YES
124	a	926.99	1.28899	YES	YES
125	a	930.42	1.14845	YES	YES
126	a	933.78	0.39922	YES	YES
127	a	937.04	6.73180	YES	YES
128	a	983.17	0.89090	YES	YES
129	a	984.90	1.59341	YES	YES
130	a	987.93	2.22626	YES	YES
131	a	990.96	0.76583	YES	YES
132	a	992.39	1.40641	YES	YES
133	a	993.68	2.33330	YES	YES
134	a	995.64	1.55895	YES	YES
135	a	996.18	1.63620	YES	YES
136	a	996.35	10.06183	YES	YES
137	a	999.81	0.09916	YES	YES
138	a	1001.88	0.12980	YES	YES
139	a	1001.91	1.12554	YES	YES
140	a	1003.60	0.47193	YES	YES
141	a	1007.38	0.55835	YES	YES
142	a	1007.97	6.00682	YES	YES
143	a	1008.27	0.59182	YES	YES
144	a	1009.67	0.53659	YES	YES
145	a	1015.90	13.10526	YES	YES
146	a	1025.12	1.31890	YES	YES
147	a	1044.53	1.76403	YES	YES
148	a	1045.20	0.89941	YES	YES
149	a	1045.84	6.34478	YES	YES
150	a	1046.23	12.48148	YES	YES
151	a	1047.02	4.14648	YES	YES
152	a	1048.02	0.54920	YES	YES
153	a	1049.62	0.20901	YES	YES
154	a	1064.88	1.48601	YES	YES
155	a	1066.39	0.32178	YES	YES
156	a	1070.30	0.08256	YES	YES
157	a	1071.33	0.41968	YES	YES
158	a	1073.41	0.06234	YES	YES
159	a	1109.46	7.38002	YES	YES
160	a	1135.83	12.12714	YES	YES
161	a	1163.30	5.80219	YES	YES
162	a	1164.71	0.20224	YES	YES
163	a	1165.16	0.15136	YES	YES
164	a	1165.41	0.45750	YES	YES
165	a	1166.05	0.46672	YES	YES
166	a	1167.79	0.14946	YES	YES
167	a	1167.93	0.57270	YES	YES
168	a	1202.56	0.32144	YES	YES
169	a	1234.24	2.06085	YES	YES
170	a	1235.94	0.83629	YES	YES
171	a	1258.13	4.57580	YES	YES
172	a	1268.90	8.27942	YES	YES
173	a	1319.82	0.43658	YES	YES
174	a	1334.91	1.47523	YES	YES

175	a	1338.13	2.48891	YES	YES
176	a	1339.11	0.28517	YES	YES
177	a	1339.55	0.89678	YES	YES
178	a	1340.21	1.19967	YES	YES
179	a	1341.86	6.25487	YES	YES
180	a	1343.37	1.06598	YES	YES
181	a	1344.19	1.57156	YES	YES
182	a	1346.37	2.47604	YES	YES
183	a	1346.65	2.36034	YES	YES
184	a	1347.45	3.10754	YES	YES
185	a	1348.71	1.49600	YES	YES
186	a	1350.36	1.29985	YES	YES
187	a	1351.14	0.54953	YES	YES
188	a	1353.38	0.89420	YES	YES
189	a	1359.74	5.35819	YES	YES
190	a	1370.01	2.60379	YES	YES
191	a	1373.03	4.95278	YES	YES
192	a	1384.26	1.03292	YES	YES
193	a	1385.81	3.30883	YES	YES
194	a	1386.66	0.32903	YES	YES
195	a	1387.97	3.38378	YES	YES
196	a	1389.82	8.87226	YES	YES
197	a	1390.29	5.39065	YES	YES
198	a	1392.15	11.26467	YES	YES
199	a	1392.99	1.38799	YES	YES
200	a	1395.39	4.22811	YES	YES
201	a	1396.65	1.77739	YES	YES
202	a	1397.41	3.31222	YES	YES
203	a	1398.49	13.17155	YES	YES
204	a	1398.91	2.09865	YES	YES
205	a	1399.93	0.69622	YES	YES
206	a	1400.98	2.11295	YES	YES
207	a	1401.60	1.09389	YES	YES
208	a	1402.22	13.18336	YES	YES
209	a	1403.37	17.38864	YES	YES
210	a	1404.30	7.98480	YES	YES
211	a	1404.67	1.14068	YES	YES
212	a	1406.05	2.64120	YES	YES
213	a	1406.38	7.92027	YES	YES
214	a	1407.02	6.25856	YES	YES
215	a	1407.94	22.84816	YES	YES
216	a	1408.75	43.34038	YES	YES
217	a	1408.99	9.74202	YES	YES
218	a	1410.67	16.07594	YES	YES
219	a	1410.99	0.35524	YES	YES
220	a	1412.68	4.26751	YES	YES
221	a	1413.77	7.15113	YES	YES
222	a	1414.09	2.19295	YES	YES
223	a	1416.90	11.41187	YES	YES
224	a	1418.04	19.23632	YES	YES
225	a	1420.39	34.21001	YES	YES
226	a	1424.16	14.50885	YES	YES
227	a	1424.64	19.66198	YES	YES
228	a	1425.55	12.39517	YES	YES
229	a	1426.67	9.51969	YES	YES
230	a	1428.63	32.92951	YES	YES
231	a	1430.06	16.74730	YES	YES
232	a	1432.99	16.50896	YES	YES
233	a	1433.81	12.59692	YES	YES
234	a	1434.22	17.30526	YES	YES
235	a	1436.31	16.22327	YES	YES

236	a	1439.35	4.84784	YES	YES
237	a	1444.87	1.15325	YES	YES
238	a	1445.47	0.80628	YES	YES
239	a	1447.69	0.11183	YES	YES
240	a	1452.64	4.93294	YES	YES
241	a	1454.16	2.96476	YES	YES
242	a	1456.87	3.66552	YES	YES
243	a	1483.17	5.04960	YES	YES
244	a	1483.97	6.39523	YES	YES
245	a	1485.21	1.36915	YES	YES
246	a	1498.73	10.34880	YES	YES
247	a	1500.21	6.63807	YES	YES
248	a	1502.30	9.47817	YES	YES
249	a	2929.15	51.89357	YES	YES
250	a	2941.29	53.15325	YES	YES
251	a	2942.56	18.40205	YES	YES
252	a	2942.83	17.99342	YES	YES
253	a	2946.43	35.06361	YES	YES
254	a	2947.11	11.88155	YES	YES
255	a	2947.23	19.07685	YES	YES
256	a	2947.39	22.99476	YES	YES
257	a	2948.16	26.54228	YES	YES
258	a	2952.22	71.98167	YES	YES
259	a	2952.72	31.29926	YES	YES
260	a	2954.72	27.41634	YES	YES
261	a	2954.97	18.94253	YES	YES
262	a	2956.22	21.05001	YES	YES
263	a	2957.47	35.92033	YES	YES
264	a	2959.81	25.85540	YES	YES
265	a	2960.19	17.66141	YES	YES
266	a	2960.71	24.34226	YES	YES
267	a	2965.46	22.47670	YES	YES
268	a	2966.49	26.73630	YES	YES
269	a	2972.20	40.92846	YES	YES
270	a	3008.48	14.01612	YES	YES
271	a	3013.28	10.96939	YES	YES
272	a	3015.41	4.51930	YES	YES
273	a	3019.15	7.77666	YES	YES
274	a	3020.60	4.93223	YES	YES
275	a	3021.17	4.98405	YES	YES
276	a	3021.78	12.89468	YES	YES
277	a	3022.06	10.53256	YES	YES
278	a	3022.60	5.79544	YES	YES
279	a	3024.39	9.16664	YES	YES
280	a	3026.98	9.36697	YES	YES
281	a	3027.13	3.01145	YES	YES
282	a	3032.04	4.34167	YES	YES
283	a	3033.63	4.98357	YES	YES
284	a	3044.67	2.53590	YES	YES
285	a	3044.91	3.30096	YES	YES
286	a	3045.29	6.11084	YES	YES
287	a	3047.19	8.80447	YES	YES
288	a	3052.53	8.06429	YES	YES
289	a	3055.35	11.27768	YES	YES
290	a	3056.24	10.82295	YES	YES
291	a	3057.05	2.28294	YES	YES
292	a	3058.60	6.20055	YES	YES
293	a	3059.22	13.79709	YES	YES
294	a	3062.10	7.56614	YES	YES
295	a	3066.63	8.83613	YES	YES
296	a	3067.61	6.26894	YES	YES

297	a	3071.39	2.86550	YES	YES
298	a	3072.39	6.52700	YES	YES
299	a	3074.51	6.35851	YES	YES
300	a	3075.58	1.64758	YES	YES
301	a	3079.95	6.92294	YES	YES
302	a	3083.03	5.29242	YES	YES
303	a	3084.31	4.40890	YES	YES
304	a	3084.34	6.56443	YES	YES
305	a	3087.04	1.63200	YES	YES
306	a	3093.60	3.44182	YES	YES
307	a	3096.24	0.31103	YES	YES
308	a	3103.66	1.77619	YES	YES
309	a	3118.93	0.42574	YES	YES

$end

$[\{(Ph_3P)_2C\}Al(AlCp^*)_3]^+$

Method: (RI-)BP86(D3BJ)/def2-SVP
Symmetry: c1

Cartesian coordinates in Ångström:

P	11.5946484	16.0152024	14.4152911
P	10.8001564	13.8069801	16.2123969
Al	7.8145315	12.9762972	11.7121956
Al	8.9512490	14.4445316	13.5454465
Al	8.2903909	15.6320577	11.3171186
Al	6.4010290	14.8658792	13.1346232
C	9.1480072	17.6195687	10.4981844
C	7.7163027	17.7403816	10.5875886
C	9.8489613	12.2385777	16.3217812
C	10.2773614	14.6384181	17.7622143
C	10.7962745	17.6693340	14.4440236
C	13.8751765	16.9686451	17.7089060
H	13.7103021	17.4614537	18.6784512
C	10.5079605	14.7232465	14.7867537
C	9.7079574	15.9219223	17.6775586
H	9.6194269	16.4046261	16.6933218
C	13.0170007	16.2327145	15.5502663
C	10.9921481	20.0998014	14.5384132
H	11.6210200	21.0016728	14.5711570
C	14.2906226	15.7253313	15.2201779
H	14.4554869	15.2340479	14.2520908
C	7.1330999	16.7654257	9.7056303
C	9.8827494	14.6260904	20.1644751
H	9.9383194	14.1138779	21.1365514
C	13.1482781	12.7027404	15.2497181
H	12.5810633	12.6308353	14.3102252
C	15.3468227	15.8407440	16.1345438
H	16.3367541	15.4402638	15.8721789
C	8.7963112	19.0557391	14.5419136
H	7.7011610	19.1354358	14.5668926
C	14.6127866	12.9725849	17.6276512
H	15.1919392	13.0987688	18.5542009
C	15.1422655	16.4597741	17.3788232
H	15.9745447	16.5485900	18.0927481
C	13.2601322	16.7200534	12.2317305
H	13.3720548	17.7054943	12.7050137
C	10.3431186	13.9790859	19.0087374
H	10.7323453	12.9517281	19.0739610

C	12.8151215	16.8609034	16.7981059
H	11.8323822	17.2768726	17.0572818
C	11.5937856	18.8339934	14.4859393
H	12.6904153	18.7549424	14.5118307
C	5.3790595	15.0572380	15.2327059
C	4.1916689	14.3770317	13.3502076
C	15.2017947	12.3676779	16.5062103
H	16.2400052	12.0073433	16.5565271
C	4.2868517	15.8131908	13.3257791
C	12.3866796	15.7565960	12.7791199
C	12.5460510	13.2859511	16.3871857
C	9.4466493	16.5671825	9.5644701
C	10.4702144	10.9807340	16.1838871
H	11.5239596	10.9108978	15.8820576
C	13.2854670	13.4273775	17.5752628
H	12.8396564	13.9164969	18.4517725
C	9.3932256	17.7874774	14.4787016
H	8.7584408	16.8861797	14.4470928
C	9.2404495	16.5631840	18.8356763
H	8.7941418	17.5660257	18.7619788
C	14.0145003	16.4134184	11.0893299
H	14.6984459	17.1657247	10.6697738
C	14.4682412	12.2374209	15.3140726
H	14.9290592	11.7786592	14.4266385
C	6.9544010	18.7070961	11.4460996
H	7.6197861	19.4862709	11.8621368
H	6.4633224	18.1991591	12.3036192
H	6.1584942	19.2190912	10.8680968
C	8.2027644	16.0406735	9.0760350
C	12.2551717	14.5009744	12.1568473
H	11.5587295	13.7638680	12.5818811
C	6.1539521	15.0576258	16.5180514
H	7.2477779	15.1839292	16.3516272
H	6.0077085	14.1139220	17.0775393
H	5.8346702	15.8841755	17.1832949
C	4.8755305	13.9083425	14.5304457
C	3.5947999	16.7206887	12.3531633
H	4.1826675	17.6355249	12.1430761
H	2.6132168	17.0503852	12.7570364
H	3.3975065	16.2170902	11.3886432
C	8.5026751	12.3083732	16.7383763
H	8.0180690	13.2848613	16.8612435
C	9.2345392	11.1366862	11.6704350
C	9.3360032	15.9197523	20.0800430
H	8.9697600	16.4202985	20.9888218
C	5.0254143	16.2273323	14.4874285
C	9.5917407	20.2125986	14.5672607
H	9.1200172	21.2052485	14.6168991
C	7.6379416	11.4385064	10.0087330
C	10.1718706	18.5008895	11.1484197
H	11.0258768	17.9162529	11.5394223
H	9.7501227	19.0759652	11.9916466
H	10.5833152	19.2302240	10.4183080
C	5.6734109	16.5137940	9.4725639
H	5.4491099	16.4204549	8.3910798
H	5.0526496	17.3349467	9.8749109
H	5.3360314	15.5728046	9.9637487
C	10.8149386	16.1703130	9.1026505
H	10.9016175	15.0769763	8.9446578
H	11.5888879	16.4631329	9.8341903
H	11.0689394	16.6596861	8.1376636

```
C    13.0145934   14.1970566   11.0165037
H    12.9091206   13.2123059   10.5385458
C     5.2869529   17.6393764   14.9193924
H     5.3472994   18.3330675   14.0578891
H     6.2304483   17.7239915   15.4938739
H     4.4716296   18.0140703   15.5756461
C     7.9659371   10.7328245   12.2022519
C     3.4625248   13.5450889   12.3361155
H     3.7503751   13.8123550   11.2978168
H     2.3636436   13.6805259   12.4189604
H     3.6751909   12.4682564   12.4661857
C     8.4206078    9.8838489   16.9099780
H     7.8678323    8.9646122   17.1536866
C     9.7526929    9.8090880   16.4735758
H    10.2475293    8.8319191   16.3725470
C     8.0333789   14.9934973    8.0193685
H     7.9498334   15.4560901    7.0122726
H     7.1188139   14.3942483    8.1841555
H     8.8935513   14.2988903    7.9906261
C     5.0483985   12.4820596   14.9646996
H     4.5558761   11.7847937   14.2611237
H     4.6003855   12.3083400   15.9657320
H     6.1180639   12.1942291   15.0195928
C     7.7940289   11.1352945   17.0318690
H     6.7489965   11.2002739   17.3675266
C     6.9728533   10.9266817   11.1820022
C     9.0380839   11.5719930   10.3159910
C    13.9037850   15.1465980   10.4890475
H    14.5040783   14.9061919    9.5991817
C     6.9622375   11.6505996    8.6857178
H     7.6518095   12.0740918    7.9332256
H     6.0913473   12.3347369    8.7630071
H     6.5810125   10.6888458    8.2822550
C     5.5240027   10.5442788   11.2493435
H     5.3545461    9.5449662   10.7937203
H     4.8816662   11.2635450   10.7046269
H     5.1615801   10.4928571   12.2942310
C     7.7608843   10.2242276   13.5938328
H     6.6934285   10.0449936   13.8193999
H     8.1454732   10.9466541   14.3407997
H     8.3022945    9.2694397   13.7580646
C    10.5204472   11.1265722   12.4432313
H    11.3831413   11.4010038   11.8067547
H    10.7264293   10.1261655   12.8769141
H    10.4863563   11.8414837   13.2969765
C    10.1188517   12.0800381    9.4056077
H     9.7616374   12.1693783    8.3623922
H    10.9902782   11.3935735    9.3941717
H    10.4887748   13.0812147    9.7164301

SCF energy GEOOPT =  -4248.991053956 H
ZPE =   3134. kJ/mol
FREEH energy =  3349.17 kJ/mol
FREEH entropy =   1.76131 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	20.19	0.00533	YES	YES
8	a	26.24	0.00420	YES	YES
9	a	26.76	0.01772	YES	YES
10	a	31.33	0.01887	YES	YES
11	a	35.81	0.08122	YES	YES
12	a	36.13	0.02871	YES	YES
13	a	39.88	0.01294	YES	YES
14	a	43.49	0.10775	YES	YES
15	a	44.27	0.04989	YES	YES
16	a	47.93	0.16637	YES	YES
17	a	49.26	0.05342	YES	YES
18	a	52.23	0.06271	YES	YES
19	a	53.15	0.06617	YES	YES
20	a	57.75	0.20563	YES	YES
21	a	58.61	0.08106	YES	YES
22	a	59.49	0.01217	YES	YES
23	a	64.57	0.00326	YES	YES
24	a	67.06	0.10502	YES	YES
25	a	70.15	0.05297	YES	YES
26	a	71.43	0.29486	YES	YES
27	a	72.83	0.07764	YES	YES
28	a	76.44	0.11917	YES	YES
29	a	77.16	0.28017	YES	YES
30	a	80.85	0.33608	YES	YES
31	a	83.98	0.11655	YES	YES
32	a	85.67	0.03725	YES	YES
33	a	89.97	0.10555	YES	YES
34	a	92.26	0.06375	YES	YES
35	a	93.54	0.11397	YES	YES
36	a	96.44	0.03156	YES	YES
37	a	97.39	0.15312	YES	YES
38	a	99.17	0.01773	YES	YES
39	a	102.64	0.19049	YES	YES
40	a	106.62	0.07435	YES	YES
41	a	109.66	0.10198	YES	YES
42	a	110.22	0.11900	YES	YES
43	a	112.61	0.24980	YES	YES
44	a	114.38	0.09633	YES	YES
45	a	122.03	0.00998	YES	YES
46	a	123.68	0.13956	YES	YES
47	a	125.42	0.20905	YES	YES
48	a	131.24	0.08884	YES	YES
49	a	132.80	0.50697	YES	YES
50	a	139.20	0.84481	YES	YES
51	a	143.55	0.14201	YES	YES
52	a	145.78	0.47907	YES	YES
53	a	149.65	0.70596	YES	YES
54	a	152.90	0.51787	YES	YES
55	a	156.25	0.40820	YES	YES
56	a	158.55	0.52797	YES	YES
57	a	160.17	0.20941	YES	YES
58	a	162.37	0.47487	YES	YES
59	a	165.95	0.46913	YES	YES
60	a	168.71	1.01538	YES	YES
61	a	174.00	0.83426	YES	YES
62	a	175.32	0.44557	YES	YES
63	a	177.84	0.86726	YES	YES
64	a	179.50	0.26094	YES	YES

65	a	181.48	0.22702	YES	YES
66	a	183.91	0.07273	YES	YES
67	a	185.02	0.11530	YES	YES
68	a	190.36	0.45478	YES	YES
69	a	193.44	0.90016	YES	YES
70	a	196.19	0.52400	YES	YES
71	a	202.49	0.22495	YES	YES
72	a	208.06	0.22965	YES	YES
73	a	210.55	1.73862	YES	YES
74	a	227.01	0.38483	YES	YES
75	a	232.42	0.22673	YES	YES
76	a	236.52	1.66650	YES	YES
77	a	242.07	3.96583	YES	YES
78	a	245.64	2.72240	YES	YES
79	a	246.90	1.14859	YES	YES
80	a	253.20	0.71292	YES	YES
81	a	254.90	0.48577	YES	YES
82	a	260.51	1.39460	YES	YES
83	a	262.28	0.40658	YES	YES
84	a	264.92	2.71006	YES	YES
85	a	266.27	1.75657	YES	YES
86	a	268.56	0.06541	YES	YES
87	a	268.77	0.68835	YES	YES
88	a	270.82	2.70562	YES	YES
89	a	271.90	5.87595	YES	YES
90	a	275.42	2.33396	YES	YES
91	a	275.60	2.71936	YES	YES
92	a	278.41	0.83627	YES	YES
93	a	278.97	5.62387	YES	YES
94	a	283.25	5.95073	YES	YES
95	a	286.14	4.09686	YES	YES
96	a	290.07	1.54968	YES	YES
97	a	290.44	1.67196	YES	YES
98	a	291.77	2.10342	YES	YES
99	a	337.03	81.27315	YES	YES
100	a	340.85	5.20159	YES	YES
101	a	347.87	10.46794	YES	YES
102	a	349.67	4.65066	YES	YES
103	a	354.02	24.02432	YES	YES
104	a	359.06	12.23344	YES	YES
105	a	369.54	12.11240	YES	YES
106	a	378.56	3.86304	YES	YES
107	a	387.81	12.19928	YES	YES
108	a	391.44	0.52497	YES	YES
109	a	394.02	1.61370	YES	YES
110	a	398.19	1.30410	YES	YES
111	a	402.12	2.64466	YES	YES
112	a	404.77	7.43806	YES	YES
113	a	408.99	282.45524	YES	YES
114	a	409.60	2.29727	YES	YES
115	a	413.81	300.12297	YES	YES
116	a	418.35	9.48120	YES	YES
117	a	437.45	14.93919	YES	YES
118	a	449.47	2.31755	YES	YES
119	a	452.20	65.29245	YES	YES
120	a	466.57	3.47717	YES	YES
121	a	489.80	41.75771	YES	YES
122	a	493.26	45.42292	YES	YES
123	a	503.78	30.71320	YES	YES
124	a	512.41	56.06289	YES	YES
125	a	518.31	54.02738	YES	YES

126	a	522.23	64.49844	YES	YES
127	a	544.31	0.14028	YES	YES
128	a	544.93	0.11626	YES	YES
129	a	545.49	0.14896	YES	YES
130	a	547.78	0.18333	YES	YES
131	a	548.86	0.24507	YES	YES
132	a	549.22	0.07685	YES	YES
133	a	549.51	0.05686	YES	YES
134	a	550.30	0.36693	YES	YES
135	a	550.71	0.26069	YES	YES
136	a	574.01	0.48316	YES	YES
137	a	578.11	0.52146	YES	YES
138	a	580.28	0.44803	YES	YES
139	a	584.99	1.13684	YES	YES
140	a	586.53	1.18927	YES	YES
141	a	587.60	0.75135	YES	YES
142	a	589.80	1.02136	YES	YES
143	a	593.80	7.79513	YES	YES
144	a	595.98	7.18772	YES	YES
145	a	598.38	9.39913	YES	YES
146	a	608.71	0.02124	YES	YES
147	a	609.71	0.09926	YES	YES
148	a	609.92	0.20534	YES	YES
149	a	610.90	0.15953	YES	YES
150	a	611.34	0.14160	YES	YES
151	a	612.62	0.22772	YES	YES
152	a	678.19	8.71919	YES	YES
153	a	682.51	6.36215	YES	YES
154	a	688.77	21.29445	YES	YES
155	a	692.28	22.89077	YES	YES
156	a	693.23	36.87571	YES	YES
157	a	696.13	22.45343	YES	YES
158	a	697.27	10.77164	YES	YES
159	a	700.73	7.67173	YES	YES
160	a	704.04	41.82719	YES	YES
161	a	706.57	14.24151	YES	YES
162	a	708.11	11.12411	YES	YES
163	a	711.34	17.66414	YES	YES
164	a	736.43	20.03578	YES	YES
165	a	737.59	6.04094	YES	YES
166	a	739.65	39.66481	YES	YES
167	a	741.80	6.78719	YES	YES
168	a	746.06	6.92382	YES	YES
169	a	749.18	13.98093	YES	YES
170	a	799.91	1.86342	YES	YES
171	a	800.52	1.69142	YES	YES
172	a	805.02	5.16903	YES	YES
173	a	805.34	3.05820	YES	YES
174	a	806.75	6.96785	YES	YES
175	a	808.09	1.08405	YES	YES
176	a	829.58	6.35800	YES	YES
177	a	832.87	10.42425	YES	YES
178	a	834.78	274.40251	YES	YES
179	a	837.40	100.74337	YES	YES
180	a	837.81	3.02019	YES	YES
181	a	839.74	16.26016	YES	YES
182	a	848.79	0.62402	YES	YES
183	a	908.44	1.47383	YES	YES
184	a	910.25	3.05340	YES	YES
185	a	914.54	0.93489	YES	YES
186	a	916.91	0.44789	YES	YES

187	a	919.85	0.60772	YES	YES
188	a	920.34	1.24382	YES	YES
189	a	922.59	1.67360	YES	YES
190	a	923.17	1.85717	YES	YES
191	a	927.45	0.23620	YES	YES
192	a	934.70	0.19260	YES	YES
193	a	935.74	0.78848	YES	YES
194	a	939.58	0.78663	YES	YES
195	a	962.98	1.12709	YES	YES
196	a	964.05	0.60761	YES	YES
197	a	965.36	0.83461	YES	YES
198	a	967.22	0.56394	YES	YES
199	a	969.21	0.74927	YES	YES
200	a	975.93	0.18082	YES	YES
201	a	984.46	9.63557	YES	YES
202	a	985.43	7.84062	YES	YES
203	a	985.70	2.74233	YES	YES
204	a	986.40	1.40649	YES	YES
205	a	987.27	5.95732	YES	YES
206	a	987.78	2.35711	YES	YES
207	a	989.02	0.67418	YES	YES
208	a	989.61	3.85525	YES	YES
209	a	990.23	2.00060	YES	YES
210	a	990.30	0.71702	YES	YES
211	a	990.89	2.49662	YES	YES
212	a	992.25	0.41278	YES	YES
213	a	992.61	0.16793	YES	YES
214	a	993.30	1.57900	YES	YES
215	a	993.40	0.73168	YES	YES
216	a	995.79	0.91538	YES	YES
217	a	996.26	0.89460	YES	YES
218	a	996.84	0.78883	YES	YES
219	a	998.72	0.80942	YES	YES
220	a	999.68	0.42853	YES	YES
221	a	1000.54	0.17086	YES	YES
222	a	1002.06	0.18086	YES	YES
223	a	1002.44	0.18489	YES	YES
224	a	1003.15	0.03371	YES	YES
225	a	1008.45	0.20430	YES	YES
226	a	1011.84	1.00455	YES	YES
227	a	1013.91	1.04814	YES	YES
228	a	1021.32	2.42067	YES	YES
229	a	1023.53	2.98610	YES	YES
230	a	1024.20	1.41730	YES	YES
231	a	1025.09	1.24589	YES	YES
232	a	1025.93	4.92118	YES	YES
233	a	1026.32	0.09703	YES	YES
234	a	1046.80	0.35866	YES	YES
235	a	1047.32	0.68513	YES	YES
236	a	1049.27	2.22457	YES	YES
237	a	1050.12	1.52280	YES	YES
238	a	1050.85	5.04204	YES	YES
239	a	1053.33	8.07039	YES	YES
240	a	1055.57	249.56470	YES	YES
241	a	1068.26	6.17499	YES	YES
242	a	1069.46	3.13172	YES	YES
243	a	1072.69	1.30670	YES	YES
244	a	1072.99	1.52172	YES	YES
245	a	1074.56	0.40471	YES	YES
246	a	1076.10	1.02608	YES	YES
247	a	1077.91	5.78930	YES	YES

248	a	1078.28	1.79431	YES	YES
249	a	1079.58	3.65272	YES	YES
250	a	1084.68	37.68379	YES	YES
251	a	1086.28	28.15740	YES	YES
252	a	1086.95	15.81525	YES	YES
253	a	1088.62	47.13053	YES	YES
254	a	1090.16	53.18001	YES	YES
255	a	1093.62	68.88555	YES	YES
256	a	1141.91	0.34014	YES	YES
257	a	1142.17	0.08700	YES	YES
258	a	1142.75	0.96918	YES	YES
259	a	1143.15	0.10943	YES	YES
260	a	1143.96	0.34294	YES	YES
261	a	1144.49	0.40232	YES	YES
262	a	1156.89	0.33528	YES	YES
263	a	1158.73	0.16352	YES	YES
264	a	1162.84	0.76310	YES	YES
265	a	1164.73	0.67715	YES	YES
266	a	1165.72	0.11075	YES	YES
267	a	1166.47	1.23078	YES	YES
268	a	1167.38	0.50488	YES	YES
269	a	1167.99	0.33564	YES	YES
270	a	1168.35	0.82219	YES	YES
271	a	1168.83	2.03590	YES	YES
272	a	1169.13	0.23612	YES	YES
273	a	1172.41	0.11792	YES	YES
274	a	1275.04	0.68738	YES	YES
275	a	1275.37	4.64338	YES	YES
276	a	1282.29	3.61185	YES	YES
277	a	1283.37	4.40611	YES	YES
278	a	1286.52	1.98274	YES	YES
279	a	1288.69	2.73729	YES	YES
280	a	1336.51	2.64350	YES	YES
281	a	1337.62	1.62762	YES	YES
282	a	1338.69	0.50928	YES	YES
283	a	1339.64	3.40939	YES	YES
284	a	1340.39	1.02919	YES	YES
285	a	1340.52	5.47445	YES	YES
286	a	1340.97	3.16223	YES	YES
287	a	1341.76	1.40759	YES	YES
288	a	1343.22	3.61943	YES	YES
289	a	1343.59	1.07219	YES	YES
290	a	1345.00	3.29698	YES	YES
291	a	1345.23	2.49154	YES	YES
292	a	1348.48	3.85375	YES	YES
293	a	1349.80	1.18570	YES	YES
294	a	1351.54	0.14906	YES	YES
295	a	1363.28	0.32301	YES	YES
296	a	1363.95	0.49131	YES	YES
297	a	1365.47	0.56674	YES	YES
298	a	1367.56	2.31317	YES	YES
299	a	1368.91	0.52062	YES	YES
300	a	1369.21	1.30035	YES	YES
301	a	1382.74	0.59923	YES	YES
302	a	1384.26	1.84820	YES	YES
303	a	1385.56	2.88197	YES	YES
304	a	1389.01	2.41119	YES	YES
305	a	1390.69	0.96445	YES	YES
306	a	1393.27	2.07138	YES	YES
307	a	1394.13	1.75341	YES	YES
308	a	1395.43	5.76689	YES	YES

309	a	1396.43	12.45300	YES	YES
310	a	1396.96	3.61969	YES	YES
311	a	1397.53	4.93295	YES	YES
312	a	1398.59	13.86648	YES	YES
313	a	1399.09	4.33332	YES	YES
314	a	1401.53	8.69242	YES	YES
315	a	1402.55	17.69649	YES	YES
316	a	1403.76	15.39589	YES	YES
317	a	1405.16	16.91737	YES	YES
318	a	1405.97	1.65861	YES	YES
319	a	1407.00	12.19734	YES	YES
320	a	1408.29	11.00884	YES	YES
321	a	1410.91	1.19194	YES	YES
322	a	1411.89	5.43855	YES	YES
323	a	1412.88	3.57853	YES	YES
324	a	1415.58	16.04388	YES	YES
325	a	1415.88	9.59014	YES	YES
326	a	1416.28	18.01031	YES	YES
327	a	1417.52	20.01278	YES	YES
328	a	1418.72	24.08116	YES	YES
329	a	1420.12	9.18384	YES	YES
330	a	1421.70	5.07439	YES	YES
331	a	1422.34	5.99012	YES	YES
332	a	1422.50	20.02453	YES	YES
333	a	1424.13	15.66569	YES	YES
334	a	1424.85	18.89947	YES	YES
335	a	1426.54	11.21900	YES	YES
336	a	1427.70	19.42387	YES	YES
337	a	1433.06	3.82706	YES	YES
338	a	1441.72	6.25671	YES	YES
339	a	1442.69	2.88984	YES	YES
340	a	1443.28	1.89877	YES	YES
341	a	1445.66	1.51207	YES	YES
342	a	1446.39	0.68433	YES	YES
343	a	1451.20	1.35854	YES	YES
344	a	1453.42	3.30723	YES	YES
345	a	1455.27	4.79545	YES	YES
346	a	1461.46	5.06751	YES	YES
347	a	1462.18	5.03135	YES	YES
348	a	1463.51	7.38065	YES	YES
349	a	1464.43	17.90066	YES	YES
350	a	1465.51	4.34297	YES	YES
351	a	1466.19	4.33060	YES	YES
352	a	1486.31	5.20902	YES	YES
353	a	1490.62	4.40096	YES	YES
354	a	1490.98	10.45211	YES	YES
355	a	1494.68	6.33006	YES	YES
356	a	1496.59	6.38587	YES	YES
357	a	1500.15	8.63077	YES	YES
358	a	1581.76	0.26753	YES	YES
359	a	1583.71	0.38458	YES	YES
360	a	1584.43	0.46397	YES	YES
361	a	1585.27	0.72359	YES	YES
362	a	1585.65	1.48939	YES	YES
363	a	1587.37	1.81123	YES	YES
364	a	1595.53	3.52829	YES	YES
365	a	1597.16	4.06181	YES	YES
366	a	1597.59	1.40075	YES	YES
367	a	1597.70	2.60969	YES	YES
368	a	1597.98	1.77588	YES	YES
369	a	1598.89	0.58526	YES	YES

370	a	2921.66	29.76356	YES	YES
371	a	2931.01	29.25798	YES	YES
372	a	2932.08	35.62765	YES	YES
373	a	2946.80	27.52254	YES	YES
374	a	2952.03	44.22163	YES	YES
375	a	2953.58	8.94700	YES	YES
376	a	2956.28	22.61405	YES	YES
377	a	2956.56	52.88654	YES	YES
378	a	2957.33	28.09080	YES	YES
379	a	2957.56	35.87586	YES	YES
380	a	2958.27	20.26212	YES	YES
381	a	2959.21	39.33777	YES	YES
382	a	2961.42	29.02167	YES	YES
383	a	2963.75	26.88961	YES	YES
384	a	2963.93	17.55822	YES	YES
385	a	3004.28	10.54645	YES	YES
386	a	3019.26	7.14251	YES	YES
387	a	3019.72	13.08371	YES	YES
388	a	3020.52	9.00031	YES	YES
389	a	3020.73	13.30564	YES	YES
390	a	3024.18	8.49964	YES	YES
391	a	3025.02	6.24157	YES	YES
392	a	3025.81	6.36237	YES	YES
393	a	3030.10	5.53064	YES	YES
394	a	3031.03	5.98479	YES	YES
395	a	3032.23	5.17980	YES	YES
396	a	3034.23	4.97751	YES	YES
397	a	3037.69	4.46931	YES	YES
398	a	3043.29	2.93203	YES	YES
399	a	3046.21	1.93982	YES	YES
400	a	3048.05	9.56090	YES	YES
401	a	3057.86	8.48574	YES	YES
402	a	3058.78	10.31809	YES	YES
403	a	3061.62	5.40067	YES	YES
404	a	3064.07	4.70674	YES	YES
405	a	3064.53	2.63288	YES	YES
406	a	3064.56	13.15014	YES	YES
407	a	3069.73	6.90164	YES	YES
408	a	3074.57	3.91207	YES	YES
409	a	3075.38	7.90998	YES	YES
410	a	3076.48	2.49329	YES	YES
411	a	3077.88	6.58163	YES	YES
412	a	3078.24	4.18843	YES	YES
413	a	3084.11	1.94426	YES	YES
414	a	3089.58	2.66611	YES	YES
415	a	3092.60	2.15393	YES	YES
416	a	3105.63	2.04391	YES	YES
417	a	3107.72	0.35181	YES	YES
418	a	3108.46	1.54787	YES	YES
419	a	3109.04	3.78920	YES	YES
420	a	3111.57	0.47126	YES	YES
421	a	3112.77	0.19386	YES	YES
422	a	3114.44	0.08098	YES	YES
423	a	3115.67	0.49859	YES	YES
424	a	3115.82	0.20270	YES	YES
425	a	3117.28	1.02189	YES	YES
426	a	3120.12	1.74851	YES	YES
427	a	3122.46	1.79422	YES	YES
428	a	3123.01	1.21050	YES	YES
429	a	3123.16	2.02519	YES	YES
430	a	3123.61	3.26316	YES	YES

431	a	3125.07	3.29061	YES	YES
432	a	3129.86	3.20972	YES	YES
433	a	3130.17	1.53913	YES	YES
434	a	3131.46	1.25546	YES	YES
435	a	3131.72	2.96205	YES	YES
436	a	3131.86	5.04602	YES	YES
437	a	3134.18	9.29463	YES	YES
438	a	3136.29	2.35135	YES	YES
439	a	3137.01	8.80789	YES	YES
440	a	3137.03	2.86699	YES	YES
441	a	3137.63	5.78916	YES	YES
442	a	3139.94	4.26800	YES	YES
443	a	3141.99	4.00760	YES	YES
444	a	3148.78	2.35416	YES	YES

$end

$[(dmap)_3Al(AlCp^*)_3]^+$

Method: (RI-)BP86(D3BJ)/def2-SVP
Symmetry: c1

Cartesian coordinates in Ångström:

Al	11.5405496	13.6892848	3.8435374
N	9.6010128	13.5523401	3.0963201
N	5.8806393	13.4140634	1.1099475
C	9.5027074	13.1779072	1.7942832
H	10.4668889	12.9643743	1.3037084
C	8.3024191	13.0922555	1.1072328
H	8.3257566	12.7773630	0.0576869
C	7.0797662	13.4458763	1.7572273
C	7.1976874	13.8465472	3.1244985
H	6.3210913	14.1406896	3.7133350
C	8.4454041	13.8762074	3.7326724
H	8.5384267	14.1806848	4.7846247
C	5.8194529	13.0148223	-0.2918817
H	6.4153165	13.6945039	-0.9382951
H	4.7710612	13.0494641	-0.6346337
H	6.1939610	11.9794063	-0.4389807
C	4.6631459	13.8141274	1.8050833
H	4.7167365	14.8682098	2.1533244
H	4.4623686	13.1670291	2.6857957
H	3.8050986	13.7260623	1.1166556
N	10.8383880	14.7773115	5.4784060
N	9.9486270	17.3922571	8.6702464
C	10.3723419	14.3124501	6.6667131
H	10.2516427	13.2230002	6.7487761
C	10.0636221	15.1307872	7.7460412
H	9.7117691	14.6633737	8.6731371
C	10.2151579	16.5475572	7.6341836
C	10.6742568	17.0236440	6.3662969
H	10.8202836	18.0918114	6.1686497
C	10.9784837	16.1234992	5.3580422
H	11.3897931	16.4585746	4.3918737
C	9.5091728	16.8589001	9.9537786
H	8.5479626	16.3087483	9.8622305
H	9.3574432	17.6918025	10.6616952
H	10.2634183	16.1697243	10.3911872
C	10.1361065	18.8295369	8.5055614
H	11.1906592	19.0796131	8.2603611

H	9.8737910	19.3408525	9.4476673
H	9.4871088	19.2379216	7.7017726
N	11.2538520	11.9423214	4.9274816
N	11.3366126	8.2675131	7.0005901
C	12.2898504	11.6040303	5.7400252
H	13.1178904	12.3301927	5.7590148
C	12.3478820	10.4277049	6.4679925
H	13.2288105	10.2466364	7.0945789
C	11.2983439	9.4638166	6.3480470
C	10.2155523	9.8294048	5.4897421
H	9.3599785	9.1627256	5.3306845
C	10.2340095	11.0519486	4.8291167
H	9.3973273	11.3419666	4.1780860
C	12.4773125	7.9342927	7.8463122
H	13.4258774	7.9169834	7.2675820
H	12.3255634	6.9325202	8.2835649
H	12.5933214	8.6579755	8.6811196
C	10.2607469	7.3009075	6.8179266
H	10.1637774	6.9908625	5.7550069
H	9.2822905	7.7086582	7.1512620
H	10.4749771	6.3998591	7.4179593
Al	14.1715350	14.4376987	3.9072364
Al	13.3055325	12.8149633	1.9738594
Al	12.5869773	15.3838870	2.0002709
C	14.7732445	14.8128411	6.2012081
C	15.6249307	13.7636619	5.7140817
C	16.4131811	14.2963662	4.6404511
C	16.0596785	15.6757853	4.4681633
C	15.0438564	15.9970617	5.4308061
C	14.4357419	17.3527926	5.6354272
H	14.2640019	17.8711145	4.6703684
H	15.0937396	18.0083968	6.2456404
H	13.4600913	17.2895696	6.1544197
C	16.7046909	16.6031166	3.4817110
H	16.6718907	16.1952260	2.4492188
H	17.7739772	16.7719122	3.7314534
H	16.2093968	17.5910320	3.4629566
C	17.5022257	13.5996729	3.8805520
H	17.3780090	13.7113606	2.7832816
H	17.5363606	12.5176190	4.1038032
H	18.4968790	14.0241214	4.1366825
C	15.7176942	12.3597114	6.2426541
H	15.4802537	11.5986870	5.4670348
H	15.0274454	12.2011142	7.0944268
H	16.7394730	12.1323705	6.6128638
C	13.8247570	14.7266804	7.3620266
H	13.0302404	15.4944066	7.2943018
H	14.3491784	14.8854285	8.3295619
H	13.3188929	13.7425028	7.4287878
C	12.4381800	10.7069706	1.0358145
C	13.4975178	10.4307292	1.9598993
C	14.6960451	11.0459608	1.4641110
C	14.3709659	11.7266100	0.2385012
C	12.9728835	11.5103767	-0.0246657
C	12.2396418	11.9862720	-1.2430177
H	12.5899619	12.9862191	-1.5680344
H	11.1466700	12.0561415	-1.0718503
H	12.3889436	11.2979545	-2.1029986
C	15.3270785	12.4885065	-0.6327177
H	15.7879877	11.8362673	-1.4056023
H	16.1519205	12.9329403	-0.0407434

```
H    14.8222646   13.3208585   -1.1613641
C    16.0544287   10.9146715    2.0821840
H    16.5235940    9.9427904    1.8162609
H    16.0079251   10.9647916    3.1888320
H    16.7383819   11.7145710    1.7434711
C    13.4006326    9.5821396    3.1919557
H    13.7401935    8.5408760    2.9976554
H    12.3607051    9.5220953    3.5668602
H    14.0297547    9.9782393    4.0143751
C    11.0332737   10.1935187    1.1600348
H    10.3536674   10.6625168    0.4227328
H    10.6087004   10.3784360    2.1689173
H    10.9865978    9.0962980    0.9886926
C    10.7282347   16.9108733    1.3761109
C    11.2402155   16.2197848    0.2276806
C    12.6228527   16.5865908    0.0652777
C    12.9556674   17.5180422    1.1104722
C    11.7838229   17.7183203    1.9135188
C    11.6695650   18.6809293    3.0609034
H    11.7288066   19.7338646    2.7105731
H    12.4796226   18.5498008    3.8086180
H    10.7005719   18.5732577    3.5865201
C    14.2659180   18.2298470    1.2679796
H    15.1221697   17.5872518    0.9834147
H    14.4299062   18.5574044    2.3132248
H    14.3107336   19.1385222    0.6290125
C    13.5283905   16.1438797   -1.0471971
H    13.5266520   16.8689921   -1.8896377
H    13.2144982   15.1634472   -1.4569444
H    14.5776392   16.0368705   -0.7058679
C    10.4721003   15.3391007   -0.7134049
H    10.4194300   15.7878370   -1.7280493
H     9.4333624   15.1865425   -0.3657978
H    10.9369894   14.3391112   -0.8272349
C     9.3304633   16.8286246    1.9181367
H     8.7444252   17.7450619    1.6894873
H     9.3158551   16.7030074    3.0209033
H     8.7777172   15.9711474    1.4891892

SCF energy GEOOPT =  -3285.384189018 H
ZPE =   2956. kJ/mol
FREEH energy =  3161.12 kJ/mol
FREEH entropy =   1.73098 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             16.15         0.23468       YES     YES
     8        a             18.67         0.67561       YES     YES
     9        a             20.83         0.92448       YES     YES
    10        a             21.17         0.51269       YES     YES
    11        a             23.95         1.14844       YES     YES
    12        a             28.75         0.37919       YES     YES
    13        a             30.41         0.23210       YES     YES
    14        a             34.53         0.16484       YES     YES
```

15	a	35.20	0.34741	YES	YES
16	a	38.86	0.03317	YES	YES
17	a	43.50	0.04508	YES	YES
18	a	45.86	0.20406	YES	YES
19	a	50.58	0.03866	YES	YES
20	a	52.77	0.22463	YES	YES
21	a	57.78	0.03862	YES	YES
22	a	62.09	0.15154	YES	YES
23	a	63.92	0.52967	YES	YES
24	a	67.80	0.47405	YES	YES
25	a	72.17	0.68877	YES	YES
26	a	78.86	0.91846	YES	YES
27	a	81.37	0.35022	YES	YES
28	a	84.54	0.74060	YES	YES
29	a	85.89	0.11364	YES	YES
30	a	90.70	0.28010	YES	YES
31	a	91.92	0.40325	YES	YES
32	a	94.20	0.34037	YES	YES
33	a	95.00	0.15209	YES	YES
34	a	96.95	0.31760	YES	YES
35	a	98.60	0.68266	YES	YES
36	a	103.35	0.26903	YES	YES
37	a	103.84	0.63998	YES	YES
38	a	105.52	0.18899	YES	YES
39	a	106.23	0.19160	YES	YES
40	a	109.40	0.32700	YES	YES
41	a	109.80	0.00866	YES	YES
42	a	114.27	0.44736	YES	YES
43	a	118.80	1.71134	YES	YES
44	a	120.35	0.53554	YES	YES
45	a	123.42	0.18337	YES	YES
46	a	126.62	1.96779	YES	YES
47	a	128.43	1.03716	YES	YES
48	a	129.40	0.44556	YES	YES
49	a	131.24	0.62134	YES	YES
50	a	135.30	0.71763	YES	YES
51	a	136.88	0.24414	YES	YES
52	a	139.01	0.31418	YES	YES
53	a	140.27	0.15460	YES	YES
54	a	144.73	1.16050	YES	YES
55	a	147.76	3.11404	YES	YES
56	a	149.89	0.43566	YES	YES
57	a	151.79	0.89490	YES	YES
58	a	154.67	3.04735	YES	YES
59	a	156.23	1.96232	YES	YES
60	a	157.97	0.81907	YES	YES
61	a	162.23	1.23733	YES	YES
62	a	171.08	0.40243	YES	YES
63	a	176.91	0.73280	YES	YES
64	a	178.08	0.50341	YES	YES
65	a	179.72	1.74642	YES	YES
66	a	183.86	1.00937	YES	YES
67	a	185.57	0.61795	YES	YES
68	a	187.66	0.09553	YES	YES
69	a	189.35	0.34371	YES	YES
70	a	191.48	0.04408	YES	YES
71	a	200.04	4.89040	YES	YES
72	a	202.78	4.10508	YES	YES
73	a	207.57	1.64747	YES	YES
74	a	209.71	1.24843	YES	YES
75	a	211.78	2.64556	YES	YES

76	a	240.31	4.55541	YES	YES
77	a	244.95	7.36046	YES	YES
78	a	249.18	11.18479	YES	YES
79	a	255.16	0.83521	YES	YES
80	a	256.32	2.63105	YES	YES
81	a	259.53	1.08479	YES	YES
82	a	259.72	3.97100	YES	YES
83	a	260.97	3.86373	YES	YES
84	a	263.43	0.83570	YES	YES
85	a	269.87	0.23540	YES	YES
86	a	270.28	7.54889	YES	YES
87	a	273.37	2.18545	YES	YES
88	a	274.88	3.40813	YES	YES
89	a	276.87	2.48539	YES	YES
90	a	280.56	0.33245	YES	YES
91	a	282.82	4.50799	YES	YES
92	a	288.77	0.24744	YES	YES
93	a	291.73	2.17212	YES	YES
94	a	296.55	17.92655	YES	YES
95	a	297.36	1.65548	YES	YES
96	a	301.70	10.58526	YES	YES
97	a	317.77	102.42704	YES	YES
98	a	319.24	73.98231	YES	YES
99	a	325.78	14.78045	YES	YES
100	a	329.05	33.99271	YES	YES
101	a	332.17	16.34045	YES	YES
102	a	336.79	26.53960	YES	YES
103	a	348.43	192.76560	YES	YES
104	a	352.06	26.57207	YES	YES
105	a	355.45	82.93387	YES	YES
106	a	369.51	198.61123	YES	YES
107	a	377.65	204.44573	YES	YES
108	a	400.41	22.91923	YES	YES
109	a	404.30	7.81283	YES	YES
110	a	405.22	12.28139	YES	YES
111	a	406.92	2.49184	YES	YES
112	a	410.29	6.15577	YES	YES
113	a	412.46	7.49857	YES	YES
114	a	469.63	34.93853	YES	YES
115	a	481.36	1.94768	YES	YES
116	a	481.93	1.20144	YES	YES
117	a	483.96	9.66003	YES	YES
118	a	527.01	12.63860	YES	YES
119	a	528.82	15.61288	YES	YES
120	a	530.29	8.43299	YES	YES
121	a	540.40	0.07452	YES	YES
122	a	541.76	0.07201	YES	YES
123	a	542.60	0.02068	YES	YES
124	a	543.92	0.17278	YES	YES
125	a	545.11	0.03003	YES	YES
126	a	545.30	0.12487	YES	YES
127	a	545.97	0.01762	YES	YES
128	a	547.15	0.28942	YES	YES
129	a	547.58	0.23932	YES	YES
130	a	549.79	4.22535	YES	YES
131	a	550.15	1.72677	YES	YES
132	a	550.87	7.03882	YES	YES
133	a	570.12	0.12130	YES	YES
134	a	573.69	0.29938	YES	YES
135	a	575.35	0.90599	YES	YES
136	a	577.87	0.30649	YES	YES

137	a	580.94	0.47312	YES	YES
138	a	582.65	0.60811	YES	YES
139	a	591.26	11.44198	YES	YES
140	a	592.09	10.18853	YES	YES
141	a	594.73	10.86801	YES	YES
142	a	658.23	0.33035	YES	YES
143	a	658.55	0.46346	YES	YES
144	a	659.39	0.73284	YES	YES
145	a	725.59	0.10757	YES	YES
146	a	726.72	0.34795	YES	YES
147	a	726.87	0.46435	YES	YES
148	a	762.69	1.65443	YES	YES
149	a	764.35	3.00298	YES	YES
150	a	765.02	4.84491	YES	YES
151	a	799.85	1.19058	YES	YES
152	a	800.71	2.04915	YES	YES
153	a	801.26	3.79220	YES	YES
154	a	802.11	10.81927	YES	YES
155	a	802.34	14.24814	YES	YES
156	a	803.00	4.67555	YES	YES
157	a	804.37	5.44555	YES	YES
158	a	805.44	6.87255	YES	YES
159	a	805.72	7.81977	YES	YES
160	a	810.39	11.00504	YES	YES
161	a	811.96	15.82223	YES	YES
162	a	815.37	12.90947	YES	YES
163	a	917.59	1.31419	YES	YES
164	a	918.98	0.13592	YES	YES
165	a	919.85	0.36845	YES	YES
166	a	932.04	1.15220	YES	YES
167	a	933.97	0.14621	YES	YES
168	a	934.76	0.42537	YES	YES
169	a	936.88	0.21399	YES	YES
170	a	937.39	2.54760	YES	YES
171	a	943.22	3.82858	YES	YES
172	a	949.14	23.18601	YES	YES
173	a	949.77	20.89731	YES	YES
174	a	950.16	16.68853	YES	YES
175	a	957.80	0.76354	YES	YES
176	a	961.95	0.78824	YES	YES
177	a	968.01	2.95611	YES	YES
178	a	986.01	2.35086	YES	YES
179	a	986.33	1.18261	YES	YES
180	a	987.57	0.77536	YES	YES
181	a	989.28	1.44865	YES	YES
182	a	989.80	2.62582	YES	YES
183	a	991.58	0.60697	YES	YES
184	a	995.47	1.99335	YES	YES
185	a	996.17	8.95563	YES	YES
186	a	997.58	14.13177	YES	YES
187	a	998.36	46.77064	YES	YES
188	a	998.48	35.46621	YES	YES
189	a	999.28	75.65150	YES	YES
190	a	999.76	5.92466	YES	YES
191	a	999.99	38.67703	YES	YES
192	a	1000.59	0.73257	YES	YES
193	a	1000.84	1.70902	YES	YES
194	a	1002.49	0.50291	YES	YES
195	a	1004.87	0.58687	YES	YES
196	a	1042.33	13.04774	YES	YES
197	a	1042.44	12.65937	YES	YES

198	a	1042.55	14.24635	YES	YES
199	a	1046.65	3.85375	YES	YES
200	a	1046.82	0.91876	YES	YES
201	a	1047.01	0.47007	YES	YES
202	a	1047.88	1.52444	YES	YES
203	a	1048.88	0.79678	YES	YES
204	a	1049.23	0.30108	YES	YES
205	a	1050.74	20.08371	YES	YES
206	a	1051.99	21.48420	YES	YES
207	a	1054.92	15.25438	YES	YES
208	a	1072.47	0.49406	YES	YES
209	a	1073.42	1.14370	YES	YES
210	a	1074.81	0.76512	YES	YES
211	a	1089.72	0.03586	YES	YES
212	a	1089.76	0.02114	YES	YES
213	a	1089.81	0.02207	YES	YES
214	a	1096.52	0.09650	YES	YES
215	a	1096.53	0.20750	YES	YES
216	a	1096.68	0.15894	YES	YES
217	a	1103.76	1.61263	YES	YES
218	a	1104.23	1.03349	YES	YES
219	a	1106.24	2.93535	YES	YES
220	a	1153.98	0.21563	YES	YES
221	a	1154.25	0.67103	YES	YES
222	a	1154.59	0.82413	YES	YES
223	a	1162.77	0.07280	YES	YES
224	a	1165.70	0.53681	YES	YES
225	a	1166.19	0.19530	YES	YES
226	a	1167.86	0.03436	YES	YES
227	a	1168.83	0.02557	YES	YES
228	a	1169.85	0.24039	YES	YES
229	a	1196.39	63.54687	YES	YES
230	a	1197.86	70.05787	YES	YES
231	a	1204.72	29.32484	YES	YES
232	a	1236.25	22.65385	YES	YES
233	a	1236.59	27.06766	YES	YES
234	a	1237.59	28.53154	YES	YES
235	a	1306.35	13.85591	YES	YES
236	a	1309.19	16.49232	YES	YES
237	a	1309.82	10.87071	YES	YES
238	a	1335.47	0.20682	YES	YES
239	a	1336.02	0.43922	YES	YES
240	a	1336.46	0.55592	YES	YES
241	a	1338.69	0.45652	YES	YES
242	a	1339.67	1.40453	YES	YES
243	a	1339.93	2.06255	YES	YES
244	a	1340.70	2.08091	YES	YES
245	a	1341.11	2.67566	YES	YES
246	a	1341.22	11.66240	YES	YES
247	a	1341.79	2.12689	YES	YES
248	a	1341.93	4.80819	YES	YES
249	a	1342.88	2.19439	YES	YES
250	a	1343.07	8.44793	YES	YES
251	a	1344.60	2.06696	YES	YES
252	a	1345.59	1.62589	YES	YES
253	a	1347.73	5.11665	YES	YES
254	a	1348.39	5.27784	YES	YES
255	a	1350.68	3.84307	YES	YES
256	a	1370.07	68.67081	YES	YES
257	a	1370.76	80.09658	YES	YES
258	a	1371.29	84.68327	YES	YES

259	a	1381.47	1.91365	YES	YES
260	a	1381.81	0.54046	YES	YES
261	a	1381.90	0.38454	YES	YES
262	a	1382.03	0.54733	YES	YES
263	a	1384.52	4.12671	YES	YES
264	a	1387.02	1.07152	YES	YES
265	a	1389.37	2.31465	YES	YES
266	a	1390.66	2.45892	YES	YES
267	a	1392.76	1.65229	YES	YES
268	a	1393.02	0.75108	YES	YES
269	a	1394.93	12.63996	YES	YES
270	a	1396.67	0.98695	YES	YES
271	a	1396.79	4.81094	YES	YES
272	a	1398.17	9.47098	YES	YES
273	a	1399.07	5.04848	YES	YES
274	a	1400.44	8.64885	YES	YES
275	a	1402.27	2.85116	YES	YES
276	a	1402.38	17.87009	YES	YES
277	a	1403.33	2.38906	YES	YES
278	a	1403.89	2.29383	YES	YES
279	a	1405.58	8.02438	YES	YES
280	a	1406.01	1.38821	YES	YES
281	a	1407.03	13.30695	YES	YES
282	a	1408.76	0.35426	YES	YES
283	a	1408.92	4.80273	YES	YES
284	a	1409.09	0.14617	YES	YES
285	a	1409.15	5.14904	YES	YES
286	a	1409.58	12.10980	YES	YES
287	a	1410.83	7.02200	YES	YES
288	a	1413.02	29.41551	YES	YES
289	a	1414.07	19.37951	YES	YES
290	a	1414.98	27.37160	YES	YES
291	a	1416.32	4.88313	YES	YES
292	a	1416.66	6.84813	YES	YES
293	a	1417.18	49.00611	YES	YES
294	a	1417.91	43.20908	YES	YES
295	a	1418.15	46.32014	YES	YES
296	a	1418.77	28.30335	YES	YES
297	a	1419.99	17.45599	YES	YES
298	a	1420.23	17.94694	YES	YES
299	a	1420.38	17.95295	YES	YES
300	a	1421.78	19.58315	YES	YES
301	a	1433.48	3.75699	YES	YES
302	a	1433.60	1.35884	YES	YES
303	a	1433.77	1.24053	YES	YES
304	a	1438.68	3.43348	YES	YES
305	a	1439.89	4.35813	YES	YES
306	a	1443.13	4.39513	YES	YES
307	a	1444.19	1.51335	YES	YES
308	a	1447.19	2.38557	YES	YES
309	a	1448.17	2.60279	YES	YES
310	a	1451.30	41.08948	YES	YES
311	a	1451.86	50.82269	YES	YES
312	a	1452.08	61.95838	YES	YES
313	a	1452.77	6.91591	YES	YES
314	a	1453.46	1.01673	YES	YES
315	a	1454.56	1.59641	YES	YES
316	a	1468.01	1.92169	YES	YES
317	a	1469.41	2.63793	YES	YES
318	a	1469.88	4.03689	YES	YES
319	a	1490.20	3.39597	YES	YES

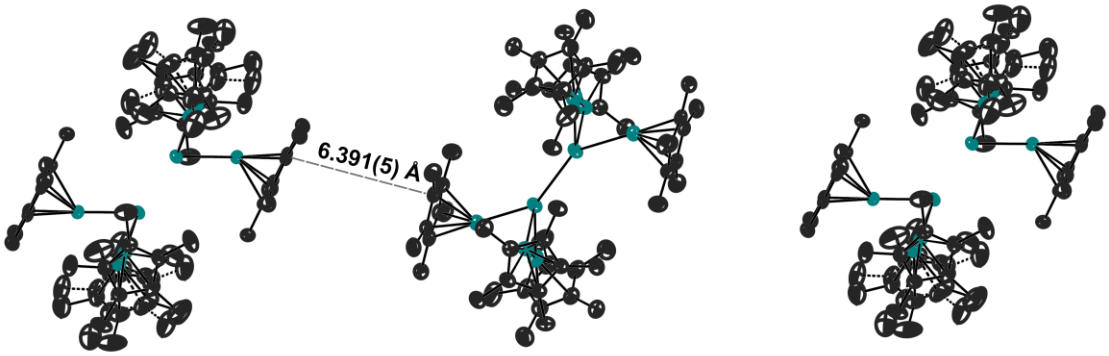
320	a	1492.99	9.68922	YES	YES
321	a	1493.70	0.62492	YES	YES
322	a	1497.26	7.92406	YES	YES
323	a	1497.94	6.80347	YES	YES
324	a	1499.01	5.12061	YES	YES
325	a	1523.76	6.34417	YES	YES
326	a	1525.24	4.47409	YES	YES
327	a	1525.78	2.39654	YES	YES
328	a	1533.20	368.70897	YES	YES
329	a	1534.14	363.28059	YES	YES
330	a	1535.31	309.80552	YES	YES
331	a	1638.30	523.98151	YES	YES
332	a	1639.36	526.12193	YES	YES
333	a	1641.33	371.18996	YES	YES
334	a	2937.01	44.48535	YES	YES
335	a	2941.94	39.47544	YES	YES
336	a	2942.01	43.05965	YES	YES
337	a	2942.28	49.19836	YES	YES
338	a	2944.97	29.97948	YES	YES
339	a	2947.08	29.55522	YES	YES
340	a	2947.61	27.38312	YES	YES
341	a	2948.29	93.79855	YES	YES
342	a	2948.33	48.03455	YES	YES
343	a	2948.67	96.28652	YES	YES
344	a	2948.78	30.94955	YES	YES
345	a	2949.12	78.04360	YES	YES
346	a	2949.95	47.49427	YES	YES
347	a	2950.41	6.40556	YES	YES
348	a	2950.49	42.47762	YES	YES
349	a	2951.67	22.47138	YES	YES
350	a	2952.07	59.48914	YES	YES
351	a	2952.19	26.97455	YES	YES
352	a	2953.15	29.74694	YES	YES
353	a	2954.05	71.09322	YES	YES
354	a	2958.63	44.02068	YES	YES
355	a	3006.75	11.00408	YES	YES
356	a	3010.76	9.61260	YES	YES
357	a	3011.77	15.87668	YES	YES
358	a	3012.21	10.70502	YES	YES
359	a	3012.43	10.10789	YES	YES
360	a	3012.69	5.57499	YES	YES
361	a	3012.87	13.29299	YES	YES
362	a	3014.14	16.61529	YES	YES
363	a	3015.79	20.07921	YES	YES
364	a	3016.22	2.68553	YES	YES
365	a	3016.65	14.77866	YES	YES
366	a	3016.69	15.76587	YES	YES
367	a	3017.68	0.12234	YES	YES
368	a	3018.09	12.45295	YES	YES
369	a	3020.17	12.48768	YES	YES
370	a	3021.64	6.84940	YES	YES
371	a	3023.74	8.81487	YES	YES
372	a	3023.98	17.57721	YES	YES
373	a	3026.71	5.14139	YES	YES
374	a	3028.39	4.23330	YES	YES
375	a	3029.40	4.24816	YES	YES
376	a	3045.62	12.12641	YES	YES
377	a	3047.71	7.07179	YES	YES
378	a	3048.84	9.36065	YES	YES
379	a	3052.56	12.13948	YES	YES
380	a	3052.91	9.61250	YES	YES

381	a	3056.86	7.64429	YES	YES
382	a	3058.27	7.57451	YES	YES
383	a	3059.40	4.05927	YES	YES
384	a	3059.44	6.48789	YES	YES
385	a	3059.93	10.72866	YES	YES
386	a	3060.41	8.21256	YES	YES
387	a	3068.61	5.44179	YES	YES
388	a	3071.41	20.31119	YES	YES
389	a	3072.45	6.57971	YES	YES
390	a	3074.96	10.23272	YES	YES
391	a	3075.55	1.59525	YES	YES
392	a	3080.07	17.86478	YES	YES
393	a	3093.56	0.61182	YES	YES
394	a	3093.68	0.60750	YES	YES
395	a	3093.95	0.53929	YES	YES
396	a	3094.94	9.80103	YES	YES
397	a	3100.70	11.18804	YES	YES
398	a	3100.72	8.90688	YES	YES
399	a	3100.94	9.37198	YES	YES
400	a	3131.01	1.03996	YES	YES
401	a	3131.54	0.97017	YES	YES
402	a	3133.43	0.88430	YES	YES
403	a	3160.01	4.10344	YES	YES
404	a	3160.13	4.62603	YES	YES
405	a	3160.41	5.56204	YES	YES
406	a	3161.08	2.20906	YES	YES
407	a	3161.13	0.99757	YES	YES
408	a	3161.14	0.67524	YES	YES

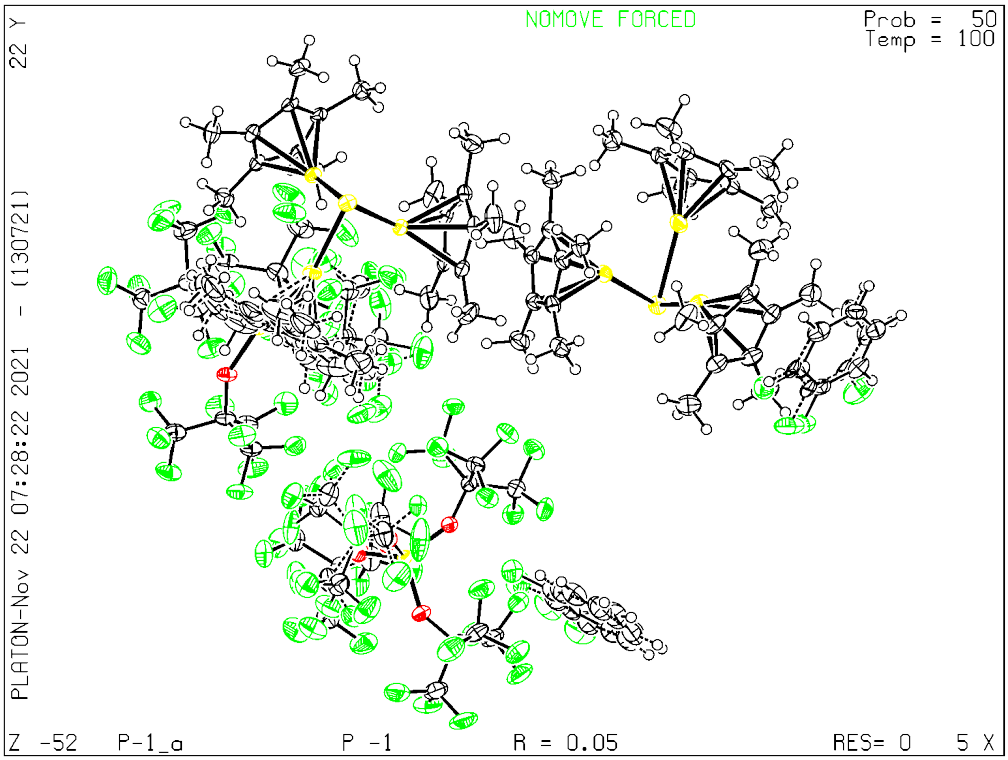
$end

S-4 Single-crystal X-ray data

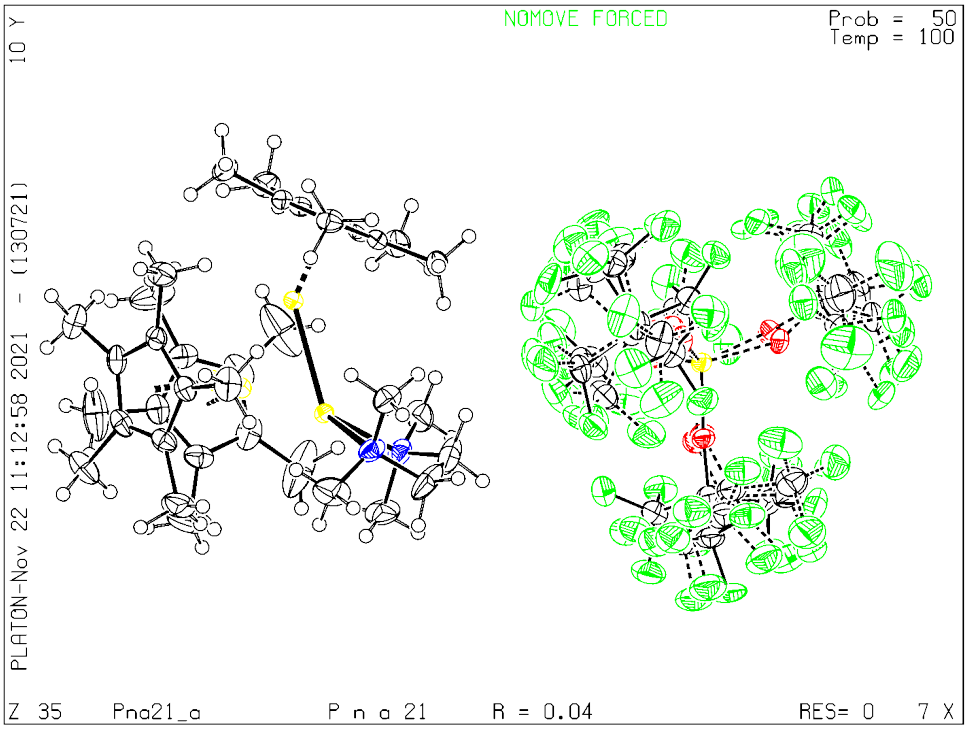
Visualization of molecular structures



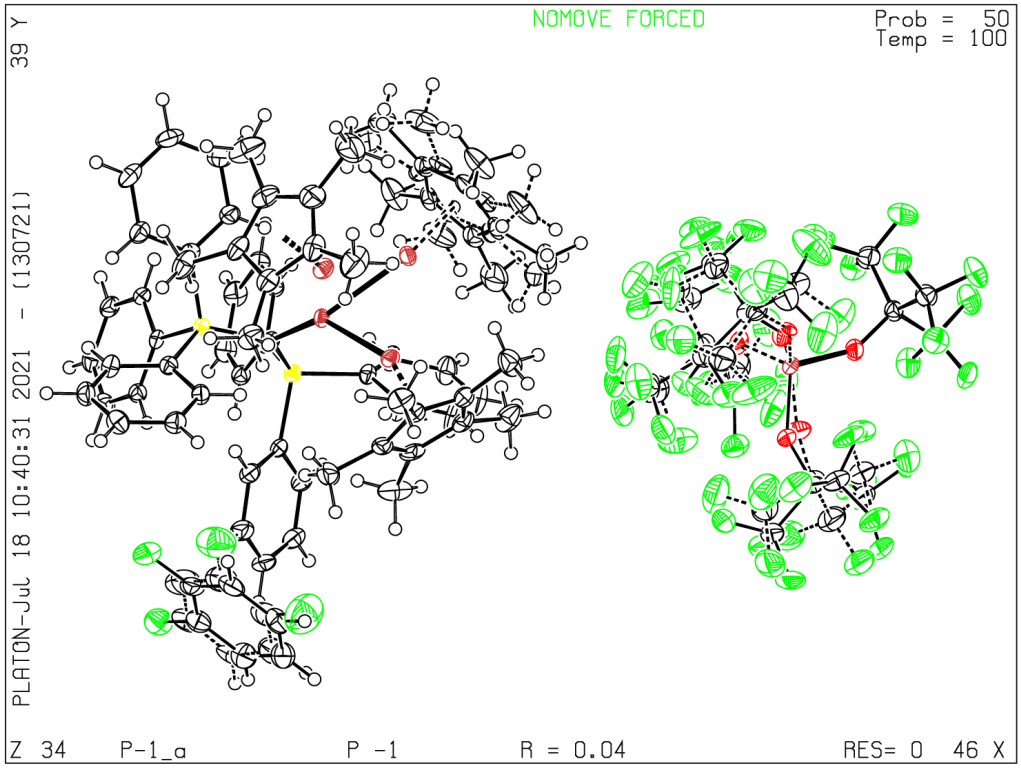
S-Figure 67: 1D chain-structure of $[Al_8Cp^*_6]^{2+}$ dimers in the molecular structure of $[Al(AlCp^*)_3]^+[pf]^-$ with alternation of the two observable bonding motifs. Hydrogen atoms, solvent molecules and [*pf*] anions omitted for chlarity. Ellipsoids shown at 50 % probability.



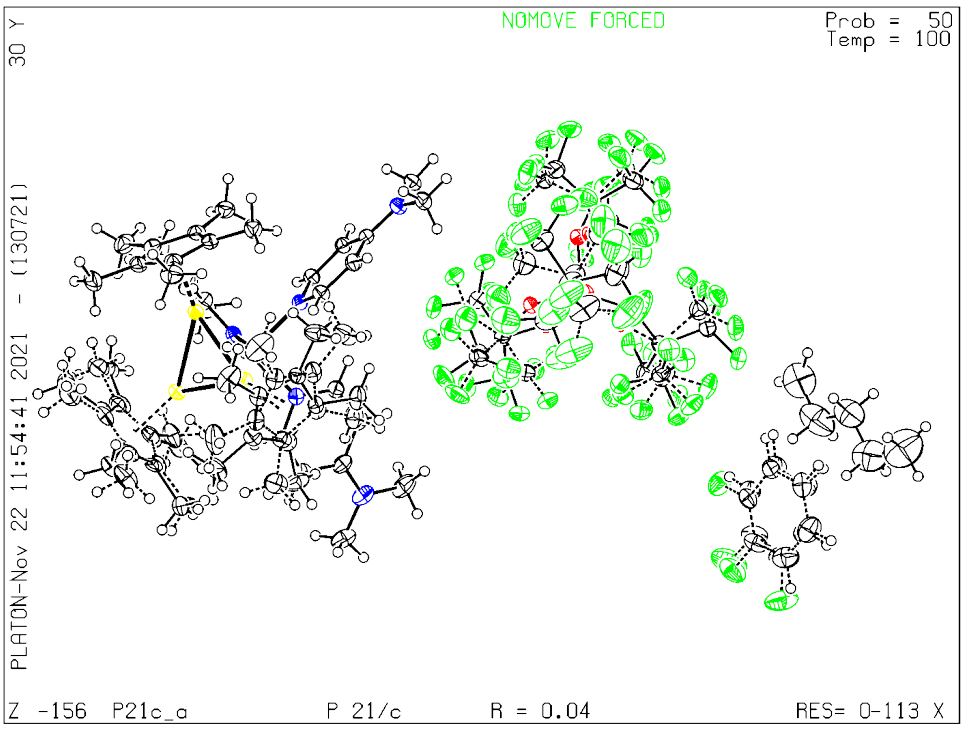
S-Figure 68: Molecular structure of $[Al(AlCp^*)_3]^+[pf]^-$. Ellipsoids shown at 50 % probability.



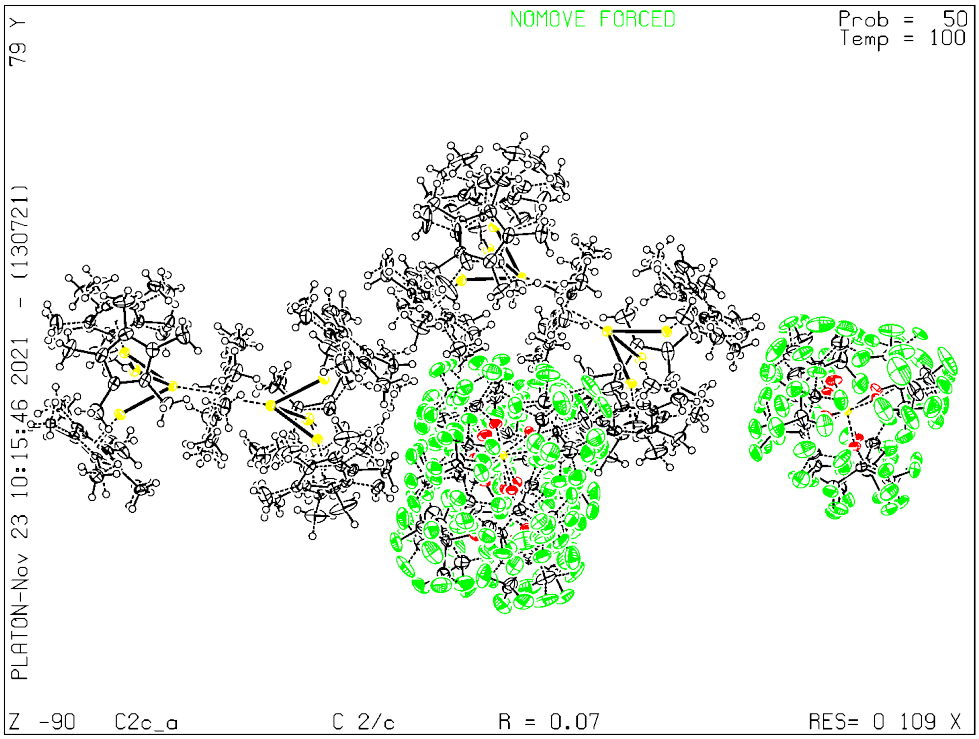
S-Figure 69: Molecular structure of [(tmeda)Al(AlCp*)$_3$]$^+$[*pf*]$^-$. Ellipsoids shown at 50 % probability.



S-Figure 70: Molecular structure of [(cdp)Al(AlCp*)$_3$]$^+$[*pf*]$^-$. Ellipsoids shown at 50 % probability.



S-Figure 71: Molecular structure of $[(dmap)_3Al(AlCp^*)_3]^+[pf]^-$. Ellipsoids shown at 50 % probability.



S-Figure 72: Molecular structure of $[Cp^*\{Al(AlCp^*)_3\}_2]^+[pf]^-$. Ellipsoids shown at 50 % probability.

Overview: Crystal data and structure refinement

S-Table 18: Crystal data and structure refinement of reported molecules

	[Al(AlCp*)$_3$][*pf*]	**[(tmeda)Al(AlCp*)$_3$][*pf*]**	**[(cdp)Al(AlCp*)$_3$][*pf*]**	**[(dmap)$_3$Al(AlCp*)$_3$][*pf*]**	**[Cp*{Al(AlCp*)$_3$}$_2$][*pf*]**
CCDC number	2123471	2123536	2123485	2123538	2124880
Empirical formula	$C_{52}O_4F_{38}Al_5H_{49}$	$C_{52}H_{61}Al_5F36N_2O_4$	$C_{89}O_4F_{38}Al_5P_2H_{79}$	$C_{75.10}H_{86.72}Al_5F_{37.33}N_6O_4$	$C_{86.02}H_{105.09}Al_9F_{35.97}O_{3.99}$
Formula weight	1594.81	1596.37	2131.40	1981.57	2129.16
Temperature [K]	100(2)	100(2)	100(2)	100(2)	100(2)
Crystal system	triclinic	orthorhombic	triclinic	monoclinic	monoclinic
Space group (number)	$P\overline{1}$ (2)	$Pna2_1$ (33)	$P\overline{1}$ (2)	$P2_1/c$ (14)	$C2/c$ (15)
***a* [Å]**	16.596(6)	34.914(7)	13.559(5)	16.361(4)	43.085(9)
***b* [Å]**	19.883(6)	11.175(2)	18.467(4)	32.286(10)	34.018(9)
***c* [Å]**	22.100(7)	17.505(4)	19.117(4)	18.454(4)	26.753(6)
α [°]	90.590(7)	90	85.951(7)	90	90
β [°]	107.669(13)	90	84.779(13)	109.236(10)	97.625(7)
γ [°]	104.381(19)	90	86.198(5)	90	90
Volume [Å^3]	6702(4)	6830(2)	4746(2)	9204(4)	38864(16)
Z	4	4	2	4	16
ρ_{calc} [gcm^{-3}]	1.581	1.552	1.491	1.430	1.455
μ [mm^{-1}]	0.230	0.223	0.216	0.184	0.210
***F*(000)**	3200	3231	2164	4049	17493
Crystal size [mm^3]	0.389×0.256×0.144	0.444×0.226×0.164	0.225×0.172×0.118	0.341×0.198×0.140	0.261×0.216×0.108
Crystal colour	purple	yellow	yellow	orange	yellow

Crystal shape	block	plate	block	block	block
Radiation	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)
2Θ range [°]	1.94 to 50.19 (0.84 Å)	3.29 to 61.06 (0.70 Å)	2.14 to 52.12 (0.81 Å)	2.92 to 52.81 (0.80 Å)	3.06 to 57.46 (0.74 Å)
Index ranges	-19 ≤ h ≤ 19 -23 ≤ k ≤ 23 -26 ≤ l ≤ 26	-49 ≤ h ≤ 49 -15 ≤ k ≤ 15 -25 ≤ l ≤ 25	-16 ≤ h ≤ 16 -22 ≤ k ≤ 22 -23 ≤ l ≤ 23	-20 ≤ h ≤ 20 -40 ≤ k ≤ 40 -23 ≤ l ≤ 23	-58 ≤ h ≤ 58 -45 ≤ k ≤ 45 -36 ≤ l ≤ 36
Reflections collected	147794	300196	113861	282906	1365671
Independent reflections	23831 R_{int} = 0.0458 R_{sigma} = 0.0345	20768 R_{int} = 0.0605 R_{sigma} = 0.0306	18769 R_{int} = 0.0524 R_{sigma} = 0.0399	18867 R_{int} = 0.0616 R_{sigma} = 0.0265	50268 R_{int} = 0.1001 R_{sigma} = 0.0313
Completeness to Θ = 25.095°	99.8 %	99.9 %	100.0 %	99.9 %	99.9 %
Data / Restraints / Parameters	23831/22815/2309	20768/18750/1675	18769/8733/1808	18867/16307/1978	50268/126060/5201
Goodness-of-fit on F^2	1.070	1.018	1.019	1.030	1.019
Final *R* indexes [*I*≥2σ(*I*)]	R_1 = 0.0494 wR_2 = 0.1136	R_1 = 0.0373 wR_2 = 0.0848	R_1 = 0.0436 wR_2 = 0.1021	R_1 = 0.0413 wR_2 = 0.1071	R_1 = 0.0713 wR_2 = 0.1872
Final *R* indexes [all data]	R_1 = 0.0760 wR_2 = 0.1269	R_1 = 0.0535 wR_2 = 0.0933	R_1 = 0.0661 wR_2 = 0.1147	R_1 = 0.0566 wR_2 = 0.1174	R_1 = 0.1265 wR_2 = 0.2309

Largest peak/hole [eÅ^{-3}]	0.58/-0.40	0.36/-0.27 -0.03(2)	0.45/-0.34	0.78/-0.28	0.93/-0.58

Coordinates, bond lengths and angles

S-Table 19: Atomic coordinates and U_{eq} [Å^2] for [Al(AlCp*)$_3$][*pf*]

Atom	*x*	*y*	*z*	U_{eq}
Al01	0.27861(5)	0.97912(4)	0.12862(4)	0.01997(19)
Al1	0.90311(6)	0.99313(5)	0.47999(4)	0.0237(2)
Al03	0.27392(6)	0.58236(4)	0.42059(4)	0.02109(19)
Al2	0.83726(6)	1.06068(4)	0.38929(4)	0.02210(19)
Al3	0.81792(6)	0.90490(4)	0.38373(4)	0.02265(19)
Al4	0.73996(6)	0.96856(5)	0.47121(4)	0.0251(2)
Al5	0.58948(6)	0.51556(5)	0.03787(4)	0.0280(2)
Al6	0.70273(6)	0.46650(5)	0.11696(5)	0.0308(2)
Al7	0.67858(6)	0.61157(5)	0.12636(4)	0.0263(2)
Al8	0.73375(6)	0.56803(5)	0.01815(5)	0.0317(2)
C1_1	0.0244(3)	0.3288(3)	0.0911(2)	0.0485(10)
C2_1	0.0883(3)	0.3687(2)	0.1431(2)	0.0491(10)
C3_1	0.1440(4)	0.3396(3)	0.1874(3)	0.0587(11)
H_1	0.187662	0.367554	0.223151	0.070
C4_1	0.1356(4)	0.2694(3)	0.1791(3)	0.0667(12)
HA_1	0.174045	0.248504	0.209235	0.080
C5_1	0.0717(4)	0.2292(3)	0.1276(3)	0.0636(11)
HB_1	0.066382	0.180556	0.122798	0.076
C6_1	0.0149(3)	0.2580(3)	0.0823(3)	0.0586(11)
HC_1	-0.028951	0.230021	0.046561	0.070
F1_1	-0.02905(19)	0.35907(19)	0.04847(14)	0.0694(10)
F2_1	0.0938(2)	0.43698(14)	0.14879(17)	0.0682(10)
O1_2	0.20108(14)	0.50870(10)	0.43239(10)	0.0307(5)
C1_2	0.1867(2)	0.43965(16)	0.43916(16)	0.0355(8)
C2_2	0.1067(2)	0.41713(18)	0.46339(18)	0.0465(9)
F1_2	0.03187(13)	0.41325(12)	0.41637(11)	0.0572(6)
F2_2	0.09964(16)	0.35480(11)	0.48678(11)	0.0604(6)
F3_2	0.11143(15)	0.46277(11)	0.50941(11)	0.0572(6)
C3_2	0.2678(2)	0.42287(17)	0.48755(18)	0.0439(9)
F4_2	0.34074(13)	0.45891(11)	0.47944(11)	0.0518(6)
F5_2	0.27106(15)	0.43908(11)	0.54772(10)	0.0561(6)
F6_2	0.26497(16)	0.35505(10)	0.48233(12)	0.0588(6)
C4_2	0.1667(3)	0.39811(17)	0.37342(18)	0.0448(9)
F7_2	0.23967(15)	0.40106(10)	0.35975(11)	0.0532(6)
F8_2	0.12641(16)	0.33067(10)	0.37249(12)	0.0609(6)
F9_2	0.11467(15)	0.42403(11)	0.32689(10)	0.0547(6)
O1_3	0.21483(13)	0.64188(10)	0.39097(10)	0.0277(5)
C1_3	0.13788(19)	0.65177(16)	0.35443(14)	0.0300(7)
C2_3	0.0624(2)	0.61761(19)	0.38094(18)	0.0421(8)
F1_3	0.03296(13)	0.54938(11)	0.36334(12)	0.0570(6)
F2_3	-0.00658(13)	0.64460(12)	0.36027(11)	0.0557(6)
F3_3	0.08903(13)	0.62605(12)	0.44397(10)	0.0529(6)
C3_3	0.1483(2)	0.73172(17)	0.35560(16)	0.0363(8)
F4_3	0.22421(13)	0.76509(10)	0.34859(10)	0.0431(5)
F5_3	0.14653(13)	0.75697(10)	0.41132(9)	0.0459(5)
F6_3	0.08425(14)	0.74868(11)	0.30959(10)	0.0514(6)
C4_3	0.1154(2)	0.62180(19)	0.28419(16)	0.0412(8)
F7_3	0.16528(14)	0.66208(12)	0.25449(10)	0.0504(5)

F8_3	0.03119(13)	0.61613(12)	0.25038(10)	0.0547(6)
F9_3	0.12804(14)	0.55855(11)	0.28227(10)	0.0522(6)
O1_4	0.32214(13)	0.55937(10)	0.36744(10)	0.0259(5)
C1_4	0.39137(19)	0.57477(15)	0.34492(14)	0.0260(6)
C2_4	0.3938(2)	0.64186(16)	0.30983(15)	0.0311(7)
F1_4	0.33161(13)	0.63003(10)	0.25316(9)	0.0425(5)
F2_4	0.47112(12)	0.66741(10)	0.29976(10)	0.0401(5)
F3_4	0.38044(13)	0.69151(9)	0.34328(10)	0.0398(5)
C3_4	0.4802(2)	0.58490(16)	0.39955(15)	0.0315(7)
F4_4	0.47233(12)	0.53967(10)	0.44212(9)	0.0386(5)
F5_4	0.50663(12)	0.64891(10)	0.42990(9)	0.0399(5)
F6_4	0.54438(12)	0.57660(11)	0.37765(9)	0.0414(5)
C4_4	0.3798(2)	0.51248(17)	0.29745(16)	0.0345(7)
F7_4	0.39781(14)	0.45793(9)	0.32770(10)	0.0440(5)
F8_4	0.43079(13)	0.52819(11)	0.26001(10)	0.0454(5)
F9_4	0.29703(13)	0.49159(10)	0.25893(9)	0.0406(5)
O1_6	0.34429(13)	1.06058(10)	0.16257(9)	0.0275(5)
C1_6	0.37419(19)	1.10861(16)	0.21342(14)	0.0282(7)
C2_6	0.3992(2)	1.07403(18)	0.27654(16)	0.0406(8)
F1_6	0.47233(14)	1.05454(12)	0.28469(11)	0.0598(6)
F2_6	0.41046(16)	1.11561(12)	0.32785(9)	0.0586(6)
F3_6	0.33676(14)	1.01683(10)	0.27552(9)	0.0492(5)
C3_6	0.3045(2)	1.14797(18)	0.21369(17)	0.0390(8)
F4_6	0.26389(14)	1.16091(12)	0.15543(10)	0.0550(6)
F5_6	0.24322(13)	1.10994(12)	0.23605(10)	0.0524(6)
F6_6	0.33924(15)	1.20849(11)	0.25021(11)	0.0588(6)
C4_6	0.4572(2)	1.16129(18)	0.20746(17)	0.0416(8)
F7_6	0.43522(15)	1.20383(11)	0.16283(11)	0.0571(6)
F8_6	0.50457(13)	1.20121(11)	0.26224(11)	0.0539(6)
F9_6	0.50871(13)	1.12869(12)	0.19127(12)	0.0590(6)
O1_8	0.27443(14)	0.97530(11)	0.04977(9)	0.0282(5)
C1_8	0.2703(2)	1.00833(17)	-0.00367(14)	0.0326(7)
C2_8	0.2437(2)	1.07722(18)	0.00000(16)	0.0374(8)
F1_8	0.31234(14)	1.12880(10)	0.03336(10)	0.0485(5)
F2_8	0.21238(13)	1.09894(11)	-0.05766(9)	0.0501(6)
F3_8	0.18389(13)	1.07084(11)	0.02883(10)	0.0454(5)
C3_8	0.1983(3)	0.9584(2)	-0.06001(17)	0.0542(10)
F4_8	0.20577(19)	0.89341(13)	-0.05525(11)	0.0735(8)
F5_8	0.11862(15)	0.95855(13)	-0.05932(11)	0.0633(7)
F6_8	0.2047(2)	0.97708(16)	-0.11647(10)	0.0871(9)
C4_8	0.3595(3)	1.0235(2)	-0.0155(2)	0.0586(11)
F7_8	0.3726(2)	0.96435(16)	-0.03583(14)	0.0839(9)
F8_8	0.36530(18)	1.06851(15)	-0.05972(13)	0.0801(9)
F9_8	0.42483(14)	1.05106(14)	0.03811(13)	0.0689(7)
C1_11	0.87330(18)	1.11092(14)	0.30847(14)	0.0239(6)
C2_11	0.78131(18)	1.10066(14)	0.29785(13)	0.0227(6)
C3_11	0.77183(18)	1.14010(14)	0.34837(13)	0.0231(6)
C4_11	0.85713(19)	1.17528(15)	0.38937(14)	0.0246(6)
C5_11	0.91919(18)	1.15680(14)	0.36495(14)	0.0237(6)
C6_11	1.01800(19)	1.18084(17)	0.39234(17)	0.0343(8)
H6A_11	1.042932	1.195079	0.358091	0.051
H6B_11	1.040430	1.142557	0.412283	0.051
H6C_11	1.034694	1.220478	0.424387	0.051
C7_11	0.8758(2)	1.22524(17)	0.44631(15)	0.0353(8)

H7A_11	0.856803	1.266958	0.432203	0.053
H7B_11	0.938895	1.238523	0.469244	0.053
H7C_11	0.843956	1.202872	0.474671	0.053
C8_11	0.6865(2)	1.14679(18)	0.35440(16)	0.0334(7)
H8A_11	0.671206	1.186658	0.332501	0.050
H8B_11	0.692180	1.153971	0.399594	0.050
H8C_11	0.640381	1.104105	0.335027	0.050
C9_11	0.7063(2)	1.06068(16)	0.24177(15)	0.0316(7)
H9A_11	0.670564	1.091675	0.221340	0.047
H9B_11	0.670130	1.021677	0.256487	0.047
H9C_11	0.729471	1.042687	0.210986	0.047
C10_11	0.9165(2)	1.08235(17)	0.26693(16)	0.0335(7)
H10A_11	0.872637	1.045943	0.235379	0.050
H10B_11	0.962358	1.062519	0.293469	0.050
H10C_11	0.942767	1.120014	0.244939	0.050
C1_12	0.87554(19)	0.85910(15)	0.31983(14)	0.0267(7)
C2_12	0.87178(19)	0.81582(15)	0.36988(14)	0.0277(7)
C3_12	0.7827(2)	0.78950(15)	0.36634(15)	0.0292(7)
C4_12	0.73094(19)	0.81741(15)	0.31412(15)	0.0279(7)
C5_12	0.78834(19)	0.86029(15)	0.28514(14)	0.0264(7)
C6_12	0.7586(3)	0.89518(18)	0.22547(16)	0.0463(10)
H6A_12	0.809021	0.929117	0.219573	0.070
H6B_12	0.715134	0.919165	0.229194	0.070
H6C_12	0.732204	0.860007	0.188732	0.070
C7_12	0.6324(2)	0.80143(19)	0.2899(2)	0.0477(10)
H7A_12	0.614836	0.845088	0.283740	0.072
H7B_12	0.608043	0.776429	0.321095	0.072
H7C_12	0.610100	0.772393	0.249241	0.072
C8_12	0.7502(3)	0.73921(18)	0.40922(19)	0.0522(11)
H8A_12	0.688119	0.735835	0.402573	0.078
H8B_12	0.784180	0.755752	0.453779	0.078
H8C_12	0.756992	0.693187	0.399304	0.078
C9_12	0.9493(2)	0.8004(2)	0.41850(17)	0.0475(10)
H9A_12	0.950448	0.752343	0.409508	0.071
H9B_12	0.944454	0.806220	0.461235	0.071
H9C_12	1.003474	0.832618	0.416404	0.071
C10_12	0.9587(2)	0.8971(2)	0.30756(19)	0.0480(10)
H10A_12	0.989597	0.863313	0.300036	0.072
H10B_12	0.996288	0.929675	0.344690	0.072
H10C_12	0.944471	0.922899	0.269959	0.072
C1_13	0.8435(2)	0.55956(18)	-0.01357(18)	0.0430(9)
C2_13	0.8585(2)	0.63089(18)	0.00986(16)	0.0371(8)
C3_13	0.7896(2)	0.65577(16)	-0.03113(15)	0.0318(7)
C4_13	0.7338(2)	0.60043(17)	-0.07848(16)	0.0369(8)
C5_13	0.7669(2)	0.54160(18)	-0.06763(17)	0.0400(8)
C6_13	0.7307(3)	0.47140(19)	-0.1061(2)	0.0563(11)
H_13	0.733368	0.434406	-0.077129	0.084
HA_13	0.765637	0.467844	-0.134057	0.084
HB_13	0.669684	0.466379	-0.131942	0.084
C7_13	0.6532(3)	0.6050(2)	-0.13055(17)	0.0502(10)
HC_13	0.624727	0.635979	-0.115023	0.075
HD_13	0.612639	0.558424	-0.143388	0.075
HE_13	0.669705	0.623553	-0.167280	0.075
C8_13	0.7779(2)	0.72802(17)	-0.02850(17)	0.0389(8)

HF_13	0.819882	0.755072	0.010584	0.058
HG_13	0.718045	0.725502	-0.028704	0.058
HH_13	0.787976	0.750700	-0.065680	0.058
C9_13	0.9350(2)	0.6718(2)	0.06413(18)	0.0516(10)
HI_13	0.941509	0.645420	0.101746	0.077
HJ_13	0.924946	0.716569	0.074016	0.077
HK_13	0.988595	0.680110	0.052058	0.077
C10_13	0.9046(3)	0.5143(3)	0.0127(3)	0.0747(15)
HL_13	0.870187	0.467265	0.015430	0.112
HM_13	0.943766	0.534364	0.055313	0.112
HN_13	0.939442	0.511860	-0.015574	0.112
C1_14	0.6750(2)	0.38837(16)	0.18445(15)	0.0340(7)
C2_14	0.7642(2)	0.42791(15)	0.20788(15)	0.0326(7)
C3_14	0.8064(2)	0.41575(16)	0.16291(16)	0.0337(7)
C4_14	0.7436(2)	0.36898(16)	0.11209(15)	0.0339(7)
C5_14	0.6627(2)	0.35227(17)	0.12501(15)	0.0344(8)
C6_14	0.5784(2)	0.3039(2)	0.08342(18)	0.0509(10)
H_14	0.529119	0.322307	0.084218	0.076
HA_14	0.571137	0.257691	0.099356	0.076
HB_14	0.579989	0.300196	0.039565	0.076
C7_14	0.7582(3)	0.3399(2)	0.05432(17)	0.0473(9)
HC_14	0.751253	0.289638	0.055790	0.071
HD_14	0.817583	0.362753	0.053902	0.071
HE_14	0.715314	0.348532	0.015649	0.071
C8_14	0.9029(2)	0.4440(2)	0.1718(2)	0.0477(10)
HF_14	0.936993	0.423660	0.207702	0.071
HG_14	0.919581	0.494799	0.180481	0.071
HH_14	0.914851	0.431695	0.132874	0.071
C9_14	0.8089(3)	0.47018(18)	0.27135(16)	0.0460(9)
HI_14	0.838989	0.442202	0.302099	0.069
HJ_14	0.765135	0.483863	0.286616	0.069
HK_14	0.851726	0.512042	0.266722	0.069
C10_14	0.6062(2)	0.3830(2)	0.21665(18)	0.0467(9)
HL_14	0.626090	0.420775	0.250963	0.070
HM_14	0.596029	0.337966	0.234555	0.070
HN_14	0.551485	0.386859	0.185449	0.070
C1_15	0.60531(19)	0.66967(15)	0.16707(14)	0.0269(7)
C2_15	0.6637(2)	0.64437(16)	0.21789(14)	0.0286(7)
C3_15	0.75050(19)	0.67560(16)	0.21737(14)	0.0283(7)
C4_15	0.74587(19)	0.71992(15)	0.16705(14)	0.0278(7)
C5_15	0.65614(19)	0.71669(15)	0.13617(14)	0.0271(7)
C6_15	0.6189(2)	0.75470(18)	0.08036(16)	0.0374(8)
H_15	0.593752	0.789372	0.094285	0.056
HA_15	0.573046	0.721304	0.047063	0.056
HB_15	0.665602	0.778187	0.063376	0.056
C7_15	0.8242(2)	0.76525(17)	0.15348(17)	0.0361(8)
HC_15	0.868080	0.739115	0.157197	0.054
HD_15	0.849407	0.806702	0.184213	0.054
HE_15	0.806163	0.779533	0.110168	0.054
C8_15	0.8343(2)	0.66740(18)	0.26366(16)	0.0361(8)
HF_15	0.820713	0.630807	0.291162	0.054
HG_15	0.866388	0.711539	0.289917	0.054
HH_15	0.870429	0.654501	0.240070	0.054
C9_15	0.6372(2)	0.59493(18)	0.26318(17)	0.0399(8)

HI_15	0.617190	0.618864	0.292559	0.060
HJ_15	0.687433	0.578420	0.287501	0.060
HK_15	0.589453	0.555102	0.239167	0.060
C10_15	0.5068(2)	0.64957(19)	0.14918(17)	0.0386(8)
HL_15	0.487777	0.687001	0.165342	0.058
HM_15	0.487310	0.606500	0.167914	0.058
HN_15	0.481183	0.642148	0.102648	0.058
O1_16	0.3584(5)	0.6197(5)	0.4899(4)	0.0238(11)
C1_16	0.3831(3)	0.6598(3)	0.5457(3)	0.0286(9)
C2_16	0.4737(4)	0.6508(3)	0.5858(3)	0.0537(14)
F1_16	0.53546(19)	0.6832(2)	0.56440(17)	0.0803(13)
F2_16	0.4936(5)	0.6722(3)	0.6485(2)	0.0631(16)
F3_16	0.4696(3)	0.5822(2)	0.58354(18)	0.0808(14)
C3_16	0.3181(4)	0.6375(3)	0.5833(3)	0.0416(12)
F4_16	0.23514(19)	0.6281(2)	0.54441(15)	0.0586(9)
F5_16	0.3222(3)	0.57888(15)	0.60863(15)	0.0695(11)
F6_16	0.3301(6)	0.6861(4)	0.6302(3)	0.0500(15)
C4_16	0.3905(3)	0.7368(3)	0.5324(2)	0.0390(11)
F7_16	0.3133(2)	0.75023(15)	0.51401(13)	0.0550(9)
F8_16	0.4396(7)	0.7814(5)	0.5840(4)	0.0580(18)
F9_16	0.4286(3)	0.75190(17)	0.48738(19)	0.0731(12)
O1_17	0.350(2)	0.6192(18)	0.4899(12)	0.032(3)
C1_17	0.3844(9)	0.6593(8)	0.5459(9)	0.0347(19)
C2_17	0.4567(9)	0.6318(7)	0.5939(7)	0.043(2)
F1_17	0.4156(9)	0.5755(5)	0.6174(5)	0.070(3)
F2_17	0.5100(15)	0.6856(11)	0.6370(9)	0.069(5)
F3_17	0.5114(5)	0.6171(5)	0.5659(4)	0.0298(19)
C3_17	0.4249(8)	0.7362(8)	0.5366(7)	0.043(3)
F4_17	0.3748(7)	0.7547(5)	0.4833(5)	0.045(3)
F5_17	0.5076(6)	0.7398(6)	0.5331(5)	0.060(3)
F6_17	0.436(2)	0.7793(18)	0.5863(12)	0.054(5)
C4_17	0.3106(9)	0.6545(7)	0.5763(8)	0.041(2)
F7_17	0.2589(6)	0.6942(6)	0.5453(5)	0.061(3)
F8_17	0.340(2)	0.6764(16)	0.6376(9)	0.052(4)
F9_17	0.2588(7)	0.5904(5)	0.5666(5)	0.046(2)
O1_18	0.3180(3)	0.9112(3)	0.1626(2)	0.0291(9)
C1_18	0.3673(3)	0.8662(2)	0.16153(18)	0.0312(8)
C2_18	0.4644(2)	0.9069(2)	0.1722(2)	0.0412(10)
F1_18	0.50477(14)	0.93073(13)	0.23357(13)	0.0500(7)
F2_18	0.5103(4)	0.8666(4)	0.1568(3)	0.0579(13)
F3_18	0.4683(4)	0.9607(2)	0.1378(3)	0.0566(13)
C3_18	0.3317(3)	0.8198(2)	0.0973(2)	0.0499(11)
F4_18	0.2443(2)	0.8013(3)	0.07778(17)	0.0637(12)
F5_18	0.3581(2)	0.85336(18)	0.05231(13)	0.0641(9)
F6_18	0.3584(4)	0.7614(3)	0.1019(3)	0.0720(14)
C4_18	0.3632(3)	0.8197(2)	0.2170(2)	0.0398(10)
F7_18	0.28654(15)	0.77151(13)	0.20175(15)	0.0601(9)
F8_18	0.4263(4)	0.7861(2)	0.2315(3)	0.0534(12)
F9_18	0.3711(2)	0.85727(18)	0.26947(14)	0.0503(8)
O1_19	0.316(3)	0.909(2)	0.156(2)	0.032(6)
C1_19	0.3653(15)	0.8631(13)	0.1566(9)	0.039(4)
C2_19	0.3084(14)	0.7944(12)	0.1149(11)	0.053(5)
F1_19	0.2551(15)	0.7564(11)	0.1434(13)	0.072(6)
F2_19	0.358(3)	0.755(2)	0.104(3)	0.063(8)

F3_19	0.260(2)	0.8083(19)	0.0589(11)	0.056(7)
C3_19	0.4424(15)	0.8960(13)	0.1312(10)	0.046(4)
F4_19	0.477(4)	0.9630(16)	0.152(2)	0.048(8)
F5_19	0.4140(17)	0.8918(13)	0.0676(9)	0.053(5)
F6_19	0.506(3)	0.863(3)	0.148(2)	0.050(8)
C4_19	0.4014(14)	0.8448(11)	0.2262(9)	0.043(4)
F7_19	0.4668(12)	0.8976(10)	0.2593(9)	0.048(5)
F8_19	0.431(3)	0.7879(17)	0.227(2)	0.047(8)
F9_19	0.3385(15)	0.8327(15)	0.2534(13)	0.045(6)
C1_20	0.7577(6)	0.2402(6)	0.2188(5)	0.0359(19)
C2_20	0.8195(8)	0.2814(8)	0.2701(5)	0.033(2)
C3_20	0.9065(8)	0.2958(11)	0.2758(7)	0.040(3)
H_20	0.949394	0.323949	0.311753	0.048
C4_20	0.9312(6)	0.2690(8)	0.2287(6)	0.039(2)
HA_20	0.991510	0.278725	0.232188	0.047
C5_20	0.8689(6)	0.2281(9)	0.1766(6)	0.043(2)
HB_20	0.886464	0.210563	0.143865	0.051
C6_20	0.7818(5)	0.2125(5)	0.1716(4)	0.041(2)
HC_20	0.738839	0.183220	0.136375	0.049
F1_20	0.6727(7)	0.2268(8)	0.2150(7)	0.055(2)
F2_20	0.7943(2)	0.30873(15)	0.31478(15)	0.0486(10)
C1_21	0.7683(12)	0.2272(12)	0.1760(10)	0.036(5)
C2_21	0.7525(17)	0.2535(15)	0.2274(12)	0.032(5)
C3_21	0.820(2)	0.291(2)	0.2778(14)	0.032(6)
H_21	0.809033	0.308584	0.313410	0.038
C4_21	0.9050(19)	0.302(3)	0.277(2)	0.037(7)
HA_21	0.952282	0.328187	0.311834	0.044
C5_21	0.9209(16)	0.275(3)	0.2256(19)	0.050(8)
HB_21	0.979384	0.283171	0.224750	0.060
C6_21	0.8527(14)	0.236(2)	0.1753(17)	0.045(6)
HC_21	0.863965	0.215547	0.140656	0.054
F1_21	0.7018(7)	0.1904(5)	0.1270(4)	0.074(4)
F2_21	0.6691(19)	0.241(2)	0.227(2)	0.059(7)
C1_22	0.0132(16)	0.2949(12)	0.0876(11)	0.056(3)
C2_22	0.0596(17)	0.3572(11)	0.1236(12)	0.057(3)
C3_22	0.128(2)	0.3572(15)	0.1774(14)	0.058(3)
H_22	0.161694	0.399351	0.203189	0.070
C4_22	0.147(2)	0.2952(18)	0.1930(16)	0.061(3)
HA_22	0.195376	0.295505	0.229810	0.073
C5_22	0.100(2)	0.2324(16)	0.1578(17)	0.059(3)
HB_22	0.113942	0.190155	0.171122	0.071
C6_22	0.033(2)	0.2323(13)	0.1027(16)	0.057(2)
HC_22	0.000521	0.190430	0.076000	0.068
F1_22	-0.0533(14)	0.2968(15)	0.0355(10)	0.082(5)
F2_22	0.0392(17)	0.4170(11)	0.1075(13)	0.067(4)
C1_23	0.6729(4)	0.8943(2)	0.5271(2)	0.0423(11)
C2_23	0.6100(3)	0.9054(3)	0.4717(2)	0.0411(11)
C3_23	0.6120(3)	0.9768(3)	0.4739(2)	0.0426(11)
C4_23	0.6771(4)	1.0107(2)	0.5315(3)	0.0425(11)
C5_23	0.7141(3)	0.9595(3)	0.5634(2)	0.0419(11)
C6_23	0.7868(4)	0.9713(4)	0.6263(2)	0.0757(18)
H6A_23	0.834189	0.952775	0.621586	0.114
H6B_23	0.763950	0.947514	0.658639	0.114
H6C_23	0.809303	1.021446	0.639555	0.114

C7_23	0.7007(5)	1.0864(3)	0.5553(4)	0.0869(19)
H7A_23	0.674938	1.112577	0.520619	0.130
H7B_23	0.764637	1.104874	0.570001	0.130
H7C_23	0.677957	1.091166	0.590721	0.130
C8_23	0.5487(4)	1.0085(4)	0.4263(4)	0.0817(18)
H8A_23	0.574352	1.058848	0.428286	0.123
H8B_23	0.493741	1.000161	0.436515	0.123
H8C_23	0.536922	0.987187	0.383290	0.123
C9_23	0.5468(4)	0.8503(4)	0.4201(3)	0.081(2)
H9A_23	0.544755	0.866918	0.378164	0.121
H9B_23	0.488192	0.840650	0.424627	0.121
H9C_23	0.566451	0.807477	0.423848	0.121
C10_23	0.6932(5)	0.8265(3)	0.5465(4)	0.0773(17)
H10A_23	0.667962	0.791610	0.509457	0.116
H10B_23	0.667830	0.810123	0.580063	0.116
H10C_23	0.756836	0.833454	0.562449	0.116
C1_10	0.7131(15)	0.9425(11)	0.5629(10)	0.051(3)
C2_10	0.6564(14)	0.8934(10)	0.5114(10)	0.047(3)
C3_10	0.6018(14)	0.9272(11)	0.4669(10)	0.047(3)
C4_10	0.6247(18)	0.9986(11)	0.4898(11)	0.051(3)
C5_10	0.691(2)	1.0062(11)	0.5498(12)	0.056(3)
C6_10	0.736(2)	1.0744(12)	0.5914(14)	0.080(4)
H6A_10	0.744582	1.112607	0.564486	0.120
H6B_10	0.792407	1.071917	0.620522	0.120
H6C_10	0.698533	1.082810	0.616209	0.120
C7_10	0.581(2)	1.0532(16)	0.4591(15)	0.072(3)
H7A_10	0.571676	1.048949	0.413066	0.107
H7B_10	0.618594	1.099692	0.477538	0.107
H7C_10	0.524433	1.046579	0.466575	0.107
C8_10	0.5299(16)	0.8949(18)	0.4061(11)	0.080(4)
H8A_10	0.512869	0.931780	0.380096	0.120
H8B_10	0.479101	0.866753	0.416338	0.120
H8C_10	0.551023	0.865103	0.382191	0.120
C9_10	0.653(2)	0.8170(11)	0.5074(17)	0.077(4)
H9A_10	0.622489	0.796528	0.463301	0.115
H9B_10	0.621123	0.793305	0.535317	0.115
H9C_10	0.712606	0.811439	0.520890	0.115
C10_10	0.7799(18)	0.9274(18)	0.6207(12)	0.073(4)
H10A_10	0.811333	0.897332	0.607506	0.109
H10B_10	0.750171	0.903843	0.649828	0.109
H10C_10	0.821575	0.971289	0.642473	0.109
O1_24	0.17891(12)	0.97230(11)	0.14075(10)	0.0271(5)
C1_24	0.10045(17)	0.93213(15)	0.14050(14)	0.0263(6)
C2_24	0.0533(2)	0.97982(17)	0.16523(16)	0.0346(7)
F1_24	0.08736(13)	0.99470(11)	0.22829(9)	0.0450(5)
F2_24	-0.03275(11)	0.94999(11)	0.15275(10)	0.0463(5)
F3_24	0.06117(12)	1.03948(10)	0.13882(10)	0.0449(5)
C3_24	0.0439(2)	0.89983(18)	0.07183(16)	0.0364(8)
F4_24	0.09121(13)	0.87215(11)	0.04450(9)	0.0468(5)
F5_24	0.01751(13)	0.94835(11)	0.03584(9)	0.0492(5)
F6_24	-0.02733(13)	0.85026(11)	0.07039(10)	0.0527(6)
C4_24	0.11068(19)	0.87215(17)	0.18448(15)	0.0313(7)
F7_24	0.12921(12)	0.82098(10)	0.15730(10)	0.0412(5)
F8_24	0.03774(12)	0.84449(10)	0.19950(10)	0.0437(5)

F9_24	0.17524(12)	0.89557(10)	0.23873(9)	0.0427(5)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

S-Table 20: Bond lengths and angles for [Al(AlCp*)$_3$][*pf*]

Atom–Atom	**Length [Å]**
Al01–O1_19	1.72(3)
Al01–O1_8	1.723(2)
Al01–O1_6	1.725(2)
Al01–O1_18	1.725(4)
Al01–O1_24	1.728(2)
Al1–Al3	2.5431(14)
Al1–Al2	2.5437(13)
Al1–Al4	2.5749(15)
Al03–O1_17	1.68(2)
Al03–O1_4	1.723(2)
Al03–O1_3	1.730(2)
Al03–O1_2	1.730(2)
Al03–O1_16	1.738(7)
Al2–C3_11	2.185(3)
Al2–C2_11	2.200(3)
Al2–C4_11	2.220(3)
Al2–C1_11	2.221(3)
Al2–C5_11	2.228(3)
Al3–C4_12	2.197(3)
Al3–C5_12	2.207(3)
Al3–C3_12	2.221(3)
Al3–C1_12	2.228(3)
Al3–C2_12	2.230(3)
Al4–C2_10	2.17(2)
Al4–C3_23	2.188(5)
Al4–C4_23	2.196(6)
Al4–C5_23	2.206(5)
Al4–C3_10	2.21(2)
Al4–C2_23	2.213(5)
Al4–C1_23	2.235(5)
Al4–C1_10	2.24(2)
Al4–C4_10	2.29(3)
Al4–C5_10	2.31(3)
Al5–Al8	2.5324(15)
Al5–Al7	2.5340(15)
Al5–Al6	2.5478(14)
Al5–Al5$^{\#1}$	2.838(2)
Al6–C3_14	2.198(3)
Al6–C2_14	2.201(3)
Al6–C4_14	2.219(3)
Al6–C1_14	2.227(3)
Al6–C5_14	2.227(3)
Al7–C3_15	2.197(3)
Al7–C4_15	2.203(3)
Al7–C2_15	2.221(3)
Al7–C1_15	2.228(3)
Al7–C5_15	2.232(3)
Al7–Al8	2.9978(15)
Al8–C1_13	2.182(3)
Al8–C2_13	2.199(3)
Al8–C5_13	2.220(3)
Al8–C3_13	2.222(3)
Al8–C4_13	2.237(3)
C1_1–F1_1	1.344(5)
C1_1–C2_1	1.378(6)
C1_1–C6_1	1.382(6)
C2_1–F2_1	1.340(5)
C2_1–C3_1	1.369(6)
C3_1–C4_1	1.373(7)
C3_1–H_1	0.9500
C4_1–C5_1	1.374(7)
C4_1–HA_1	0.9500
C5_1–C6_1	1.388(7)
C5_1–HB_1	0.9500
C6_1–HC_1	0.9500
O1_2–C1_2	1.352(4)
C1_2–C2_2	1.546(5)
C1_2–C3_2	1.556(5)
C1_2–C4_2	1.565(5)
C2_2–F3_2	1.327(4)
C2_2–F2_2	1.340(4)
C2_2–F1_2	1.340(4)
C3_2–F4_2	1.310(4)
C3_2–F6_2	1.340(4)
C3_2–F5_2	1.347(4)
C4_2–F7_2	1.323(4)
C4_2–F9_2	1.327(4)
C4_2–F8_2	1.338(4)
O1_3–C1_3	1.350(3)
C1_3–C2_3	1.550(5)
C1_3–C3_3	1.555(4)
C1_3–C4_3	1.557(4)
C2_3–F3_3	1.322(4)
C2_3–F1_3	1.332(4)
C2_3–F2_3	1.342(4)
C3_3–F4_3	1.325(4)
C3_3–F5_3	1.336(4)
C3_3–F6_3	1.344(4)
C4_3–F9_3	1.327(4)
C4_3–F7_3	1.330(4)
C4_3–F8_3	1.346(4)
O1_4–C1_4	1.355(3)
C1_4–C2_4	1.548(4)
C1_4–C4_4	1.550(4)
C1_4–C3_4	1.561(4)

C2_4–F3_4	1.328(4)	C9_11–H9A_11	0.9800
C2_4–F1_4	1.333(4)	C9_11–H9B_11	0.9800
C2_4–F2_4	1.344(3)	C9_11–H9C_11	0.9800
C3_4–F4_4	1.321(3)	C10_11–H10A_11	0.9800
C3_4–F5_4	1.337(4)	C10_11–H10B_11	0.9800
C3_4–F6_4	1.340(3)	C10_11–H10C_11	0.9800
C4_4–F7_4	1.330(4)	C1_12–C2_12	1.415(4)
C4_4–F9_4	1.335(4)	C1_12–C5_12	1.424(4)
C4_4–F8_4	1.341(4)	C1_12–C10_12	1.504(4)
O1_6–C1_6	1.351(4)	C2_12–C3_12	1.418(4)
C1_6–C2_6	1.549(4)	C2_12–C9_12	1.506(4)
C1_6–C3_6	1.550(4)	C3_12–C4_12	1.423(4)
C1_6–C4_6	1.552(4)	C3_12–C8_12	1.500(4)
C2_6–F1_6	1.327(4)	C4_12–C5_12	1.422(4)
C2_6–F3_6	1.329(4)	C4_12–C7_12	1.507(4)
C2_6–F2_6	1.334(4)	C5_12–C6_12	1.503(4)
C3_6–F4_6	1.321(4)	C6_12–H6A_12	0.9800
C3_6–F5_6	1.335(4)	C6_12–H6B_12	0.9800
C3_6–F6_6	1.336(4)	C6_12–H6C_12	0.9800
C4_6–F9_6	1.317(4)	C7_12–H7A_12	0.9800
C4_6–F7_6	1.332(4)	C7_12–H7B_12	0.9800
C4_6–F8_6	1.344(4)	C7_12–H7C_12	0.9800
O1_8–C1_8	1.349(4)	C8_12–H8A_12	0.9800
C1_8–C4_8	1.538(5)	C8_12–H8B_12	0.9800
C1_8–C2_8	1.548(5)	C8_12–H8C_12	0.9800
C1_8–C3_8	1.564(5)	C9_12–H9A_12	0.9800
C2_8–F3_8	1.315(4)	C9_12–H9B_12	0.9800
C2_8–F1_8	1.337(4)	C9_12–H9C_12	0.9800
C2_8–F2_8	1.342(4)	C10_12–H10A_12	0.9800
C3_8–F5_8	1.328(5)	C10_12–H10B_12	0.9800
C3_8–F4_8	1.330(4)	C10_12–H10C_12	0.9800
C3_8–F6_8	1.333(4)	C1_13–C5_13	1.419(5)
C4_8–F9_8	1.339(5)	C1_13–C2_13	1.439(5)
C4_8–F8_8	1.341(4)	C1_13–C10_13	1.511(5)
C4_8–F7_8	1.345(5)	C2_13–C3_13	1.427(4)
C1_11–C5_11	1.423(4)	C2_13–C9_13	1.502(5)
C1_11–C2_11	1.433(4)	C3_13–C4_13	1.430(5)
C1_11–C10_11	1.507(4)	C3_13–C8_13	1.499(4)
C2_11–C3_11	1.427(4)	C4_13–C5_13	1.405(5)
C2_11–C9_11	1.506(4)	C4_13–C7_13	1.500(5)
C3_11–C4_11	1.425(4)	C5_13–C6_13	1.510(5)
C3_11–C8_11	1.499(4)	C6_13–H_13	0.9800
C4_11–C5_11	1.417(4)	C6_13–HA_13	0.9800
C4_11–C7_11	1.500(4)	C6_13–HB_13	0.9800
C5_11–C6_11	1.512(4)	C7_13–HC_13	0.9800
C6_11–H6A_11	0.9800	C7_13–HD_13	0.9800
C6_11–H6B_11	0.9800	C7_13–HE_13	0.9800
C6_11–H6C_11	0.9800	C8_13–HF_13	0.9800
C7_11–H7A_11	0.9800	C8_13–HG_13	0.9800
C7_11–H7B_11	0.9800	C8_13–HH_13	0.9800
C7_11–H7C_11	0.9800	C9_13–HI_13	0.9800
C8_11–H8A_11	0.9800	C9_13–HJ_13	0.9800
C8_11–H8B_11	0.9800	C9_13–HK_13	0.9800
C8_11–H8C_11	0.9800	C10_13–HL_13	0.9800

C10_13–HM_13	0.9800	C1_16–C4_16	1.544(6)
C10_13–HN_13	0.9800	C1_16–C2_16	1.552(6)
C1_14–C2_14	1.424(4)	C2_16–F1_16	1.289(7)
C1_14–C5_14	1.424(4)	C2_16–F3_16	1.349(6)
C1_14–C10_14	1.502(5)	C2_16–F2_16	1.360(7)
C2_14–C3_14	1.427(5)	C3_16–F5_16	1.307(6)
C2_14–C9_14	1.503(4)	C3_16–F6_16	1.344(7)
C3_14–C4_14	1.414(4)	C3_16–F4_16	1.350(6)
C3_14–C8_14	1.511(4)	C4_16–F7_16	1.316(6)
C4_14–C5_14	1.416(4)	C4_16–F9_16	1.332(6)
C4_14–C7_14	1.505(5)	C4_16–F8_16	1.344(7)
C5_14–C6_14	1.503(4)	O1_17–C1_17	1.349(13)
C6_14–H_14	0.9800	C1_17–C4_17	1.549(12)
C6_14–HA_14	0.9800	C1_17–C3_17	1.553(12)
C6_14–HB_14	0.9800	C1_17–C2_17	1.558(12)
C7_14–HC_14	0.9800	C2_17–F3_17	1.328(12)
C7_14–HD_14	0.9800	C2_17–F2_17	1.353(13)
C7_14–HE_14	0.9800	C2_17–F1_17	1.355(12)
C8_14–HF_14	0.9800	C3_17–F6_17	1.326(13)
C8_14–HG_14	0.9800	C3_17–F4_17	1.333(12)
C8_14–HH_14	0.9800	C3_17–F5_17	1.382(12)
C9_14–HI_14	0.9800	C4_17–F8_17	1.322(13)
C9_14–HJ_14	0.9800	C4_17–F9_17	1.323(12)
C9_14–HK_14	0.9800	C4_17–F7_17	1.348(12)
C10_14–HL_14	0.9800	O1_18–C1_18	1.358(4)
C10_14–HM_14	0.9800	C1_18–C4_18	1.550(5)
C10_14–HN_14	0.9800	C1_18–C3_18	1.552(5)
C1_15–C5_15	1.422(4)	C1_18–C2_18	1.557(5)
C1_15–C2_15	1.431(4)	C2_18–F3_18	1.319(6)
C1_15–C10_15	1.506(4)	C2_18–F1_18	1.338(5)
C2_15–C3_15	1.424(4)	C2_18–F2_18	1.339(6)
C2_15–C9_15	1.495(4)	C3_18–F5_18	1.326(5)
C3_15–C4_15	1.422(4)	C3_18–F4_18	1.333(5)
C3_15–C8_15	1.503(4)	C3_18–F6_18	1.337(6)
C4_15–C5_15	1.422(4)	C4_18–F9_18	1.327(5)
C4_15–C7_15	1.500(4)	C4_18–F7_18	1.334(4)
C5_15–C6_15	1.504(4)	C4_18–F8_18	1.339(5)
C6_15–H_15	0.9800	O1_19–C1_19	1.353(14)
C6_15–HA_15	0.9800	C1_19–C3_19	1.551(13)
C6_15–HB_15	0.9800	C1_19–C2_19	1.552(13)
C7_15–HC_15	0.9800	C1_19–C4_19	1.555(13)
C7_15–HD_15	0.9800	C2_19–F1_19	1.329(13)
C7_15–HE_15	0.9800	C2_19–F3_19	1.330(13)
C8_15–HF_15	0.9800	C2_19–F2_19	1.334(14)
C8_15–HG_15	0.9800	C3_19–F4_19	1.329(14)
C8_15–HH_15	0.9800	C3_19–F6_19	1.332(14)
C9_15–HI_15	0.9800	C3_19–F5_19	1.335(13)
C9_15–HJ_15	0.9800	C4_19–F7_19	1.325(13)
C9_15–HK_15	0.9800	C4_19–F9_19	1.329(13)
C10_15–HL_15	0.9800	C4_19–F8_19	1.334(14)
C10_15–HM_15	0.9800	C1_20–F1_20	1.345(7)
C10_15–HN_15	0.9800	C1_20–C2_20	1.366(7)
O1_16–C1_16	1.354(6)	C1_20–C6_20	1.378(8)
C1_16–C3_16	1.537(6)	C2_20–F2_20	1.340(9)

C2_20–C3_20	1.366(7)
C3_20–C4_20	1.374(8)
C3_20–H_20	0.9500
C4_20–C5_20	1.377(8)
C4_20–HA_20	0.9500
C5_20–C6_20	1.371(8)
C5_20–HB_20	0.9500
C6_20–HC_20	0.9500
C1_21–F1_21	1.335(14)
C1_21–C2_21	1.366(12)
C1_21–C6_21	1.374(13)
C2_21–F2_21	1.345(13)
C2_21–C3_21	1.365(13)
C3_21–C4_21	1.370(13)
C3_21–H_21	0.9500
C4_21–C5_21	1.374(13)
C4_21–HA_21	0.9500
C5_21–C6_21	1.378(13)
C5_21–HB_21	0.9500
C6_21–HC_21	0.9500
C1_22–F1_22	1.340(14)
C1_22–C2_22	1.376(13)
C1_22–C6_22	1.382(13)
C2_22–F2_22	1.339(14)
C2_22–C3_22	1.374(13)
C3_22–C4_22	1.370(14)
C3_22–H_22	0.9500
C4_22–C5_22	1.379(14)
C4_22–HA_22	0.9500
C5_22–C6_22	1.383(14)
C5_22–HB_22	0.9500
C6_22–HC_22	0.9500
C1_23–C2_23	1.408(6)
C1_23–C5_23	1.413(6)
C1_23–C10_23	1.505(6)
C2_23–C3_23	1.410(6)
C2_23–C9_23	1.511(6)
C3_23–C4_23	1.424(6)
C3_23–C8_23	1.511(6)
C4_23–C5_23	1.404(6)
C4_23–C7_23	1.505(6)
C5_23–C6_23	1.508(6)
C6_23–H6A_23	0.9800
C6_23–H6B_23	0.9800
C6_23–H6C_23	0.9800
C7_23–H7A_23	0.9800
C7_23–H7B_23	0.9800
C7_23–H7C_23	0.9800
C8_23–H8A_23	0.9800
C8_23–H8B_23	0.9800
C8_23–H8C_23	0.9800
C9_23–H9A_23	0.9800
C9_23–H9B_23	0.9800
C9_23–H9C_23	0.9800
C10_23–H10A_23	0.9800
C10_23–H10B_23	0.9800
C10_23–H10C_23	0.9800
C1_10–C5_10	1.411(12)
C1_10–C2_10	1.416(13)
C1_10–C10_10	1.505(13)
C2_10–C3_10	1.421(12)
C2_10–C9_10	1.506(13)
C3_10–C4_10	1.419(12)
C3_10–C8_10	1.507(13)
C4_10–C5_10	1.422(13)
C4_10–C7_10	1.509(12)
C5_10–C6_10	1.515(13)
C6_10–H6A_10	0.9800
C6_10–H6B_10	0.9800
C6_10–H6C_10	0.9800
C7_10–H7A_10	0.9800
C7_10–H7B_10	0.9800
C7_10–H7C_10	0.9800
C8_10–H8A_10	0.9800
C8_10–H8B_10	0.9800
C8_10–H8C_10	0.9800
C9_10–H9A_10	0.9800
C9_10–H9B_10	0.9800
C9_10–H9C_10	0.9800
C10_10–H10A_10	0.9800
C10_10–H10B_10	0.9800
C10_10–H10C_10	0.9800
O1_24–C1_24	1.346(3)
C1_24–C3_24	1.553(4)
C1_24–C4_24	1.556(4)
C1_24–C2_24	1.558(4)
C2_24–F3_24	1.322(4)
C2_24–F1_24	1.334(4)
C2_24–F2_24	1.343(4)
C3_24–F6_24	1.329(4)
C3_24–F5_24	1.330(4)
C3_24–F4_24	1.335(4)
C4_24–F7_24	1.321(4)
C4_24–F9_24	1.328(4)
C4_24–F8_24	1.340(3)

Atom–Atom–Atom	**Angle [°]**
O1_19–Al01–O1_8	103.2(15)
O1_19–Al01–O1_6	117.2(16)
O1_8–Al01–O1_6	106.33(11)
O1_8–Al01–O1_18	108.11(19)
O1_6–Al01–O1_18	113.9(2)
O1_8–Al01–O1_24	114.77(11)
O1_6–Al01–O1_24	106.27(11)
O1_18–Al01–O1_24	107.60(19)
Al3–Al1–Al2	73.14(4)
Al3–Al1–Al4	73.12(4)
Al2–Al1–Al4	74.56(4)

O1_17–Al03–O1_4	110.9(11)	C1_10–Al4–C4_10	61.8(7)
O1_17–Al03–O1_3	107.4(13)	C2_10–Al4–C5_10	60.5(7)
O1_4–Al03–O1_3	111.30(11)	C3_10–Al4–C5_10	60.3(7)
O1_17–Al03–O1_2	110.9(13)	C1_10–Al4–C5_10	36.0(5)
O1_4–Al03–O1_2	108.81(11)	C4_10–Al4–C5_10	36.0(5)
O1_3–Al03–O1_2	107.40(11)	C2_10–Al4–Al1	132.8(5)
O1_4–Al03–O1_16	106.7(3)	C3_23–Al4–Al1	164.72(15)
O1_3–Al03–O1_16	109.6(3)	C4_23–Al4–Al1	130.02(14)
O1_2–Al03–O1_16	113.0(3)	C5_23–Al4–Al1	114.31(14)
C3_11–Al2–C2_11	37.98(10)	C3_10–Al4–Al1	169.2(5)
C3_11–Al2–C4_11	37.74(10)	C2_23–Al4–Al1	156.49(15)
C2_11–Al2–C4_11	63.06(11)	C1_23–Al4–Al1	125.21(14)
C3_11–Al2–C1_11	63.16(11)	C1_10–Al4–Al1	113.6(6)
C2_11–Al2–C1_11	37.83(10)	C4_10–Al4–Al1	152.2(6)
C4_11–Al2–C1_11	62.59(11)	C5_10–Al4–Al1	123.4(6)
C3_11–Al2–C5_11	62.71(11)	Al8–Al5–Al7	72.56(4)
C2_11–Al2–C5_11	62.77(11)	Al8–Al5–Al6	74.09(5)
C4_11–Al2–C5_11	37.16(10)	Al7–Al5–Al6	72.99(5)
C1_11–Al2–C5_11	37.30(10)	Al8–Al5–Al5	134.65(6)
C3_11–Al2–Al1	153.98(9)	Al7–Al5–Al5	130.30(6)
C2_11–Al2–Al1	167.73(9)	Al6–Al5–Al5	143.48(6)
C4_11–Al2–Al1	127.70(9)	C3_14–Al6–C2_14	37.87(12)
C1_11–Al2–Al1	137.36(9)	C3_14–Al6–C4_14	37.33(12)
C5_11–Al2–Al1	121.01(9)	C2_14–Al6–C4_14	62.66(12)
C4_12–Al3–C5_12	37.69(11)	C3_14–Al6–C1_14	62.86(12)
C4_12–Al3–C3_12	37.58(11)	C2_14–Al6–C1_14	37.51(11)
C5_12–Al3–C3_12	62.64(11)	C4_14–Al6–C1_14	62.46(12)
C4_12–Al3–C1_12	62.62(11)	C3_14–Al6–C5_14	62.36(12)
C5_12–Al3–C1_12	37.44(11)	C2_14–Al6–C5_14	62.42(12)
C3_12–Al3–C1_12	62.18(11)	C4_14–Al6–C5_14	37.15(12)
C4_12–Al3–C2_12	62.49(11)	C1_14–Al6–C5_14	37.29(12)
C5_12–Al3–C2_12	62.35(11)	C3_14–Al6–Al5	165.30(10)
C3_12–Al3–C2_12	37.16(11)	C2_14–Al6–Al5	156.20(10)
C1_12–Al3–C2_12	37.02(11)	C4_14–Al6–Al5	131.99(10)
C4_12–Al3–Al1	168.13(9)	C1_14–Al6–Al5	125.64(10)
C5_12–Al3–Al1	154.12(9)	C5_14–Al6–Al5	115.81(9)
C3_12–Al3–Al1	135.22(9)	C3_15–Al7–C4_15	37.70(11)
C1_12–Al3–Al1	125.78(9)	C3_15–Al7–C2_15	37.59(11)
C2_12–Al3–Al1	118.01(9)	C4_15–Al7–C2_15	62.88(11)
C3_23–Al4–C4_23	37.92(18)	C3_15–Al7–C1_15	62.61(11)
C3_23–Al4–C5_23	62.32(18)	C4_15–Al7–C1_15	62.50(11)
C4_23–Al4–C5_23	37.19(17)	C2_15–Al7–C1_15	37.51(11)
C2_10–Al4–C3_10	37.9(5)	C3_15–Al7–C5_15	62.64(11)
C3_23–Al4–C2_23	37.36(17)	C4_15–Al7–C5_15	37.40(11)
C4_23–Al4–C2_23	62.67(18)	C2_15–Al7–C5_15	62.59(11)
C5_23–Al4–C2_23	61.84(17)	C1_15–Al7–C5_15	37.20(11)
C3_23–Al4–C1_23	62.25(17)	C3_15–Al7–Al5	166.77(10)
C4_23–Al4–C1_23	62.43(18)	C4_15–Al7–Al5	155.39(9)
C5_23–Al4–C1_23	37.08(16)	C2_15–Al7–Al5	133.84(9)
C2_23–Al4–C1_23	36.91(16)	C1_15–Al7–Al5	117.38(9)
C2_10–Al4–C1_10	37.4(5)	C5_15–Al7–Al5	126.32(9)
C3_10–Al4–C1_10	62.5(6)	C3_15–Al7–Al8	133.05(9)
C2_10–Al4–C4_10	62.2(7)	C4_15–Al7–Al8	113.39(9)
C3_10–Al4–C4_10	36.8(5)	C2_15–Al7–Al8	169.01(9)

C1_15–Al7–Al8	151.79(9)	F1_2–C2_2–C1_2	111.0(3)
C5_15–Al7–Al8	121.56(9)	F4_2–C3_2–F6_2	108.3(3)
Al5–Al7–Al8	53.70(4)	F4_2–C3_2–F5_2	107.9(3)
C1_13–Al8–C2_13	38.37(13)	F6_2–C3_2–F5_2	107.0(3)
C1_13–Al8–C5_13	37.59(13)	F4_2–C3_2–C1_2	111.0(3)
C2_13–Al8–C5_13	63.52(13)	F6_2–C3_2–C1_2	112.2(3)
C1_13–Al8–C3_13	62.80(12)	F5_2–C3_2–C1_2	110.2(3)
C2_13–Al8–C3_13	37.67(12)	F7_2–C4_2–F9_2	108.1(3)
C5_13–Al8–C3_13	62.43(12)	F7_2–C4_2–F8_2	107.3(3)
C1_13–Al8–C4_13	62.15(13)	F9_2–C4_2–F8_2	107.1(3)
C2_13–Al8–C4_13	62.94(13)	F7_2–C4_2–C1_2	111.0(3)
C5_13–Al8–C4_13	36.73(12)	F9_2–C4_2–C1_2	110.7(3)
C3_13–Al8–C4_13	37.41(12)	F8_2–C4_2–C1_2	112.3(3)
C1_13–Al8–Al5	151.92(11)	C1_3–O1_3–Al03	146.7(2)
C2_13–Al8–Al5	169.65(10)	O1_3–C1_3–C2_3	111.0(3)
C5_13–Al8–Al5	125.12(11)	O1_3–C1_3–C3_3	107.5(2)
C3_13–Al8–Al5	137.81(9)	C2_3–C1_3–C3_3	109.1(3)
C4_13–Al8–Al5	119.61(10)	O1_3–C1_3–C4_3	110.8(2)
C1_13–Al8–Al7	146.04(12)	C2_3–C1_3–C4_3	109.8(3)
C2_13–Al8–Al7	117.04(10)	C3_3–C1_3–C4_3	108.5(3)
C5_13–Al8–Al7	174.65(10)	F3_3–C2_3–F1_3	107.8(3)
C3_13–Al8–Al7	114.41(9)	F3_3–C2_3–F2_3	107.2(3)
C4_13–Al8–Al7	138.14(9)	F1_3–C2_3–F2_3	106.8(3)
Al5–Al8–Al7	53.75(4)	F3_3–C2_3–C1_3	111.0(3)
F1_1–C1_1–C2_1	119.6(4)	F1_3–C2_3–C1_3	111.2(3)
F1_1–C1_1–C6_1	119.7(5)	F2_3–C2_3–C1_3	112.6(3)
C2_1–C1_1–C6_1	120.6(4)	F4_3–C3_3–F5_3	107.3(3)
F2_1–C2_1–C3_1	121.2(5)	F4_3–C3_3–F6_3	107.7(3)
F2_1–C2_1–C1_1	117.6(4)	F5_3–C3_3–F6_3	107.1(3)
C3_1–C2_1–C1_1	121.2(4)	F4_3–C3_3–C1_3	111.1(3)
C2_1–C3_1–C4_1	118.8(5)	F5_3–C3_3–C1_3	110.6(3)
C2_1–C3_1–H_1	120.6	F6_3–C3_3–C1_3	112.8(3)
C4_1–C3_1–H_1	120.6	F9_3–C4_3–F7_3	108.0(3)
C3_1–C4_1–C5_1	120.3(5)	F9_3–C4_3–F8_3	107.2(3)
C3_1–C4_1–HA_1	119.8	F7_3–C4_3–F8_3	107.6(3)
C5_1–C4_1–HA_1	119.8	F9_3–C4_3–C1_3	110.6(3)
C4_1–C5_1–C6_1	121.5(5)	F7_3–C4_3–C1_3	111.4(3)
C4_1–C5_1–HB_1	119.3	F8_3–C4_3–C1_3	111.9(3)
C6_1–C5_1–HB_1	119.3	C1_4–O1_4–Al03	147.29(19)
C1_1–C6_1–C5_1	117.5(5)	O1_4–C1_4–C2_4	110.7(2)
C1_1–C6_1–HC_1	121.2	O1_4–C1_4–C4_4	107.2(2)
C5_1–C6_1–HC_1	121.2	C2_4–C1_4–C4_4	109.4(2)
C1_2–O1_2–Al03	145.1(2)	O1_4–C1_4–C3_4	111.7(2)
O1_2–C1_2–C2_2	107.8(3)	C2_4–C1_4–C3_4	108.9(2)
O1_2–C1_2–C3_2	111.4(3)	C4_4–C1_4–C3_4	108.8(2)
C2_2–C1_2–C3_2	109.5(3)	F3_4–C2_4–F1_4	107.4(2)
O1_2–C1_2–C4_2	110.0(3)	F3_4–C2_4–F2_4	107.6(2)
C2_2–C1_2–C4_2	109.5(3)	F1_4–C2_4–F2_4	107.4(2)
C3_2–C1_2–C4_2	108.5(3)	F3_4–C2_4–C1_4	110.9(2)
F3_2–C2_2–F2_2	107.2(3)	F1_4–C2_4–C1_4	111.3(2)
F3_2–C2_2–F1_2	107.1(3)	F2_4–C2_4–C1_4	112.1(2)
F2_2–C2_2–F1_2	107.3(3)	F4_4–C3_4–F5_4	107.7(3)
F3_2–C2_2–C1_2	111.1(3)	F4_4–C3_4–F6_4	107.7(2)
F2_2–C2_2–C1_2	112.8(3)	F5_4–C3_4–F6_4	107.2(2)

F4_4–C3_4–C1_4	110.9(2)	F9_8–C4_8–F7_8	108.3(3)
F5_4–C3_4–C1_4	111.0(2)	F8_8–C4_8–F7_8	107.5(3)
F6_4–C3_4–C1_4	112.2(2)	F9_8–C4_8–C1_8	110.8(3)
F7_4–C4_4–F9_4	107.0(3)	F8_8–C4_8–C1_8	112.4(3)
F7_4–C4_4–F8_4	107.7(3)	F7_8–C4_8–C1_8	110.4(3)
F9_4–C4_4–F8_4	106.9(3)	C5_11–C1_11–C2_11	107.7(2)
F7_4–C4_4–C1_4	111.5(3)	C5_11–C1_11–C10_11	124.6(3)
F9_4–C4_4–C1_4	110.6(3)	C2_11–C1_11–C10_11	127.7(3)
F8_4–C4_4–C1_4	112.9(3)	C5_11–C1_11–Al2	71.62(16)
C1_6–O1_6–Al01	147.3(2)	C2_11–C1_11–Al2	70.27(15)
O1_6–C1_6–C2_6	110.9(3)	C10_11–C1_11–Al2	125.9(2)
O1_6–C1_6–C3_6	110.8(2)	C3_11–C2_11–C1_11	107.6(2)
C2_6–C1_6–C3_6	109.7(3)	C3_11–C2_11–C9_11	124.5(3)
O1_6–C1_6–C4_6	107.2(3)	C1_11–C2_11–C9_11	127.7(3)
C2_6–C1_6–C4_6	109.1(3)	C3_11–C2_11–Al2	70.46(16)
C3_6–C1_6–C4_6	109.2(3)	C1_11–C2_11–Al2	71.90(15)
F1_6–C2_6–F3_6	106.8(3)	C9_11–C2_11–Al2	126.5(2)
F1_6–C2_6–F2_6	107.9(3)	C4_11–C3_11–C2_11	108.3(2)
F3_6–C2_6–F2_6	107.2(3)	C4_11–C3_11–C8_11	126.2(3)
F1_6–C2_6–C1_6	111.0(3)	C2_11–C3_11–C8_11	125.4(3)
F3_6–C2_6–C1_6	110.4(3)	C4_11–C3_11–Al2	72.44(16)
F2_6–C2_6–C1_6	113.1(3)	C2_11–C3_11–Al2	71.55(15)
F4_6–C3_6–F5_6	106.9(3)	C8_11–C3_11–Al2	124.9(2)
F4_6–C3_6–F6_6	108.1(3)	C5_11–C4_11–C3_11	107.8(2)
F5_6–C3_6–F6_6	107.0(3)	C5_11–C4_11–C7_11	127.1(3)
F4_6–C3_6–C1_6	111.1(3)	C3_11–C4_11–C7_11	125.0(3)
F5_6–C3_6–C1_6	110.9(3)	C5_11–C4_11–Al2	71.75(16)
F6_6–C3_6–C1_6	112.4(3)	C3_11–C4_11–Al2	69.82(16)
F9_6–C4_6–F7_6	107.7(3)	C7_11–C4_11–Al2	126.0(2)
F9_6–C4_6–F8_6	107.6(3)	C4_11–C5_11–C1_11	108.6(2)
F7_6–C4_6–F8_6	107.4(3)	C4_11–C5_11–C6_11	127.3(3)
F9_6–C4_6–C1_6	111.0(3)	C1_11–C5_11–C6_11	124.1(3)
F7_6–C4_6–C1_6	110.6(3)	C4_11–C5_11–Al2	71.10(16)
F8_6–C4_6–C1_6	112.3(3)	C1_11–C5_11–Al2	71.09(16)
C1_8–O1_8–Al01	148.1(2)	C6_11–C5_11–Al2	124.1(2)
O1_8–C1_8–C4_8	109.7(3)	C5_11–C6_11–H6A_11	109.5
O1_8–C1_8–C2_8	112.2(3)	C5_11–C6_11–H6B_11	109.5
C4_8–C1_8–C2_8	109.6(3)	H6A_11–C6_11–H6B_11	109.5
O1_8–C1_8–C3_8	107.1(3)		
C4_8–C1_8–C3_8	110.0(3)	C5_11–C6_11–H6C_11	109.5
C2_8–C1_8–C3_8	108.2(3)	H6A_11–C6_11–H6C_11	109.5
F3_8–C2_8–F1_8	106.7(3)		
F3_8–C2_8–F2_8	108.1(3)	H6B_11–C6_11–H6C_11	109.5
F1_8–C2_8–F2_8	106.6(3)		
F3_8–C2_8–C1_8	111.3(3)	C4_11–C7_11–H7A_11	109.5
F1_8–C2_8–C1_8	111.1(3)	C4_11–C7_11–H7B_11	109.5
F2_8–C2_8–C1_8	112.7(3)	H7A_11–C7_11–H7B_11	109.5
F5_8–C3_8–F4_8	108.1(3)		
F5_8–C3_8–F6_8	107.6(3)	C4_11–C7_11–H7C_11	109.5
F4_8–C3_8–F6_8	108.1(3)	H7A_11–C7_11–H7C_11	109.5
F5_8–C3_8–C1_8	110.8(3)		
F4_8–C3_8–C1_8	110.3(3)	H7B_11–C7_11–H7C_11	109.5
F6_8–C3_8–C1_8	111.8(3)		
F9_8–C4_8–F8_8	107.3(4)	C3_11–C8_11–H8A_11	109.5

C3_11–C8_11–H8B_11	109.5	C4_12–C5_12–C6_12	124.4(3)
H8A_11–C8_11–H8B_11	109.5	C1_12–C5_12–C6_12	127.6(3)
C3_11–C8_11–H8C_11	109.5	C4_12–C5_12–Al3	70.77(17)
H8A_11–C8_11–H8C_11	109.5	C1_12–C5_12–Al3	72.09(17)
H8B_11–C8_11–H8C_11	109.5	C6_12–C5_12–Al3	126.2(2)
C2_11–C9_11–H9A_11	109.5	C5_12–C6_12–H6A_12	109.5
C2_11–C9_11–H9B_11	109.5	C5_12–C6_12–H6B_12	109.5
H9A_11–C9_11–H9B_11	109.5	H6A_12–C6_12–H6B_12	109.5
C2_11–C9_11–H9C_11	109.5	C5_12–C6_12–H6C_12	109.5
H9A_11–C9_11–H9C_11	109.5	H6A_12–C6_12–H6C_12	109.5
H9B_11–C9_11–H9C_11	109.5	H6B_12–C6_12–H6C_12	109.5
C1_11–C10_11–H10A_11	109.5	C4_12–C7_12–H7A_12	109.5
C1_11–C10_11–H10B_11	109.5	C4_12–C7_12–H7B_12	109.5
H10A_11–C10_11–H10B_11	109.5	H7A_12–C7_12–H7B_12	109.5
C1_11–C10_11–H10C_11	109.5	C4_12–C7_12–H7C_12	109.5
H10A_11–C10_11–H10C_11	109.5	H7A_12–C7_12–H7C_12	109.5
H10B_11–C10_11–H10C_11	109.5	H7B_12–C7_12–H7C_12	109.5
C2_12–C1_12–C5_12	108.0(3)	C3_12–C8_12–H8A_12	109.5
C2_12–C1_12–C10_12	124.6(3)	C3_12–C8_12–H8B_12	109.5
C5_12–C1_12–C10_12	127.4(3)	H8A_12–C8_12–H8B_12	109.5
C2_12–C1_12–Al3	71.55(16)	C3_12–C8_12–H8C_12	109.5
C5_12–C1_12–Al3	70.47(17)	H8A_12–C8_12–H8C_12	109.5
C10_12–C1_12–Al3	123.0(2)	H8B_12–C8_12–H8C_12	109.5
C1_12–C2_12–C3_12	108.4(3)	C2_12–C9_12–H9A_12	109.5
C1_12–C2_12–C9_12	125.7(3)	C2_12–C9_12–H9B_12	109.5
C3_12–C2_12–C9_12	125.9(3)	H9A_12–C9_12–H9B_12	109.5
C1_12–C2_12–Al3	71.43(16)	C2_12–C9_12–H9C_12	109.5
C3_12–C2_12–Al3	71.09(16)	H9A_12–C9_12–H9C_12	109.5
C9_12–C2_12–Al3	123.3(2)	H9B_12–C9_12–H9C_12	109.5
C2_12–C3_12–C4_12	107.8(3)	C1_12–C10_12–H10A_12	109.5
C2_12–C3_12–C8_12	125.2(3)	C1_12–C10_12–H10B_12	109.5
C4_12–C3_12–C8_12	126.9(3)	H10A_12–C10_12–H10B_12	109.5
C2_12–C3_12–Al3	71.74(16)	C1_12–C10_12–H10C_12	109.5
C4_12–C3_12–Al3	70.28(16)	H10A_12–C10_12–H10C_12	109.5
C8_12–C3_12–Al3	125.1(2)	H10B_12–C10_12–H10C_12	109.5
C5_12–C4_12–C3_12	108.0(3)	C5_13–C1_13–C2_13	109.0(3)
C5_12–C4_12–C7_12	124.9(3)		
C3_12–C4_12–C7_12	127.0(3)		
C5_12–C4_12–Al3	71.54(17)		
C3_12–C4_12–Al3	72.14(17)		
C7_12–C4_12–Al3	125.1(2)		
C4_12–C5_12–C1_12	107.8(3)		

C5_13–C1_13–C10_13	126.4(4)	C1_13–C10_13–HM_13	109.5
C2_13–C1_13–C10_13	124.5(4)	HL_13–C10_13–HM_13	109.5
C5_13–C1_13–Al8	72.69(19)	C1_13–C10_13–HN_13	109.5
C2_13–C1_13–Al8	71.45(17)	HL_13–C10_13–HN_13	109.5
C10_13–C1_13–Al8	125.8(2)	HM_13–C10_13–HN_13	109.5
C3_13–C2_13–C1_13	106.3(3)	C2_14–C1_14–C5_14	107.4(3)
C3_13–C2_13–C9_13	127.2(3)	C2_14–C1_14–C10_14	127.1(3)
C1_13–C2_13–C9_13	126.4(3)	C5_14–C1_14–C10_14	125.5(3)
C3_13–C2_13–Al8	72.04(18)	C2_14–C1_14–Al6	70.24(17)
C1_13–C2_13–Al8	70.18(18)	C5_14–C1_14–Al6	71.37(18)
C9_13–C2_13–Al8	125.5(2)	C10_14–C1_14–Al6	125.2(2)
C2_13–C3_13–C4_13	108.3(3)	C1_14–C2_14–C3_14	108.1(3)
C2_13–C3_13–C8_13	127.2(3)	C1_14–C2_14–C9_14	126.4(3)
C4_13–C3_13–C8_13	124.5(3)	C3_14–C2_14–C9_14	125.4(3)
C2_13–C3_13–Al8	70.29(18)	C1_14–C2_14–Al6	72.25(17)
C4_13–C3_13–Al8	71.87(18)	C3_14–C2_14–Al6	70.96(17)
C8_13–C3_13–Al8	125.8(2)	C9_14–C2_14–Al6	126.5(2)
C5_13–C4_13–C3_13	108.6(3)	C4_14–C3_14–C2_14	108.0(3)
C5_13–C4_13–C7_13	126.2(3)	C4_14–C3_14–C8_14	126.8(3)
C3_13–C4_13–C7_13	125.2(3)	C2_14–C3_14–C8_14	125.0(3)
C5_13–C4_13–Al8	70.99(19)	C4_14–C3_14–Al6	72.14(18)
C3_13–C4_13–Al8	70.71(18)	C2_14–C3_14–Al6	71.17(17)
C7_13–C4_13–Al8	123.9(2)	C8_14–C3_14–Al6	126.0(2)
C4_13–C5_13–C1_13	107.8(3)	C3_14–C4_14–C5_14	108.1(3)
C4_13–C5_13–C6_13	127.6(4)	C3_14–C4_14–C7_14	127.1(3)
C1_13–C5_13–C6_13	124.6(3)	C5_14–C4_14–C7_14	124.7(3)
C4_13–C5_13–Al8	72.28(19)	C3_14–C4_14–Al6	70.53(18)
C1_13–C5_13–Al8	69.73(19)	C5_14–C4_14–Al6	71.76(19)
C6_13–C5_13–Al8	124.3(2)	C7_14–C4_14–Al6	124.3(2)
C5_13–C6_13–H_13	109.5	C4_14–C5_14–C1_14	108.5(3)
C5_13–C6_13–HA_13	109.5	C4_14–C5_14–C6_14	125.8(3)
H_13–C6_13–HA_13	109.5	C1_14–C5_14–C6_14	125.7(3)
C5_13–C6_13–HB_13	109.5	C4_14–C5_14–Al6	71.09(18)
H_13–C6_13–HB_13	109.5	C1_14–C5_14–Al6	71.34(18)
HA_13–C6_13–HB_13	109.5	C6_14–C5_14–Al6	124.0(2)
C4_13–C7_13–HC_13	109.5	C5_14–C6_14–H_14	109.5
C4_13–C7_13–HD_13	109.5	C5_14–C6_14–HA_14	109.5
HC_13–C7_13–HD_13	109.5	H_14–C6_14–HA_14	109.5
C4_13–C7_13–HE_13	109.5	C5_14–C6_14–HB_14	109.5
HC_13–C7_13–HE_13	109.5	H_14–C6_14–HB_14	109.5
HD_13–C7_13–HE_13	109.5	HA_14–C6_14–HB_14	109.5
C3_13–C8_13–HF_13	109.5	C4_14–C7_14–HC_14	109.5
C3_13–C8_13–HG_13	109.5	C4_14–C7_14–HD_14	109.5
HF_13–C8_13–HG_13	109.5	HC_14–C7_14–HD_14	109.5
C3_13–C8_13–HH_13	109.5	C4_14–C7_14–HE_14	109.5
HF_13–C8_13–HH_13	109.5	HC_14–C7_14–HE_14	109.5
HG_13–C8_13–HH_13	109.5	HD_14–C7_14–HE_14	109.5
C2_13–C9_13–HI_13	109.5	C3_14–C8_14–HF_14	109.5
C2_13–C9_13–HJ_13	109.5	C3_14–C8_14–HG_14	109.5
HI_13–C9_13–HJ_13	109.5	HF_14–C8_14–HG_14	109.5
C2_13–C9_13–HK_13	109.5	C3_14–C8_14–HH_14	109.5
HI_13–C9_13–HK_13	109.5		
HJ_13–C9_13–HK_13	109.5		
C1_13–C10_13–HL_13	109.5		

HF_14–C8_14–HH_14	109.5
HG_14–C8_14–HH_14	109.5
C2_14–C9_14–HI_14	109.5
C2_14–C9_14–HJ_14	109.5
HI_14–C9_14–HJ_14	109.5
C2_14–C9_14–HK_14	109.5
HI_14–C9_14–HK_14	109.5
HJ_14–C9_14–HK_14	109.5
C1_14–C10_14–HL_14	109.5
C1_14–C10_14–HM_14	109.5
HL_14–C10_14–HM_14	109.5
C1_14–C10_14–HN_14	109.5
HL_14–C10_14–HN_14	109.5
HM_14–C10_14–HN_14	109.5
C5_15–C1_15–C2_15	108.4(3)
C5_15–C1_15–C10_15	125.9(3)
C2_15–C1_15–C10_15	125.8(3)
C5_15–C1_15–Al7	71.55(17)
C2_15–C1_15–Al7	71.00(16)
C10_15–C1_15–Al7	123.0(2)
C3_15–C2_15–C1_15	107.3(3)
C3_15–C2_15–C9_15	127.0(3)
C1_15–C2_15–C9_15	125.6(3)
C3_15–C2_15–Al7	70.27(16)
C1_15–C2_15–Al7	71.49(16)
C9_15–C2_15–Al7	124.1(2)
C4_15–C3_15–C2_15	108.4(3)
C4_15–C3_15–C8_15	124.6(3)
C2_15–C3_15–C8_15	126.9(3)
C4_15–C3_15–Al7	71.37(17)
C2_15–C3_15–Al7	72.14(17)
C8_15–C3_15–Al7	124.9(2)
C3_15–C4_15–C5_15	108.1(3)
C3_15–C4_15–C7_15	124.4(3)
C5_15–C4_15–C7_15	127.3(3)
C3_15–C4_15–Al7	70.92(17)
C5_15–C4_15–Al7	72.40(17)
C7_15–C4_15–Al7	125.6(2)
C4_15–C5_15–C1_15	107.8(3)
C4_15–C5_15–C6_15	127.5(3)
C1_15–C5_15–C6_15	124.7(3)
C4_15–C5_15–Al7	70.19(17)
C1_15–C5_15–Al7	71.26(17)
C6_15–C5_15–Al7	123.6(2)
C5_15–C6_15–H_15	109.5
C5_15–C6_15–HA_15	109.5
H_15–C6_15–HA_15	109.5
C5_15–C6_15–HB_15	109.5
H_15–C6_15–HB_15	109.5
HA_15–C6_15–HB_15	109.5
C4_15–C7_15–HC_15	109.5
C4_15–C7_15–HD_15	109.5
HC_15–C7_15–HD_15	109.5
C4_15–C7_15–HE_15	109.5
HC_15–C7_15–HE_15	109.5
HD_15–C7_15–HE_15	109.5
C3_15–C8_15–HF_15	109.5
C3_15–C8_15–HG_15	109.5
HF_15–C8_15–HG_15	109.5
C3_15–C8_15–HH_15	109.5
HF_15–C8_15–HH_15	109.5
HG_15–C8_15–HH_15	109.5
C2_15–C9_15–HI_15	109.5
C2_15–C9_15–HJ_15	109.5
HI_15–C9_15–HJ_15	109.5
C2_15–C9_15–HK_15	109.5
HI_15–C9_15–HK_15	109.5
HJ_15–C9_15–HK_15	109.5
C1_15–C10_15–HL_15	109.5
C1_15–C10_15–HM_15	109.5
HL_15–C10_15–HM_15	109.5
C1_15–C10_15–HN_15	109.5
HL_15–C10_15–HN_15	109.5
HM_15–C10_15–HN_15	109.5
C1_16–O1_16–Al03	146.6(7)
O1_16–C1_16–C3_16	112.2(5)
O1_16–C1_16–C4_16	109.6(6)
C3_16–C1_16–C4_16	109.0(4)
O1_16–C1_16–C2_16	106.9(5)
C3_16–C1_16–C2_16	108.9(4)
C4_16–C1_16–C2_16	110.3(4)
F1_16–C2_16–F3_16	109.0(5)
F1_16–C2_16–F2_16	109.9(5)
F3_16–C2_16–F2_16	105.8(5)
F1_16–C2_16–C1_16	111.9(5)
F3_16–C2_16–C1_16	108.2(5)
F2_16–C2_16–C1_16	111.8(5)
F5_16–C3_16–F6_16	107.9(5)
F5_16–C3_16–F4_16	106.7(5)
F6_16–C3_16–F4_16	106.4(5)
F5_16–C3_16–C1_16	112.9(4)
F6_16–C3_16–C1_16	112.4(6)
F4_16–C3_16–C1_16	110.2(4)
F7_16–C4_16–F9_16	109.3(5)
F7_16–C4_16–F8_16	106.4(6)
F9_16–C4_16–F8_16	106.8(6)
F7_16–C4_16–C1_16	111.9(4)
F9_16–C4_16–C1_16	109.6(4)
F8_16–C4_16–C1_16	112.7(6)
C1_17–O1_17–Al03	157(3)
O1_17–C1_17–C4_17	108.1(16)
O1_17–C1_17–C3_17	111.3(17)

C4_17–C1_17–C3_17	110.7(11)	F1_19–C2_19–F3_19	108.4(18)
O1_17–C1_17–C2_17	111.4(17)	F1_19–C2_19–F2_19	108(2)
C4_17–C1_17–C2_17	106.6(10)	F3_19–C2_19–F2_19	108(2)
C3_17–C1_17–C2_17	108.6(10)	F1_19–C2_19–C1_19	111.2(15)
F3_17–C2_17–F2_17	101.7(14)	F3_19–C2_19–C1_19	110.4(17)
F3_17–C2_17–F1_17	112.5(12)	F2_19–C2_19–C1_19	111(2)
F2_17–C2_17–F1_17	116.4(15)	F4_19–C3_19–F6_19	108(2)
F3_17–C2_17–C1_17	110.9(11)	F4_19–C3_19–F5_19	107.7(19)
F2_17–C2_17–C1_17	107.9(14)	F6_19–C3_19–F5_19	107(2)
F1_17–C2_17–C1_17	107.3(10)	F4_19–C3_19–C1_19	111.6(19)
F6_17–C3_17–F4_17	110.6(17)	F6_19–C3_19–C1_19	112.3(19)
F6_17–C3_17–F5_17	106.7(17)	F5_19–C3_19–C1_19	110.0(15)
F4_17–C3_17–F5_17	111.1(12)	F7_19–C4_19–F9_19	109.2(17)
F6_17–C3_17–C1_17	111.7(18)	F7_19–C4_19–F8_19	109(2)
F4_17–C3_17–C1_17	110.0(11)	F9_19–C4_19–F8_19	108(2)
F5_17–C3_17–C1_17	106.7(10)	F7_19–C4_19–C1_19	109.3(14)
F8_17–C4_17–F9_17	110.6(17)	F9_19–C4_19–C1_19	110.2(16)
F8_17–C4_17–F7_17	108.4(16)	F8_19–C4_19–C1_19	110.7(19)
F9_17–C4_17–F7_17	105.1(12)	F1_20–C1_20–C2_20	119.0(7)
F8_17–C4_17–C1_17	113.5(17)	F1_20–C1_20–C6_20	120.4(7)
F9_17–C4_17–C1_17	110.7(11)	C2_20–C1_20–C6_20	120.7(6)
F7_17–C4_17–C1_17	108.1(11)	F2_20–C2_20–C3_20	119.8(9)
C1_18–O1_18–Al01	147.2(4)	F2_20–C2_20–C1_20	119.6(8)
O1_18–C1_18–C4_18	107.2(4)	C3_20–C2_20–C1_20	120.6(7)
O1_18–C1_18–C3_18	111.3(3)	C2_20–C3_20–C4_20	119.2(7)
C4_18–C1_18–C3_18	109.7(3)	C2_20–C3_20–H_20	120.4
O1_18–C1_18–C2_18	110.4(4)	C4_20–C3_20–H_20	120.4
C4_18–C1_18–C2_18	109.0(3)	C3_20–C4_20–C5_20	120.3(7)
C3_18–C1_18–C2_18	109.2(3)	C3_20–C4_20–HA_20	119.8
F3_18–C2_18–F1_18	108.1(4)	C5_20–C4_20–HA_20	119.8
F3_18–C2_18–F2_18	108.5(4)	C6_20–C5_20–C4_20	120.4(7)
F1_18–C2_18–F2_18	106.9(4)	C6_20–C5_20–HB_20	119.8
F3_18–C2_18–C1_18	110.5(4)	C4_20–C5_20–HB_20	119.8
F1_18–C2_18–C1_18	110.6(3)	C5_20–C6_20–C1_20	118.8(6)
F2_18–C2_18–C1_18	112.1(4)	C5_20–C6_20–HC_20	120.6
F5_18–C3_18–F4_18	108.2(4)	C1_20–C6_20–HC_20	120.6
F5_18–C3_18–F6_18	107.1(5)	F1_21–C1_21–C2_21	120.2(15)
F4_18–C3_18–F6_18	107.6(5)	F1_21–C1_21–C6_21	119.2(16)
F5_18–C3_18–C1_18	111.3(4)	C2_21–C1_21–C6_21	120.5(14)
F4_18–C3_18–C1_18	110.1(4)	F2_21–C2_21–C3_21	121.0(16)
F6_18–C3_18–C1_18	112.4(4)	F2_21–C2_21–C1_21	118.7(15)
F9_18–C4_18–F7_18	107.4(4)	C3_21–C2_21–C1_21	120.3(14)
F9_18–C4_18–F8_18	107.6(4)	C2_21–C3_21–C4_21	120.1(16)
F7_18–C4_18–F8_18	107.2(4)	C2_21–C3_21–H_21	119.9
F9_18–C4_18–C1_18	111.2(3)	C4_21–C3_21–H_21	119.9
F7_18–C4_18–C1_18	110.6(3)	C3_21–C4_21–C5_21	119.5(17)
F8_18–C4_18–C1_18	112.6(4)	C3_21–C4_21–HA_21	120.2
C1_19–O1_19–Al01	153(3)	C5_21–C4_21–HA_21	120.2
O1_19–C1_19–C3_19	110.0(19)	C4_21–C5_21–C6_21	120.6(17)
O1_19–C1_19–C2_19	111(2)	C4_21–C5_21–HB_21	119.7
C3_19–C1_19–C2_19	109.5(14)	C6_21–C5_21–HB_21	119.7
O1_19–C1_19–C4_19	109.0(19)	C1_21–C6_21–C5_21	118.8(16)
C3_19–C1_19–C4_19	110.0(14)	C1_21–C6_21–HC_21	120.6
C2_19–C1_19–C4_19	107.9(14)	C5_21–C6_21–HC_21	120.6

F1_22–C1_22–C2_22	117.0(16)
F1_22–C1_22–C6_22	119.9(17)
C2_22–C1_22–C6_22	123.2(15)
F2_22–C2_22–C3_22	119.8(17)
F2_22–C2_22–C1_22	121.6(17)
C3_22–C2_22–C1_22	118.6(14)
C4_22–C3_22–C2_22	118.6(17)
C4_22–C3_22–H_22	120.7
C2_22–C3_22–H_22	120.7
C3_22–C4_22–C5_22	123.2(18)
C3_22–C4_22–HA_22	118.4
C5_22–C4_22–HA_22	118.4
C4_22–C5_22–C6_22	118.4(17)
C4_22–C5_22–HB_22	120.8
C6_22–C5_22–HB_22	120.8
C1_22–C6_22–C5_22	117.9(16)
C1_22–C6_22–HC_22	121.0
C5_22–C6_22–HC_22	121.0
C2_23–C1_23–C5_23	107.2(4)
C2_23–C1_23–C10_23	127.8(5)
C5_23–C1_23–C10_23	125.0(5)
C2_23–C1_23–Al4	70.7(2)
C5_23–C1_23–Al4	70.3(3)
C10_23–C1_23–Al4	125.2(4)
C1_23–C2_23–C3_23	108.5(4)
C1_23–C2_23–C9_23	126.3(5)
C3_23–C2_23–C9_23	125.1(5)
C1_23–C2_23–Al4	72.4(2)
C3_23–C2_23–Al4	70.3(3)
C9_23–C2_23–Al4	125.7(3)
C2_23–C3_23–C4_23	108.0(4)
C2_23–C3_23–C8_23	124.8(5)
C4_23–C3_23–C8_23	126.9(5)
C2_23–C3_23–Al4	72.3(3)
C4_23–C3_23–Al4	71.3(3)
C8_23–C3_23–Al4	127.0(4)
C5_23–C4_23–C3_23	107.0(4)
C5_23–C4_23–C7_23	125.9(5)
C3_23–C4_23–C7_23	127.0(5)
C5_23–C4_23–Al4	71.8(3)
C3_23–C4_23–Al4	70.7(3)
C7_23–C4_23–Al4	123.9(4)
C4_23–C5_23–C1_23	109.3(4)
C4_23–C5_23–C6_23	126.0(5)
C1_23–C5_23–C6_23	124.7(5)
C4_23–C5_23–Al4	71.0(3)
C1_23–C5_23–Al4	72.6(3)
C6_23–C5_23–Al4	122.4(4)
C5_23–C6_23–H6A_23	109.5
C5_23–C6_23–H6B_23	109.5
H6A_23–C6_23–H6B_23	109.5
C5_23–C6_23–H6C_23	109.5
H6A_23–C6_23–H6C_23	109.5
H6B_23–C6_23–H6C_23	109.5
C4_23–C7_23–H7A_23	109.5
C4_23–C7_23–H7B_23	109.5
H7A_23–C7_23–H7B_23	109.5
C4_23–C7_23–H7C_23	109.5
H7A_23–C7_23–H7C_23	109.5
H7B_23–C7_23–H7C_23	109.5
C3_23–C8_23–H8A_23	109.5
C3_23–C8_23–H8B_23	109.5
H8A_23–C8_23–H8B_23	109.5
C3_23–C8_23–H8C_23	109.5
H8A_23–C8_23–H8C_23	109.5
H8B_23–C8_23–H8C_23	109.5
C2_23–C9_23–H9A_23	109.5
C2_23–C9_23–H9B_23	109.5
H9A_23–C9_23–H9B_23	109.5
C2_23–C9_23–H9C_23	109.5
H9A_23–C9_23–H9C_23	109.5
H9B_23–C9_23–H9C_23	109.5
C1_23–C10_23–H10A_23	109.5
C1_23–C10_23–H10B_23	109.5
H10A_23–C10_23–H10B_23	109.5
C1_23–C10_23–H10C_23	109.5
H10A_23–C10_23–H10C_23	109.5
H10B_23–C10_23–H10C_23	109.5
C5_10–C1_10–C2_10	106.1(11)
C5_10–C1_10–C10_10	128.0(16)
C2_10–C1_10–C10_10	125.9(16)
C5_10–C1_10–Al4	74.7(15)
C2_10–C1_10–Al4	68.4(8)
C10_10–C1_10–Al4	123.5(15)
C1_10–C2_10–C3_10	109.0(11)
C1_10–C2_10–C9_10	124.5(16)
C3_10–C2_10–C9_10	126.4(15)
C1_10–C2_10–Al4	74.2(9)
C3_10–C2_10–Al4	72.6(8)

C9_10–C2_10–Al4	121.8(14)	C2_10–C9_10–H9B_10	109.5
C4_10–C3_10–C2_10	108.2(11)	H9A_10–C9_10–H9B_10	109.5
C4_10–C3_10–C8_10	124.3(15)	C2_10–C9_10–H9C_10	109.5
C2_10–C3_10–C8_10	127.5(15)	H9A_10–C9_10–H9C_10	109.5
C4_10–C3_10–Al4	74.7(13)	H9B_10–C9_10–H9C_10	109.5
C2_10–C3_10–Al4	69.5(8)	C1_10–C10_10–H10A_10	109.5
C8_10–C3_10–Al4	122.8(14)	C1_10–C10_10–H10B_10	109.5
C3_10–C4_10–C5_10	106.1(11)	H10A_10–C10_10–H10B_10	109.5
C3_10–C4_10–C7_10	126.3(16)	C1_10–C10_10–H10C_10	109.5
C5_10–C4_10–C7_10	127.4(16)	H10A_10–C10_10–H10C_10	109.5
C3_10–C4_10–Al4	68.6(12)	H10B_10–C10_10–H10C_10	109.5
C5_10–C4_10–Al4	73.0(16)	C1_24–O1_24–Al01	149.0(2)
C7_10–C4_10–Al4	126.9(19)	O1_24–C1_24–C3_24	110.6(2)
C1_10–C5_10–C4_10	110.4(12)	O1_24–C1_24–C4_24	111.5(2)
C1_10–C5_10–C6_10	125.2(15)	C3_24–C1_24–C4_24	108.8(2)
C4_10–C5_10–C6_10	124.3(15)	O1_24–C1_24–C2_24	107.4(2)
C1_10–C5_10–Al4	69.2(13)	C3_24–C1_24–C2_24	109.1(2)
C4_10–C5_10–Al4	71.0(16)	C4_24–C1_24–C2_24	109.4(2)
C6_10–C5_10–Al4	124(2)	F3_24–C2_24–F1_24	107.7(3)
C5_10–C6_10–H6A_10	109.5	F3_24–C2_24–F2_24	107.4(2)
C5_10–C6_10–H6B_10	109.5	F1_24–C2_24–F2_24	106.8(3)
H6A_10–C6_10–H6B_10	109.5	F3_24–C2_24–C1_24	111.1(3)
C5_10–C6_10–H6C_10	109.5	F1_24–C2_24–C1_24	111.1(2)
H6A_10–C6_10–H6C_10	109.5	F2_24–C2_24–C1_24	112.6(3)
H6B_10–C6_10–H6C_10	109.5	F6_24–C3_24–F5_24	107.4(3)
C4_10–C7_10–H7A_10	109.5	F6_24–C3_24–F4_24	108.1(3)
C4_10–C7_10–H7B_10	109.5	F5_24–C3_24–F4_24	107.4(3)
H7A_10–C7_10–H7B_10	109.5	F6_24–C3_24–C1_24	112.9(3)
C4_10–C7_10–H7C_10	109.5	F5_24–C3_24–C1_24	110.8(3)
H7A_10–C7_10–H7C_10	109.5	F4_24–C3_24–C1_24	109.9(2)
H7B_10–C7_10–H7C_10	109.5	F7_24–C4_24–F9_24	107.6(2)
C3_10–C8_10–H8A_10	109.5	F7_24–C4_24–F8_24	107.3(3)
C3_10–C8_10–H8B_10	109.5	F9_24–C4_24–F8_24	107.4(2)
H8A_10–C8_10–H8B_10	109.5	F7_24–C4_24–C1_24	111.7(3)
C3_10–C8_10–H8C_10	109.5	F9_24–C4_24–C1_24	110.5(2)
H8A_10–C8_10–H8C_10	109.5	F8_24–C4_24–C1_24	112.2(2)
H8B_10–C8_10–H8C_10	109.5		
C2_10–C9_10–H9A_10	109.5		

Symmetry transformations used to generate equivalent atoms:
#1: 1-X, 1-Y, -Z;

S-Table 21: Torsion angles for [Al(AlCp*)$_3$][*pf*]

Atom–Atom–Atom–Atom	Torsion Angle [°]
F1_1–C1_1–C2_1–F2_1	0.2(6)
C6_1–C1_1–C2_1–F2_1	−179.8(4)
F1_1–C1_1–C2_1–C3_1	−180.0(4)
C6_1–C1_1–C2_1–C3_1	0.0(6)
F2_1–C2_1–C3_1–C4_1	−179.9(5)
C1_1–C2_1–C3_1–C4_1	0.3(6)
C2_1–C3_1–C4_1–C5_1	−0.6(8)
C3_1–C4_1–C5_1–C6_1	0.6(8)
F1_1–C1_1–C6_1–C5_1	180.0(4)
C2_1–C1_1–C6_1–C5_1	0.0(6)
C4_1–C5_1–C6_1–C1_1	−0.3(7)
O1_17–Al03–O1_2–C1_2	−83.7(13)
O1_4–Al03–O1_2–C1_2	38.6(4)
O1_3–Al03–O1_2–C1_2	159.2(4)
O1_16–Al03–O1_2–C1_2	−79.8(5)
Al03–O1_2–C1_2–C2_2	167.5(3)
Al03–O1_2–C1_2–C3_2	47.3(5)
Al03–O1_2–C1_2–C4_2	−73.1(4)
O1_2–C1_2–C2_2–F3_2	−44.0(4)
C3_2–C1_2–C2_2–F3_2	77.4(4)
C4_2–C1_2–C2_2–F3_2	−163.7(3)
O1_2–C1_2–C2_2–F2_2	−164.4(3)
C3_2–C1_2–C2_2–F2_2	−43.0(4)
C4_2–C1_2–C2_2–F2_2	75.9(4)
O1_2–C1_2–C2_2–F1_2	75.1(3)
C3_2–C1_2–C2_2–F1_2	−163.5(3)
C4_2–C1_2–C2_2–F1_2	−44.6(4)
O1_2–C1_2–C3_2–F4_2	−41.8(4)
C2_2–C1_2–C3_2–F4_2	−161.0(3)
C4_2–C1_2–C3_2–F4_2	79.5(3)
O1_2–C1_2–C3_2–F6_2	−163.1(3)
C2_2–C1_2–C3_2–F6_2	77.8(4)
C4_2–C1_2–C3_2–F6_2	−41.8(4)
O1_2–C1_2–C3_2–F5_2	77.8(3)
C2_2–C1_2–C3_2–F5_2	−41.4(3)
C4_2–C1_2–C3_2–F5_2	−161.0(3)
O1_2–C1_2–C4_2–F7_2	79.0(4)
C2_2–C1_2–C4_2–F7_2	−162.7(3)
C3_2–C1_2–C4_2–F7_2	−43.1(3)
O1_2–C1_2–C4_2–F9_2	−41.1(4)
C2_2–C1_2–C4_2–F9_2	77.2(3)
C3_2–C1_2–C4_2–F9_2	−163.2(3)
O1_2–C1_2–C4_2–F8_2	−160.8(3)
C2_2–C1_2–C4_2–F8_2	−42.5(4)
C3_2–C1_2–C4_2–F8_2	77.0(4)
O1_17–Al03–O1_3–C1_3	−153.1(13)
O1_4–Al03–O1_3–C1_3	85.2(4)
O1_2–Al03–O1_3–C1_3	−33.8(4)
O1_16–Al03–O1_3–C1_3	−156.9(5)
Al03–O1_3–C1_3–C2_3	61.8(5)
Al03–O1_3–C1_3–C3_3	−178.9(3)
Al03–O1_3–C1_3–C4_3	−60.5(5)
O1_3–C1_3–C2_3–F3_3	39.1(4)

C3_3–C1_3–C2_3–F3_3	−79.2(3)
C4_3–C1_3–C2_3–F3_3	162.0(3)
O1_3–C1_3–C2_3–F1_3	−80.9(3)
C3_3–C1_3–C2_3–F1_3	160.8(3)
C4_3–C1_3–C2_3–F1_3	42.0(4)
O1_3–C1_3–C2_3–F2_3	159.3(3)
C3_3–C1_3–C2_3–F2_3	41.0(4)
C4_3–C1_3–C2_3–F2_3	−77.8(3)
O1_3–C1_3–C3_3–F4_3	44.0(3)
C2_3–C1_3–C3_3–F4_3	164.5(3)
C4_3–C1_3–C3_3–F4_3	−75.9(3)
O1_3–C1_3–C3_3–F5_3	−75.0(3)
C2_3–C1_3–C3_3–F5_3	45.5(3)
C4_3–C1_3–C3_3–F5_3	165.1(3)
O1_3–C1_3–C3_3–F6_3	165.1(3)
C2_3–C1_3–C3_3–F6_3	−74.4(3)
C4_3–C1_3–C3_3–F6_3	45.2(4)
O1_3–C1_3–C4_3–F9_3	46.1(4)
C2_3–C1_3–C4_3–F9_3	−76.9(3)
C3_3–C1_3–C4_3–F9_3	163.9(3)
O1_3–C1_3–C4_3–F7_3	−74.0(3)
C2_3–C1_3–C4_3–F7_3	163.0(3)
C3_3–C1_3–C4_3–F7_3	43.9(3)
O1_3–C1_3–C4_3–F8_3	165.6(3)
C2_3–C1_3–C4_3–F8_3	42.5(4)
C3_3–C1_3–C4_3–F8_3	−76.6(3)
O1_17–Al03–O1_4–C1_4	−34.6(14)
O1_3–Al03–O1_4–C1_4	85.0(4)
O1_2–Al03–O1_4–C1_4	−156.9(3)
O1_16–Al03–O1_4–C1_4	−34.6(5)
Al03–O1_4–C1_4–C2_4	−67.9(4)
Al03–O1_4–C1_4–C4_4	172.7(3)
Al03–O1_4–C1_4–C3_4	53.6(4)
O1_4–C1_4–C2_4–F3_4	45.6(3)
C4_4–C1_4–C2_4–F3_4	163.6(2)
C3_4–C1_4–C2_4–F3_4	−77.7(3)
O1_4–C1_4–C2_4–F1_4	−73.9(3)
C4_4–C1_4–C2_4–F1_4	44.1(3)
C3_4–C1_4–C2_4–F1_4	162.9(2)
O1_4–C1_4–C2_4–F2_4	165.8(2)
C4_4–C1_4–C2_4–F2_4	−76.2(3)
C3_4–C1_4–C2_4–F2_4	42.6(3)
O1_4–C1_4–C3_4–F4_4	38.4(3)
C2_4–C1_4–C3_4–F4_4	161.0(2)
C4_4–C1_4–C3_4–F4_4	−79.9(3)
O1_4–C1_4–C3_4–F5_4	−81.2(3)
C2_4–C1_4–C3_4–F5_4	41.4(3)
C4_4–C1_4–C3_4–F5_4	160.6(2)
O1_4–C1_4–C3_4–F6_4	158.9(2)
C2_4–C1_4–C3_4–F6_4	−78.5(3)
C4_4–C1_4–C3_4–F6_4	40.6(3)
O1_4–C1_4–C4_4–F7_4	−74.6(3)
C2_4–C1_4–C4_4–F7_4	165.2(2)
C3_4–C1_4–C4_4–F7_4	46.4(3)

O1_4–C1_4–C4_4–F9_4	44.4(3)
C2_4–C1_4–C4_4–F9_4	−75.8(3)
C3_4–C1_4–C4_4–F9_4	165.4(2)
O1_4–C1_4–C4_4–F8_4	164.1(2)
C2_4–C1_4–C4_4–F8_4	43.9(3)
C3_4–C1_4–C4_4–F8_4	−74.9(3)
O1_19–Al01–O1_6–C1_6	−76.2(17)
O1_8–Al01–O1_6–C1_6	169.2(3)
O1_18–Al01–O1_6–C1_6	−71.8(4)
O1_24–Al01–O1_6–C1_6	46.5(4)
Al01–O1_6–C1_6–C2_6	43.9(5)
Al01–O1_6–C1_6–C3_6	−78.1(4)
Al01–O1_6–C1_6–C4_6	162.9(3)
O1_6–C1_6–C2_6–F1_6	72.4(3)
C3_6–C1_6–C2_6–F1_6	−165.0(3)
C4_6–C1_6–C2_6–F1_6	−45.5(4)
O1_6–C1_6–C2_6–F3_6	−46.0(4)
C3_6–C1_6–C2_6–F3_6	76.7(3)
C4_6–C1_6–C2_6–F3_6	−163.8(3)
O1_6–C1_6–C2_6–F2_6	−166.1(3)
C3_6–C1_6–C2_6–F2_6	−43.4(4)
C4_6–C1_6–C2_6–F2_6	76.1(3)
O1_6–C1_6–C3_6–F4_6	−39.4(4)
C2_6–C1_6–C3_6–F4_6	−162.1(3)
C4_6–C1_6–C3_6–F4_6	78.3(3)
O1_6–C1_6–C3_6–F5_6	79.4(3)
C2_6–C1_6–C3_6–F5_6	−43.3(3)
C4_6–C1_6–C3_6–F5_6	−162.8(3)
O1_6–C1_6–C3_6–F6_6	−160.8(3)
C2_6–C1_6–C3_6–F6_6	76.5(3)
C4_6–C1_6–C3_6–F6_6	−43.0(4)
O1_6–C1_6–C4_6–F9_6	−44.4(4)
C2_6–C1_6–C4_6–F9_6	75.8(3)
C3_6–C1_6–C4_6–F9_6	−164.4(3)
O1_6–C1_6–C4_6–F7_6	75.1(3)
C2_6–C1_6–C4_6–F7_6	−164.8(3)
C3_6–C1_6–C4_6–F7_6	−44.9(4)
O1_6–C1_6–C4_6–F8_6	−164.9(3)
C2_6–C1_6–C4_6–F8_6	−44.8(4)
C3_6–C1_6–C4_6–F8_6	75.1(3)
O1_19–Al01–O1_8–C1_8	−162.1(17)
O1_6–Al01–O1_8–C1_8	−38.2(4)
O1_18–Al01–O1_8–C1_8	−160.9(4)
O1_24–Al01–O1_8–C1_8	79.0(4)
Al01–O1_8–C1_8–C4_8	107.1(4)
Al01–O1_8–C1_8–C2_8	−14.9(5)
Al01–O1_8–C1_8–C3_8	−133.6(4)
O1_8–C1_8–C2_8–F3_8	−38.4(4)
C4_8–C1_8–C2_8–F3_8	−160.5(3)
C3_8–C1_8–C2_8–F3_8	79.6(3)
O1_8–C1_8–C2_8–F1_8	80.4(3)
C4_8–C1_8–C2_8–F1_8	−41.7(4)
C3_8–C1_8–C2_8–F1_8	−161.6(3)
O1_8–C1_8–C2_8–F2_8	−160.0(3)

C4_8–C1_8–C2_8–F2_8	77.8(4)
C3_8–C1_8–C2_8–F2_8	−42.1(4)
O1_8–C1_8–C3_8–F5_8	76.7(3)
C4_8–C1_8–C3_8–F5_8	−164.2(3)
C2_8–C1_8–C3_8–F5_8	−44.5(4)
O1_8–C1_8–C3_8–F4_8	−43.0(4)
C4_8–C1_8–C3_8–F4_8	76.1(4)
C2_8–C1_8–C3_8–F4_8	−164.2(3)
O1_8–C1_8–C3_8–F6_8	−163.3(3)
C4_8–C1_8–C3_8–F6_8	−44.2(4)
C2_8–C1_8–C3_8–F6_8	75.6(4)
O1_8–C1_8–C4_8–F9_8	−47.0(4)
C2_8–C1_8–C4_8–F9_8	76.7(4)
C3_8–C1_8–C4_8–F9_8	−164.5(3)
O1_8–C1_8–C4_8–F8_8	−167.0(3)
C2_8–C1_8–C4_8–F8_8	−43.4(5)
C3_8–C1_8–C4_8–F8_8	75.5(4)
O1_8–C1_8–C4_8–F7_8	73.0(4)
C2_8–C1_8–C4_8–F7_8	−163.4(3)
C3_8–C1_8–C4_8–F7_8	−44.5(4)
C5_11–C1_11–C2_11–C3_11	−0.4(3)
C10_11–C1_11–C2_11–C3_11	−177.6(3)
Al2–C1_11–C2_11–C3_11	61.79(18)
C5_11–C1_11–C2_11–C9_11	175.2(3)
C10_11–C1_11–C2_11–C9_11	−2.0(5)
Al2–C1_11–C2_11–C9_11	−122.6(3)
C5_11–C1_11–C2_11–Al2	−62.22(19)
C10_11–C1_11–C2_11–Al2	120.7(3)
C1_11–C2_11–C3_11–C4_11	0.9(3)
C9_11–C2_11–C3_11–C4_11	−174.9(3)
Al2–C2_11–C3_11–C4_11	63.58(19)
C1_11–C2_11–C3_11–C8_11	177.1(3)
C9_11–C2_11–C3_11–C8_11	1.4(4)
Al2–C2_11–C3_11–C8_11	−120.1(3)
C1_11–C2_11–C3_11–Al2	−62.73(18)
C9_11–C2_11–C3_11–Al2	121.5(3)
C2_11–C3_11–C4_11–C5_11	−1.0(3)
C8_11–C3_11–C4_11–C5_11	−177.2(3)
Al2–C3_11–C4_11–C5_11	62.1(2)
C2_11–C3_11–C4_11–C7_11	176.6(3)
C8_11–C3_11–C4_11–C7_11	0.3(5)

Al2–C3_11–C4_11–C7_11	−120.4(3)
C2_11–C3_11–C4_11–Al2	−63.01(19)
C8_11–C3_11–C4_11–Al2	120.8(3)
C3_11–C4_11–C5_11–C1_11	0.7(3)
C7_11–C4_11–C5_11–C1_11	−176.8(3)
Al2–C4_11–C5_11–C1_11	61.51(19)
C3_11–C4_11–C5_11–C6_11	−179.7(3)
C7_11–C4_11–C5_11–C6_11	2.8(5)
Al2–C4_11–C5_11–C6_11	−118.9(3)
C3_11–C4_11–C5_11–Al2	−60.82(19)
C7_11–C4_11–C5_11–Al2	121.7(3)
C2_11–C1_11–C5_11–C4_11	−0.2(3)
C10_11–C1_11–C5_11–C4_11	177.1(3)
Al2–C1_11–C5_11–C4_11	−61.5(2)
C2_11–C1_11–C5_11–C6_11	−179.8(3)
C10_11–C1_11–C5_11–C6_11	−2.5(4)
Al2–C1_11–C5_11–C6_11	118.9(3)
C2_11–C1_11–C5_11–Al2	61.35(18)
C10_11–C1_11–C5_11–Al2	−121.4(3)
C5_12–C1_12–C2_12–C3_12	0.5(3)
C10_12–C1_12–C2_12–C3_12	179.8(3)
Al3–C1_12–C2_12–C3_12	61.86(19)
C5_12–C1_12–C2_12–C9_12	−179.6(3)
C10_12–C1_12–C2_12–C9_12	−0.3(5)
Al3–C1_12–C2_12–C9_12	−118.2(3)
C5_12–C1_12–C2_12–Al3	−61.4(2)
C10_12–C1_12–C2_12–Al3	117.9(3)
C1_12–C2_12–C3_12–C4_12	−0.7(3)
C9_12–C2_12–C3_12–C4_12	179.3(3)
Al3–C2_12–C3_12–C4_12	61.4(2)
C1_12–C2_12–C3_12–C8_12	177.4(3)
C9_12–C2_12–C3_12–C8_12	−2.6(5)
Al3–C2_12–C3_12–C8_12	−120.6(3)
C1_12–C2_12–C3_12–Al3	−62.08(19)
C9_12–C2_12–C3_12–Al3	118.0(3)

C2_12–C3_12–C4_12–C5_12	0.7(3)
C8_12–C3_12–C4_12–C5_12	−177.4(3)
Al3–C3_12–C4_12–C5_12	63.0(2)
C2_12–C3_12–C4_12–C7_12	176.8(3)
C8_12–C3_12–C4_12–C7_12	−1.2(5)
Al3–C3_12–C4_12–C7_12	−120.9(3)
C2_12–C3_12–C4_12–Al3	−62.3(2)
C8_12–C3_12–C4_12–Al3	119.7(3)
C3_12–C4_12–C5_12–C1_12	−0.4(3)
C7_12–C4_12–C5_12–C1_12	−176.6(3)
Al3–C4_12–C5_12–C1_12	63.0(2)
C3_12–C4_12–C5_12–C6_12	175.4(3)
C7_12–C4_12–C5_12–C6_12	−0.8(5)
Al3–C4_12–C5_12–C6_12	−121.2(3)
C3_12–C4_12–C5_12–Al3	−63.4(2)
C7_12–C4_12–C5_12–Al3	120.4(3)
C2_12–C1_12–C5_12–C4_12	−0.1(3)
C10_12–C1_12–C5_12–C4_12	−179.3(3)
Al3–C1_12–C5_12–C4_12	−62.1(2)
C2_12–C1_12–C5_12–C6_12	−175.7(3)
C10_12–C1_12–C5_12–C6_12	5.1(5)
Al3–C1_12–C5_12–C6_12	122.3(3)
C2_12–C1_12–C5_12–Al3	62.1(2)
C10_12–C1_12–C5_12–Al3	−117.2(3)
C5_13–C1_13–C2_13–C3_13	0.0(3)
C10_13–C1_13–C2_13–C3_13	175.3(3)
Al8–C1_13–C2_13–C3_13	−63.4(2)
C5_13–C1_13–C2_13–C9_13	−176.5(3)
C10_13–C1_13–C2_13–C9_13	−1.2(5)
Al8–C1_13–C2_13–C9_13	120.1(3)
C5_13–C1_13–C2_13–Al8	63.4(2)
C10_13–C1_13–C2_13–Al8	−121.3(3)
C1_13–C2_13–C3_13–C4_13	0.0(3)
C9_13–C2_13–C3_13–C4_13	176.5(3)

Al8–C2_13–C3_13–C4_13	−62.2(2)
C1_13–C2_13–C3_13–C8_13	−177.2(3)
C9_13–C2_13–C3_13–C8_13	−0.7(5)
Al8–C2_13–C3_13–C8_13	120.6(3)
C1_13–C2_13–C3_13–Al8	62.2(2)
C9_13–C2_13–C3_13–Al8	−121.3(3)
C2_13–C3_13–C4_13–C5_13	0.0(4)
C8_13–C3_13–C4_13–C5_13	177.3(3)
Al8–C3_13–C4_13–C5_13	−61.2(2)
C2_13–C3_13–C4_13–C7_13	179.7(3)
C8_13–C3_13–C4_13–C7_13	−3.0(5)
Al8–C3_13–C4_13–C7_13	118.5(3)
C2_13–C3_13–C4_13–Al8	61.2(2)
C8_13–C3_13–C4_13–Al8	−121.5(3)
C3_13–C4_13–C5_13–C1_13	0.0(4)
C7_13–C4_13–C5_13–C1_13	−179.6(3)
Al8–C4_13–C5_13–C1_13	−61.0(2)
C3_13–C4_13–C5_13–C6_13	−178.9(3)
C7_13–C4_13–C5_13–C6_13	1.4(6)
Al8–C4_13–C5_13–C6_13	120.0(4)
C3_13–C4_13–C5_13–Al8	61.0(2)
C7_13–C4_13–C5_13–Al8	−118.6(3)
C2_13–C1_13–C5_13–C4_13	0.0(4)
C10_13–C1_13–C5_13–C4_13	−175.2(3)
Al8–C1_13–C5_13–C4_13	62.6(2)
C2_13–C1_13–C5_13–C6_13	179.0(3)
C10_13–C1_13–C5_13–C6_13	3.8(5)
Al8–C1_13–C5_13–C6_13	−118.4(3)
C2_13–C1_13–C5_13–Al8	−62.7(2)
C10_13–C1_13–C5_13–Al8	122.2(3)
C5_14–C1_14–C2_14–C3_14	−0.2(3)
C10_14–C1_14–C2_14–C3_14	177.9(3)
Al6–C1_14–C2_14–C3_14	−62.3(2)
C5_14–C1_14–C2_14–C9_14	−175.3(3)
C10_14–C1_14–C2_14–C9_14	2.9(5)

Al6–C1_14–C2_14–C9_14	122.6(3)
C5_14–C1_14–C2_14–Al6	62.1(2)
C10_14–C1_14–C2_14–Al6	−119.8(3)
C1_14–C2_14–C3_14–C4_14	0.0(3)
C9_14–C2_14–C3_14–C4_14	175.1(3)
Al6–C2_14–C3_14–C4_14	−63.2(2)
C1_14–C2_14–C3_14–C8_14	−175.6(3)
C9_14–C2_14–C3_14–C8_14	−0.5(5)
Al6–C2_14–C3_14–C8_14	121.3(3)
C1_14–C2_14–C3_14–Al6	63.1(2)
C9_14–C2_14–C3_14–Al6	−121.7(3)
C2_14–C3_14–C4_14–C5_14	0.3(3)
C8_14–C3_14–C4_14–C5_14	175.7(3)
Al6–C3_14–C4_14–C5_14	−62.3(2)
C2_14–C3_14–C4_14–C7_14	−178.7(3)
C8_14–C3_14–C4_14–C7_14	−3.2(5)
Al6–C3_14–C4_14–C7_14	118.8(3)
C2_14–C3_14–C4_14–Al6	62.5(2)
C8_14–C3_14–C4_14–Al6	−122.0(3)
C3_14–C4_14–C5_14–C1_14	−0.4(4)
C7_14–C4_14–C5_14–C1_14	178.6(3)
Al6–C4_14–C5_14–C1_14	−61.9(2)
C3_14–C4_14–C5_14–C6_14	−179.7(3)
C7_14–C4_14–C5_14–C6_14	−0.7(5)
Al6–C4_14–C5_14–C6_14	118.8(3)
C3_14–C4_14–C5_14–Al6	61.5(2)
C7_14–C4_14–C5_14–Al6	−119.5(3)
C2_14–C1_14–C5_14–C4_14	0.4(3)
C10_14–C1_14–C5_14–C4_14	−177.8(3)
Al6–C1_14–C5_14–C4_14	61.7(2)
C2_14–C1_14–C5_14–C6_14	179.7(3)
C10_14–C1_14–C5_14–C6_14	1.5(5)
Al6–C1_14–C5_14–C6_14	−118.9(3)
C2_14–C1_14–C5_14–Al6	−61.4(2)
C10_14–C1_14–C5_14–Al6	120.5(3)

C5_15–C1_15–C2_15–C3_15	−0.7(3)
C10_15–C1_15–C2_15–C3_15	179.0(3)
Al7–C1_15–C2_15–C3_15	61.49(19)
C5_15–C1_15–C2_15–C9_15	178.6(3)
C10_15–C1_15–C2_15–C9_15	−1.7(5)
Al7–C1_15–C2_15–C9_15	−119.2(3)
C5_15–C1_15–C2_15–Al7	−62.2(2)
C10_15–C1_15–C2_15–Al7	117.5(3)
C1_15–C2_15–C3_15–C4_15	0.3(3)
C9_15–C2_15–C3_15–C4_15	−179.0(3)
Al7–C2_15–C3_15–C4_15	62.6(2)
C1_15–C2_15–C3_15–C8_15	177.1(3)
C9_15–C2_15–C3_15–C8_15	−2.2(5)
Al7–C2_15–C3_15–C8_15	−120.6(3)
C1_15–C2_15–C3_15–Al7	−62.3(2)
C9_15–C2_15–C3_15–Al7	118.4(3)
C2_15–C3_15–C4_15–C5_15	0.2(3)
C8_15–C3_15–C4_15–C5_15	−176.7(3)
Al7–C3_15–C4_15–C5_15	63.3(2)
C2_15–C3_15–C4_15–C7_15	176.3(3)
C8_15–C3_15–C4_15–C7_15	−0.6(5)
Al7–C3_15–C4_15–C7_15	−120.6(3)
C2_15–C3_15–C4_15–Al7	−63.0(2)
C8_15–C3_15–C4_15–Al7	120.0(3)
C3_15–C4_15–C5_15–C1_15	−0.6(3)
C7_15–C4_15–C5_15–C1_15	−176.6(3)
Al7–C4_15–C5_15–C1_15	61.7(2)
C3_15–C4_15–C5_15–C6_15	179.9(3)
C7_15–C4_15–C5_15–C6_15	4.0(5)
Al7–C4_15–C5_15–C6_15	−117.8(3)
C3_15–C4_15–C5_15–Al7	−62.3(2)
C7_15–C4_15–C5_15–Al7	121.7(3)
C2_15–C1_15–C5_15–C4_15	0.8(3)
C10_15–C1_15–C5_15–C4_15	−178.9(3)
Al7–C1_15–C5_15–C4_15	−61.0(2)

C2_15–C1_15–C5_15–C6_15	−179.7(3)
C10_15–C1_15–C5_15–C6_15	0.6(5)
Al7–C1_15–C5_15–C6_15	118.5(3)
C2_15–C1_15–C5_15–Al7	61.8(2)
C10_15–C1_15–C5_15–Al7	−117.9(3)
O1_4–Al03–O1_16–C1_16	162.6(12)
O1_3–Al03–O1_16–C1_16	41.9(14)
O1_2–Al03–O1_16–C1_16	−77.8(14)
Al03–O1_16–C1_16–C3_16	48.1(15)
Al03–O1_16–C1_16–C4_16	−73.1(14)
Al03–O1_16–C1_16–C2_16	167.4(12)
O1_16–C1_16–C2_16–F1_16	73.6(6)
C3_16–C1_16–C2_16–F1_16	−165.0(5)
C4_16–C1_16–C2_16–F1_16	−45.4(6)
O1_16–C1_16–C2_16–F3_16	−46.5(7)
C3_16–C1_16–C2_16–F3_16	74.9(6)
C4_16–C1_16–C2_16–F3_16	−165.6(5)
O1_16–C1_16–C2_16–F2_16	−162.6(6)
C3_16–C1_16–C2_16–F2_16	−41.2(7)
C4_16–C1_16–C2_16–F2_16	78.3(6)
O1_16–C1_16–C3_16–F5_16	72.6(7)
C4_16–C1_16–C3_16–F5_16	−165.9(5)
C2_16–C1_16–C3_16–F5_16	−45.5(6)
O1_16–C1_16–C3_16–F6_16	−165.1(7)
C4_16–C1_16–C3_16–F6_16	−43.5(7)
C2_16–C1_16–C3_16–F6_16	76.8(6)
O1_16–C1_16–C3_16–F4_16	−46.7(7)
C4_16–C1_16–C3_16–F4_16	74.9(5)
C2_16–C1_16–C3_16–F4_16	−164.8(5)

O1_16–C1_16–C4_16–F7_16	79.6(6)
C3_16–C1_16–C4_16–F7_16	−43.5(6)
C2_16–C1_16–C4_16–F7_16	−163.0(4)
O1_16–C1_16–C4_16–F9_16	−41.7(7)
C3_16–C1_16–C4_16–F9_16	−164.9(5)
C2_16–C1_16–C4_16–F9_16	75.7(6)
O1_16–C1_16–C4_16–F8_16	−160.5(7)
C3_16–C1_16–C4_16–F8_16	76.3(7)
C2_16–C1_16–C4_16–F8_16	−43.2(7)
O1_4–Al03–O1_17–C1_17	156(7)
O1_3–Al03–O1_17–C1_17	34(7)
O1_2–Al03–O1_17–C1_17	−83(7)
Al03–O1_17–C1_17–C4_17	37(7)
Al03–O1_17–C1_17–C3_17	−85(7)
Al03–O1_17–C1_17–C2_17	154(7)
O1_17–C1_17–C2_17–F3_17	46(2)
C4_17–C1_17–C2_17–F3_17	164.0(12)
C3_17–C1_17–C2_17–F3_17	−76.7(14)
O1_17–C1_17–C2_17–F2_17	157(2)
C4_17–C1_17–C2_17–F2_17	−85.4(16)
C3_17–C1_17–C2_17–F2_17	33.9(17)
O1_17–C1_17–C2_17–F1_17	−76.9(19)
C4_17–C1_17–C2_17–F1_17	40.8(14)
C3_17–C1_17–C2_17–F1_17	160.1(12)
O1_17–C1_17–C3_17–F6_17	162(2)
C4_17–C1_17–C3_17–F6_17	41(2)
C2_17–C1_17–C3_17–F6_17	−75(2)
O1_17–C1_17–C3_17–F4_17	39(2)

C4_17–C1_17–C3_17–F4_17	−81.7(15)
C2_17–C1_17–C3_17–F4_17	161.6(13)
O1_17–C1_17–C3_17–F5_17	−82.0(18)
C4_17–C1_17–C3_17–F5_17	157.7(12)
C2_17–C1_17–C3_17–F5_17	41.0(14)
O1_17–C1_17–C4_17–F8_17	164(2)
C3_17–C1_17–C4_17–F8_17	−74.2(19)
C2_17–C1_17–C4_17–F8_17	44(2)
O1_17–C1_17–C4_17–F9_17	38(2)
C3_17–C1_17–C4_17–F9_17	160.7(13)
C2_17–C1_17–C4_17–F9_17	−81.4(14)
O1_17–C1_17–C4_17–F7_17	−76(2)
C3_17–C1_17–C4_17–F7_17	46.0(15)
C2_17–C1_17–C4_17–F7_17	163.9(13)
O1_8–Al01–O1_18–C1_18	26.3(8)
O1_6–Al01–O1_18–C1_18	−91.7(7)
O1_24–Al01–O1_18–C1_18	150.8(7)
Al01–O1_18–C1_18–C4_18	179.8(6)
Al01–O1_18–C1_18–C3_18	−60.3(8)
Al01–O1_18–C1_18–C2_18	61.2(8)
O1_18–C1_18–C2_18–F3_18	−44.2(5)
C4_18–C1_18–C2_18–F3_18	−161.7(4)
C3_18–C1_18–C2_18–F3_18	78.5(5)
O1_18–C1_18–C2_18–F1_18	75.5(4)
C4_18–C1_18–C2_18–F1_18	−42.0(4)
C3_18–C1_18–C2_18–F1_18	−161.8(3)
O1_18–C1_18–C2_18–F2_18	−165.3(4)
C4_18–C1_18–C2_18–F2_18	77.2(5)

C3_18–C1_18–C2_18–F2_18	−42.6(5)
O1_18–C1_18–C3_18–F5_18	80.8(4)
C4_18–C1_18–C3_18–F5_18	−160.8(3)
C2_18–C1_18–C3_18–F5_18	−41.4(4)
O1_18–C1_18–C3_18–F4_18	−39.2(5)
C4_18–C1_18–C3_18–F4_18	79.3(5)
C2_18–C1_18–C3_18–F4_18	−161.3(4)
O1_18–C1_18–C3_18–F6_18	−159.1(5)
C4_18–C1_18–C3_18–F6_18	−40.7(6)
C2_18–C1_18–C3_18–F6_18	78.7(6)
O1_18–C1_18–C4_18–F9_18	−42.8(5)
C3_18–C1_18–C4_18–F9_18	−163.7(3)
C2_18–C1_18–C4_18–F9_18	76.8(4)
O1_18–C1_18–C4_18–F7_18	76.4(4)
C3_18–C1_18–C4_18–F7_18	−44.5(4)
C2_18–C1_18–C4_18–F7_18	−164.0(3)
O1_18–C1_18–C4_18–F8_18	−163.6(4)
C3_18–C1_18–C4_18–F8_18	75.4(5)
C2_18–C1_18–C4_18–F8_18	−44.1(5)
O1_8–Al01–O1_19–C1_19	33(8)
O1_6–Al01–O1_19–C1_19	−83(7)
Al01–O1_19–C1_19–C3_19	23(8)
Al01–O1_19–C1_19–C2_19	−98(7)
Al01–O1_19–C1_19–C4_19	143(7)
O1_19–C1_19–C2_19–F1_19	−74(3)
C3_19–C1_19–C2_19–F1_19	165(2)
C4_19–C1_19–C2_19–F1_19	45(2)
O1_19–C1_19–C2_19–F3_19	47(3)

C3_19–C1_19–C2_19–F3_19	−75(2)
C4_19–C1_19–C2_19–F3_19	166(2)
O1_19–C1_19–C2_19–F2_19	166(3)
C3_19–C1_19–C2_19–F2_19	45(3)
C4_19–C1_19–C2_19–F2_19	−75(3)
O1_19–C1_19–C3_19–F4_19	40(3)
C2_19–C1_19–C3_19–F4_19	162(3)
C4_19–C1_19–C3_19–F4_19	−80(3)
O1_19–C1_19–C3_19–F6_19	162(3)
C2_19–C1_19–C3_19–F6_19	−76(3)
C4_19–C1_19–C3_19–F6_19	42(3)
O1_19–C1_19–C3_19–F5_19	−79(3)
C2_19–C1_19–C3_19–F5_19	42(2)
C4_19–C1_19–C3_19–F5_19	161(2)
O1_19–C1_19–C4_19–F7_19	−76(3)
C3_19–C1_19–C4_19–F7_19	45(2)
C2_19–C1_19–C4_19–F7_19	164.3(19)
O1_19–C1_19–C4_19–F9_19	44(3)
C3_19–C1_19–C4_19–F9_19	165(2)
C2_19–C1_19–C4_19–F9_19	−76(2)
O1_19–C1_19–C4_19–F8_19	164(3)
C3_19–C1_19–C4_19–F8_19	−75(3)
C2_19–C1_19–C4_19–F8_19	44(3)
F1_20–C1_20–C2_20–F2_20	−1.5(15)
C6_20–C1_20–C2_20–F2_20	178.8(13)
F1_20–C1_20–C2_20–C3_20	179.6(11)
C6_20–C1_20–C2_20–C3_20	−0.1(9)

F2_20–C2_20–C3_20–C4_20	−178.2(18)
C1_20–C2_20–C3_20–C4_20	0.7(15)
C2_20–C3_20–C4_20–C5_20	0(2)
C3_20–C4_20–C5_20–C6_20	−1(2)
C4_20–C5_20–C6_20–C1_20	1.9(18)
F1_20–C1_20–C6_20–C5_20	179.1(12)
C2_20–C1_20–C6_20–C5_20	−1.2(12)
F1_21–C1_21–C2_21–F2_21	0(3)
C6_21–C1_21–C2_21–F2_21	−177(3)
F1_21–C1_21–C2_21–C3_21	179(2)
C6_21–C1_21–C2_21–C3_21	2(2)
F2_21–C2_21–C3_21–C4_21	179(3)
C1_21–C2_21–C3_21–C4_21	0(2)
C2_21–C3_21–C4_21–C5_21	−1(4)
C3_21–C4_21–C5_21–C6_21	−1(6)
F1_21–C1_21–C6_21–C5_21	179(4)
C2_21–C1_21–C6_21–C5_21	−3(5)
C4_21–C5_21–C6_21–C1_21	3(6)
F1_22–C1_22–C2_22–F2_22	0(3)
C6_22–C1_22–C2_22–F2_22	180(3)
F1_22–C1_22–C2_22–C3_22	180(2)
C6_22–C1_22–C2_22–C3_22	0(2)
F2_22–C2_22–C3_22–C4_22	180(3)
C1_22–C2_22–C3_22–C4_22	0(2)
C2_22–C3_22–C4_22–C5_22	−1(5)
C3_22–C4_22–C5_22–C6_22	3(6)
F1_22–C1_22–C6_22–C5_22	−178(3)

C2_22–C1_22–C6_22–C5_22	2(4)
C4_22–C5_22–C6_22–C1_22	−3(5)
C5_23–C1_23–C2_23–C3_23	−0.2(4)
C10_23–C1_23–C2_23–C3_23	178.5(5)
Al4–C1_23–C2_23–C3_23	−61.4(3)
C5_23–C1_23–C2_23–C9_23	−177.0(5)
C10_23–C1_23–C2_23–C9_23	1.8(7)
Al4–C1_23–C2_23–C9_23	121.8(5)
C5_23–C1_23–C2_23–Al4	61.2(3)
C10_23–C1_23–C2_23–Al4	−120.1(5)
C1_23–C2_23–C3_23–C4_23	−0.1(5)
C9_23–C2_23–C3_23–C4_23	176.7(5)
Al4–C2_23–C3_23–C4_23	−62.8(4)
C1_23–C2_23–C3_23–C8_23	−174.1(5)
C9_23–C2_23–C3_23–C8_23	2.7(7)
Al4–C2_23–C3_23–C8_23	123.2(5)
C1_23–C2_23–C3_23–Al4	62.7(3)
C9_23–C2_23–C3_23–Al4	−120.5(4)
C2_23–C3_23–C4_23–C5_23	0.4(6)
C8_23–C3_23–C4_23–C5_23	174.2(5)
Al4–C3_23–C4_23–C5_23	−63.1(4)
C2_23–C3_23–C4_23–C7_23	−178.1(5)
C8_23–C3_23–C4_23–C7_23	−4.3(9)
Al4–C3_23–C4_23–C7_23	118.5(6)
C2_23–C3_23–C4_23–Al4	63.4(3)
C8_23–C3_23–C4_23–Al4	−122.7(5)
C3_23–C4_23–C5_23–C1_23	−0.5(6)
C7_23–C4_23–C5_23–C1_23	178.0(5)
Al4–C4_23–C5_23–C1_23	−62.9(3)
C3_23–C4_23–C5_23–C6_23	179.2(5)
C7_23–C4_23–C5_23–C6_23	−2.3(9)
Al4–C4_23–C5_23–C6_23	116.8(5)
C3_23–C4_23–C5_23–Al4	62.4(4)
C7_23–C4_23–C5_23–Al4	−119.2(6)

C2_23–C1_23–C5_23–C4_23	0.5(5)
C10_23–C1_23–C5_23–C4_23	−178.3(5)
Al4–C1_23–C5_23–C4_23	61.9(4)
C2_23–C1_23–C5_23–C6_23	−179.2(5)
C10_23–C1_23–C5_23–C6_23	2.0(7)
Al4–C1_23–C5_23–C6_23	−117.8(5)
C2_23–C1_23–C5_23–Al4	−61.4(3)
C10_23–C1_23–C5_23–Al4	119.8(5)
C5_10–C1_10–C2_10–C3_10	1.1(16)
C10_10–C1_10–C2_10–C3_10	179(2)
Al4–C1_10–C2_10–C3_10	−64.8(7)
C5_10–C1_10–C2_10–C9_10	−176(2)
C10_10–C1_10–C2_10–C9_10	2(2)
Al4–C1_10–C2_10–C9_10	118.0(17)
C5_10–C1_10–C2_10–Al4	65.8(17)
C10_10–C1_10–C2_10–Al4	−116.5(19)
C1_10–C2_10–C3_10–C4_10	0.7(15)
C9_10–C2_10–C3_10–C4_10	178(2)
Al4–C2_10–C3_10–C4_10	−65.1(15)
C1_10–C2_10–C3_10–C8_10	−177.9(19)
C9_10–C2_10–C3_10–C8_10	−1(2)
Al4–C2_10–C3_10–C8_10	116.2(18)
C1_10–C2_10–C3_10–Al4	65.8(8)
C9_10–C2_10–C3_10–Al4	−117.1(18)
C2_10–C3_10–C4_10–C5_10	−2(3)
C8_10–C3_10–C4_10–C5_10	177(2)
Al4–C3_10–C4_10–C5_10	−64(2)
C2_10–C3_10–C4_10–C7_10	−177(2)
C8_10–C3_10–C4_10–C7_10	1(4)
Al4–C3_10–C4_10–C7_10	121(3)
C2_10–C3_10–C4_10–Al4	61.8(10)
C8_10–C3_10–C4_10–Al4	−120(2)
C2_10–C1_10–C5_10–C4_10	−2(3)
C10_10–C1_10–C5_10–C4_10	180(3)

Al4–C1_10–C5_10–C4_10	59(2)
C2_10–C1_10–C5_10–C6_10	−179(3)
C10_10–C1_10–C5_10–C6_10	3(5)
Al4–C1_10–C5_10–C6_10	−118(3)
C2_10–C1_10–C5_10–Al4	−61.5(10)
C10_10–C1_10–C5_10–Al4	121(2)
C3_10–C4_10–C5_10–C1_10	3(3)
C7_10–C4_10–C5_10–C1_10	178(3)
Al4–C4_10–C5_10–C1_10	−58(2)
C3_10–C4_10–C5_10–C6_10	180(3)
C7_10–C4_10–C5_10–C6_10	−5(5)
Al4–C4_10–C5_10–C6_10	119(3)
C3_10–C4_10–C5_10–Al4	60.9(18)
C7_10–C4_10–C5_10–Al4	−124(3)
O1_8–Al01–O1_24–C1_24	76.5(4)
O1_6–Al01–O1_24–C1_24	−166.2(4)
O1_18–Al01–O1_24–C1_24	−43.8(4)
Al01–O1_24–C1_24–C3_24	−64.4(4)
Al01–O1_24–C1_24–C4_24	56.7(5)
Al01–O1_24–C1_24–C2_24	176.5(3)
O1_24–C1_24–C2_24–F3_24	44.4(3)
C3_24–C1_24–C2_24–F3_24	−75.6(3)
C4_24–C1_24–C2_24–F3_24	165.5(2)
O1_24–C1_24–C2_24–F1_24	−75.4(3)
C3_24–C1_24–C2_24–F1_24	164.6(2)
C4_24–C1_24–C2_24–F1_24	45.7(3)
O1_24–C1_24–C2_24–F2_24	164.9(2)
C3_24–C1_24–C2_24–F2_24	44.9(3)
C4_24–C1_24–C2_24–F2_24	−74.0(3)
O1_24–C1_24–C3_24–F6_24	168.7(3)
C4_24–C1_24–C3_24–F6_24	46.0(3)

C2_24–C1_24–C3_24–F6_24	−73.3(3)
O1_24–C1_24–C3_24–F5_24	−70.7(3)
C4_24–C1_24–C3_24–F5_24	166.6(2)
C2_24–C1_24–C3_24–F5_24	47.3(3)
O1_24–C1_24–C3_24–F4_24	47.9(3)
C4_24–C1_24–C3_24–F4_24	−74.8(3)
C2_24–C1_24–C3_24–F4_24	165.9(2)
O1_24–C1_24–C4_24–F7_24	−77.4(3)
C3_24–C1_24–C4_24–F7_24	44.8(3)
C2_24–C1_24–C4_24–F7_24	163.9(2)
O1_24–C1_24–C4_24–F9_24	42.3(3)
C3_24–C1_24–C4_24–F9_24	164.5(2)
C2_24–C1_24–C4_24–F9_24	−76.4(3)
O1_24–C1_24–C4_24–F8_24	162.0(3)
C3_24–C1_24–C4_24–F8_24	−75.8(3)
C2_24–C1_24–C4_24–F8_24	43.3(3)

S-Table 22: Atomic coordinates and U_{eq} [Å^2] for [(cdp)Al(AlCp*)$_3$][*pf*]

Atom	***x***	***y***	***z***	U_{eq}
P001	0.30381(4)	0.17736(3)	0.23585(3)	0.01685(12)
P002	0.36928(4)	0.30372(3)	0.14523(3)	0.01724(12)
Al03	0.99256(5)	0.72243(4)	0.25113(3)	0.01710(14)
Al4	0.54973(5)	0.19572(4)	0.41209(4)	0.02459(16)
Al1	0.48389(5)	0.25520(4)	0.29033(4)	0.01743(14)
Al2	0.54136(5)	0.34371(4)	0.37787(4)	0.02162(16)
Al3	0.67768(5)	0.25021(4)	0.30386(4)	0.01992(15)
F008	1.12217(11)	0.93928(8)	0.21194(8)	0.0379(4)
F009	1.16927(10)	0.84016(9)	0.31700(8)	0.0386(4)
F00A	0.97720(12)	0.93541(8)	0.17712(8)	0.0396(4)
F00B	1.05419(12)	0.82928(9)	0.40046(8)	0.0414(4)
F00C	0.86823(11)	0.82481(9)	0.35715(9)	0.0419(4)
F00D	0.99992(13)	1.00392(8)	0.25985(9)	0.0444(4)
F00E	0.83417(11)	0.91172(9)	0.28086(9)	0.0438(4)
F00I	0.89695(13)	0.93505(9)	0.37533(9)	0.0484(4)
O00O	1.01227(12)	0.81365(9)	0.25210(9)	0.0245(4)
F00P	1.10079(13)	0.93569(9)	0.36357(9)	0.0449(4)

C1	0.43603(17)	0.38688(12)	0.14086(12)	0.0207(5)
C2	0.53842(19)	0.38027(15)	0.13833(18)	0.0445(8)
H2	0.570989	0.334325	0.149502	0.053
C01U	1.00482(17)	0.87440(13)	0.28832(13)	0.0232(5)
C3	0.5940(2)	0.44005(17)	0.1196(2)	0.0600(11)
H3	0.664355	0.434662	0.116617	0.072
C23	0.03379(17)	0.20327(13)	0.15427(13)	0.0256(5)
H23	-0.030849	0.223102	0.168269	0.031
C24	0.10853(16)	0.20272(13)	0.19929(12)	0.0216(5)
H24	0.094628	0.221631	0.244319	0.026
C25	0.36845(16)	0.08778(12)	0.23070(12)	0.0202(5)
C26	0.47156(17)	0.07946(13)	0.22821(12)	0.0223(5)
H26	0.509172	0.121149	0.227568	0.027
C27	0.51986(18)	0.01085(13)	0.22666(13)	0.0276(5)
H27	0.590226	0.005902	0.224789	0.033
C28	0.46584(19)	-0.05054(14)	0.22785(14)	0.0301(6)
H28	0.498885	-0.097523	0.227338	0.036
C29	0.36330(19)	-0.04275(14)	0.22977(14)	0.0295(6)
H29	0.326079	-0.084667	0.230733	0.035
C30	0.31451(18)	0.02562(13)	0.23032(13)	0.0251(5)
H30	0.244303	0.030367	0.230432	0.030
C31	0.23730(16)	0.18057(13)	0.32291(12)	0.0218(5)
C32	0.22321(17)	0.24734(14)	0.35316(13)	0.0268(5)
H32	0.256309	0.288027	0.331638	0.032
C33	0.16127(19)	0.25498(17)	0.41445(14)	0.0359(6)
H33	0.151191	0.300963	0.434185	0.043
C34	0.1141(2)	0.19557(18)	0.44692(14)	0.0389(7)
H34	0.071639	0.200717	0.488859	0.047
C02C	1.02542(19)	0.93929(14)	0.23385(14)	0.0294(6)
C02E	1.08359(19)	0.87004(14)	0.34312(13)	0.0298(6)
C02K	0.89974(19)	0.88720(15)	0.32617(15)	0.0330(6)
C4	0.5472(2)	0.50731(15)	0.10543(17)	0.0411(7)
H4	0.585167	0.548676	0.094521	0.049
C35	0.12915(19)	0.12872(16)	0.41789(14)	0.0349(6)
H35	0.097804	0.087771	0.440517	0.042
C36	0.18966(17)	0.12107(14)	0.35602(13)	0.0276(5)
H36	0.198700	0.075146	0.336114	0.033
C37	0.38124(16)	0.24785(12)	0.21983(11)	0.0177(5)
C48	0.5492(3)	0.2039(2)	0.59475(17)	0.0675(11)
H48A	0.609842	0.230581	0.587954	0.101
H48B	0.550636	0.171732	0.637713	0.101
H48C	0.491298	0.238477	0.599044	0.101
C49	0.7298(2)	0.1209(2)	0.51558(17)	0.0548(9)
H49A	0.771565	0.086742	0.487077	0.082
H49B	0.733190	0.106118	0.565599	0.082
H49C	0.753556	0.169914	0.505938	0.082
C50	0.6444(2)	0.02571(15)	0.40043(15)	0.0374(6)
H50A	0.607783	-0.018196	0.399749	0.056
H50B	0.709411	0.012589	0.417893	0.056
H50C	0.653498	0.048642	0.352659	0.056
C51	0.4118(2)	0.05148(16)	0.41463(14)	0.0375(7)
H51A	0.403055	0.077960	0.369145	0.056
H51B	0.347582	0.049634	0.442472	0.056
H51C	0.438933	0.001883	0.406888	0.056

C52	0.3499(2)	0.16706(18)	0.52842(18)	0.0554(9)
H52A	0.327024	0.205006	0.494131	0.083
H52B	0.348405	0.187060	0.574674	0.083
H52C	0.306356	0.126482	0.531425	0.083
C53	0.4547(2)	0.14031(15)	0.50535(14)	0.0351(6)
C54	0.5429(2)	0.15904(15)	0.53231(14)	0.0398(7)
C55	0.6242(2)	0.12087(15)	0.49736(14)	0.0339(6)
C56	0.58713(18)	0.07790(14)	0.44788(13)	0.0267(5)
C57	0.48216(18)	0.08971(14)	0.45350(13)	0.0278(6)
C58	0.8054(2)	0.38449(16)	0.21465(17)	0.0435(7)
H58A	0.817418	0.390732	0.163313	0.065
H58B	0.856905	0.407466	0.236537	0.065
H58C	0.740216	0.407247	0.229505	0.065
C59	0.8872(2)	0.31089(16)	0.35584(16)	0.0400(7)
H59A	0.958429	0.297647	0.355716	0.060
H59B	0.853969	0.296626	0.401952	0.060
H59C	0.876965	0.363567	0.346332	0.060
C60	0.8794(2)	0.14087(16)	0.35269(15)	0.0381(7)
H60A	0.838042	0.098918	0.358597	0.057
H60B	0.879904	0.162560	0.397969	0.057
H60C	0.947231	0.125000	0.335820	0.057
C61	0.7812(2)	0.10727(16)	0.21392(16)	0.0418(7)
H61A	0.721345	0.109718	0.188486	0.063
H61B	0.773446	0.072570	0.254970	0.063
H61C	0.838696	0.091324	0.182720	0.063
C62	0.7451(2)	0.2533(2)	0.12514(14)	0.0456(8)
H62A	0.734310	0.304678	0.109397	0.068
H62B	0.683164	0.228888	0.125037	0.068
H62C	0.796417	0.230085	0.093225	0.068
C63	0.80795(17)	0.30477(14)	0.23703(13)	0.0273(5)
C64	0.84485(16)	0.27238(14)	0.30003(13)	0.0252(5)
C65	0.83786(17)	0.19618(14)	0.30014(13)	0.0256(5)
C66	0.79655(17)	0.18105(14)	0.23777(13)	0.0262(5)
C67	0.77816(17)	0.24772(15)	0.19856(13)	0.0284(6)
C5	0.4462(2)	0.51444(14)	0.10703(15)	0.0349(6)
H5	0.413996	0.560558	0.095929	0.042
C6	0.39023(18)	0.45436(13)	0.12488(14)	0.0292(6)
H6	0.319938	0.459743	0.126105	0.035
C7	0.24291(16)	0.33742(12)	0.13168(12)	0.0190(5)
C8	0.18898(17)	0.37229(13)	0.18679(13)	0.0238(5)
H8	0.216702	0.374247	0.230453	0.029
C9	0.09484(18)	0.40412(13)	0.17776(14)	0.0293(6)
H9	0.058172	0.427687	0.215316	0.035
C10	0.05455(18)	0.40153(14)	0.11432(15)	0.0325(6)
H10	-0.009175	0.424351	0.107981	0.039
C11	0.10637(18)	0.36594(14)	0.06003(14)	0.0297(6)
H11	0.077443	0.363259	0.016922	0.036
C12	0.20092(17)	0.33393(13)	0.06821(13)	0.0225(5)
H12	0.236674	0.309800	0.030638	0.027
C13	0.42365(16)	0.26596(13)	0.06380(12)	0.0203(5)
C14	0.46450(17)	0.19498(13)	0.06468(13)	0.0256(5)
H14	0.460881	0.165196	0.107326	0.031
C15	0.51054(19)	0.16736(15)	0.00363(14)	0.0332(6)
H15	0.537332	0.118485	0.004401	0.040

C16	0.51761(18)	0.21068(15)	-0.05832(14)	0.0326(6)
H16	0.549185	0.191597	-0.100086	0.039
C17	0.47879(18)	0.28163(15)	-0.05950(13)	0.0295(6)
H17	0.483908	0.311429	-0.102100	0.035
C18	0.43234(17)	0.30962(14)	0.00120(12)	0.0242(5)
H18	0.406336	0.358702	0.000206	0.029
C19	0.20417(16)	0.17450(12)	0.17879(12)	0.0181(5)
C20	0.22286(17)	0.14564(12)	0.11299(12)	0.0208(5)
H20	0.287316	0.125623	0.098777	0.025
C21	0.14752(18)	0.14604(13)	0.06813(13)	0.0250(5)
H21	0.160609	0.126538	0.023319	0.030
C22	0.05330(18)	0.17496(14)	0.08896(13)	0.0272(5)
H22	0.001927	0.175349	0.058280	0.033
C1_3	0.4306(4)	0.4398(3)	0.3916(3)	0.0274(12)
C2_3	0.4500(4)	0.4076(3)	0.4586(3)	0.0269(12)
C3_3	0.5527(4)	0.4148(3)	0.4664(3)	0.0296(13)
C4_3	0.5942(3)	0.4508(3)	0.4038(3)	0.0294(11)
C5_3	0.5196(4)	0.4666(2)	0.3577(2)	0.0288(10)
C6_3	0.5311(4)	0.5070(2)	0.2858(2)	0.0529(13)
H6A_3	0.600841	0.503355	0.267194	0.079
H6B_3	0.509247	0.558325	0.290088	0.079
H6C_3	0.490449	0.485577	0.253772	0.079
C7_3	0.7011(3)	0.4718(3)	0.3901(3)	0.0557(15)
H7A_3	0.725080	0.463668	0.341212	0.084
H7B_3	0.742567	0.442091	0.421892	0.084
H7C_3	0.704685	0.523338	0.398411	0.084
C8_3	0.6076(4)	0.3908(3)	0.5295(3)	0.0497(13)
H8A_3	0.658651	0.352675	0.516941	0.074
H8B_3	0.561074	0.371644	0.567502	0.074
H8C_3	0.639065	0.432295	0.545308	0.074
C9_3	0.3747(4)	0.3736(2)	0.5108(3)	0.0493(13)
H9A_3	0.340643	0.337669	0.488164	0.074
H9B_3	0.326233	0.411390	0.528171	0.074
H9C_3	0.408049	0.349638	0.550391	0.074
C10_3	0.3333(3)	0.4470(2)	0.3586(3)	0.0468(13)
H10A_3	0.313189	0.498578	0.350127	0.070
H10B_3	0.282448	0.423390	0.390373	0.070
H10C_3	0.340977	0.423588	0.313795	0.070
C1_4	0.4924(8)	0.4055(4)	0.4784(4)	0.026(2)
C2_4	0.4176(6)	0.4219(4)	0.4321(5)	0.0229(19)
C3_4	0.4586(7)	0.4590(5)	0.3710(4)	0.018(2)
C4_4	0.5603(6)	0.4648(5)	0.3797(4)	0.0185(19)
C5_4	0.5819(7)	0.4323(6)	0.4460(5)	0.020(2)
C6_4	0.6804(6)	0.4285(5)	0.4762(6)	0.051(3)
H6A_4	0.724571	0.461276	0.447925	0.076
H6B_4	0.709720	0.378596	0.475737	0.076
H6C_4	0.671274	0.443218	0.524770	0.076
C7_4	0.6288(7)	0.5080(5)	0.3273(5)	0.046(2)
H7A_4	0.697899	0.496144	0.337252	0.069
H7B_4	0.612907	0.560137	0.331440	0.069
H7C_4	0.619848	0.495479	0.279376	0.069
C8_4	0.4046(7)	0.4887(5)	0.3085(4)	0.044(2)
H8A_4	0.453049	0.500970	0.268874	0.066
H8B_4	0.363727	0.532486	0.320823	0.066

H8C_4	0.362151	0.451974	0.295149	0.066
C9_4	0.3094(6)	0.4032(5)	0.4455(6)	0.052(3)
H9A_4	0.269425	0.445235	0.463260	0.078
H9B_4	0.303952	0.361800	0.480358	0.078
H9C_4	0.285212	0.390453	0.401418	0.078
C10_4	0.4799(9)	0.3702(5)	0.5523(4)	0.057(3)
H10A_4	0.446699	0.324736	0.551622	0.086
H10B_4	0.439650	0.403216	0.582917	0.086
H10C_4	0.545175	0.359822	0.570136	0.086
C1_1	0.6936(3)	-0.0299(3)	0.0544(2)	0.0341(10)
C2_1	0.6837(4)	-0.0008(4)	-0.0129(3)	0.0329(11)
C3_1	0.7585(4)	0.0358(4)	-0.0500(3)	0.0366(13)
H3_1	0.750849	0.056086	-0.096429	0.044
C4_1	0.8449(4)	0.0425(4)	-0.0188(3)	0.0386(11)
H4_1	0.897456	0.067383	-0.044144	0.046
C5_1	0.8559(4)	0.0139(3)	0.0480(2)	0.0355(10)
H5_1	0.915840	0.018927	0.068866	0.043
C6_1	0.7796(3)	-0.0226(2)	0.0855(2)	0.0365(10)
H6_1	0.786788	-0.042248	0.132165	0.044
F1_1	0.61901(16)	-0.06587(12)	0.08901(11)	0.0513(7)
F2_1	0.59869(15)	-0.00978(12)	-0.04306(11)	0.0436(6)
C1_2	0.8190(13)	0.0184(14)	0.0425(10)	0.050(6)
C2_2	0.7409(13)	-0.0151(12)	0.0786(9)	0.055(6)
C3_2	0.6585(15)	-0.0229(16)	0.0452(12)	0.061(7)
H3_2	0.603242	-0.045072	0.070061	0.073
C4_2	0.654(2)	0.001(2)	-0.0236(13)	0.052(6)
H4_2	0.596871	-0.005938	-0.046861	0.063
C5_2	0.732(2)	0.034(2)	-0.0593(13)	0.052(7)
H5_2	0.730238	0.049241	-0.107712	0.062
C6_2	0.813(2)	0.046(2)	-0.0253(12)	0.055(7)
H6_2	0.865195	0.073249	-0.048421	0.066
F1_2	0.9015(11)	0.0256(10)	0.0723(8)	0.093(5)
F2_2	0.7464(10)	-0.0401(7)	0.1458(6)	0.075(4)
O1_5	0.8701(3)	0.7076(3)	0.2410(2)	0.0259(6)
C1_5	0.7980(2)	0.70599(17)	0.19693(16)	0.0277(6)
C2_5	0.8156(2)	0.75822(17)	0.13047(16)	0.0324(7)
F1_5	0.88296(12)	0.72940(11)	0.08376(9)	0.0403(5)
F2_5	0.7334(3)	0.7754(2)	0.0975(2)	0.0465(9)
F3_5	0.84930(17)	0.81991(10)	0.14715(11)	0.0444(5)
C3_5	0.6978(2)	0.7297(2)	0.23833(18)	0.0439(9)
F4_5	0.69208(14)	0.69821(16)	0.30318(10)	0.0543(6)
F5_5	0.69001(14)	0.80109(12)	0.24328(12)	0.0580(6)
F6_5	0.6187(2)	0.7112(2)	0.20790(16)	0.0622(9)
C4_5	0.7938(3)	0.62733(19)	0.1736(2)	0.0411(8)
F7_5	0.75581(18)	0.58382(12)	0.22557(12)	0.0583(6)
F8_5	0.73749(17)	0.62543(15)	0.11910(13)	0.0522(6)
F9_5	0.88369(14)	0.59959(10)	0.15336(12)	0.0467(5)
O1_7	1.0227(11)	0.6774(5)	0.3271(6)	0.028(2)
C1_7	1.0099(5)	0.6199(4)	0.3748(4)	0.0268(11)
C2_7	1.0862(6)	0.6236(4)	0.4294(4)	0.0436(15)
F1_7	1.0567(8)	0.6756(5)	0.4734(5)	0.073(2)
F2_7	1.0980(9)	0.5614(4)	0.4687(5)	0.0564(18)
F3_7	1.1732(5)	0.6395(5)	0.3993(4)	0.0616(17)
C3_7	1.0277(5)	0.5473(3)	0.3388(3)	0.0332(12)

F4_7	0.9849(4)	0.5516(3)	0.2786(3)	0.0419(10)
F5_7	1.1248(4)	0.5330(3)	0.3219(3)	0.0521(12)
F6_7	0.9946(5)	0.4906(3)	0.3790(3)	0.0479(12)
C4_7	0.9028(5)	0.6231(5)	0.4120(4)	0.0370(14)
F7_7	0.8401(5)	0.5994(4)	0.3708(4)	0.0428(12)
F8_7	0.8938(8)	0.5827(4)	0.4733(4)	0.0448(14)
F9_7	0.8747(6)	0.6911(4)	0.4254(5)	0.051(2)
O1_6	0.874(3)	0.709(3)	0.246(2)	0.030(5)
C1_6	0.7937(17)	0.7087(9)	0.2091(10)	0.035(3)
C2_6	0.7965(15)	0.6378(10)	0.1696(11)	0.042(4)
F1_6	0.8621(15)	0.6433(14)	0.1134(10)	0.069(5)
F2_6	0.7067(15)	0.6256(15)	0.1510(11)	0.051(5)
F3_6	0.8265(18)	0.5819(10)	0.2115(12)	0.060(5)
C3_6	0.6973(17)	0.7113(11)	0.2594(10)	0.040(4)
F4_6	0.6998(14)	0.7602(13)	0.3063(10)	0.060(5)
F5_6	0.6858(17)	0.6464(12)	0.2929(13)	0.070(6)
F6_6	0.620(2)	0.731(2)	0.2222(17)	0.066(7)
C4_6	0.7919(15)	0.7738(10)	0.1537(11)	0.044(4)
F7_6	0.7592(17)	0.8346(10)	0.1836(13)	0.071(5)
F8_6	0.732(3)	0.763(2)	0.104(2)	0.049(8)
F9_6	0.8824(14)	0.7838(14)	0.1229(12)	0.056(5)
O1_8	1.027(2)	0.6835(12)	0.3341(13)	0.014(3)
C1_8	1.0231(11)	0.6245(8)	0.3803(8)	0.027(2)
C2_8	1.0872(11)	0.6380(10)	0.4407(9)	0.035(3)
F1_8	1.0413(12)	0.6860(9)	0.4826(9)	0.037(3)
F2_8	1.107(2)	0.5785(10)	0.4815(11)	0.053(4)
F3_8	1.1725(11)	0.6642(11)	0.4147(10)	0.055(4)
C3_8	1.0614(15)	0.5534(7)	0.3459(7)	0.041(3)
F4_8	1.0282(19)	0.5515(7)	0.2835(6)	0.059(4)
F5_8	1.1606(14)	0.5489(10)	0.3364(10)	0.072(5)
F6_8	1.0350(15)	0.4943(7)	0.3851(8)	0.054(3)
C4_8	0.9141(12)	0.6174(10)	0.4104(10)	0.037(3)
F7_8	0.8621(16)	0.5836(12)	0.3678(11)	0.068(5)
F8_8	0.916(2)	0.5786(13)	0.4722(10)	0.063(5)
F9_8	0.8638(11)	0.6807(10)	0.4217(11)	0.034(3)
O1_9	1.06349(17)	0.68870(12)	0.17882(15)	0.0227(5)
C1_9	1.1523(2)	0.68874(15)	0.14008(14)	0.0228(6)
C2_9	1.2382(2)	0.66508(17)	0.18711(15)	0.0333(7)
F1_9	1.24202(15)	0.59401(11)	0.20324(11)	0.0494(6)
F2_9	1.32727(19)	0.6806(2)	0.1556(2)	0.0446(9)
F3_9	1.2256(3)	0.69908(17)	0.24663(14)	0.0451(8)
C3_9	1.1705(2)	0.76499(16)	0.10384(15)	0.0319(7)
F4_9	1.08577(17)	0.79594(12)	0.08148(15)	0.0470(6)
F5_9	1.20110(14)	0.80893(10)	0.14879(11)	0.0436(5)
F6_9	1.23841(14)	0.76370(12)	0.04900(12)	0.0405(5)
C4_9	1.1495(2)	0.63368(16)	0.08310(15)	0.0332(7)
F7_9	1.09408(14)	0.66121(13)	0.03208(10)	0.0447(5)
F8_9	1.24023(15)	0.61653(12)	0.05158(11)	0.0445(5)
F9_9	1.11115(17)	0.57302(11)	0.10870(11)	0.0516(6)
O1_10	1.059(2)	0.7082(19)	0.181(2)	0.034(6)
C1_10	1.1440(18)	0.6904(10)	0.1424(11)	0.035(3)
C2_10	1.1569(17)	0.6080(10)	0.1326(13)	0.049(4)
F1_10	1.198(2)	0.5725(15)	0.1865(14)	0.067(6)
F2_10	1.220(2)	0.5900(16)	0.0789(14)	0.057(6)

F3_10	1.0699(18)	0.5799(16)	0.132(2)	0.073(7)
C3_10	1.1469(17)	0.7340(12)	0.0699(11)	0.046(4)
F4_10	1.117(2)	0.8033(12)	0.077(2)	0.055(7)
F5_10	1.084(2)	0.7089(18)	0.0293(13)	0.058(6)
F6_10	1.2400(18)	0.7298(19)	0.0401(17)	0.061(7)
C4_10	1.2324(19)	0.7108(13)	0.1815(13)	0.041(4)
F7_10	1.234(2)	0.7822(13)	0.1836(17)	0.062(6)
F8_10	1.319(2)	0.688(3)	0.148(3)	0.043(8)
F9_10	1.228(4)	0.679(2)	0.2464(17)	0.045(7)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

S-Table 23: Bond lengths and angles for [(cdp)Al(AlCp*)$_3$][*pf*]

Atom–Atom	**Length [Å]**
P001–C37	1.720(2)
P001–C19	1.818(2)
P001–C31	1.822(2)
P001–C25	1.825(2)
P002–C37	1.714(2)
P002–C7	1.819(2)
P002–C13	1.825(2)
P002–C1	1.827(2)
Al03–O1_10	1.57(3)
Al03–O1_6	1.66(3)
Al03–O1_7	1.691(10)
Al03–O00O	1.7246(17)
Al03–O1_5	1.730(3)
Al03–O1_9	1.739(2)
Al03–O1_8	1.78(2)
Al4–C56	2.273(3)
Al4–C57	2.277(3)
Al4–C53	2.320(3)
Al4–C55	2.321(3)
Al4–C54	2.345(3)
Al4–Al1	2.7035(11)
Al4–Al3	2.7546(11)
Al4–Al2	2.7622(12)
Al1–C37	2.041(2)
Al1–Al2	2.6215(10)
Al1–Al3	2.6585(13)
Al2–C3_3	2.236(6)
Al2–C2_3	2.241(4)
Al2–C4_3	2.250(5)
Al2–C1_3	2.262(5)
Al2–C4_4	2.272(8)
Al2–C5_3	2.278(5)
Al2–C5_4	2.286(11)
Al2–C1_4	2.327(8)
Al2–C3_4	2.342(9)
Al2–C2_4	2.356(7)
Al3–C64	2.324(2)
Al3–C66	2.326(2)
Al3–C63	2.326(3)

Al3–C65	2.326(2)
Al3–C67	2.327(2)
F008–C02C	1.340(3)
F009–C02E	1.323(3)
F00A–C02C	1.325(3)
F00B–C02E	1.331(3)
F00C–C02K	1.336(3)
F00D–C02C	1.338(3)
F00E–C02K	1.333(3)
F00I–C02K	1.331(3)
O00O–C01U	1.353(3)
F00P–C02E	1.341(3)
C1–C6	1.382(3)
C1–C2	1.382(3)
C2–C3	1.385(4)
C2–H2	0.9500
C01U–C02K	1.550(3)
C01U–C02C	1.554(3)
C01U–C02E	1.557(3)
C3–C4	1.378(4)
C3–H3	0.9500
C23–C22	1.384(4)
C23–C24	1.387(3)
C23–H23	0.9500
C24–C19	1.398(3)
C24–H24	0.9500
C25–C26	1.393(3)
C25–C30	1.402(3)
C26–C27	1.388(3)
C26–H26	0.9500
C27–C28	1.388(4)
C27–H27	0.9500
C28–C29	1.386(4)
C28–H28	0.9500
C29–C30	1.386(3)
C29–H29	0.9500
C30–H30	0.9500
C31–C32	1.393(3)
C31–C36	1.395(3)
C32–C33	1.388(3)
C32–H32	0.9500
C33–C34	1.387(4)
C33–H33	0.9500
C34–C35	1.384(4)
C34–H34	0.9500
C4–C5	1.365(4)
C4–H4	0.9500
C35–C36	1.387(4)
C35–H35	0.9500
C36–H36	0.9500
C48–C54	1.512(4)
C48–H48A	0.9800
C48–H48B	0.9800
C48–H48C	0.9800

C49–C55	1.504(4)
C49–H49A	0.9800
C49–H49B	0.9800
C49–H49C	0.9800
C50–C56	1.500(4)
C50–H50A	0.9800
C50–H50B	0.9800
C50–H50C	0.9800
C51–C57	1.501(4)
C51–H51A	0.9800
C51–H51B	0.9800
C51–H51C	0.9800
C52–C53	1.510(4)
C52–H52A	0.9800
C52–H52B	0.9800
C52–H52C	0.9800
C53–C54	1.416(4)
C53–C57	1.418(4)
C54–C55	1.411(4)
C55–C56	1.423(4)
C56–C57	1.421(3)
C58–C63	1.503(4)
C58–H58A	0.9800
C58–H58B	0.9800
C58–H58C	0.9800
C59–C64	1.499(4)
C59–H59A	0.9800
C59–H59B	0.9800
C59–H59C	0.9800
C60–C65	1.500(4)
C60–H60A	0.9800
C60–H60B	0.9800
C60–H60C	0.9800
C61–C66	1.500(4)
C61–H61A	0.9800
C61–H61B	0.9800
C61–H61C	0.9800
C62–C67	1.506(4)
C62–H62A	0.9800
C62–H62B	0.9800
C62–H62C	0.9800
C63–C64	1.424(3)
C63–C67	1.426(4)
C64–C65	1.417(3)
C65–C66	1.415(3)
C66–C67	1.415(4)
C5–C6	1.391(4)
C5–H5	0.9500
C6–H6	0.9500
C7–C12	1.394(3)
C7–C8	1.397(3)
C8–C9	1.390(3)
C8–H8	0.9500
C9–C10	1.380(4)

C9–H9	0.9500
C10–C11	1.380(4)
C10–H10	0.9500
C11–C12	1.393(3)
C11–H11	0.9500
C12–H12	0.9500
C13–C14	1.388(3)
C13–C18	1.395(3)
C14–C15	1.386(3)
C14–H14	0.9500
C15–C16	1.381(4)
C15–H15	0.9500
C16–C17	1.379(4)
C16–H16	0.9500
C17–C18	1.385(3)
C17–H17	0.9500
C18–H18	0.9500
C19–C20	1.396(3)
C20–C21	1.392(3)
C20–H20	0.9500
C21–C22	1.387(3)
C21–H21	0.9500
C22–H22	0.9500
C1_3–C2_3	1.413(7)
C1_3–C5_3	1.418(6)
C1_3–C10_3	1.508(6)
C2_3–C3_3	1.429(6)
C2_3–C9_3	1.498(6)
C3_3–C4_3	1.417(7)
C3_3–C8_3	1.500(6)
C4_3–C5_3	1.404(6)
C4_3–C7_3	1.521(6)
C5_3–C6_3	1.518(6)
C6_3–H6A_3	0.9800
C6_3–H6B_3	0.9800
C6_3–H6C_3	0.9800
C7_3–H7A_3	0.9800
C7_3–H7B_3	0.9800
C7_3–H7C_3	0.9800
C8_3–H8A_3	0.9800
C8_3–H8B_3	0.9800
C8_3–H8C_3	0.9800
C9_3–H9A_3	0.9800
C9_3–H9B_3	0.9800
C9_3–H9C_3	0.9800
C10_3–H10A_3	0.9800
C10_3–H10B_3	0.9800
C10_3–H10C_3	0.9800
C1_4–C2_4	1.411(9)
C1_4–C5_4	1.414(10)
C1_4–C10_4	1.513(9)
C2_4–C3_4	1.401(9)
C2_4–C9_4	1.524(9)
C3_4–C4_4	1.417(9)

C3_4–C8_4	1.509(9)
C4_4–C5_4	1.411(9)
C4_4–C7_4	1.522(9)
C5_4–C6_4	1.498(9)
C6_4–H6A_4	0.9800
C6_4–H6B_4	0.9800
C6_4–H6C_4	0.9800
C7_4–H7A_4	0.9800
C7_4–H7B_4	0.9800
C7_4–H7C_4	0.9800
C8_4–H8A_4	0.9800
C8_4–H8B_4	0.9800
C8_4–H8C_4	0.9800
C9_4–H9A_4	0.9800
C9_4–H9B_4	0.9800
C9_4–H9C_4	0.9800
C10_4–H10A_4	0.9800
C10_4–H10B_4	0.9800
C10_4–H10C_4	0.9800
C1_1–F1_1	1.344(5)
C1_1–C2_1	1.372(5)
C1_1–C6_1	1.376(5)
C2_1–F2_1	1.360(5)
C2_1–C3_1	1.371(5)
C3_1–C4_1	1.380(5)
C3_1–H3_1	0.9500
C4_1–C5_1	1.364(5)
C4_1–H4_1	0.9500
C5_1–C6_1	1.388(5)
C5_1–H5_1	0.9500
C6_1–H6_1	0.9500
C1_2–F1_2	1.319(14)
C1_2–C6_2	1.366(13)
C1_2–C2_2	1.369(13)
C2_2–F2_2	1.340(14)
C2_2–C3_2	1.357(13)
C3_2–C4_2	1.363(14)
C3_2–H3_2	0.9500
C4_2–C5_2	1.364(14)
C4_2–H4_2	0.9500
C5_2–C6_2	1.363(14)
C5_2–H5_2	0.9500
C6_2–H6_2	0.9500
O1_5–C1_5	1.351(3)
C1_5–C2_5	1.550(4)
C1_5–C4_5	1.555(4)
C1_5–C3_5	1.561(4)
C2_5–F3_5	1.325(3)
C2_5–F1_5	1.330(3)
C2_5–F2_5	1.338(4)
C3_5–F5_5	1.325(4)
C3_5–F4_5	1.330(4)
C3_5–F6_5	1.341(4)
C4_5–F7_5	1.321(4)

C4_5–F9_5	1.326(4)
C4_5–F8_5	1.350(4)
O1_7–C1_7	1.359(6)
C1_7–C2_7	1.543(6)
C1_7–C3_7	1.545(6)
C1_7–C4_7	1.557(6)
C2_7–F3_7	1.308(7)
C2_7–F2_7	1.336(6)
C2_7–F1_7	1.339(6)
C3_7–F4_7	1.331(6)
C3_7–F6_7	1.332(6)
C3_7–F5_7	1.339(5)
C4_7–F7_7	1.324(7)
C4_7–F9_7	1.325(6)
C4_7–F8_7	1.344(6)
O1_6–C1_6	1.348(15)
C1_6–C4_6	1.547(13)
C1_6–C3_6	1.550(13)
C1_6–C2_6	1.554(13)
C2_6–F3_6	1.327(13)
C2_6–F1_6	1.333(13)
C2_6–F2_6	1.336(14)
C3_6–F4_6	1.322(13)
C3_6–F5_6	1.329(13)
C3_6–F6_6	1.338(14)
C4_6–F7_6	1.328(13)
C4_6–F9_6	1.330(13)
C4_6–F8_6	1.332(14)
O1_8–C1_8	1.353(13)
C1_8–C3_8	1.547(11)
C1_8–C4_8	1.548(12)
C1_8–C2_8	1.551(11)
C2_8–F1_8	1.323(12)
C2_8–F3_8	1.325(12)
C2_8–F2_8	1.329(12)
C3_8–F4_8	1.316(11)
C3_8–F6_8	1.330(11)
C3_8–F5_8	1.339(11)
C4_8–F9_8	1.334(12)
C4_8–F7_8	1.335(12)
C4_8–F8_8	1.340(13)
O1_9–C1_9	1.355(3)
C1_9–C4_9	1.546(4)
C1_9–C3_9	1.549(4)
C1_9–C2_9	1.557(4)
C2_9–F1_9	1.326(4)
C2_9–F3_9	1.330(4)
C2_9–F2_9	1.339(4)
C3_9–F6_9	1.331(3)
C3_9–F5_9	1.333(3)
C3_9–F4_9	1.341(4)
C4_9–F9_9	1.311(3)
C4_9–F7_9	1.337(3)
C4_9–F8_9	1.348(3)

O1_10–C1_10	1.349(15)
C1_10–C2_10	1.544(13)
C1_10–C4_10	1.548(13)
C1_10–C3_10	1.551(13)
C2_10–F2_10	1.320(13)
C2_10–F3_10	1.322(13)
C2_10–F1_10	1.331(14)
C3_10–F4_10	1.330(14)
C3_10–F5_10	1.331(13)
C3_10–F6_10	1.337(13)
C4_10–F7_10	1.325(13)
C4_10–F9_10	1.332(14)
C4_10–F8_10	1.337(14)

Atom–Atom–Atom	**Angle [°]**
C37–P001–C19	117.42(10)
C37–P001–C31	110.89(11)
C19–P001–C31	102.70(10)
C37–P001–C25	113.47(11)
C19–P001–C25	103.80(10)
C31–P001–C25	107.57(11)
C37–P002–C7	114.86(11)
C37–P002–C13	115.03(11)
C7–P002–C13	107.81(10)
C37–P002–C1	115.04(11)
C7–P002–C1	103.06(10)
C13–P002–C1	99.31(11)
O1_10–Al03–O1_6	113(2)
O1_10–Al03–O00O	96.8(14)
O1_6–Al03–O00O	111.9(17)
O1_7–Al03–O00O	110.6(4)
O1_7–Al03–O1_5	107.7(5)
O00O–Al03–O1_5	112.25(17)
O1_7–Al03–O1_9	111.4(5)
O00O–Al03–O1_9	107.84(10)
O1_5–Al03–O1_9	106.99(18)
O1_10–Al03–O1_8	121.4(17)
O1_6–Al03–O1_8	108.1(18)
O00O–Al03–O1_8	105.0(9)
C56–Al4–C57	36.40(9)
C56–Al4–C53	60.17(9)
C57–Al4–C53	35.93(10)
C56–Al4–C55	36.06(9)
C57–Al4–C55	59.81(9)
C53–Al4–C55	59.29(10)
C56–Al4–C54	59.51(10)
C57–Al4–C54	59.26(10)
C53–Al4–C54	35.34(10)
C55–Al4–C54	35.19(10)
C56–Al4–Al1	130.89(7)
C57–Al4–Al1	115.12(7)
C53–Al4–Al1	126.40(8)
C55–Al4–Al1	164.73(8)
C54–Al4–Al1	157.45(9)

C56–Al4–Al3	114.16(7)
C57–Al4–Al3	140.55(8)
C53–Al4–Al3	174.02(8)
C55–Al4–Al3	115.16(8)
C54–Al4–Al3	141.27(9)
Al1–Al4–Al3	58.29(3)
C56–Al4–Al2	168.31(7)
C57–Al4–Al2	153.43(7)
C53–Al4–Al2	124.09(8)
C55–Al4–Al2	134.13(8)
C54–Al4–Al2	116.59(8)
Al1–Al4–Al2	57.31(3)
Al3–Al4–Al2	61.02(3)
C37–Al1–Al2	141.71(7)
C37–Al1–Al3	143.43(7)
Al2–Al1–Al3	64.07(3)
C37–Al1–Al4	143.93(7)
Al2–Al1–Al4	62.47(3)
Al3–Al1–Al4	61.82(3)
C3_3–Al2–C2_3	37.24(17)
C3_3–Al2–C4_3	36.82(17)
C2_3–Al2–C4_3	61.51(17)
C3_3–Al2–C1_3	61.15(18)
C2_3–Al2–C1_3	36.58(18)
C4_3–Al2–C1_3	60.58(17)
C3_3–Al2–C5_3	61.09(18)
C2_3–Al2–C5_3	61.26(17)
C4_3–Al2–C5_3	36.11(16)
C1_3–Al2–C5_3	36.40(16)
C4_4–Al2–C5_4	36.1(2)
C4_4–Al2–C1_4	59.1(3)
C5_4–Al2–C1_4	35.7(3)
C4_4–Al2–C3_4	35.7(2)
C5_4–Al2–C3_4	59.8(3)
C1_4–Al2–C3_4	58.7(3)
C4_4–Al2–C2_4	58.5(3)
C5_4–Al2–C2_4	59.1(3)
C1_4–Al2–C2_4	35.1(2)
C3_4–Al2–C2_4	34.7(2)
C3_3–Al2–Al1	165.54(16)
C2_3–Al2–Al1	129.16(13)
C4_3–Al2–Al1	152.60(17)
C1_3–Al2–Al1	111.05(13)
C4_4–Al2–Al1	137.2(2)
C5_3–Al2–Al1	120.95(13)
C5_4–Al2–Al1	172.8(2)
C1_4–Al2–Al1	144.1(3)
C3_4–Al2–Al1	113.3(2)
C2_4–Al2–Al1	116.8(2)
C3_3–Al2–Al4	116.12(15)
C2_3–Al2–Al4	113.04(13)
C4_3–Al2–Al4	144.67(16)
C1_3–Al2–Al4	137.69(15)
C4_4–Al2–Al4	162.4(2)

C5_3–Al2–Al4	173.90(14)
C5_4–Al2–Al4	126.7(2)
C1_4–Al2–Al4	109.50(19)
C3_4–Al2–Al4	152.9(2)
C2_4–Al2–Al4	121.2(2)
Al1–Al2–Al4	60.22(3)
C64–Al3–C66	59.13(9)
C64–Al3–C63	35.66(9)
C66–Al3–C63	59.24(9)
C64–Al3–C65	35.47(9)
C66–Al3–C65	35.42(8)
C63–Al3–C65	59.20(9)
C64–Al3–C67	59.26(9)
C66–Al3–C67	35.42(9)
C63–Al3–C67	35.69(9)
C65–Al3–C67	59.02(9)
C64–Al3–Al1	166.25(7)
C66–Al3–Al1	124.63(7)
C63–Al3–Al1	132.09(7)
C65–Al3–Al1	155.09(7)
C67–Al3–Al1	114.95(7)
C64–Al3–Al4	130.90(7)
C66–Al3–Al4	125.05(7)
C63–Al3–Al4	164.79(7)
C65–Al3–Al4	114.54(7)
C67–Al3–Al4	156.02(8)
Al1–Al3–Al4	59.89(3)
C64–Al3–Al2	117.85(7)
C66–Al3–Al2	175.28(7)
C63–Al3–Al2	116.11(7)
C65–Al3–Al2	144.18(7)
C67–Al3–Al2	140.37(8)
Al1–Al3–Al2	57.32(3)
Al4–Al3–Al2	59.62(3)
C01U–O00O–Al03	148.28(16)
C6–C1–C2	118.7(2)
C6–C1–P002	121.73(18)
C2–C1–P002	118.07(19)
C1–C2–C3	120.6(3)
C1–C2–H2	119.7
C3–C2–H2	119.7
O00O–C01U–C02K	111.7(2)
O00O–C01U–C02C	106.9(2)
C02K–C01U–C02C	108.9(2)
O00O–C01U–C02E	110.68(19)
C02K–C01U–C02E	109.6(2)
C02C–C01U–C02E	108.9(2)
C4–C3–C2	120.0(3)
C4–C3–H3	120.0
C2–C3–H3	120.0
C22–C23–C24	120.1(2)
C22–C23–H23	120.0
C24–C23–H23	120.0
C23–C24–C19	120.4(2)

C23–C24–H24	119.8
C19–C24–H24	119.8
C26–C25–C30	118.7(2)
C26–C25–P001	121.08(17)
C30–C25–P001	120.20(17)
C27–C26–C25	120.6(2)
C27–C26–H26	119.7
C25–C26–H26	119.7
C28–C27–C26	120.3(2)
C28–C27–H27	119.9
C26–C27–H27	119.9
C29–C28–C27	119.5(2)
C29–C28–H28	120.3
C27–C28–H28	120.3
C28–C29–C30	120.6(2)
C28–C29–H29	119.7
C30–C29–H29	119.7
C29–C30–C25	120.2(2)
C29–C30–H30	119.9
C25–C30–H30	119.9
C32–C31–C36	118.9(2)
C32–C31–P001	118.32(18)
C36–C31–P001	122.29(19)
C33–C32–C31	120.6(2)
C33–C32–H32	119.7
C31–C32–H32	119.7
C34–C33–C32	120.1(3)
C34–C33–H33	120.0
C32–C33–H33	120.0
C35–C34–C33	119.6(2)
C35–C34–H34	120.2
C33–C34–H34	120.2
F00A–C02C–F00D	107.7(2)
F00A–C02C–F008	106.8(2)
F00D–C02C–F008	106.9(2)
F00A–C02C–C01U	111.5(2)
F00D–C02C–C01U	113.0(2)
F008–C02C–C01U	110.7(2)
F009–C02E–F00B	107.2(2)
F009–C02E–F00P	107.6(2)
F00B–C02E–F00P	107.6(2)
F009–C02E–C01U	111.1(2)
F00B–C02E–C01U	110.9(2)
F00P–C02E–C01U	112.3(2)
F00I–C02K–F00E	107.4(2)
F00I–C02K–F00C	107.9(2)
F00E–C02K–F00C	107.1(2)
F00I–C02K–C01U	112.7(2)
F00E–C02K–C01U	111.4(2)
F00C–C02K–C01U	110.2(2)
C5–C4–C3	119.9(3)
C5–C4–H4	120.0
C3–C4–H4	120.0
C34–C35–C36	120.5(3)

C34–C35–H35	119.8
C36–C35–H35	119.8
C35–C36–C31	120.3(2)
C35–C36–H36	119.9
C31–C36–H36	119.9
P002–C37–P001	117.97(13)
P002–C37–Al1	125.48(12)
P001–C37–Al1	116.51(12)
C54–C48–H48A	109.5
C54–C48–H48B	109.5
H48A–C48–H48B	109.5
C54–C48–H48C	109.5
H48A–C48–H48C	109.5
H48B–C48–H48C	109.5
C55–C49–H49A	109.5
C55–C49–H49B	109.5
H49A–C49–H49B	109.5
C55–C49–H49C	109.5
H49A–C49–H49C	109.5
H49B–C49–H49C	109.5
C56–C50–H50A	109.5
C56–C50–H50B	109.5
H50A–C50–H50B	109.5
C56–C50–H50C	109.5
H50A–C50–H50C	109.5
H50B–C50–H50C	109.5
C57–C51–H51A	109.5
C57–C51–H51B	109.5
H51A–C51–H51B	109.5
C57–C51–H51C	109.5
H51A–C51–H51C	109.5
H51B–C51–H51C	109.5
C53–C52–H52A	109.5
C53–C52–H52B	109.5
H52A–C52–H52B	109.5
C53–C52–H52C	109.5
H52A–C52–H52C	109.5
H52B–C52–H52C	109.5
C54–C53–C57	107.5(2)
C54–C53–C52	126.9(3)
C57–C53–C52	125.6(3)
C54–C53–Al4	73.28(15)
C57–C53–Al4	70.38(14)
C52–C53–Al4	123.09(19)
C55–C54–C53	108.6(2)
C55–C54–C48	124.7(3)
C53–C54–C48	126.2(3)
C55–C54–Al4	71.46(15)
C53–C54–Al4	71.37(15)
C48–C54–Al4	129.4(2)
C54–C55–C56	108.1(2)
C54–C55–C49	124.8(3)
C56–C55–C49	126.9(3)
C54–C55–Al4	73.35(16)

C56–C55–Al4	70.14(14)
C49–C55–Al4	126.8(2)
C57–C56–C55	107.5(2)
C57–C56–C50	124.5(2)
C55–C56–C50	128.0(2)
C57–C56–Al4	71.97(14)
C55–C56–Al4	73.80(15)
C50–C56–Al4	122.36(17)
C53–C57–C56	108.4(2)
C53–C57–C51	125.7(2)
C56–C57–C51	125.8(2)
C53–C57–Al4	73.69(15)
C56–C57–Al4	71.64(14)
C51–C57–Al4	123.59(17)
C63–C58–H58A	109.5
C63–C58–H58B	109.5
H58A–C58–H58B	109.5
C63–C58–H58C	109.5
H58A–C58–H58C	109.5
H58B–C58–H58C	109.5
C64–C59–H59A	109.5
C64–C59–H59B	109.5
H59A–C59–H59B	109.5
C64–C59–H59C	109.5
H59A–C59–H59C	109.5
H59B–C59–H59C	109.5
C65–C60–H60A	109.5
C65–C60–H60B	109.5
H60A–C60–H60B	109.5
C65–C60–H60C	109.5
H60A–C60–H60C	109.5
H60B–C60–H60C	109.5
C66–C61–H61A	109.5
C66–C61–H61B	109.5
H61A–C61–H61B	109.5
C66–C61–H61C	109.5
H61A–C61–H61C	109.5
H61B–C61–H61C	109.5
C67–C62–H62A	109.5
C67–C62–H62B	109.5
H62A–C62–H62B	109.5
C67–C62–H62C	109.5
H62A–C62–H62C	109.5
H62B–C62–H62C	109.5
C64–C63–C67	107.6(2)
C64–C63–C58	125.5(2)
C67–C63–C58	126.9(2)
C64–C63–Al3	72.08(14)
C67–C63–Al3	72.19(14)
C58–C63–Al3	123.14(17)
C65–C64–C63	108.0(2)
C65–C64–C59	125.3(2)
C63–C64–C59	126.7(2)
C65–C64–Al3	72.37(13)

C63–C64–Al3	72.26(13)
C59–C64–Al3	122.69(17)
C66–C65–C64	108.2(2)
C66–C65–C60	125.9(2)
C64–C65–C60	125.4(2)
C66–C65–Al3	72.27(13)
C64–C65–Al3	72.16(13)
C60–C65–Al3	127.29(18)
C67–C66–C65	108.2(2)
C67–C66–C61	125.1(2)
C65–C66–C61	126.6(2)
C67–C66–Al3	72.34(14)
C65–C66–Al3	72.31(13)
C61–C66–Al3	124.42(17)
C66–C67–C63	108.0(2)
C66–C67–C62	123.9(3)
C63–C67–C62	127.7(3)
C66–C67–Al3	72.24(14)
C63–C67–Al3	72.11(14)
C62–C67–Al3	127.19(17)
C4–C5–C6	120.1(2)
C4–C5–H5	119.9
C6–C5–H5	119.9
C1–C6–C5	120.6(2)
C1–C6–H6	119.7
C5–C6–H6	119.7
C12–C7–C8	119.5(2)
C12–C7–P002	123.09(18)
C8–C7–P002	117.29(17)
C9–C8–C7	120.0(2)
C9–C8–H8	120.0
C7–C8–H8	120.0
C10–C9–C8	120.1(2)
C10–C9–H9	120.0
C8–C9–H9	120.0
C9–C10–C11	120.3(2)
C9–C10–H10	119.8
C11–C10–H10	119.8
C10–C11–C12	120.2(2)
C10–C11–H11	119.9
C12–C11–H11	119.9
C11–C12–C7	119.8(2)
C11–C12–H12	120.1
C7–C12–H12	120.1
C14–C13–C18	119.1(2)
C14–C13–P002	120.15(18)
C18–C13–P002	120.56(18)
C15–C14–C13	120.3(2)
C15–C14–H14	119.8
C13–C14–H14	119.8
C16–C15–C14	120.2(2)
C16–C15–H15	119.9
C14–C15–H15	119.9
C17–C16–C15	119.9(2)

C17–C16–H16	120.0
C15–C16–H16	120.0
C16–C17–C18	120.3(2)
C16–C17–H17	119.9
C18–C17–H17	119.9
C17–C18–C13	120.2(2)
C17–C18–H18	119.9
C13–C18–H18	119.9
C20–C19–C24	119.1(2)
C20–C19–P001	120.29(17)
C24–C19–P001	120.61(17)
C21–C20–C19	120.3(2)
C21–C20–H20	119.8
C19–C20–H20	119.8
C22–C21–C20	119.9(2)
C22–C21–H21	120.1
C20–C21–H21	120.1
C23–C22–C21	120.3(2)
C23–C22–H22	119.9
C21–C22–H22	119.9
C2_3–C1_3–C5_3	108.9(4)
C2_3–C1_3–C10_3	127.9(5)
C5_3–C1_3–C10_3	123.2(6)
C2_3–C1_3–Al2	70.9(3)
C5_3–C1_3–Al2	72.4(3)
C10_3–C1_3–Al2	123.0(3)
C1_3–C2_3–C3_3	107.2(4)
C1_3–C2_3–C9_3	125.2(5)
C3_3–C2_3–C9_3	127.6(5)
C1_3–C2_3–Al2	72.5(3)
C3_3–C2_3–Al2	71.2(3)
C9_3–C2_3–Al2	122.4(3)
C4_3–C3_3–C2_3	107.6(4)
C4_3–C3_3–C8_3	125.3(5)
C2_3–C3_3–C8_3	127.2(6)
C4_3–C3_3–Al2	72.1(3)
C2_3–C3_3–Al2	71.5(3)
C8_3–C3_3–Al2	122.9(4)
C5_3–C4_3–C3_3	108.9(5)
C5_3–C4_3–C7_3	125.6(6)
C3_3–C4_3–C7_3	125.5(5)
C5_3–C4_3–Al2	73.0(3)
C3_3–C4_3–Al2	71.1(3)
C7_3–C4_3–Al2	124.0(3)
C4_3–C5_3–C1_3	107.5(5)
C4_3–C5_3–C6_3	126.4(5)
C1_3–C5_3–C6_3	126.1(5)
C4_3–C5_3–Al2	70.9(3)
C1_3–C5_3–Al2	71.2(3)
C6_3–C5_3–Al2	124.9(3)
C5_3–C6_3–H6A_3	109.5
C5_3–C6_3–H6B_3	109.5
H6A_3–C6_3–H6B_3	109.5
C5_3–C6_3–H6C_3	109.5

H6A_3–C6_3–H6C_3	109.5
H6B_3–C6_3–H6C_3	109.5
C4_3–C7_3–H7A_3	109.5
C4_3–C7_3–H7B_3	109.5
H7A_3–C7_3–H7B_3	109.5
C4_3–C7_3–H7C_3	109.5
H7A_3–C7_3–H7C_3	109.5
H7B_3–C7_3–H7C_3	109.5
C3_3–C8_3–H8A_3	109.5
C3_3–C8_3–H8B_3	109.5
H8A_3–C8_3–H8B_3	109.5
C3_3–C8_3–H8C_3	109.5
H8A_3–C8_3–H8C_3	109.5
H8B_3–C8_3–H8C_3	109.5
C2_3–C9_3–H9A_3	109.5
C2_3–C9_3–H9B_3	109.5
H9A_3–C9_3–H9B_3	109.5
C2_3–C9_3–H9C_3	109.5
H9A_3–C9_3–H9C_3	109.5
H9B_3–C9_3–H9C_3	109.5
C1_3–C10_3–H10A_3	109.5
C1_3–C10_3–H10B_3	109.5
H10A_3–C10_3–H10B_3	109.5
C1_3–C10_3–H10C_3	109.5
H10A_3–C10_3–H10C_3	109.5
H10B_3–C10_3–H10C_3	109.5
C2_4–C1_4–C5_4	108.3(7)
C2_4–C1_4–C10_4	126.9(9)
C5_4–C1_4–C10_4	124.7(9)
C2_4–C1_4–Al2	73.6(4)
C5_4–C1_4–Al2	70.6(6)
C10_4–C1_4–Al2	124.8(6)
C3_4–C2_4–C1_4	108.9(7)
C3_4–C2_4–C9_4	124.9(9)
C1_4–C2_4–C9_4	126.3(9)
C3_4–C2_4–Al2	72.1(4)
C1_4–C2_4–Al2	71.3(4)
C9_4–C2_4–Al2	122.9(5)
C2_4–C3_4–C4_4	106.8(6)
C2_4–C3_4–C8_4	126.8(9)
C4_4–C3_4–C8_4	126.3(8)
C2_4–C3_4–Al2	73.2(4)
C4_4–C3_4–Al2	69.4(5)
C8_4–C3_4–Al2	123.4(6)
C5_4–C4_4–C3_4	109.3(6)
C5_4–C4_4–C7_4	127.4(9)
C3_4–C4_4–C7_4	122.9(8)
C5_4–C4_4–Al2	72.5(6)
C3_4–C4_4–Al2	74.8(5)
C7_4–C4_4–Al2	124.6(6)
C4_4–C5_4–C1_4	106.7(7)

C4_4–C5_4–C6_4	126.2(9)
C1_4–C5_4–C6_4	127.1(9)
C4_4–C5_4–Al2	71.4(6)
C1_4–C5_4–Al2	73.7(5)
C6_4–C5_4–Al2	120.9(7)
C5_4–C6_4–H6A_4	109.5
C5_4–C6_4–H6B_4	109.5
H6A_4–C6_4–H6B_4	109.5
C5_4–C6_4–H6C_4	109.5
H6A_4–C6_4–H6C_4	109.5
H6B_4–C6_4–H6C_4	109.5
C4_4–C7_4–H7A_4	109.5
C4_4–C7_4–H7B_4	109.5
H7A_4–C7_4–H7B_4	109.5
C4_4–C7_4–H7C_4	109.5
H7A_4–C7_4–H7C_4	109.5
H7B_4–C7_4–H7C_4	109.5
C3_4–C8_4–H8A_4	109.5
C3_4–C8_4–H8B_4	109.5
H8A_4–C8_4–H8B_4	109.5
C3_4–C8_4–H8C_4	109.5
H8A_4–C8_4–H8C_4	109.5
H8B_4–C8_4–H8C_4	109.5
C2_4–C9_4–H9A_4	109.5
C2_4–C9_4–H9B_4	109.5
H9A_4–C9_4–H9B_4	109.5
C2_4–C9_4–H9C_4	109.5
H9A_4–C9_4–H9C_4	109.5
H9B_4–C9_4–H9C_4	109.5
C1_4–C10_4–H10A_4	109.5
C1_4–C10_4–H10B_4	109.5
H10A_4–C10_4–H10B_4	109.5
C1_4–C10_4–H10C_4	109.5
H10A_4–C10_4–H10C_4	109.5
H10B_4–C10_4–H10C_4	109.5
F1_1–C1_1–C2_1	119.4(4)
F1_1–C1_1–C6_1	120.6(4)
C2_1–C1_1–C6_1	119.9(4)
F2_1–C2_1–C3_1	120.0(4)
F2_1–C2_1–C1_1	118.9(4)
C3_1–C2_1–C1_1	121.1(4)
C2_1–C3_1–C4_1	118.8(4)
C2_1–C3_1–H3_1	120.6
C4_1–C3_1–H3_1	120.6
C5_1–C4_1–C3_1	120.8(4)
C5_1–C4_1–H4_1	119.6
C3_1–C4_1–H4_1	119.6
C4_1–C5_1–C6_1	120.1(4)
C4_1–C5_1–H5_1	120.0
C6_1–C5_1–H5_1	120.0
C1_1–C6_1–C5_1	119.3(4)

C1_1–C6_1–H6_1	120.4
C5_1–C6_1–H6_1	120.4
F1_2–C1_2–C6_2	118.0(15)
F1_2–C1_2–C2_2	121.1(15)
C6_2–C1_2–C2_2	120.9(14)
F2_2–C2_2–C3_2	120.8(15)
F2_2–C2_2–C1_2	120.3(14)
C3_2–C2_2–C1_2	119.0(14)
C2_2–C3_2–C4_2	120.6(16)
C2_2–C3_2–H3_2	119.7
C4_2–C3_2–H3_2	119.7
C3_2–C4_2–C5_2	120.2(17)
C3_2–C4_2–H4_2	119.9
C5_2–C4_2–H4_2	119.9
C6_2–C5_2–C4_2	119.9(17)
C6_2–C5_2–H5_2	120.1
C4_2–C5_2–H5_2	120.1
C5_2–C6_2–C1_2	119.3(16)
C5_2–C6_2–H6_2	120.4
C1_2–C6_2–H6_2	120.4
C1_5–O1_5–Al03	147.8(3)
O1_5–C1_5–C2_5	112.0(3)
O1_5–C1_5–C4_5	109.5(3)
C2_5–C1_5–C4_5	108.8(2)
O1_5–C1_5–C3_5	107.4(3)
C2_5–C1_5–C3_5	109.3(3)
C4_5–C1_5–C3_5	109.9(3)
F3_5–C2_5–F1_5	107.0(3)
F3_5–C2_5–F2_5	107.3(3)
F1_5–C2_5–F2_5	107.1(3)
F3_5–C2_5–C1_5	110.6(2)
F1_5–C2_5–C1_5	111.3(2)
F2_5–C2_5–C1_5	113.2(3)
F5_5–C3_5–F4_5	108.0(3)
F5_5–C3_5–F6_5	107.8(3)
F4_5–C3_5–F6_5	106.9(3)
F5_5–C3_5–C1_5	110.7(3)
F4_5–C3_5–C1_5	110.6(3)
F6_5–C3_5–C1_5	112.6(3)
F7_5–C4_5–F9_5	107.7(3)
F7_5–C4_5–F8_5	107.5(3)
F9_5–C4_5–F8_5	107.4(3)
F7_5–C4_5–C1_5	111.3(3)
F9_5–C4_5–C1_5	111.0(3)
F8_5–C4_5–C1_5	111.7(3)
C1_7–O1_7–Al03	148.8(10)
O1_7–C1_7–C2_7	107.3(7)
O1_7–C1_7–C3_7	110.9(6)
C2_7–C1_7–C3_7	109.5(4)
O1_7–C1_7–C4_7	111.1(7)
C2_7–C1_7–C4_7	109.9(5)
C3_7–C1_7–C4_7	108.2(5)
F3_7–C2_7–F2_7	107.8(7)
F3_7–C2_7–F1_7	107.2(6)

F2_7–C2_7–F1_7	107.2(6)
F3_7–C2_7–C1_7	111.5(6)
F2_7–C2_7–C1_7	112.8(6)
F1_7–C2_7–C1_7	110.1(6)
F4_7–C3_7–F6_7	108.8(5)
F4_7–C3_7–F5_7	106.2(4)
F6_7–C3_7–F5_7	107.3(4)
F4_7–C3_7–C1_7	110.3(5)
F6_7–C3_7–C1_7	113.3(5)
F5_7–C3_7–C1_7	110.5(4)
F7_7–C4_7–F9_7	108.5(6)
F7_7–C4_7–F8_7	107.1(7)
F9_7–C4_7–F8_7	107.5(6)
F7_7–C4_7–C1_7	110.2(5)
F9_7–C4_7–C1_7	109.6(6)
F8_7–C4_7–C1_7	113.8(6)
C1_6–O1_6–Al03	152(3)
O1_6–C1_6–C4_6	110.5(19)
O1_6–C1_6–C3_6	110.7(19)
C4_6–C1_6–C3_6	110.3(13)
O1_6–C1_6–C2_6	110.0(19)
C4_6–C1_6–C2_6	107.8(13)
C3_6–C1_6–C2_6	107.5(12)
F3_6–C2_6–F1_6	108.2(17)
F3_6–C2_6–F2_6	108.3(17)
F1_6–C2_6–F2_6	111.1(17)
F3_6–C2_6–C1_6	109.2(15)
F1_6–C2_6–C1_6	108.7(15)
F2_6–C2_6–C1_6	111.2(15)
F4_6–C3_6–F5_6	109.0(18)
F4_6–C3_6–F6_6	106.7(17)
F5_6–C3_6–F6_6	110.8(19)
F4_6–C3_6–C1_6	111.2(15)
F5_6–C3_6–C1_6	109.7(15)
F6_6–C3_6–C1_6	109.4(17)
F7_6–C4_6–F9_6	107.8(17)
F7_6–C4_6–F8_6	108(2)
F9_6–C4_6–F8_6	109(2)
F7_6–C4_6–C1_6	110.6(15)
F9_6–C4_6–C1_6	110.8(15)
F8_6–C4_6–C1_6	110.5(19)
C1_8–O1_8–Al03	146(2)
O1_8–C1_8–C3_8	112.6(14)
O1_8–C1_8–C4_8	108.3(14)
C3_8–C1_8–C4_8	109.0(10)
O1_8–C1_8–C2_8	107.6(14)
C3_8–C1_8–C2_8	109.9(10)
C4_8–C1_8–C2_8	109.4(10)
F1_8–C2_8–F3_8	107.7(12)
F1_8–C2_8–F2_8	106.3(13)
F3_8–C2_8–F2_8	108.1(14)
F1_8–C2_8–C1_8	110.8(12)
F3_8–C2_8–C1_8	110.2(11)
F2_8–C2_8–C1_8	113.4(13)

F4_8–C3_8–F6_8	108.7(11)
F4_8–C3_8–F5_8	107.1(10)
F6_8–C3_8–F5_8	106.8(10)
F4_8–C3_8–C1_8	110.6(11)
F6_8–C3_8–C1_8	112.5(12)
F5_8–C3_8–C1_8	110.9(10)
F9_8–C4_8–F7_8	106.0(13)
F9_8–C4_8–F8_8	108.1(15)
F7_8–C4_8–F8_8	109.3(16)
F9_8–C4_8–C1_8	114.3(13)
F7_8–C4_8–C1_8	112.1(12)
F8_8–C4_8–C1_8	106.8(14)
C1_9–O1_9–Al03	145.7(2)
O1_9–C1_9–C4_9	107.1(2)
O1_9–C1_9–C3_9	111.1(2)
C4_9–C1_9–C3_9	109.2(2)
O1_9–C1_9–C2_9	110.7(2)
C4_9–C1_9–C2_9	109.6(2)
C3_9–C1_9–C2_9	109.2(2)
F1_9–C2_9–F3_9	108.4(3)
F1_9–C2_9–F2_9	106.7(3)
F3_9–C2_9–F2_9	107.4(3)
F1_9–C2_9–C1_9	111.4(2)
F3_9–C2_9–C1_9	110.2(3)
F2_9–C2_9–C1_9	112.5(3)
F6_9–C3_9–F5_9	107.0(2)
F6_9–C3_9–F4_9	108.1(3)
F5_9–C3_9–F4_9	107.0(3)
F6_9–C3_9–C1_9	113.5(2)
F5_9–C3_9–C1_9	111.0(2)
F4_9–C3_9–C1_9	110.0(2)
F9_9–C4_9–F7_9	106.9(2)
F9_9–C4_9–F8_9	107.8(2)
F7_9–C4_9–F8_9	106.4(2)
F9_9–C4_9–C1_9	112.2(2)
F7_9–C4_9–C1_9	110.7(2)
F8_9–C4_9–C1_9	112.5(2)
C1_10–O1_10–Al03	155(3)
O1_10–C1_10–C2_10	111.8(17)
O1_10–C1_10–C4_10	108.8(18)
C2_10–C1_10–C4_10	107.4(13)
O1_10–C1_10–C3_10	109.8(17)
C2_10–C1_10–C3_10	110.4(14)
C4_10–C1_10–C3_10	108.6(14)
F2_10–C2_10–F3_10	112.8(19)
F2_10–C2_10–F1_10	101.8(18)
F3_10–C2_10–F1_10	105.0(18)
F2_10–C2_10–C1_10	114.4(16)
F3_10–C2_10–C1_10	110.9(16)
F1_10–C2_10–C1_10	111.2(16)
F4_10–C3_10–F5_10	105.5(18)
F4_10–C3_10–F6_10	109.6(18)
F5_10–C3_10–F6_10	111.7(19)
F4_10–C3_10–C1_10	110.8(18)

F5_10–C3_10–C1_10	110.7(16)
F6_10–C3_10–C1_10	108.5(16)
F7_10–C4_10–F9_10	110(2)
F7_10–C4_10–F8_10	107(2)
F9_10–C4_10–F8_10	107(2)
F7_10–C4_10–C1_10	111.1(16)
F9_10–C4_10–C1_10	110.6(19)
F8_10–C4_10–C1_10	111(2)

S-Table 24: Atomic coordinates and U_{eq} [Å^2] for [(tmeda)Al(AlCp*)$_3$][*pf*]

Atom	***x***	***y***	***z***	U_{eq}
Al01	0.30558(2)	0.39777(6)	0.51897(4)	0.01950(13)
Al02	0.30246(2)	0.21407(6)	0.41418(4)	0.02094(14)
Al03	0.53801(2)	0.77577(6)	0.46777(4)	0.02226(14)
Al04	0.36392(2)	0.25029(6)	0.50722(4)	0.02042(13)
Al05	0.29818(2)	0.16320(6)	0.57091(4)	0.02061(13)
N1	0.41219(7)	0.2861(2)	0.43764(14)	0.0356(5)
N2	0.40977(6)	0.2287(2)	0.58899(14)	0.0330(5)
C1	0.42262(11)	0.1760(3)	0.3967(2)	0.0509(8)
H1A	0.446466	0.188954	0.368345	0.076
H1B	0.402117	0.154678	0.360957	0.076
H1C	0.426239	0.110816	0.433475	0.076
C2	0.40384(11)	0.3800(3)	0.3812(2)	0.0488(8)
H2A	0.425579	0.388111	0.346132	0.073
H2B	0.399519	0.456128	0.407537	0.073
H2C	0.380856	0.358215	0.352176	0.073
C3	0.44387(9)	0.3287(4)	0.4877(2)	0.0575(11)
H3A	0.468109	0.331105	0.458354	0.069
H3B	0.438231	0.410577	0.506051	0.069
C4	0.44794(8)	0.2467(4)	0.5535(2)	0.0573(11)
H4A	0.465877	0.281277	0.591304	0.069
H4B	0.458397	0.168979	0.536129	0.069
C5	0.40773(11)	0.1076(3)	0.6235(2)	0.0541(9)
H5A	0.428428	0.098292	0.660857	0.081
H5B	0.410454	0.047059	0.583379	0.081
H5C	0.382975	0.097526	0.649075	0.081
C6	0.40361(8)	0.3183(3)	0.65041(18)	0.0385(6)
H6A	0.421222	0.302280	0.692771	0.058
H6B	0.377136	0.313107	0.668721	0.058
H6C	0.408395	0.398774	0.630254	0.058
O1_1	0.50557(8)	0.7465(3)	0.39474(16)	0.0266(6)
C1_1	0.47808(13)	0.7887(4)	0.3482(3)	0.0262(8)
C2_1	0.49265(14)	0.8953(5)	0.2986(3)	0.0363(10)
F1_1	0.49328(7)	0.9951(2)	0.33931(18)	0.0465(6)
F2_1	0.47039(8)	0.9138(3)	0.23790(16)	0.0535(7)
F3_1	0.52790(14)	0.8745(9)	0.2744(5)	0.0513(14)
C3_1	0.46578(13)	0.6855(4)	0.2932(3)	0.0449(9)
F4_1	0.46309(9)	0.5834(2)	0.33147(19)	0.0629(9)
F5_1	0.49175(10)	0.6695(3)	0.23813(16)	0.0624(8)
F6_1	0.43194(9)	0.7065(3)	0.26030(19)	0.0679(9)
C4_1	0.44277(11)	0.8290(5)	0.3949(3)	0.0402(9)
F7_1	0.42380(11)	0.7372(4)	0.4234(2)	0.0650(11)
F8_1	0.41786(7)	0.8945(3)	0.35378(18)	0.0571(8)

F9_1	0.45349(7)	0.8973(3)	0.45348(14)	0.0494(7)
O1_2	0.5593(6)	0.9065(16)	0.4448(11)	0.027(2)
C1_2	0.5794(3)	1.0020(10)	0.4699(5)	0.0294(15)
C2_2	0.5856(3)	1.0885(7)	0.4009(6)	0.0528(17)
F1_2	0.5537(2)	1.1495(5)	0.3869(4)	0.076(2)
F2_2	0.6138(6)	1.1672(14)	0.4158(14)	0.068(4)
F3_2	0.5939(5)	1.0254(17)	0.3383(6)	0.065(3)
C3_2	0.61895(17)	0.9615(6)	0.5008(4)	0.0410(14)
F4_2	0.6151(6)	0.8654(12)	0.5457(10)	0.053(3)
F5_2	0.64221(13)	0.9348(6)	0.4424(4)	0.0606(16)
F6_2	0.6361(2)	1.0453(8)	0.5416(5)	0.060(2)
C4_2	0.5574(2)	1.0686(7)	0.5328(5)	0.0512(17)
F7_2	0.5618(3)	1.0099(9)	0.6000(5)	0.063(2)
F8_2	0.5684(6)	1.1836(11)	0.5394(10)	0.087(5)
F9_2	0.5200(3)	1.0722(12)	0.5175(9)	0.075(3)
O1_3	0.51655(11)	0.7850(5)	0.5564(2)	0.0251(8)
C1_3	0.50387(13)	0.7279(4)	0.6193(2)	0.0248(7)
C2_3	0.48853(16)	0.6006(4)	0.6001(3)	0.0319(9)
F1_3	0.51662(13)	0.5223(4)	0.5922(2)	0.0440(8)
F2_3	0.46413(18)	0.5575(8)	0.6521(3)	0.0468(11)
F3_3	0.46967(12)	0.6032(5)	0.5336(2)	0.0437(9)
C3_3	0.47063(12)	0.8024(4)	0.6544(2)	0.0351(8)
F4_3	0.4795(2)	0.9186(5)	0.6548(4)	0.0464(11)
F5_3	0.43909(6)	0.7923(2)	0.61223(15)	0.0448(6)
F6_3	0.46214(8)	0.7709(3)	0.72539(15)	0.0561(7)
C4_3	0.53641(13)	0.7166(4)	0.6795(2)	0.0389(9)
F7_3	0.54295(18)	0.8204(4)	0.7136(4)	0.0510(12)
F8_3	0.52747(9)	0.6370(3)	0.73444(15)	0.0589(8)
F9_3	0.56867(6)	0.6789(2)	0.64747(15)	0.0470(6)
O1_4	0.56820(8)	0.6531(3)	0.47023(17)	0.0253(6)
C1_4	0.58914(10)	0.5738(3)	0.4301(2)	0.0281(6)
C2_4	0.61845(11)	0.6401(4)	0.3783(2)	0.0361(7)
F1_4	0.64743(7)	0.6833(3)	0.41806(16)	0.0501(6)
F2_4	0.63286(8)	0.5689(3)	0.32333(16)	0.0492(7)
F3_4	0.60137(14)	0.7323(3)	0.3431(2)	0.0427(8)
C3_4	0.56324(11)	0.4923(3)	0.3799(2)	0.0369(7)
F4_4	0.53167(7)	0.4617(2)	0.41741(16)	0.0462(6)
F5_4	0.55218(7)	0.5493(2)	0.31669(13)	0.0451(6)
F6_4	0.58090(8)	0.3918(2)	0.35788(16)	0.0530(7)
C4_4	0.61125(11)	0.4940(4)	0.4882(2)	0.0358(7)
F7_4	0.58703(11)	0.4173(3)	0.5217(2)	0.0527(8)
F8_4	0.63925(8)	0.4318(3)	0.45413(18)	0.0484(7)
F9_4	0.62677(7)	0.5625(2)	0.54283(14)	0.0467(6)
O1_5	0.5607(9)	0.911(2)	0.4558(19)	0.031(4)
C1_5	0.5785(4)	1.0085(13)	0.4844(7)	0.032(2)
C2_5	0.5491(3)	1.1049(8)	0.5065(7)	0.0382(19)
F1_5	0.5356(2)	1.1627(7)	0.4469(6)	0.062(2)
F2_5	0.5653(6)	1.1842(14)	0.5560(11)	0.053(3)
F3_5	0.5197(4)	1.0567(18)	0.5446(9)	0.053(3)
C3_5	0.6021(3)	0.9753(9)	0.5560(6)	0.0371(18)
F4_5	0.6205(8)	0.8706(16)	0.5435(16)	0.052(4)
F5_5	0.5810(2)	0.9635(7)	0.6178(4)	0.0492(18)
F6_5	0.6294(3)	1.0544(11)	0.5727(6)	0.050(2)
C4_5	0.6057(4)	1.0572(13)	0.4224(7)	0.044(2)

F7_5	0.6372(3)	0.9916(14)	0.4153(7)	0.050(2)
F8_5	0.6184(7)	1.1684(17)	0.4385(14)	0.064(5)
F9_5	0.5877(5)	1.0605(14)	0.3544(8)	0.062(3)
O1_6	0.4976(3)	0.7855(11)	0.4141(7)	0.033(2)
C1_6	0.4790(5)	0.7674(13)	0.3472(10)	0.033(2)
C2_6	0.4358(4)	0.7827(12)	0.3620(8)	0.044(2)
F1_6	0.4221(4)	0.6877(10)	0.3989(8)	0.051(3)
F2_6	0.4158(3)	0.7979(12)	0.2970(7)	0.068(3)
F3_6	0.4290(4)	0.8777(9)	0.4052(7)	0.056(3)
C3_6	0.4916(6)	0.8623(14)	0.2885(10)	0.048(3)
F4_6	0.5297(6)	0.871(3)	0.2908(19)	0.060(5)
F5_6	0.4755(4)	0.9685(9)	0.3010(7)	0.059(3)
F6_6	0.4842(5)	0.8301(14)	0.2173(6)	0.081(4)
C4_6	0.4863(4)	0.6394(11)	0.3167(7)	0.045(2)
F7_6	0.5200(3)	0.6331(9)	0.2807(7)	0.068(3)
F8_6	0.4600(4)	0.6088(11)	0.2651(7)	0.075(3)
F9_6	0.4872(3)	0.5621(7)	0.3732(5)	0.050(2)
O1_7	0.5691(7)	0.9037(19)	0.453(2)	0.032(4)
C1_7	0.5765(5)	1.0204(17)	0.4670(10)	0.038(3)
C2_7	0.5908(5)	1.0344(17)	0.5488(10)	0.062(3)
F1_7	0.5613(9)	1.034(3)	0.5986(18)	0.121(10)
F2_7	0.6096(5)	1.1391(16)	0.5601(13)	0.123(7)
F3_7	0.6165(6)	0.950(2)	0.5652(12)	0.107(7)
C3_7	0.6089(6)	1.062(2)	0.4121(12)	0.048(3)
F4_7	0.6034(8)	1.023(3)	0.3422(13)	0.063(5)
F5_7	0.6425(6)	1.018(2)	0.4337(18)	0.089(8)
F6_7	0.6110(12)	1.181(2)	0.411(3)	0.066(8)
C4_7	0.5405(4)	1.0984(14)	0.4549(9)	0.048(3)
F7_7	0.5335(4)	1.1114(14)	0.3799(8)	0.070(4)
F8_7	0.5421(3)	1.2049(9)	0.4879(10)	0.061(4)
F9_7	0.5103(3)	1.0403(10)	0.4845(9)	0.054(3)
O1_8	0.5273(5)	0.772(3)	0.5635(13)	0.028(4)
C1_8	0.5036(6)	0.735(2)	0.6203(12)	0.035(3)
C2_8	0.4705(5)	0.8246(19)	0.6326(10)	0.040(3)
F1_8	0.4841(10)	0.921(3)	0.667(2)	0.050(6)
F2_8	0.4422(4)	0.7798(14)	0.6754(9)	0.069(4)
F3_8	0.4545(3)	0.8572(12)	0.5667(6)	0.051(3)
C3_8	0.4867(7)	0.612(2)	0.5993(15)	0.041(4)
F4_8	0.5120(7)	0.540(2)	0.5664(13)	0.062(5)
F5_8	0.4590(7)	0.622(3)	0.5469(14)	0.062(6)
F6_8	0.4717(10)	0.555(4)	0.6591(18)	0.065(7)
C4_8	0.5266(5)	0.7221(19)	0.6957(10)	0.047(4)
F7_8	0.5505(4)	0.6270(15)	0.6892(8)	0.069(4)
F8_8	0.5041(4)	0.7082(15)	0.7562(6)	0.059(4)
F9_8	0.5497(10)	0.815(3)	0.706(2)	0.066(7)
C1_9	0.25280(8)	0.2152(3)	0.32834(17)	0.0370(6)
C2_9	0.28447(10)	0.2632(3)	0.28955(17)	0.0419(7)
C3_9	0.31293(9)	0.1738(3)	0.28443(16)	0.0399(7)
C4_9	0.29887(9)	0.0703(3)	0.32059(16)	0.0343(6)
C5_9	0.26156(8)	0.0955(3)	0.34747(15)	0.0320(6)
C6_9	0.23409(14)	0.0096(5)	0.3838(2)	0.0735(15)
H6A_9	0.212465	-0.004444	0.349269	0.110
H6B_9	0.224665	0.043319	0.431949	0.110
H6C_9	0.247184	-0.066337	0.394006	0.110

C7_9	0.31945(14)	-0.0469(4)	0.3284(3)	0.0750(15)
H7A_9	0.331819	-0.067090	0.279834	0.113
H7B_9	0.301070	-0.109655	0.341947	0.113
H7C_9	0.338913	-0.040411	0.368533	0.113
C8_9	0.34921(12)	0.1824(7)	0.2385(2)	0.095(2)
H8A_9	0.366385	0.116662	0.252541	0.142
H8B_9	0.361801	0.259043	0.249061	0.142
H8C_9	0.343082	0.177243	0.183970	0.142
C9_9	0.2880(2)	0.3859(4)	0.2553(3)	0.092(2)
H9A_9	0.295072	0.378875	0.201273	0.139
H9B_9	0.307730	0.431113	0.282564	0.139
H9C_9	0.263386	0.427655	0.259533	0.139
C10_9	0.21533(12)	0.2757(5)	0.3452(3)	0.0766(16)
H10A_9	0.194192	0.224110	0.328714	0.115
H10B_9	0.214086	0.351944	0.317610	0.115
H10C_9	0.213265	0.290583	0.400197	0.115
C1_10	0.26240(7)	0.1469(2)	0.68057(14)	0.0264(5)
C2_10	0.24501(7)	0.0768(2)	0.62233(15)	0.0299(5)
C3_10	0.27043(8)	-0.0185(2)	0.60434(15)	0.0318(5)
C4_10	0.30329(8)	-0.0073(2)	0.65131(16)	0.0312(5)
C5_10	0.29847(8)	0.0940(2)	0.69821(15)	0.0276(5)
C6_10	0.32424(10)	0.1384(3)	0.76099(16)	0.0415(7)
H6A_10	0.349567	0.101485	0.755799	0.062
H6B_10	0.313236	0.116980	0.810652	0.062
H6C_10	0.326690	0.225551	0.757422	0.062
C7_10	0.33543(11)	-0.0974(3)	0.6534(2)	0.0507(8)
H7A_10	0.352414	-0.079547	0.696517	0.076
H7B_10	0.349986	-0.093257	0.605645	0.076
H7C_10	0.324755	-0.177942	0.659521	0.076
C8_10	0.26344(12)	-0.1250(3)	0.5534(2)	0.0482(8)
H8A_10	0.265154	-0.198546	0.583700	0.072
H8B_10	0.282753	-0.126697	0.512835	0.072
H8C_10	0.237870	-0.118872	0.530698	0.072
C9_10	0.20565(8)	0.0970(3)	0.5904(2)	0.0444(7)
H9A_10	0.187280	0.104767	0.632493	0.067
H9B_10	0.198423	0.028973	0.558179	0.067
H9C_10	0.205524	0.170423	0.559851	0.067
C10_10	0.24461(10)	0.2505(3)	0.72119(18)	0.0405(7)
H10A_10	0.235510	0.224619	0.771494	0.061
H10B_10	0.222984	0.280859	0.691216	0.061
H10C_10	0.263684	0.314125	0.727506	0.061
C1_11	0.26536(7)	0.5410(2)	0.56820(15)	0.0249(5)
C2_11	0.27073(7)	0.5660(2)	0.48922(14)	0.0255(5)
C3_11	0.30993(7)	0.5953(2)	0.47762(14)	0.0248(5)
C4_11	0.32864(7)	0.5883(2)	0.54933(14)	0.0234(4)
C5_11	0.30142(7)	0.5541(2)	0.60552(14)	0.0239(5)
C6_11	0.30902(8)	0.5382(3)	0.68906(15)	0.0318(5)
H6A_11	0.331559	0.585176	0.703656	0.048
H6B_11	0.313725	0.453391	0.699873	0.048
H6C_11	0.286758	0.565515	0.718346	0.048
C7_11	0.37022(7)	0.6163(2)	0.56245(17)	0.0324(6)
H7A_11	0.375190	0.700067	0.549120	0.049
H7B_11	0.386053	0.564053	0.530451	0.049
H7C_11	0.376547	0.603101	0.616340	0.049

C8_11	0.32771(9)	0.6326(3)	0.40327(17)	0.0373(6)
H8A_11	0.319813	0.714550	0.390995	0.056
H8B_11	0.319252	0.578434	0.362613	0.056
H8C_11	0.355671	0.629255	0.407654	0.056
C9_11	0.23936(8)	0.5740(3)	0.43087(18)	0.0378(6)
H9A_11	0.227485	0.653331	0.433288	0.057
H9B_11	0.220012	0.512618	0.441405	0.057
H9C_11	0.250096	0.561170	0.379787	0.057
C10_11	0.22722(8)	0.5179(3)	0.60488(19)	0.0371(6)
H10A_11	0.209271	0.581496	0.590592	0.056
H10B_11	0.230218	0.516527	0.660536	0.056
H10C_11	0.217266	0.440573	0.587466	0.056
O1_12	0.5616(7)	0.647(3)	0.4290(18)	0.034(3)
C1_12	0.5957(6)	0.5889(19)	0.4199(12)	0.0410(18)
C2_12	0.5891(7)	0.478(2)	0.3679(14)	0.045(2)
F1_12	0.5881(9)	0.510(3)	0.2941(13)	0.059(4)
F2_12	0.6168(7)	0.397(2)	0.3766(17)	0.062(4)
F3_12	0.5560(6)	0.426(2)	0.3870(17)	0.059(4)
C3_12	0.6106(7)	0.544(2)	0.4973(13)	0.046(2)
F4_12	0.6078(7)	0.630(2)	0.5489(13)	0.051(3)
F5_12	0.5949(11)	0.444(3)	0.525(3)	0.054(4)
F6_12	0.6480(6)	0.520(3)	0.4920(17)	0.061(4)
C4_12	0.6259(7)	0.674(2)	0.3848(16)	0.044(2)
F7_12	0.6392(9)	0.764(3)	0.4267(17)	0.044(4)
F8_12	0.6580(7)	0.617(2)	0.3643(18)	0.051(4)
F9_12	0.6110(9)	0.729(4)	0.3241(19)	0.046(4)
O1_13	0.5651(7)	0.661(3)	0.4487(16)	0.036(3)
C1_13	0.6003(5)	0.6068(15)	0.4463(9)	0.0408(17)
C2_13	0.6103(6)	0.5951(18)	0.3606(11)	0.048(2)
F1_13	0.5908(6)	0.5033(17)	0.3312(12)	0.064(3)
F2_13	0.6476(6)	0.577(3)	0.3487(15)	0.065(4)
F3_13	0.6028(11)	0.7022(19)	0.3288(17)	0.056(4)
C3_13	0.6322(5)	0.6802(17)	0.4862(11)	0.053(2)
F4_13	0.6171(6)	0.7183(18)	0.5534(9)	0.069(4)
F5_13	0.6439(7)	0.771(2)	0.4438(13)	0.063(4)
F6_13	0.6613(5)	0.6114(17)	0.5068(14)	0.074(4)
C4_13	0.5977(6)	0.4850(17)	0.4866(12)	0.048(2)
F7_13	0.5982(6)	0.5017(16)	0.5633(9)	0.060(3)
F8_13	0.6281(6)	0.412(2)	0.4758(14)	0.060(4)
F9_13	0.5666(4)	0.4272(13)	0.4614(11)	0.052(3)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

S-Table 25: Bond lengths and angles for [(tmeda)Al(AlCp*)$_3$][*pf*]

Atom–Atom	Length [Å]
Al01–C1_11	2.297(2)
Al01–C2_11	2.299(2)
Al01–C5_11	2.317(2)
Al01–C3_11	2.328(2)
Al01–C4_11	2.338(2)
Al01–Al04	2.6282(10)
Al01–Al02	2.7551(10)
Al01–Al05	2.7866(11)
Al02–C5_9	2.272(3)
Al02–C1_9	2.295(3)
Al02–C4_9	2.298(3)
Al02–C2_9	2.336(3)
Al02–C3_9	2.344(3)
Al02–Al04	2.7239(10)
Al02–Al05	2.8058(11)
Al03–O1_13	1.63(2)
Al03–O1_2	1.687(17)
Al03–O1_6	1.700(11)
Al03–O1_8	1.72(2)
Al03–O1_5	1.72(2)
Al03–O1_3	1.726(4)
Al03–O1_4	1.730(3)
Al03–O1_1	1.739(3)
Al03–O1_12	1.79(2)
Al03–O1_7	1.81(2)
Al04–N1	2.117(2)
Al04–N2	2.161(2)
Al04–Al05	2.7309(10)
Al05–C2_10	2.278(3)
Al05–C1_10	2.298(2)
Al05–C3_10	2.325(3)
Al05–C5_10	2.359(3)
Al05–C4_10	2.375(3)
N1–C1	1.470(4)
N1–C2	1.471(5)
N1–C3	1.489(4)
N2–C5	1.484(4)
N2–C4	1.484(4)
N2–C6	1.485(4)
C1–H1A	0.9800
C1–H1B	0.9800
C1–H1C	0.9800
C2–H2A	0.9800
C2–H2B	0.9800
C2–H2C	0.9800
C3–C4	1.478(6)
C3–H3A	0.9900
C3–H3B	0.9900
C4–H4A	0.9900
C4–H4B	0.9900
C5–H5A	0.9800
C5–H5B	0.9800
C5–H5C	0.9800

C6–H6A	0.9800
C6–H6B	0.9800
C6–H6C	0.9800
O1_1–C1_1	1.344(5)
C1_1–C4_1	1.546(6)
C1_1–C2_1	1.560(6)
C1_1–C3_1	1.562(6)
C2_1–F3_1	1.322(7)
C2_1–F1_1	1.324(6)
C2_1–F2_1	1.332(5)
C3_1–F4_1	1.327(5)
C3_1–F6_1	1.335(5)
C3_1–F5_1	1.335(6)
C4_1–F7_1	1.319(6)
C4_1–F9_1	1.332(6)
C4_1–F8_1	1.346(5)
O1_2–C1_2	1.350(11)
C1_2–C4_2	1.535(10)
C1_2–C3_2	1.552(10)
C1_2–C2_2	1.561(11)
C2_2–F1_2	1.329(11)
C2_2–F3_2	1.335(14)
C2_2–F2_2	1.344(14)
C3_2–F6_2	1.323(9)
C3_2–F4_2	1.338(14)
C3_2–F5_2	1.338(9)
C4_2–F9_2	1.333(12)
C4_2–F8_2	1.346(12)
C4_2–F7_2	1.355(13)
O1_3–C1_3	1.346(5)
C1_3–C3_3	1.555(5)
C1_3–C4_3	1.556(5)
C1_3–C2_3	1.557(5)
C2_3–F1_3	1.321(5)
C2_3–F2_3	1.336(5)
C2_3–F3_3	1.338(5)
C3_3–F6_3	1.326(5)
C3_3–F5_3	1.330(5)
C3_3–F4_3	1.335(6)
C4_3–F7_3	1.325(6)
C4_3–F9_3	1.327(5)
C4_3–F8_3	1.346(5)
O1_4–C1_4	1.346(4)
C1_4–C2_4	1.555(5)
C1_4–C3_4	1.556(5)
C1_4–C4_4	1.557(5)
C2_4–F1_4	1.319(5)
C2_4–F3_4	1.340(5)
C2_4–F2_4	1.346(5)
C3_4–F4_4	1.328(5)
C3_4–F5_4	1.334(5)
C3_4–F6_4	1.338(4)
C4_4–F8_4	1.339(4)
C4_4–F7_4	1.340(5)

C4_4–F9_4	1.340(5)
O1_5–C1_5	1.350(15)
C1_5–C2_5	1.538(13)
C1_5–C4_5	1.541(13)
C1_5–C3_5	1.546(14)
C2_5–F1_5	1.315(12)
C2_5–F3_5	1.339(13)
C2_5–F2_5	1.361(15)
C3_5–F5_5	1.315(11)
C3_5–F6_5	1.333(12)
C3_5–F4_5	1.352(15)
C4_5–F7_5	1.327(13)
C4_5–F9_5	1.347(15)
C4_5–F8_5	1.349(16)
O1_6–C1_6	1.354(17)
C1_6–C3_6	1.540(16)
C1_6–C2_6	1.541(16)
C1_6–C4_6	1.547(15)
C2_6–F3_6	1.325(14)
C2_6–F1_6	1.332(14)
C2_6–F2_6	1.345(15)
C3_6–F6_6	1.322(16)
C3_6–F5_6	1.331(16)
C3_6–F4_6	1.336(18)
C4_6–F9_6	1.313(14)
C4_6–F8_6	1.335(15)
C4_6–F7_6	1.338(14)
O1_7–C1_7	1.350(18)
C1_7–C2_7	1.525(16)
C1_7–C4_7	1.544(16)
C1_7–C3_7	1.554(17)
C2_7–F3_7	1.332(17)
C2_7–F1_7	1.349(18)
C2_7–F2_7	1.356(16)
C3_7–F4_7	1.312(18)
C3_7–F5_7	1.325(17)
C3_7–F6_7	1.331(18)
C4_7–F8_7	1.323(15)
C4_7–F9_7	1.342(15)
C4_7–F7_7	1.343(16)
O1_8–C1_8	1.361(19)
C1_8–C3_8	1.541(18)
C1_8–C2_8	1.546(17)
C1_8–C4_8	1.551(17)
C2_8–F1_8	1.321(18)
C2_8–F3_8	1.332(16)
C2_8–F2_8	1.336(16)
C3_8–F4_8	1.322(19)
C3_8–F6_8	1.332(19)
C3_8–F5_8	1.338(19)
C4_8–F8_8	1.325(16)
C4_8–F9_8	1.331(19)
C4_8–F7_8	1.357(17)
C1_9–C2_9	1.404(5)

C1_9–C5_9	1.413(4)
C1_9–C10_9	1.502(5)
C2_9–C3_9	1.412(5)
C2_9–C9_9	1.502(5)
C3_9–C4_9	1.407(4)
C3_9–C8_9	1.503(5)
C4_9–C5_9	1.414(4)
C4_9–C7_9	1.499(4)
C5_9–C6_9	1.499(4)
C6_9–H6A_9	0.9800
C6_9–H6B_9	0.9800
C6_9–H6C_9	0.9800
C7_9–H7A_9	0.9800
C7_9–H7B_9	0.9800
C7_9–H7C_9	0.9800
C8_9–H8A_9	0.9800
C8_9–H8B_9	0.9800
C8_9–H8C_9	0.9800
C9_9–H9A_9	0.9800
C9_9–H9B_9	0.9800
C9_9–H9C_9	0.9800
C10_9–H10A_9	0.9800
C10_9–H10B_9	0.9800
C10_9–H10C_9	0.9800
C1_10–C2_10	1.422(4)
C1_10–C5_10	1.425(4)
C1_10–C10_10	1.494(4)
C2_10–C3_10	1.422(4)
C2_10–C9_10	1.500(4)
C3_10–C4_10	1.417(4)
C3_10–C8_10	1.506(4)
C4_10–C5_10	1.408(4)
C4_10–C7_10	1.508(4)
C5_10–C6_10	1.504(4)
C6_10–H6A_10	0.9800
C6_10–H6B_10	0.9800
C6_10–H6C_10	0.9800
C7_10–H7A_10	0.9800
C7_10–H7B_10	0.9800
C7_10–H7C_10	0.9800
C8_10–H8A_10	0.9800
C8_10–H8B_10	0.9800
C8_10–H8C_10	0.9800
C9_10–H9A_10	0.9800
C9_10–H9B_10	0.9800
C9_10–H9C_10	0.9800
C10_10–H10A_10	0.9800
C10_10–H10B_10	0.9800
C10_10–H10C_10	0.9800
C1_11–C2_11	1.423(4)
C1_11–C5_11	1.426(3)
C1_11–C10_11	1.501(3)
C2_11–C3_11	1.422(3)
C2_11–C9_11	1.500(4)

C3_11–C4_11	1.417(3)
C3_11–C8_11	1.501(4)
C4_11–C5_11	1.420(3)
C4_11–C7_11	1.503(3)
C5_11–C6_11	1.497(4)
C6_11–H6A_11	0.9800
C6_11–H6B_11	0.9800
C6_11–H6C_11	0.9800
C7_11–H7A_11	0.9800
C7_11–H7B_11	0.9800
C7_11–H7C_11	0.9800
C8_11–H8A_11	0.9800
C8_11–H8B_11	0.9800
C8_11–H8C_11	0.9800
C9_11–H9A_11	0.9800
C9_11–H9B_11	0.9800
C9_11–H9C_11	0.9800
C10_11–H10A_11	0.9800
C10_11–H10B_11	0.9800
C10_11–H10C_11	0.9800
O1_12–C1_12	1.364(19)
C1_12–C3_12	1.536(18)
C1_12–C4_12	1.544(18)
C1_12–C2_12	1.560(18)
C2_12–F2_12	1.329(18)
C2_12–F3_12	1.333(19)
C2_12–F1_12	1.343(18)
C3_12–F4_12	1.323(19)
C3_12–F5_12	1.334(19)
C3_12–F6_12	1.338(19)
C4_12–F7_12	1.332(19)
C4_12–F9_12	1.333(19)
C4_12–F8_12	1.339(19)
O1_13–C1_13	1.371(18)
C1_13–C4_13	1.537(17)
C1_13–C2_13	1.545(17)
C1_13–C3_13	1.548(17)
C2_13–F1_13	1.333(18)
C2_13–F2_13	1.335(17)
C2_13–F3_13	1.345(18)
C3_13–F5_13	1.318(18)
C3_13–F6_13	1.324(17)
C3_13–F4_13	1.358(18)
C4_13–F9_13	1.337(17)
C4_13–F8_13	1.350(17)
C4_13–F7_13	1.356(18)

Atom–Atom–Atom	**Angle [°]**
C1_11–Al01–C2_11	36.07(9)
C1_11–Al01–C5_11	36.00(9)
C2_11–Al01–C5_11	59.90(9)
C1_11–Al01–C3_11	59.72(9)
C2_11–Al01–C3_11	35.79(8)
C5_11–Al01–C3_11	59.50(9)

C1_11–Al01–C4_11	59.37(8)
C2_11–Al01–C4_11	59.27(9)
C5_11–Al01–C4_11	35.52(8)
C3_11–Al01–C4_11	35.36(9)
C1_11–Al01–Al04	160.07(7)
C2_11–Al01–Al04	154.85(7)
C5_11–Al01–Al04	124.93(7)
C3_11–Al01–Al04	121.31(7)
C4_11–Al01–Al04	108.78(7)
C1_11–Al01–Al02	138.15(7)
C2_11–Al01–Al02	115.95(7)
C5_11–Al01–Al02	174.09(7)
C3_11–Al01–Al02	120.14(7)
C4_11–Al01–Al02	147.53(7)
Al04–Al01–Al02	60.74(3)
C1_11–Al01–Al05	118.46(7)
C2_11–Al01–Al05	142.57(7)
C5_11–Al01–Al05	119.35(7)
C3_11–Al01–Al05	178.15(7)
C4_11–Al01–Al05	144.55(7)
Al04–Al01–Al05	60.49(3)
Al02–Al01–Al05	60.83(3)
C5_9–Al02–C1_9	36.04(11)
C5_9–Al02–C4_9	36.03(10)
C1_9–Al02–C4_9	59.72(10)
C5_9–Al02–C2_9	59.19(10)
C1_9–Al02–C2_9	35.29(12)
C4_9–Al02–C2_9	58.92(11)
C5_9–Al02–C3_9	59.19(10)
C1_9–Al02–C3_9	58.96(11)
C4_9–Al02–C3_9	35.27(11)
C2_9–Al02–C3_9	35.11(12)
C5_9–Al02–Al04	152.79(8)
C1_9–Al02–Al04	170.39(9)
C4_9–Al02–Al04	124.97(8)
C2_9–Al02–Al04	137.34(9)
C3_9–Al02–Al04	119.02(8)
C5_9–Al02–Al01	143.30(8)
C1_9–Al02–Al01	117.49(8)
C4_9–Al02–Al01	176.13(8)
C2_9–Al02–Al01	117.22(8)
C3_9–Al02–Al01	141.45(9)
Al04–Al02–Al01	57.33(2)
C5_9–Al02–Al05	110.55(8)
C1_9–Al02–Al05	126.96(9)
C4_9–Al02–Al05	123.53(8)
C2_9–Al02–Al05	161.19(10)
C3_9–Al02–Al05	156.47(10)
Al04–Al02–Al05	59.17(3)
Al01–Al02–Al05	60.14(3)
O1_6–Al03–O1_8	111.1(7)
O1_6–Al03–O1_5	105.0(12)
O1_8–Al03–O1_5	103.8(14)
O1_2–Al03–O1_3	110.7(7)

O1_2–Al03–O1_4	115.1(8)
O1_3–Al03–O1_4	106.81(18)
O1_2–Al03–O1_1	105.9(6)
O1_3–Al03–O1_1	112.92(18)
O1_4–Al03–O1_1	105.44(16)
O1_6–Al03–O1_12	103.0(10)
O1_8–Al03–O1_12	116.8(14)
O1_5–Al03–O1_12	116.6(15)
O1_13–Al03–O1_7	104.2(14)
N1–Al04–N2	79.19(10)
N1–Al04–Al01	122.92(8)
N2–Al04–Al01	126.32(7)
N1–Al04–Al02	108.12(8)
N2–Al04–Al02	164.36(8)
Al01–Al04–Al02	61.93(3)
N1–Al04–Al05	166.18(8)
N2–Al04–Al05	108.21(8)
Al01–Al04–Al05	62.63(3)
Al02–Al04–Al05	61.91(3)
C2_10–Al05–C1_10	36.21(9)
C2_10–Al05–C3_10	35.96(10)
C1_10–Al05–C3_10	59.60(9)
C2_10–Al05–C5_10	59.42(9)
C1_10–Al05–C5_10	35.62(9)
C3_10–Al05–C5_10	58.51(9)
C2_10–Al05–C4_10	59.14(10)
C1_10–Al05–C4_10	58.82(9)
C3_10–Al05–C4_10	35.07(10)
C5_10–Al05–C4_10	34.61(9)
C2_10–Al05–Al04	175.79(8)
C1_10–Al05–Al04	145.73(7)
C3_10–Al05–Al04	139.84(8)
C5_10–Al05–Al04	119.93(7)
C4_10–Al05–Al04	117.69(8)
C2_10–Al05–Al01	127.10(8)
C1_10–Al05–Al01	113.42(7)
C3_10–Al05–Al01	160.47(8)
C5_10–Al05–Al01	128.04(7)
C4_10–Al05–Al01	160.20(8)
Al04–Al05–Al01	56.88(2)
C2_10–Al05–Al02	121.04(7)
C1_10–Al05–Al02	149.53(7)
C3_10–Al05–Al02	116.44(7)
C5_10–Al05–Al02	171.87(7)
C4_10–Al05–Al02	137.55(7)
Al04–Al05–Al02	58.92(3)
Al01–Al05–Al02	59.03(2)
C1–N1–C2	108.6(3)
C1–N1–C3	111.7(3)
C2–N1–C3	108.3(3)
C1–N1–Al04	108.6(2)
C2–N1–Al04	111.32(19)
C3–N1–Al04	108.26(19)
C5–N2–C4	109.7(3)

C5–N2–C6	108.3(3)
C4–N2–C6	110.0(2)
C5–N2–Al04	109.63(19)
C4–N2–Al04	111.9(2)
C6–N2–Al04	107.27(16)
N1–C1–H1A	109.5
N1–C1–H1B	109.5
H1A–C1–H1B	109.5
N1–C1–H1C	109.5
H1A–C1–H1C	109.5
H1B–C1–H1C	109.5
N1–C2–H2A	109.5
N1–C2–H2B	109.5
H2A–C2–H2B	109.5
N1–C2–H2C	109.5
H2A–C2–H2C	109.5
H2B–C2–H2C	109.5
C4–C3–N1	109.4(3)
C4–C3–H3A	109.8
N1–C3–H3A	109.8
C4–C3–H3B	109.8
N1–C3–H3B	109.8
H3A–C3–H3B	108.3
C3–C4–N2	108.9(3)
C3–C4–H4A	109.9
N2–C4–H4A	109.9
C3–C4–H4B	109.9
N2–C4–H4B	109.9
H4A–C4–H4B	108.3
N2–C5–H5A	109.5
N2–C5–H5B	109.5
H5A–C5–H5B	109.5
N2–C5–H5C	109.5
H5A–C5–H5C	109.5
H5B–C5–H5C	109.5
N2–C6–H6A	109.5
N2–C6–H6B	109.5
H6A–C6–H6B	109.5
N2–C6–H6C	109.5
H6A–C6–H6C	109.5
H6B–C6–H6C	109.5
C1_1–O1_1–Al03	147.6(3)
O1_1–C1_1–C4_1	110.6(4)
O1_1–C1_1–C2_1	111.9(4)
C4_1–C1_1–C2_1	109.4(4)
O1_1–C1_1–C3_1	108.1(4)
C4_1–C1_1–C3_1	108.8(4)
C2_1–C1_1–C3_1	108.0(4)
F3_1–C2_1–F1_1	107.7(6)
F3_1–C2_1–F2_1	108.4(5)
F1_1–C2_1–F2_1	108.0(4)
F3_1–C2_1–C1_1	110.3(5)
F1_1–C2_1–C1_1	110.4(4)
F2_1–C2_1–C1_1	111.9(4)

F4_1–C3_1–F6_1	107.9(4)
F4_1–C3_1–F5_1	107.3(4)
F6_1–C3_1–F5_1	108.2(4)
F4_1–C3_1–C1_1	110.0(4)
F6_1–C3_1–C1_1	112.3(4)
F5_1–C3_1–C1_1	110.9(4)
F7_1–C4_1–F9_1	107.1(4)
F7_1–C4_1–F8_1	107.5(4)
F9_1–C4_1–F8_1	106.3(4)
F7_1–C4_1–C1_1	112.0(5)
F9_1–C4_1–C1_1	110.5(3)
F8_1–C4_1–C1_1	113.1(3)
C1_2–O1_2–Al03	146.7(15)
O1_2–C1_2–C4_2	110.9(12)
O1_2–C1_2–C3_2	110.2(11)
C4_2–C1_2–C3_2	109.6(7)
O1_2–C1_2–C2_2	108.2(11)
C4_2–C1_2–C2_2	109.0(8)
C3_2–C1_2–C2_2	108.9(7)
F1_2–C2_2–F3_2	107.4(10)
F1_2–C2_2–F2_2	108.3(11)
F3_2–C2_2–F2_2	110.3(13)
F1_2–C2_2–C1_2	110.1(8)
F3_2–C2_2–C1_2	109.7(10)
F2_2–C2_2–C1_2	111.0(11)
F6_2–C3_2–F4_2	107.2(11)
F6_2–C3_2–F5_2	107.2(6)
F4_2–C3_2–F5_2	109.3(9)
F6_2–C3_2–C1_2	112.7(7)
F4_2–C3_2–C1_2	110.4(10)
F5_2–C3_2–C1_2	109.8(6)
F9_2–C4_2–F8_2	105.5(12)
F9_2–C4_2–F7_2	107.5(9)
F8_2–C4_2–F7_2	110.9(10)
F9_2–C4_2–C1_2	111.0(9)
F8_2–C4_2–C1_2	112.4(10)
F7_2–C4_2–C1_2	109.4(8)
C1_3–O1_3–Al03	148.1(4)
O1_3–C1_3–C3_3	108.3(4)
O1_3–C1_3–C4_3	110.6(4)
C3_3–C1_3–C4_3	108.7(3)
O1_3–C1_3–C2_3	111.7(4)
C3_3–C1_3–C2_3	108.5(4)
C4_3–C1_3–C2_3	108.8(4)
F1_3–C2_3–F2_3	107.8(5)
F1_3–C2_3–F3_3	106.8(4)
F2_3–C2_3–F3_3	106.7(4)
F1_3–C2_3–C1_3	111.8(4)
F2_3–C2_3–C1_3	113.7(5)
F3_3–C2_3–C1_3	109.7(4)
F6_3–C3_3–F5_3	108.2(4)
F6_3–C3_3–F4_3	107.8(5)
F5_3–C3_3–F4_3	106.1(4)
F6_3–C3_3–C1_3	113.3(4)

F5_3–C3_3–C1_3	110.7(3)
F4_3–C3_3–C1_3	110.5(4)
F7_3–C4_3–F9_3	108.8(4)
F7_3–C4_3–F8_3	107.3(4)
F9_3–C4_3–F8_3	106.9(4)
F7_3–C4_3–C1_3	111.1(4)
F9_3–C4_3–C1_3	111.0(3)
F8_3–C4_3–C1_3	111.6(4)
C1_4–O1_4–Al03	147.1(3)
O1_4–C1_4–C2_4	110.4(3)
O1_4–C1_4–C3_4	111.4(3)
C2_4–C1_4–C3_4	109.4(3)
O1_4–C1_4–C4_4	107.8(3)
C2_4–C1_4–C4_4	109.1(3)
C3_4–C1_4–C4_4	108.7(3)
F1_4–C2_4–F3_4	107.6(4)
F1_4–C2_4–F2_4	107.9(3)
F3_4–C2_4–F2_4	107.0(3)
F1_4–C2_4–C1_4	111.8(3)
F3_4–C2_4–C1_4	110.0(3)
F2_4–C2_4–C1_4	112.4(3)
F4_4–C3_4–F5_4	107.0(3)
F4_4–C3_4–F6_4	108.0(3)
F5_4–C3_4–F6_4	107.2(3)
F4_4–C3_4–C1_4	110.7(3)
F5_4–C3_4–C1_4	110.9(3)
F6_4–C3_4–C1_4	112.7(3)
F8_4–C4_4–F7_4	108.9(3)
F8_4–C4_4–F9_4	108.6(3)
F7_4–C4_4–F9_4	107.9(4)
F8_4–C4_4–C1_4	111.7(3)
F7_4–C4_4–C1_4	109.9(3)
F9_4–C4_4–C1_4	109.8(3)
C1_5–O1_5–Al03	151(2)
O1_5–C1_5–C2_5	110.5(17)
O1_5–C1_5–C4_5	108.0(17)
C2_5–C1_5–C4_5	109.9(10)
O1_5–C1_5–C3_5	110.6(17)
C2_5–C1_5–C3_5	108.7(10)
C4_5–C1_5–C3_5	109.1(10)
F1_5–C2_5–F3_5	108.5(10)
F1_5–C2_5–F2_5	109.5(11)
F3_5–C2_5–F2_5	105.2(14)
F1_5–C2_5–C1_5	112.6(10)
F3_5–C2_5–C1_5	110.8(11)
F2_5–C2_5–C1_5	109.9(12)
F5_5–C3_5–F6_5	106.7(9)
F5_5–C3_5–F4_5	108.3(13)
F6_5–C3_5–F4_5	105.6(15)
F5_5–C3_5–C1_5	113.1(9)
F6_5–C3_5–C1_5	113.6(11)
F4_5–C3_5–C1_5	109.2(14)
F7_5–C4_5–F9_5	108.6(12)
F7_5–C4_5–F8_5	104.9(14)

F9_5–C4_5–F8_5	108.2(14)
F7_5–C4_5–C1_5	112.4(11)
F9_5–C4_5–C1_5	110.1(12)
F8_5–C4_5–C1_5	112.4(14)
C1_6–O1_6–Al03	150.0(11)
O1_6–C1_6–C3_6	109.7(13)
O1_6–C1_6–C2_6	107.8(12)
C3_6–C1_6–C2_6	108.3(13)
O1_6–C1_6–C4_6	110.9(12)
C3_6–C1_6–C4_6	111.1(12)
C2_6–C1_6–C4_6	108.8(12)
F3_6–C2_6–F1_6	107.3(12)
F3_6–C2_6–F2_6	106.8(12)
F1_6–C2_6–F2_6	109.0(13)
F3_6–C2_6–C1_6	111.1(12)
F1_6–C2_6–C1_6	110.1(12)
F2_6–C2_6–C1_6	112.3(12)
F6_6–C3_6–F5_6	108.4(15)
F6_6–C3_6–F4_6	104(2)
F5_6–C3_6–F4_6	110(2)
F6_6–C3_6–C1_6	112.7(14)
F5_6–C3_6–C1_6	112.7(13)
F4_6–C3_6–C1_6	108.4(19)
F9_6–C4_6–F8_6	110.9(12)
F9_6–C4_6–F7_6	107.4(11)
F8_6–C4_6–F7_6	105.9(12)
F9_6–C4_6–C1_6	110.7(11)
F8_6–C4_6–C1_6	110.9(12)
F7_6–C4_6–C1_6	110.9(11)
C1_7–O1_7–Al03	148(2)
O1_7–C1_7–C2_7	109.0(19)
O1_7–C1_7–C4_7	111.5(16)
C2_7–C1_7–C4_7	109.7(14)
O1_7–C1_7–C3_7	108.4(17)
C2_7–C1_7–C3_7	108.1(14)
C4_7–C1_7–C3_7	110.0(13)
F3_7–C2_7–F1_7	112(2)
F3_7–C2_7–F2_7	104.8(17)
F1_7–C2_7–F2_7	106(2)
F3_7–C2_7–C1_7	110.5(15)
F1_7–C2_7–C1_7	110.9(19)
F2_7–C2_7–C1_7	112.6(16)
F4_7–C3_7–F5_7	106(2)
F4_7–C3_7–F6_7	109(2)
F5_7–C3_7–F6_7	109(2)
F4_7–C3_7–C1_7	111.8(18)
F5_7–C3_7–C1_7	111.1(18)
F6_7–C3_7–C1_7	110(2)
F8_7–C4_7–F9_7	107.5(12)
F8_7–C4_7–F7_7	109.7(15)
F9_7–C4_7–F7_7	106.7(14)
F8_7–C4_7–C1_7	114.4(13)
F9_7–C4_7–C1_7	108.3(13)
F7_7–C4_7–C1_7	110.0(12)

C1_8–O1_8–Al03	149(2)
O1_8–C1_8–C3_8	109.4(18)
O1_8–C1_8–C2_8	110.9(16)
C3_8–C1_8–C2_8	109.2(16)
O1_8–C1_8–C4_8	109.5(16)
C3_8–C1_8–C4_8	108.6(16)
C2_8–C1_8–C4_8	109.1(14)
F1_8–C2_8–F3_8	109(2)
F1_8–C2_8–F2_8	109(2)
F3_8–C2_8–F2_8	106.1(15)
F1_8–C2_8–C1_8	109(2)
F3_8–C2_8–C1_8	111.8(14)
F2_8–C2_8–C1_8	112.6(16)
F4_8–C3_8–F6_8	108(2)
F4_8–C3_8–F5_8	104(2)
F6_8–C3_8–F5_8	107(2)
F4_8–C3_8–C1_8	113(2)
F6_8–C3_8–C1_8	113(2)
F5_8–C3_8–C1_8	111(2)
F8_8–C4_8–F9_8	110(2)
F8_8–C4_8–F7_8	109.9(16)
F9_8–C4_8–F7_8	104(2)
F8_8–C4_8–C1_8	112.6(15)
F9_8–C4_8–C1_8	111(2)
F7_8–C4_8–C1_8	108.6(15)
C2_9–C1_9–C5_9	107.8(3)
C2_9–C1_9–C10_9	127.5(4)
C5_9–C1_9–C10_9	124.6(4)
C2_9–C1_9–Al02	73.96(16)
C5_9–C1_9–Al02	71.09(15)
C10_9–C1_9–Al02	122.2(2)
C1_9–C2_9–C3_9	108.4(3)
C1_9–C2_9–C9_9	127.3(4)
C3_9–C2_9–C9_9	124.3(4)
C1_9–C2_9–Al02	70.75(16)
C3_9–C2_9–Al02	72.76(16)
C9_9–C2_9–Al02	124.5(2)
C4_9–C3_9–C2_9	107.9(3)
C4_9–C3_9–C8_9	126.0(4)
C2_9–C3_9–C8_9	125.5(4)
C4_9–C3_9–Al02	70.59(16)
C2_9–C3_9–Al02	72.12(16)
C8_9–C3_9–Al02	129.6(2)
C3_9–C4_9–C5_9	107.9(3)
C3_9–C4_9–C7_9	126.3(4)
C5_9–C4_9–C7_9	125.8(3)
C3_9–C4_9–Al02	74.14(16)
C5_9–C4_9–Al02	70.95(15)
C7_9–C4_9–Al02	121.3(2)
C1_9–C5_9–C4_9	108.0(3)
C1_9–C5_9–C6_9	124.7(3)
C4_9–C5_9–C6_9	127.1(3)
C1_9–C5_9–Al02	72.87(15)
C4_9–C5_9–Al02	73.02(15)

C6_9–C5_9–Al02	123.9(2)
C5_9–C6_9–H6A_9	109.5
C5_9–C6_9–H6B_9	109.5
H6A_9–C6_9–H6B_9	109.5
C5_9–C6_9–H6C_9	109.5
H6A_9–C6_9–H6C_9	109.5
H6B_9–C6_9–H6C_9	109.5
C4_9–C7_9–H7A_9	109.5
C4_9–C7_9–H7B_9	109.5
H7A_9–C7_9–H7B_9	109.5
C4_9–C7_9–H7C_9	109.5
H7A_9–C7_9–H7C_9	109.5
H7B_9–C7_9–H7C_9	109.5
C3_9–C8_9–H8A_9	109.5
C3_9–C8_9–H8B_9	109.5
H8A_9–C8_9–H8B_9	109.5
C3_9–C8_9–H8C_9	109.5
H8A_9–C8_9–H8C_9	109.5
H8B_9–C8_9–H8C_9	109.5
C2_9–C9_9–H9A_9	109.5
C2_9–C9_9–H9B_9	109.5
H9A_9–C9_9–H9B_9	109.5
C2_9–C9_9–H9C_9	109.5
H9A_9–C9_9–H9C_9	109.5
H9B_9–C9_9–H9C_9	109.5
C1_9–C10_9–H10A_9	109.5
C1_9–C10_9–H10B_9	109.5
H10A_9–C10_9–H10B_9	109.5
C1_9–C10_9–H10C_9	109.5
H10A_9–C10_9–H10C_9	109.5
H10B_9–C10_9–H10C_9	109.5
C2_10–C1_10–C5_10	107.7(2)
C2_10–C1_10–C10_10	126.2(3)
C5_10–C1_10–C10_10	125.9(3)
C2_10–C1_10–Al05	71.15(14)
C5_10–C1_10–Al05	74.53(14)
C10_10–C1_10–Al05	124.21(18)
C3_10–C2_10–C1_10	107.8(2)
C3_10–C2_10–C9_10	127.0(3)
C1_10–C2_10–C9_10	125.1(3)
C3_10–C2_10–Al05	73.81(15)
C1_10–C2_10–Al05	72.64(14)
C9_10–C2_10–Al05	122.39(19)
C4_10–C3_10–C2_10	108.1(2)
C4_10–C3_10–C8_10	123.0(3)
C2_10–C3_10–C8_10	128.4(3)
C4_10–C3_10–Al05	74.40(15)
C2_10–C3_10–Al05	70.23(14)
C8_10–C3_10–Al05	127.5(2)
C5_10–C4_10–C3_10	108.2(2)
C5_10–C4_10–C7_10	127.7(3)

C3_10–C4_10–C7_10	123.9(3)
C5_10–C4_10–Al05	72.06(15)
C3_10–C4_10–Al05	70.53(15)
C7_10–C4_10–Al05	127.3(2)
C4_10–C5_10–C1_10	108.2(2)
C4_10–C5_10–C6_10	128.3(3)
C1_10–C5_10–C6_10	123.4(3)
C4_10–C5_10–Al05	73.33(15)
C1_10–C5_10–Al05	69.85(14)
C6_10–C5_10–Al05	125.78(18)
C5_10–C6_10–H6A_10	109.5
C5_10–C6_10–H6B_10	109.5
H6A_10–C6_10–H6B_10	109.5
C5_10–C6_10–H6C_10	109.5
H6A_10–C6_10–H6C_10	109.5
H6B_10–C6_10–H6C_10	109.5
C4_10–C7_10–H7A_10	109.5
C4_10–C7_10–H7B_10	109.5
H7A_10–C7_10–H7B_10	109.5
C4_10–C7_10–H7C_10	109.5
H7A_10–C7_10–H7C_10	109.5
H7B_10–C7_10–H7C_10	109.5
C3_10–C8_10–H8A_10	109.5
C3_10–C8_10–H8B_10	109.5
H8A_10–C8_10–H8B_10	109.5
C3_10–C8_10–H8C_10	109.5
H8A_10–C8_10–H8C_10	109.5
H8B_10–C8_10–H8C_10	109.5
C2_10–C9_10–H9A_10	109.5
C2_10–C9_10–H9B_10	109.5
H9A_10–C9_10–H9B_10	109.5
C2_10–C9_10–H9C_10	109.5
H9A_10–C9_10–H9C_10	109.5
H9B_10–C9_10–H9C_10	109.5
C1_10–C10_10–H10A_10	109.5
C1_10–C10_10–H10B_10	109.5
H10A_10–C10_10–H10B_10	109.5
C1_10–C10_10–H10C_10	109.5

H10A_10–C10_10–H10C_10	109.5
H10B_10–C10_10–H10C_10	109.5
C2_11–C1_11–C5_11	108.0(2)
C2_11–C1_11–C10_11	124.5(2)
C5_11–C1_11–C10_11	127.2(2)
C2_11–C1_11–Al01	72.03(14)
C5_11–C1_11–Al01	72.76(13)
C10_11–C1_11–Al01	125.66(18)
C3_11–C2_11–C1_11	108.1(2)
C3_11–C2_11–C9_11	126.3(2)
C1_11–C2_11–C9_11	125.2(2)
C3_11–C2_11–Al01	73.22(13)
C1_11–C2_11–Al01	71.90(13)
C9_11–C2_11–Al01	126.11(18)
C4_11–C3_11–C2_11	107.7(2)
C4_11–C3_11–C8_11	126.3(2)
C2_11–C3_11–C8_11	125.9(2)
C4_11–C3_11–Al01	72.70(13)
C2_11–C3_11–Al01	70.99(13)
C8_11–C3_11–Al01	124.06(18)
C3_11–C4_11–C5_11	108.6(2)
C3_11–C4_11–C7_11	124.7(2)
C5_11–C4_11–C7_11	126.6(2)
C3_11–C4_11–Al01	71.94(13)
C5_11–C4_11–Al01	71.43(13)
C7_11–C4_11–Al01	123.86(17)
C4_11–C5_11–C1_11	107.5(2)
C4_11–C5_11–C6_11	126.2(2)
C1_11–C5_11–C6_11	126.3(2)
C4_11–C5_11–Al01	73.04(13)
C1_11–C5_11–Al01	71.24(14)
C6_11–C5_11–Al01	122.55(17)
C5_11–C6_11–H6A_11	109.5
C5_11–C6_11–H6B_11	109.5
H6A_11–C6_11–H6B_11	109.5
C5_11–C6_11–H6C_11	109.5
H6A_11–C6_11–H6C_11	109.5
H6B_11–C6_11–H6C_11	109.5
C4_11–C7_11–H7A_11	109.5
C4_11–C7_11–H7B_11	109.5
H7A_11–C7_11–H7B_11	109.5
C4_11–C7_11–H7C_11	109.5
H7A_11–C7_11–H7C_11	109.5
H7B_11–C7_11–H7C_11	109.5
C3_11–C8_11–H8A_11	109.5
C3_11–C8_11–H8B_11	109.5

H8A_11–C8_11–H8B_11	109.5
C3_11–C8_11–H8C_11	109.5
H8A_11–C8_11–H8C_11	109.5
H8B_11–C8_11–H8C_11	109.5
C2_11–C9_11–H9A_11	109.5
C2_11–C9_11–H9B_11	109.5
H9A_11–C9_11–H9B_11	109.5
C2_11–C9_11–H9C_11	109.5
H9A_11–C9_11–H9C_11	109.5
H9B_11–C9_11–H9C_11	109.5
C1_11–C10_11–H10A_11	109.5
C1_11–C10_11–H10B_11	109.5
H10A_11–C10_11–H10B_11	109.5
C1_11–C10_11–H10C_11	109.5
H10A_11–C10_11–H10C_11	109.5
H10B_11–C10_11–H10C_11	109.5
C1_12–O1_12–Al03	146(2)
O1_12–C1_12–C3_12	110.4(19)
O1_12–C1_12–C4_12	110.4(19)
C3_12–C1_12–C4_12	108.7(16)
O1_12–C1_12–C2_12	108.7(18)
C3_12–C1_12–C2_12	107.7(16)
C4_12–C1_12–C2_12	110.9(16)
F2_12–C2_12–F3_12	108(2)
F2_12–C2_12–F1_12	108(2)
F3_12–C2_12–F1_12	110(2)
F2_12–C2_12–C1_12	111.3(19)
F3_12–C2_12–C1_12	109.1(19)
F1_12–C2_12–C1_12	110.3(19)
F4_12–C3_12–F5_12	110(2)
F4_12–C3_12–F6_12	105(2)
F5_12–C3_12–F6_12	105(2)
F4_12–C3_12–C1_12	109.8(18)
F5_12–C3_12–C1_12	117(2)
F6_12–C3_12–C1_12	109.6(19)
F7_12–C4_12–F9_12	103(2)
F7_12–C4_12–F8_12	102(2)
F9_12–C4_12–F8_12	109(2)
F7_12–C4_12–C1_12	119(2)
F9_12–C4_12–C1_12	109(2)
F8_12–C4_12–C1_12	112.9(19)
C1_13–O1_13–Al03	151(2)

O1_13–C1_13–C4_13	108.7(17)
O1_13–C1_13–C2_13	105.6(16)
C4_13–C1_13–C2_13	112.6(14)
O1_13–C1_13–C3_13	113.4(18)
C4_13–C1_13–C3_13	107.8(13)
C2_13–C1_13–C3_13	108.8(14)
F1_13–C2_13–F2_13	108.6(19)
F1_13–C2_13–F3_13	115(2)
F2_13–C2_13–F3_13	105(2)
F1_13–C2_13–C1_13	109.0(16)
F2_13–C2_13–C1_13	112.5(17)
F3_13–C2_13–C1_13	106.5(18)
F5_13–C3_13–F6_13	111.1(19)
F5_13–C3_13–F4_13	111.6(19)
F6_13–C3_13–F4_13	104.1(17)
F5_13–C3_13–C1_13	112.0(15)
F6_13–C3_13–C1_13	111.5(16)
F4_13–C3_13–C1_13	106.1(15)
F9_13–C4_13–F8_13	107.6(18)
F9_13–C4_13–F7_13	113.8(18)
F8_13–C4_13–F7_13	102.3(17)
F9_13–C4_13–C1_13	109.0(14)
F8_13–C4_13–C1_13	114.8(17)
F7_13–C4_13–C1_13	109.4(15)

S-Table 26:Atomic coordinates and U_{eq} [Å^2] for [(dmap)$_3$Al(AlCp*)$_3$][*pf*]

Atom	***x***	***y***	***z***	U_{eq}
Al1	0.77743(3)	0.42561(2)	0.21828(3)	0.02125(11)
Al2	0.94651(3)	0.44660(2)	0.22427(3)	0.02336(12)
Al3	0.84953(4)	0.39974(2)	0.10793(3)	0.02502(12)
Al4	0.81356(4)	0.48009(2)	0.11493(3)	0.02592(12)
Al5	0.43527(3)	0.64134(2)	0.40006(3)	0.02358(12)
N1	0.81127(12)	0.26316(5)	0.40746(10)	0.0350(4)
N2	0.76714(10)	0.53354(5)	0.49437(9)	0.0292(3)
N3	0.38279(11)	0.39275(6)	0.07709(11)	0.0391(4)
C1	0.35097(14)	0.37036(7)	0.00479(14)	0.0451(5)
H1A	0.362128	0.386659	-0.035774	0.068
H1B	0.288571	0.365697	-0.008432	0.068
H1C	0.380779	0.343649	0.009854	0.068
C2	0.32283(14)	0.39957(9)	0.11945(15)	0.0510(6)
H2A	0.328197	0.428177	0.138179	0.077
H2B	0.336550	0.380472	0.163104	0.077
H2C	0.263451	0.394634	0.085518	0.077
C3	0.74978(13)	0.51592(7)	0.56060(11)	0.0327(4)
H3A	0.790086	0.493086	0.581596	0.049
H3B	0.690214	0.505515	0.544782	0.049
H3C	0.757364	0.537334	0.599918	0.049
C4	0.76923(13)	0.57841(6)	0.48700(12)	0.0339(4)
H4A	0.824451	0.586733	0.481421	0.051
H4B	0.763135	0.591420	0.532929	0.051
H4C	0.721504	0.587269	0.441691	0.051
C5	0.89620(16)	0.25006(8)	0.45732(16)	0.0542(7)

H5A	0.923383	0.272648	0.492492	0.081
H5B	0.932426	0.242940	0.426128	0.081
H5C	0.890043	0.225779	0.486962	0.081
C6	0.73628(16)	0.23815(6)	0.40499(13)	0.0396(5)
H6A	0.705979	0.229491	0.352016	0.059
H6B	0.697053	0.254528	0.423879	0.059
H6C	0.755378	0.213612	0.437429	0.059
C1_6	-0.0631(3)	0.64723(15)	0.4093(3)	0.0947(15)
H1A_6	-0.031006	0.665181	0.449330	0.114
H1B_6	-0.054802	0.618122	0.414541	0.114
C2_6	-0.1235(3)	0.66393(15)	0.3414(3)	0.0990(16)
H2A_6	-0.181208	0.652031	0.334922	0.119
H2B_6	-0.106704	0.654957	0.296920	0.119
C3_6	-0.1311(3)	0.71129(13)	0.3396(2)	0.0802(12)
H3A_6	-0.073705	0.723113	0.344326	0.096
H3B_6	-0.145684	0.720273	0.385152	0.096
C4_6	-0.1987(3)	0.72979(19)	0.2673(3)	0.1073(17)
H4A_6	-0.255990	0.717779	0.262141	0.129
H4B_6	-0.183616	0.721263	0.221769	0.129
C5_6	-0.2062(4)	0.7782(2)	0.2673(4)	0.129(2)
H5A_6	-0.255334	0.787037	0.223126	0.193
H5B_6	-0.152822	0.790537	0.263990	0.193
H5C_6	-0.215180	0.787301	0.314795	0.193
N1_7	0.77304(9)	0.45741(4)	0.31224(8)	0.0227(3)
C1_7	0.76340(11)	0.44190(6)	0.37745(10)	0.0245(4)
H1_7	0.757306	0.412770	0.380772	0.029
C2_7	0.76190(11)	0.46538(6)	0.43831(10)	0.0260(4)
H2_7	0.755368	0.452457	0.482328	0.031
C3_7	0.77006(11)	0.50908(6)	0.43619(10)	0.0246(4)
C4_7	0.78142(12)	0.52520(6)	0.36881(10)	0.0272(4)
H4_7	0.788282	0.554168	0.363812	0.033
C5_7	0.78250(12)	0.49897(5)	0.31090(10)	0.0261(4)
H5_7	0.790454	0.510804	0.266566	0.031
N1_8	0.64536(10)	0.42370(4)	0.17286(8)	0.0236(3)
C1_8	0.58715(12)	0.43230(6)	0.20882(11)	0.0278(4)
H1_8	0.607753	0.445282	0.257698	0.033
C2_8	0.50100(12)	0.42350(6)	0.17930(11)	0.0311(4)
H2_8	0.463794	0.430573	0.207513	0.037
C3_8	0.46649(12)	0.40390(6)	0.10694(11)	0.0304(4)
C4_8	0.52644(12)	0.39706(6)	0.06785(11)	0.0315(4)
H4_8	0.507510	0.385380	0.017806	0.038
C5_8	0.61155(12)	0.40722(6)	0.10194(10)	0.0283(4)
H5_8	0.649781	0.402349	0.073694	0.034
N1_9	0.77962(9)	0.37099(4)	0.27440(8)	0.0230(3)
C1_9	0.71190(12)	0.34679(5)	0.27487(10)	0.0256(4)
H1_9	0.655492	0.355020	0.243781	0.031
C2_9	0.71964(12)	0.31138(6)	0.31718(10)	0.0277(4)
H2_9	0.669419	0.295835	0.314483	0.033
C3_9	0.80136(13)	0.29776(6)	0.36467(10)	0.0286(4)
C4_9	0.87210(13)	0.32288(6)	0.36424(12)	0.0349(4)
H4_9	0.929252	0.315586	0.395017	0.042
C5_9	0.85815(12)	0.35769(6)	0.31945(11)	0.0296(4)
H5_9	0.907209	0.373620	0.320114	0.035
C1_10	1.03505(12)	0.45005(6)	0.35991(10)	0.0288(4)

C2_10	1.07331(12)	0.41988(6)	0.32528(11)	0.0294(4)
C3_10	1.09945(12)	0.43992(6)	0.26806(11)	0.0309(4)
C4_10	1.07777(12)	0.48237(6)	0.26713(10)	0.0293(4)
C5_10	1.03777(12)	0.48873(6)	0.32398(10)	0.0281(4)
C6_10	1.01013(13)	0.52973(6)	0.34698(13)	0.0368(5)
H6A_10	0.994359	0.548569	0.302893	0.055
H6B_10	1.057957	0.541695	0.388861	0.055
H6C_10	0.960071	0.525618	0.364182	0.055
C7_10	1.09714(14)	0.51472(7)	0.21667(12)	0.0394(5)
H7A_10	1.159695	0.519670	0.233137	0.059
H7B_10	1.067307	0.540519	0.220604	0.059
H7C_10	1.077059	0.505109	0.163322	0.059
C8_10	1.14763(14)	0.42093(8)	0.21942(13)	0.0440(5)
H8A_10	1.115762	0.426120	0.165105	0.066
H8B_10	1.153042	0.390998	0.228633	0.066
H8C_10	1.205413	0.433298	0.232896	0.066
C9_10	1.08549(14)	0.37469(7)	0.34449(13)	0.0403(5)
H9A_10	1.146602	0.367357	0.356108	0.060
H9B_10	1.050087	0.358319	0.300655	0.060
H9C_10	1.067744	0.368849	0.389255	0.060
C10_10	1.00144(13)	0.44430(7)	0.42582(11)	0.0361(5)
H10A_10	0.944417	0.457367	0.413499	0.054
H10B_10	1.041550	0.457127	0.472024	0.054
H10C_10	0.996436	0.414650	0.434938	0.054
O1_13	0.41991(19)	0.59302(7)	0.35431(14)	0.0271(5)
C1_13	0.4532(4)	0.5612(2)	0.3250(4)	0.0269(13)
C2_13	0.4968(5)	0.5770(3)	0.2675(5)	0.0393(17)
F1_13	0.5748(3)	0.59309(14)	0.3038(3)	0.0496(9)
F2_13	0.5078(3)	0.54701(15)	0.2214(2)	0.0584(10)
F3_13	0.4497(6)	0.6064(2)	0.2227(6)	0.0534(18)
C3_13	0.3776(3)	0.53200(17)	0.2825(2)	0.0352(9)
F4_13	0.32649(13)	0.52478(8)	0.32360(13)	0.0389(5)
F5_13	0.32924(14)	0.54836(8)	0.21570(11)	0.0457(7)
F6_13	0.40605(17)	0.49491(8)	0.26665(15)	0.0512(7)
C4_13	0.5204(3)	0.53702(16)	0.3896(3)	0.0362(11)
F7_13	0.4828(6)	0.5136(3)	0.4290(4)	0.0487(15)
F8_13	0.56981(15)	0.51200(8)	0.36374(15)	0.0495(7)
F9_13	0.57350(13)	0.56353(8)	0.43908(12)	0.0448(6)
O1_14	0.4706(3)	0.59540(10)	0.3753(2)	0.0257(8)
C1_14	0.4601(6)	0.5646(3)	0.3230(6)	0.0245(18)
C2_14	0.5127(5)	0.5266(2)	0.3655(4)	0.0339(15)
F1_14	0.4716(9)	0.5081(4)	0.4080(5)	0.0442(18)
F2_14	0.5250(2)	0.49839(10)	0.3170(2)	0.0505(10)
F3_14	0.5900(2)	0.53816(11)	0.41212(18)	0.0440(9)
C3_14	0.4936(7)	0.5785(4)	0.2575(6)	0.035(2)
F4_14	0.4629(9)	0.6159(3)	0.2322(8)	0.0419(18)
F5_14	0.5800(4)	0.5807(2)	0.2832(4)	0.0493(13)
F6_14	0.4701(4)	0.5527(2)	0.1980(3)	0.0511(13)
C4_14	0.3636(3)	0.55129(19)	0.2892(3)	0.0312(12)
F7_14	0.31867(18)	0.57821(10)	0.23615(17)	0.0391(8)
F8_14	0.3548(2)	0.51382(13)	0.2559(2)	0.0430(10)
F9_14	0.32636(18)	0.54946(12)	0.34308(18)	0.0341(7)
O1_15	0.3312(2)	0.65627(10)	0.39666(18)	0.0264(6)
C1_15	0.2462(4)	0.6590(2)	0.3543(4)	0.0253(13)

C2_15	0.2043(3)	0.61584(13)	0.3319(2)	0.0310(9)
F1_15	0.22356(16)	0.60010(6)	0.27267(11)	0.0364(5)
F2_15	0.11785(15)	0.61689(7)	0.31205(14)	0.0427(6)
F3_15	0.2338(2)	0.58931(8)	0.39008(15)	0.0399(6)
C3_15	0.1995(3)	0.68159(12)	0.4038(2)	0.0326(8)
F4_15	0.24520(17)	0.71436(8)	0.43974(14)	0.0430(7)
F5_15	0.1893(2)	0.65645(13)	0.4578(2)	0.0429(8)
F6_15	0.12070(13)	0.69521(7)	0.36227(12)	0.0409(6)
C4_15	0.2345(5)	0.6841(2)	0.2801(5)	0.0328(16)
F7_15	0.2496(2)	0.72450(14)	0.2951(3)	0.0440(9)
F8_15	0.1554(2)	0.68092(11)	0.2282(2)	0.0427(8)
F9_15	0.2912(5)	0.6711(4)	0.2467(5)	0.0361(14)
O1_16	0.3270(3)	0.64031(13)	0.3775(3)	0.0249(9)
C1_16	0.2504(6)	0.6612(3)	0.3544(6)	0.0264(19)
C2_16	0.1754(4)	0.62882(19)	0.3333(3)	0.0348(13)
F1_16	0.1659(2)	0.61152(10)	0.26537(18)	0.0437(9)
F2_16	0.09983(19)	0.64562(12)	0.3297(2)	0.0481(10)
F3_16	0.1928(3)	0.59845(13)	0.3856(2)	0.0424(9)
C3_16	0.2424(4)	0.6895(2)	0.4206(3)	0.0361(12)
F4_16	0.3176(2)	0.70864(10)	0.45387(18)	0.0458(9)
F5_16	0.2247(4)	0.66650(17)	0.4737(3)	0.0480(12)
F6_16	0.1808(2)	0.71782(10)	0.3957(2)	0.0476(10)
C4_16	0.2424(7)	0.6885(3)	0.2826(6)	0.031(2)
F7_16	0.2869(3)	0.72331(19)	0.3023(4)	0.0396(12)
F8_16	0.1601(3)	0.69860(16)	0.2442(3)	0.0456(12)
F9_16	0.2720(8)	0.6684(6)	0.2335(8)	0.043(3)
O1_17	0.5006(6)	0.6402(3)	0.4929(4)	0.0257(13)
C1_17	0.5043(5)	0.6354(2)	0.5672(5)	0.0287(15)
C2_17	0.4947(4)	0.6777(2)	0.6043(4)	0.0421(14)
F1_17	0.5665(3)	0.70023(18)	0.6166(4)	0.0543(12)
F2_17	0.4800(3)	0.6734(2)	0.6707(3)	0.0580(14)
F3_17	0.4289(2)	0.69911(10)	0.5567(4)	0.0502(10)
C3_17	0.4316(7)	0.6067(3)	0.5741(5)	0.037(2)
F4_17	0.4199(12)	0.5756(5)	0.5242(7)	0.0421(19)
F5_17	0.3567(8)	0.6266(5)	0.5589(7)	0.0423(19)
F6_17	0.4506(6)	0.5897(2)	0.6441(4)	0.0526(15)
C4_17	0.5928(5)	0.6159(2)	0.6125(4)	0.0403(15)
F7_17	0.5950(2)	0.57550(14)	0.5975(3)	0.0502(10)
F8_17	0.6139(2)	0.6206(2)	0.68889(17)	0.0595(13)
F9_17	0.6556(8)	0.6337(4)	0.5922(7)	0.0452(19)
O1_18	0.4886(8)	0.6482(4)	0.4999(6)	0.0236(16)
C1_18	0.5055(7)	0.6314(3)	0.5710(6)	0.0270(18)
C2_18	0.5933(6)	0.6078(3)	0.5939(5)	0.0374(18)
F1_18	0.5830(3)	0.57171(13)	0.5572(5)	0.0491(13)
F2_18	0.6239(3)	0.6001(2)	0.6701(3)	0.0511(15)
F3_18	0.6541(11)	0.6292(6)	0.5765(9)	0.049(3)
C3_18	0.5142(5)	0.6681(2)	0.6286(4)	0.0369(16)
F4_18	0.4504(4)	0.69580(12)	0.5998(5)	0.0436(14)
F5_18	0.5893(4)	0.6879(2)	0.6422(4)	0.0464(13)
F6_18	0.5087(5)	0.65476(19)	0.6954(3)	0.0526(14)
C4_18	0.4322(8)	0.6010(4)	0.5725(8)	0.029(2)
F7_18	0.3620(10)	0.6219(6)	0.5737(10)	0.040(2)
F8_18	0.4560(9)	0.5769(2)	0.6349(6)	0.0437(16)
F9_18	0.4083(16)	0.5764(6)	0.5114(9)	0.041(3)

C1_19	0.7686(3)	0.51430(12)	-0.0026(2)	0.0292(8)
C2_19	0.6932(4)	0.5103(2)	0.0185(4)	0.0264(11)
C3_19	0.7051(4)	0.5339(3)	0.0861(5)	0.0252(12)
C4_19	0.7889(3)	0.55249(13)	0.1070(2)	0.0252(9)
C5_19	0.8275(2)	0.54064(13)	0.0514(3)	0.0281(8)
C6_19	0.9147(2)	0.55363(13)	0.0487(2)	0.0493(11)
H6A_19	0.907193	0.570693	0.003044	0.074
H6B_19	0.948778	0.528982	0.046548	0.074
H6C_19	0.944987	0.569694	0.094809	0.074
C7_19	0.8265(3)	0.58142(10)	0.1733(2)	0.0430(10)
H7A_19	0.889480	0.578033	0.193171	0.065
H7B_19	0.802110	0.575055	0.213958	0.065
H7C_19	0.812314	0.610047	0.156115	0.065
C8_19	0.6394(3)	0.53883(16)	0.1262(3)	0.0396(11)
H8A_19	0.664781	0.554761	0.173496	0.059
H8B_19	0.621957	0.511456	0.138736	0.059
H8C_19	0.588644	0.553494	0.092489	0.059
C9_19	0.6124(3)	0.48787(12)	-0.0264(3)	0.0436(10)
H9A_19	0.579795	0.480337	0.007620	0.065
H9B_19	0.627712	0.462729	-0.048829	0.065
H9C_19	0.576857	0.505856	-0.067541	0.065
C10_19	0.7847(3)	0.49518(13)	-0.0709(2)	0.0484(10)
H10A_19	0.774034	0.515802	-0.111983	0.073
H10B_19	0.745796	0.471543	-0.089156	0.073
H10C_19	0.844938	0.485739	-0.056184	0.073
C1_20	0.7667(6)	0.5561(3)	0.1227(5)	0.0337(18)
C2_20	0.8284(4)	0.5536(2)	0.0840(5)	0.0329(15)
C3_20	0.7950(5)	0.5283(2)	0.0182(5)	0.0306(17)
C4_20	0.7117(7)	0.5144(4)	0.0154(7)	0.030(2)
C5_20	0.6956(9)	0.5310(6)	0.0816(9)	0.031(2)
C6_20	0.6131(6)	0.5263(3)	0.1006(6)	0.0402(19)
H6A_20	0.582940	0.501062	0.076575	0.060
H6B_20	0.575759	0.550362	0.081149	0.060
H6C_20	0.627026	0.524491	0.156373	0.060
C7_20	0.6498(6)	0.4881(2)	-0.0447(4)	0.0460(18)
H7A_20	0.607866	0.505846	-0.081880	0.069
H7B_20	0.619216	0.469417	-0.020531	0.069
H7C_20	0.681851	0.471716	-0.071193	0.069
C8_20	0.8399(6)	0.5179(3)	-0.0385(5)	0.058(2)
H8A_20	0.851661	0.543449	-0.061989	0.088
H8B_20	0.802692	0.499786	-0.078454	0.088
H8C_20	0.894517	0.503706	-0.012072	0.088
C9_20	0.9141(5)	0.5774(2)	0.1082(6)	0.062(2)
H9A_20	0.958602	0.560538	0.097308	0.093
H9B_20	0.932022	0.583356	0.163243	0.093
H9C_20	0.906651	0.603394	0.079409	0.093
C10_20	0.7734(6)	0.5828(2)	0.1914(4)	0.0470(18)
H10A_20	0.726358	0.575902	0.211139	0.070
H10B_20	0.768976	0.612064	0.176208	0.070
H10C_20	0.829212	0.577961	0.231458	0.070
C1_21	0.9164(4)	0.3455(2)	0.0633(4)	0.0279(12)
C2_21	0.8668(5)	0.3255(3)	0.1033(5)	0.0281(13)
C3_21	0.7784(5)	0.3324(4)	0.0628(6)	0.0285(16)
C4_21	0.7730(5)	0.3570(5)	-0.0024(7)	0.0267(16)

C5_21	0.8585(5)	0.3648(3)	-0.0030(5)	0.0276(14)
C6_21	0.8819(4)	0.3885(2)	-0.0637(4)	0.0343(12)
H6A_21	0.828963	0.398313	-0.102798	0.051
H6B_21	0.913708	0.370328	-0.087583	0.051
H6C_21	0.918249	0.412234	-0.040097	0.051
C7_21	0.6891(6)	0.3692(5)	-0.0625(7)	0.0364(17)
H7A_21	0.692406	0.363370	-0.113578	0.055
H7B_21	0.678816	0.398827	-0.058026	0.055
H7C_21	0.641555	0.353268	-0.054973	0.055
C8_21	0.7041(5)	0.3138(4)	0.0823(6)	0.0327(15)
H8A_21	0.650145	0.327441	0.052080	0.049
H8B_21	0.713408	0.317694	0.137081	0.049
H8C_21	0.700396	0.284145	0.070377	0.049
C9_21	0.9050(4)	0.29978(19)	0.1743(3)	0.0344(12)
H9A_21	0.858972	0.291063	0.194077	0.052
H9B_21	0.947850	0.316241	0.213347	0.052
H9C_21	0.933087	0.275279	0.161793	0.052
C10_21	1.0129(3)	0.34413(18)	0.0825(3)	0.0370(12)
H10A_21	1.031796	0.367869	0.058966	0.056
H10B_21	1.029332	0.318385	0.062799	0.056
H10C_21	1.040592	0.345253	0.138350	0.056
C1_22	0.9147(7)	0.3549(4)	0.0470(7)	0.035(2)
C2_22	0.8810(7)	0.3312(4)	0.0958(7)	0.031(2)
C3_22	0.7892(8)	0.3337(5)	0.0659(9)	0.029(2)
C4_22	0.7665(8)	0.3590(8)	-0.0008(12)	0.031(3)
C5_22	0.8446(8)	0.3721(5)	-0.0118(8)	0.032(2)
C6_22	0.8517(9)	0.3985(4)	-0.0774(6)	0.052(2)
H6A_22	0.794721	0.410089	-0.105916	0.078
H6B_22	0.872095	0.381459	-0.111890	0.078
H6C_22	0.892717	0.421153	-0.056880	0.078
C7_22	0.6782(10)	0.3700(7)	-0.0553(10)	0.051(4)
H7A_22	0.680128	0.397476	-0.077206	0.077
H7B_22	0.636391	0.370160	-0.027562	0.077
H7C_22	0.660443	0.349451	-0.096710	0.077
C8_22	0.7271(9)	0.3124(6)	0.0982(9)	0.043(3)
H8A_22	0.689095	0.332967	0.109559	0.065
H8B_22	0.759694	0.297753	0.145414	0.065
H8C_22	0.692191	0.292453	0.060569	0.065
C9_22	0.9340(8)	0.3067(4)	0.1644(6)	0.049(2)
H9A_22	0.948116	0.279657	0.147566	0.073
H9B_22	0.900752	0.302775	0.199402	0.073
H9C_22	0.987548	0.321720	0.190947	0.073
C10_22	1.0093(6)	0.3597(4)	0.0551(8)	0.060(3)
H10A_22	1.022238	0.343188	0.015697	0.090
H10B_22	1.045266	0.350258	0.106064	0.090
H10C_22	1.021666	0.388973	0.048751	0.090
C1_24	-0.1126(12)	0.6840(5)	0.0778(8)	0.042(3)
C2_24	-0.1560(12)	0.7171(5)	0.0368(9)	0.049(3)
C3_24	-0.1389(18)	0.7556(5)	0.0681(14)	0.058(3)
H3_24	-0.167811	0.779040	0.039952	0.070
C4_24	-0.0795(19)	0.7608(7)	0.1407(15)	0.053(3)
H4_24	-0.069371	0.787497	0.163556	0.063
C5_24	-0.036(2)	0.7271(7)	0.1795(14)	0.044(3)
H5_24	0.006481	0.730604	0.228908	0.053

C6_24	-0.0517(14)	0.6886(6)	0.1477(9)	0.036(3)
H6_24	-0.020533	0.665325	0.174305	0.044
F1_24	-0.1295(14)	0.6472(5)	0.0411(12)	0.083(5)
F2_24	-0.2110(4)	0.70817(19)	-0.0347(3)	0.073(2)
O1_25	0.47688(17)	0.67680(9)	0.35237(17)	0.0442(7)
C1_25	0.53034(19)	0.70906(9)	0.35457(17)	0.0395(6)
C2_25	0.4938(2)	0.74934(10)	0.3769(2)	0.0607(7)
F1_25	0.42702(19)	0.76352(10)	0.31898(19)	0.0942(10)
F2_25	0.55286(19)	0.77968(6)	0.39615(17)	0.0820(7)
F3_25	0.46461(17)	0.74259(9)	0.43426(16)	0.0730(8)
C3_25	0.62086(16)	0.70068(8)	0.41207(16)	0.0425(6)
F4_25	0.6438(3)	0.66134(12)	0.4105(2)	0.0610(9)
F5_25	0.62544(14)	0.70912(8)	0.48391(11)	0.0518(6)
F6_25	0.6822(2)	0.72357(11)	0.3970(3)	0.0680(12)
C4_25	0.53606(19)	0.71395(10)	0.27254(17)	0.0536(7)
F7_25	0.58625(15)	0.68439(7)	0.25910(13)	0.0659(6)
F8_25	0.56972(19)	0.74988(9)	0.26208(16)	0.0673(8)
F9_25	0.4598(3)	0.70961(12)	0.21976(17)	0.0783(10)
O1_26	0.4635(11)	0.6869(5)	0.3636(12)	0.030(2)
C1_26	0.5323(10)	0.7113(5)	0.3662(8)	0.0428(16)
C2_26	0.6168(8)	0.6882(4)	0.3690(8)	0.0440(19)
F1_26	0.6142(8)	0.6730(4)	0.3017(8)	0.058(3)
F2_26	0.6865(13)	0.7126(7)	0.3948(15)	0.040(3)
F3_26	0.6285(17)	0.6558(7)	0.4159(15)	0.042(3)
C3_26	0.5561(9)	0.7383(4)	0.4408(8)	0.0521(19)
F4_26	0.4883(9)	0.7502(6)	0.4590(11)	0.063(3)
F5_26	0.6045(11)	0.7176(5)	0.5019(8)	0.062(3)
F6_26	0.5969(10)	0.7728(4)	0.4346(11)	0.070(3)
C4_26	0.5053(10)	0.7400(5)	0.2954(9)	0.063(2)
F7_26	0.4478(11)	0.7684(6)	0.2998(12)	0.082(4)
F8_26	0.5737(11)	0.7603(7)	0.2897(12)	0.070(4)
F9_26	0.4630(19)	0.7227(8)	0.2289(12)	0.074(4)
C1_23	-0.0557(10)	0.6891(4)	0.1318(6)	0.0338(18)
C2_23	-0.1187(7)	0.6889(3)	0.0610(5)	0.0374(16)
C3_23	-0.1573(10)	0.7241(4)	0.0306(7)	0.055(2)
H3_23	-0.200455	0.723651	-0.018670	0.066
C4_23	-0.1362(12)	0.7603(4)	0.0684(9)	0.055(2)
H4_23	-0.165085	0.785010	0.046191	0.066
C5_23	-0.0728(12)	0.7614(4)	0.1393(10)	0.0443(18)
H5_23	-0.057315	0.786996	0.165672	0.053
C6_23	-0.0319(13)	0.7254(4)	0.1719(9)	0.037(2)
H6_23	0.011607	0.725700	0.221012	0.045
F1_23	-0.0200(2)	0.65383(10)	0.1642(2)	0.0517(12)
F2_23	-0.1409(7)	0.6520(4)	0.0249(8)	0.062(2)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

S-Table 27: Bond lengths and angles for [(dmap)3Al(AlCp*)3][pf]

Atom–Atom	**Length [Å]**		
Al1–N1_7	2.0365(16)	Al2–C4_10	2.3350(19)
Al1–N1_9	2.0396(16)	Al2–C3_10	2.372(2)
Al1–N1_8	2.0450(17)	Al2–C5_10	2.3780(19)
Al1–Al3	2.7964(9)	Al2–C2_10	2.444(2)
Al1–Al4	2.7970(9)	Al2–C1_10	2.4470(19)
Al1–Al2	2.8148(10)	Al2–Al4	2.6607(9)
		Al2–Al3	2.6780(9)

Al3–C2_22	2.299(14)	C6–H6C	0.9800
Al3–C1_22	2.301(12)	C1_6–C2_6	1.422(7)
Al3–C1_21	2.353(8)	C1_6–H1A_6	0.9500
Al3–C5_22	2.359(18)	C1_6–H1B_6	0.9500
Al3–C3_22	2.370(17)	C2_6–C3_6	1.533(6)
Al3–C5_21	2.384(12)	C2_6–H2A_6	0.9900
Al3–C4_22	2.41(3)	C2_6–H2B_6	0.9900
Al3–C2_21	2.419(9)	C3_6–C4_6	1.545(6)
Al3–C4_21	2.436(15)	C3_6–H3A_6	0.9900
Al3–C3_21	2.477(12)	C3_6–H3B_6	0.9900
Al3–Al4	2.6727(11)	C4_6–C5_6	1.568(7)
Al4–C3_20	2.311(6)	C4_6–H4A_6	0.9900
Al4–C4_20	2.315(15)	C4_6–H4B_6	0.9900
Al4–C1_19	2.327(4)	C5_6–H5A_6	0.9800
Al4–C5_19	2.330(3)	C5_6–H5B_6	0.9800
Al4–C4_19	2.368(4)	C5_6–H5C_6	0.9800
Al4–C2_19	2.385(8)	N1_7–C5_7	1.352(2)
Al4–C3_19	2.414(10)	N1_7–C1_7	1.360(2)
Al4–C5_20	2.45(2)	C1_7–C2_7	1.362(2)
Al4–C2_20	2.471(6)	C1_7–H1_7	0.9500
Al5–O1_16	1.681(4)	C2_7–C3_7	1.419(3)
Al5–O1_17	1.695(8)	C2_7–H2_7	0.9500
Al5–O1_14	1.708(3)	C3_7–C4_7	1.416(3)
Al5–O1_25	1.716(3)	C4_7–C5_7	1.368(3)
Al5–O1_26	1.742(18)	C4_7–H4_7	0.9500
Al5–O1_15	1.751(3)	C5_7–H5_7	0.9500
Al5–O1_13	1.752(2)	N1_8–C5_8	1.351(2)
Al5–O1_18	1.774(11)	N1_8–C1_8	1.357(2)
N1–C3_9	1.347(2)	C1_8–C2_8	1.363(3)
N1–C5	1.454(3)	C1_8–H1_8	0.9500
N1–C6	1.457(3)	C2_8–C3_8	1.416(3)
N2–C3_7	1.346(2)	C2_8–H2_8	0.9500
N2–C4	1.457(3)	C3_8–C4_8	1.413(3)
N2–C3	1.458(3)	C4_8–C5_8	1.366(3)
N3–C3_8	1.346(3)	C4_8–H4_8	0.9500
N3–C1	1.455(3)	C5_8–H5_8	0.9500
N3–C2	1.458(3)	N1_9–C5_9	1.350(2)
C1–H1A	0.9800	N1_9–C1_9	1.358(2)
C1–H1B	0.9800	C1_9–C2_9	1.367(2)
C1–H1C	0.9800	C1_9–H1_9	0.9500
C2–H2A	0.9800	C2_9–C3_9	1.406(3)
C2–H2B	0.9800	C2_9–H2_9	0.9500
C2–H2C	0.9800	C3_9–C4_9	1.415(3)
C3–H3A	0.9800	C4_9–C5_9	1.369(3)
C3–H3B	0.9800	C4_9–H4_9	0.9500
C3–H3C	0.9800	C5_9–H5_9	0.9500
C4–H4A	0.9800	C1_10–C2_10	1.419(3)
C4–H4B	0.9800	C1_10–C5_10	1.422(3)
C4–H4C	0.9800	C1_10–C10_10	1.502(3)
C5–H5A	0.9800	C2_10–C3_10	1.419(3)
C5–H5B	0.9800	C2_10–C9_10	1.499(3)
C5–H5C	0.9800	C3_10–C4_10	1.414(3)
C6–H6A	0.9800	C3_10–C8_10	1.506(3)
C6–H6B	0.9800	C4_10–C5_10	1.423(3)

C4_10–C7_10	1.501(3)	C4_15–F9_15	1.337(8)
C5_10–C6_10	1.504(3)	C4_15–F7_15	1.339(7)
C6_10–H6A_10	0.9800	O1_16–C1_16	1.361(10)
C6_10–H6B_10	0.9800	C1_16–C4_16	1.560(10)
C6_10–H6C_10	0.9800	C1_16–C2_16	1.561(10)
C7_10–H7A_10	0.9800	C1_16–C3_16	1.566(10)
C7_10–H7B_10	0.9800	C2_16–F2_16	1.332(7)
C7_10–H7C_10	0.9800	C2_16–F1_16	1.334(7)
C8_10–H8A_10	0.9800	C2_16–F3_16	1.339(7)
C8_10–H8B_10	0.9800	C3_16–F6_16	1.325(7)
C8_10–H8C_10	0.9800	C3_16–F4_16	1.331(7)
C9_10–H9A_10	0.9800	C3_16–F5_16	1.336(7)
C9_10–H9B_10	0.9800	C4_16–F7_16	1.322(10)
C9_10–H9C_10	0.9800	C4_16–F9_16	1.331(11)
C10_10–H10A_10	0.9800	C4_16–F8_16	1.337(10)
C10_10–H10B_10	0.9800	O1_17–C1_17	1.360(8)
C10_10–H10C_10	0.9800	C1_17–C3_17	1.547(8)
O1_13–C1_13	1.355(7)	C1_17–C4_17	1.548(8)
C1_13–C4_13	1.541(7)	C1_17–C2_17	1.558(8)
C1_13–C2_13	1.547(8)	C2_17–F2_17	1.332(6)
C1_13–C3_13	1.547(8)	C2_17–F1_17	1.335(7)
C2_13–F3_13	1.326(8)	C2_17–F3_17	1.336(6)
C2_13–F1_13	1.336(8)	C3_17–F5_17	1.328(9)
C2_13–F2_13	1.340(8)	C3_17–F4_17	1.333(9)
C3_13–F4_13	1.322(4)	C3_17–F6_17	1.343(8)
C3_13–F5_13	1.334(5)	C4_17–F9_17	1.335(8)
C3_13–F6_13	1.351(5)	C4_17–F7_17	1.336(7)
C4_13–F7_13	1.333(7)	C4_17–F8_17	1.345(6)
C4_13–F8_13	1.337(5)	O1_18–C1_18	1.363(10)
C4_13–F9_13	1.341(5)	C1_18–C2_18	1.555(10)
O1_14–C1_14	1.358(9)	C1_18–C4_18	1.557(10)
C1_14–C3_14	1.549(10)	C1_18–C3_18	1.568(9)
C1_14–C2_14	1.553(10)	C2_18–F1_18	1.331(8)
C1_14–C4_14	1.555(9)	C2_18–F3_18	1.334(10)
C2_14–F3_14	1.327(7)	C2_18–F2_18	1.352(8)
C2_14–F1_14	1.332(10)	C3_18–F5_18	1.333(8)
C2_14–F2_14	1.338(7)	C3_18–F6_18	1.336(7)
C3_14–F6_14	1.330(10)	C3_18–F4_18	1.344(7)
C3_14–F4_14	1.333(11)	C4_18–F9_18	1.328(11)
C3_14–F5_14	1.337(10)	C4_18–F8_18	1.336(10)
C4_14–F9_14	1.327(6)	C4_18–F7_18	1.338(10)
C4_14–F7_14	1.335(6)	C1_19–C2_19	1.417(5)
C4_14–F8_14	1.344(6)	C1_19–C5_19	1.419(5)
O1_15–C1_15	1.355(7)	C1_19–C10_19	1.503(5)
C1_15–C4_15	1.548(8)	C2_19–C3_19	1.419(6)
C1_15–C2_15	1.549(7)	C2_19–C9_19	1.494(6)
C1_15–C3_15	1.553(7)	C3_19–C4_19	1.428(6)
C2_15–F3_15	1.333(5)	C3_19–C8_19	1.501(6)
C2_15–F1_15	1.333(5)	C4_19–C5_19	1.424(5)
C2_15–F2_15	1.340(4)	C4_19–C7_19	1.501(5)
C3_15–F5_15	1.338(5)	C5_19–C6_19	1.503(5)
C3_15–F4_15	1.339(4)	C6_19–H6A_19	0.9800
C3_15–F6_15	1.339(5)	C6_19–H6B_19	0.9800
C4_15–F8_15	1.336(8)	C6_19–H6C_19	0.9800

C7_19–H7A_19	0.9800	C8_21–H8B_21	0.9800
C7_19–H7B_19	0.9800	C8_21–H8C_21	0.9800
C7_19–H7C_19	0.9800	C9_21–H9A_21	0.9800
C8_19–H8A_19	0.9800	C9_21–H9B_21	0.9800
C8_19–H8B_19	0.9800	C9_21–H9C_21	0.9800
C8_19–H8C_19	0.9800	C10_21–H10A_21	0.9800
C9_19–H9A_19	0.9800	C10_21–H10B_21	0.9800
C9_19–H9B_19	0.9800	C10_21–H10C_21	0.9800
C9_19–H9C_19	0.9800	C1_22–C5_22	1.408(9)
C10_19–H10A_19	0.9800	C1_22–C2_22	1.423(9)
C10_19–H10B_19	0.9800	C1_22–C10_22	1.513(10)
C10_19–H10C_19	0.9800	C2_22–C3_22	1.423(10)
C1_20–C5_20	1.416(11)	C2_22–C9_22	1.502(10)
C1_20–C2_20	1.417(8)	C3_22–C4_22	1.422(11)
C1_20–C10_20	1.509(8)	C3_22–C8_22	1.502(11)
C2_20–C3_20	1.414(9)	C4_22–C5_22	1.421(11)
C2_20–C9_20	1.531(9)	C4_22–C7_22	1.506(11)
C3_20–C4_20	1.419(10)	C5_22–C6_22	1.518(10)
C3_20–C8_20	1.502(8)	C6_22–H6A_22	0.9800
C4_20–C5_20	1.436(11)	C6_22–H6B_22	0.9800
C4_20–C7_20	1.496(10)	C6_22–H6C_22	0.9800
C5_20–C6_20	1.509(11)	C7_22–H7A_22	0.9800
C6_20–H6A_20	0.9800	C7_22–H7B_22	0.9800
C6_20–H6B_20	0.9800	C7_22–H7C_22	0.9800
C6_20–H6C_20	0.9800	C8_22–H8A_22	0.9800
C7_20–H7A_20	0.9800	C8_22–H8B_22	0.9800
C7_20–H7B_20	0.9800	C8_22–H8C_22	0.9800
C7_20–H7C_20	0.9800	C9_22–H9A_22	0.9800
C8_20–H8A_20	0.9800	C9_22–H9B_22	0.9800
C8_20–H8B_20	0.9800	C9_22–H9C_22	0.9800
C8_20–H8C_20	0.9800	C10_22–H10A_22	0.9800
C9_20–H9A_20	0.9800	C10_22–H10B_22	0.9800
C9_20–H9B_20	0.9800	C10_22–H10C_22	0.9800
C9_20–H9C_20	0.9800	C1_24–F1_24	1.349(11)
C10_20–H10A_20	0.9800	C1_24–C6_24	1.354(10)
C10_20–H10B_20	0.9800	C1_24–C2_24	1.367(11)
C10_20–H10C_20	0.9800	C2_24–C3_24	1.360(11)
C1_21–C5_21	1.420(6)	C2_24–F2_24	1.362(13)
C1_21–C2_21	1.420(6)	C3_24–C4_24	1.382(12)
C1_21–C10_21	1.500(6)	C3_24–H3_24	0.9500
C2_21–C3_21	1.410(7)	C4_24–C5_24	1.369(12)
C2_21–C9_21	1.502(7)	C4_24–H4_24	0.9500
C3_21–C4_21	1.422(7)	C5_24–C6_24	1.362(12)
C3_21–C8_21	1.500(7)	C5_24–H5_24	0.9500
C4_21–C5_21	1.425(7)	C6_24–H6_24	0.9500
C4_21–C7_21	1.504(7)	O1_25–C1_25	1.352(3)
C5_21–C6_21	1.507(7)	C1_25–C3_25	1.535(4)
C6_21–H6A_21	0.9800	C1_25–C2_25	1.543(4)
C6_21–H6B_21	0.9800	C1_25–C4_25	1.555(4)
C6_21–H6C_21	0.9800	C2_25–F3_25	1.315(4)
C7_21–H7A_21	0.9800	C2_25–F1_25	1.333(4)
C7_21–H7B_21	0.9800	C2_25–F2_25	1.339(4)
C7_21–H7C_21	0.9800	C3_25–F4_25	1.328(5)
C8_21–H8A_21	0.9800	C3_25–F5_25	1.331(4)

C3_25–F6_25	1.346(4)
C4_25–F9_25	1.314(4)
C4_25–F8_25	1.325(4)
C4_25–F7_25	1.335(4)
O1_26–C1_26	1.362(13)
C1_26–C4_26	1.545(12)
C1_26–C2_26	1.556(12)
C1_26–C3_26	1.566(12)
C2_26–F1_26	1.323(12)
C2_26–F3_26	1.331(13)
C2_26–F2_26	1.338(13)
C3_26–F4_26	1.318(12)
C3_26–F6_26	1.324(12)
C3_26–F5_26	1.326(12)
C4_26–F9_26	1.319(13)
C4_26–F8_26	1.330(12)
C4_26–F7_26	1.335(13)
C1_23–F1_23	1.329(10)
C1_23–C6_23	1.372(8)
C1_23–C2_23	1.373(8)
C2_23–C3_23	1.330(9)
C2_23–F2_23	1.353(8)
C3_23–C4_23	1.347(10)
C3_23–H3_23	0.9500
C4_23–C5_23	1.376(10)
C4_23–H4_23	0.9500
C5_23–C6_23	1.377(9)
C5_23–H5_23	0.9500
C6_23–H6_23	0.9500

Atom–Atom–Atom	**Angle [°]**
N1_7–Al1–N1_9	90.19(6)
N1_7–Al1–N1_8	92.03(6)
N1_9–Al1–N1_8	91.23(6)
N1_7–Al1–Al3	155.82(5)
N1_9–Al1–Al3	99.80(5)
N1_8–Al1–Al3	109.56(5)
N1_7–Al1–Al4	109.77(5)
N1_9–Al1–Al4	156.58(5)
N1_8–Al1–Al4	99.88(5)
Al3–Al1–Al4	57.09(2)
N1_7–Al1–Al2	98.92(5)
N1_9–Al1–Al2	109.61(5)
N1_8–Al1–Al2	156.27(5)
Al3–Al1–Al2	57.01(2)
Al4–Al1–Al2	56.60(2)
C4_10–Al2–C3_10	34.96(7)
C4_10–Al2–C5_10	35.12(6)
C3_10–Al2–C5_10	57.69(6)
C4_10–Al2–C2_10	57.41(7)
C3_10–Al2–C2_10	34.23(7)
C5_10–Al2–C2_10	56.84(7)
C4_10–Al2–C1_10	57.49(7)
C3_10–Al2–C1_10	56.85(6)
C5_10–Al2–C1_10	34.23(6)
C2_10–Al2–C1_10	33.72(6)
C4_10–Al2–Al4	119.13(6)
C3_10–Al2–Al4	143.35(6)
C5_10–Al2–Al4	120.16(6)
C2_10–Al2–Al4	176.49(5)
C1_10–Al2–Al4	144.86(5)
C4_10–Al2–Al3	141.90(5)
C3_10–Al2–Al3	120.10(5)
C5_10–Al2–Al3	177.01(5)
C2_10–Al2–Al3	122.80(5)
C1_10–Al2–Al3	147.20(5)
Al4–Al2–Al3	60.08(3)
C4_10–Al2–Al1	156.16(5)
C3_10–Al2–Al1	154.71(6)
C5_10–Al2–Al1	121.76(5)
C2_10–Al2–Al1	121.41(5)
C1_10–Al2–Al1	107.10(5)
Al4–Al2–Al1	61.36(2)
Al3–Al2–Al1	61.15(2)
C2_22–Al3–C1_22	36.0(3)
C2_22–Al3–C5_22	58.9(4)
C1_22–Al3–C5_22	35.1(3)
C2_22–Al3–C3_22	35.4(3)
C1_22–Al3–C3_22	58.9(4)
C5_22–Al3–C3_22	58.1(4)
C1_21–Al3–C5_21	34.88(18)
C2_22–Al3–C4_22	58.4(5)
C1_22–Al3–C4_22	58.3(5)
C5_22–Al3–C4_22	34.7(4)
C3_22–Al3–C4_22	34.6(4)
C1_21–Al3–C2_21	34.60(18)
C5_21–Al3–C2_21	57.3(2)
C1_21–Al3–C4_21	57.1(3)
C5_21–Al3–C4_21	34.4(2)
C2_21–Al3–C4_21	56.2(3)
C1_21–Al3–C3_21	56.7(3)
C5_21–Al3–C3_21	56.7(3)
C2_21–Al3–C3_21	33.4(2)
C4_21–Al3–C3_21	33.6(2)
C2_22–Al3–Al4	177.1(3)
C1_22–Al3–Al4	141.2(3)
C1_21–Al3–Al4	150.99(18)
C5_22–Al3–Al4	118.2(3)
C3_22–Al3–Al4	144.5(3)
C5_21–Al3–Al4	125.32(19)
C4_22–Al3–Al4	119.8(5)
C2_21–Al3–Al4	173.66(18)
C4_21–Al3–Al4	121.9(3)
C3_21–Al3–Al4	141.4(2)
C2_22–Al3–Al2	121.9(3)
C1_22–Al3–Al2	120.0(3)
C1_21–Al3–Al2	118.69(16)
C5_22–Al3–Al2	142.5(3)

C3_22–Al3–Al2	147.5(3)	O1_17–Al5–O1_25	107.9(4)
C5_21–Al3–Al2	140.17(18)	O1_16–Al5–O1_26	108.2(6)
C4_22–Al3–Al2	177.0(3)	O1_14–Al5–O1_26	118.3(5)
C2_21–Al3–Al2	122.90(19)	O1_17–Al5–O1_15	108.9(3)
C4_21–Al3–Al2	174.5(2)	O1_25–Al5–O1_15	110.09(15)
C3_21–Al3–Al2	148.6(2)	O1_17–Al5–O1_13	114.2(3)
Al4–Al3–Al2	59.64(2)	O1_25–Al5–O1_13	111.42(12)
C3_20–Al4–C4_20	35.7(3)	O1_15–Al5–O1_13	104.16(15)
C1_19–Al4–C5_19	35.48(12)	O1_16–Al5–O1_18	112.1(4)
C1_19–Al4–C4_19	58.59(13)	O1_14–Al5–O1_18	107.0(3)
C5_19–Al4–C4_19	35.28(13)	O1_26–Al5–O1_18	101.1(8)
C1_19–Al4–C2_19	34.96(15)	C3_9–N1–C5	121.18(18)
C5_19–Al4–C2_19	58.34(17)	C3_9–N1–C6	120.27(18)
C4_19–Al4–C2_19	57.89(17)	C5–N1–C6	118.55(17)
C1_19–Al4–C3_19	57.9(2)	C3_7–N2–C4	120.07(16)
C5_19–Al4–C3_19	58.1(2)	C3_7–N2–C3	120.49(16)
C4_19–Al4–C3_19	34.72(17)	C4–N2–C3	118.90(15)
C2_19–Al4–C3_19	34.40(19)	C3_8–N3–C1	121.11(19)
C3_20–Al4–C5_20	57.5(4)	C3_8–N3–C2	120.91(19)
C4_20–Al4–C5_20	34.9(3)	C1–N3–C2	117.77(18)
C3_20–Al4–C2_20	34.2(2)	N3–C1–H1A	109.5
C4_20–Al4–C2_20	57.1(3)	N3–C1–H1B	109.5
C5_20–Al4–C2_20	55.1(3)	H1A–C1–H1B	109.5
C3_20–Al4–Al2	136.5(2)	N3–C1–H1C	109.5
C4_20–Al4–Al2	172.3(3)	H1A–C1–H1C	109.5
C1_19–Al4–Al2	145.92(11)	H1B–C1–H1C	109.5
C5_19–Al4–Al2	122.11(10)	N3–C2–H2A	109.5
C4_19–Al4–Al2	121.87(10)	N3–C2–H2B	109.5
C2_19–Al4–Al2	179.03(14)	H2A–C2–H2B	109.5
C3_19–Al4–Al2	144.85(15)	N3–C2–H2C	109.5
C5_20–Al4–Al2	147.3(3)	H2A–C2–H2C	109.5
C2_20–Al4–Al2	116.58(16)	H2B–C2–H2C	109.5
C3_20–Al4–Al3	126.3(2)	N2–C3–H3A	109.5
C4_20–Al4–Al3	122.6(3)	N2–C3–H3B	109.5
C1_19–Al4–Al3	115.00(10)	H3A–C3–H3B	109.5
C5_19–Al4–Al3	136.92(12)	N2–C3–H3C	109.5
C4_19–Al4–Al3	172.20(12)	H3A–C3–H3C	109.5
C2_19–Al4–Al3	120.10(15)	H3B–C3–H3C	109.5
C3_19–Al4–Al3	147.73(14)	N2–C4–H4A	109.5
C5_20–Al4–Al3	143.6(3)	N2–C4–H4B	109.5
C2_20–Al4–Al3	151.7(2)	H4A–C4–H4B	109.5
Al2–Al4–Al3	60.28(2)	N2–C4–H4C	109.5
C3_20–Al4–Al1	161.15(19)	H4A–C4–H4C	109.5
C4_20–Al4–Al1	125.7(3)	H4B–C4–H4C	109.5
C1_19–Al4–Al1	149.44(11)	N1–C5–H5A	109.5
C5_19–Al4–Al1	161.61(12)	N1–C5–H5B	109.5
C4_19–Al4–Al1	126.36(12)	H5A–C5–H5B	109.5
C2_19–Al4–Al1	117.25(14)	N1–C5–H5C	109.5
C3_19–Al4–Al1	107.35(19)	H5A–C5–H5C	109.5
C5_20–Al4–Al1	105.4(4)	H5B–C5–H5C	109.5
C2_20–Al4–Al1	145.1(2)	N1–C6–H6A	109.5
Al2–Al4–Al1	62.03(3)	N1–C6–H6B	109.5
Al3–Al4–Al1	61.44(2)	H6A–C6–H6B	109.5
O1_16–Al5–O1_14	109.8(2)	N1–C6–H6C	109.5

H6A–C6–H6C	109.5	C1_8–C2_8–H2_8	119.7
H6B–C6–H6C	109.5	C3_8–C2_8–H2_8	119.7
C2_6–C1_6–H1A_6	120.0	N3–C3_8–C4_8	122.21(19)
C2_6–C1_6–H1B_6	120.0	N3–C3_8–C2_8	122.77(18)
H1A_6–C1_6–H1B_6	120.0	C4_8–C3_8–C2_8	115.03(17)
C1_6–C2_6–C3_6	115.1(4)	C5_8–C4_8–C3_8	120.07(18)
C1_6–C2_6–H2A_6	108.5	C5_8–C4_8–H4_8	120.0
C3_6–C2_6–H2A_6	108.5	C3_8–C4_8–H4_8	120.0
C1_6–C2_6–H2B_6	108.5	N1_8–C5_8–C4_8	124.80(18)
C3_6–C2_6–H2B_6	108.5	N1_8–C5_8–H5_8	117.6
H2A_6–C2_6–H2B_6	107.5	C4_8–C5_8–H5_8	117.6
C2_6–C3_6–C4_6	115.7(4)	C5_9–N1_9–C1_9	115.22(15)
C2_6–C3_6–H3A_6	108.4	C5_9–N1_9–Al1	116.21(12)
C4_6–C3_6–H3A_6	108.4	C1_9–N1_9–Al1	128.51(12)
C2_6–C3_6–H3B_6	108.4	N1_9–C1_9–C2_9	124.23(17)
C4_6–C3_6–H3B_6	108.4	N1_9–C1_9–H1_9	117.9
H3A_6–C3_6–H3B_6	107.4	C2_9–C1_9–H1_9	117.9
C3_6–C4_6–C5_6	114.8(5)	C1_9–C2_9–C3_9	120.52(17)
C3_6–C4_6–H4A_6	108.6	C1_9–C2_9–H2_9	119.7
C5_6–C4_6–H4A_6	108.6	C3_9–C2_9–H2_9	119.7
C3_6–C4_6–H4B_6	108.6	N1–C3_9–C2_9	122.06(18)
C5_6–C4_6–H4B_6	108.6	N1–C3_9–C4_9	122.54(18)
H4A_6–C4_6–H4B_6	107.5	C2_9–C3_9–C4_9	115.39(16)
C4_6–C5_6–H5A_6	109.5	C5_9–C4_9–C3_9	119.98(18)
C4_6–C5_6–H5B_6	109.5	C5_9–C4_9–H4_9	120.0
H5A_6–C5_6–H5B_6	109.5	C3_9–C4_9–H4_9	120.0
C4_6–C5_6–H5C_6	109.5	N1_9–C5_9–C4_9	124.64(18)
H5A_6–C5_6–H5C_6	109.5	N1_9–C5_9–H5_9	117.7
H5B_6–C5_6–H5C_6	109.5	C4_9–C5_9–H5_9	117.7
C5_7–N1_7–C1_7	115.41(15)	C2_10–C1_10–C5_10	107.87(16)
C5_7–N1_7–Al1	116.64(12)	C2_10–C1_10–C10_10	127.83(18)
C1_7–N1_7–Al1	127.94(12)	C5_10–C1_10–C10_10	124.22(17)
N1_7–C1_7–C2_7	124.32(17)	C2_10–C1_10–Al2	73.04(10)
N1_7–C1_7–H1_7	117.8	C5_10–C1_10–Al2	70.23(10)
C2_7–C1_7–H1_7	117.8	C10_10–C1_10–Al2	124.84(13)
C1_7–C2_7–C3_7	120.21(17)	C1_10–C2_10–C3_10	107.93(17)
C1_7–C2_7–H2_7	119.9	C1_10–C2_10–C9_10	127.28(18)
C3_7–C2_7–H2_7	119.9	C3_10–C2_10–C9_10	124.79(18)
N2–C3_7–C4_7	122.28(17)	C1_10–C2_10–Al2	73.24(11)
N2–C3_7–C2_7	122.21(17)	C3_10–C2_10–Al2	70.11(11)
C4_7–C3_7–C2_7	115.51(16)	C9_10–C2_10–Al2	122.49(13)
C5_7–C4_7–C3_7	119.83(17)	C4_10–C3_10–C2_10	108.36(16)
C5_7–C4_7–H4_7	120.1	C4_10–C3_10–C8_10	124.45(19)
C3_7–C4_7–H4_7	120.1	C2_10–C3_10–C8_10	127.06(19)
N1_7–C5_7–C4_7	124.69(17)	C4_10–C3_10–Al2	71.07(11)
N1_7–C5_7–H5_7	117.7	C2_10–C3_10–Al2	75.66(11)
C4_7–C5_7–H5_7	117.7	C8_10–C3_10–Al2	122.29(13)
C5_8–N1_8–C1_8	115.16(16)	C3_10–C4_10–C5_10	107.78(17)
C5_8–N1_8–Al1	116.69(12)	C3_10–C4_10–C7_10	125.34(18)
C1_8–N1_8–Al1	127.62(12)	C5_10–C4_10–C7_10	126.83(18)
N1_8–C1_8–C2_8	124.18(18)	C3_10–C4_10–Al2	73.97(11)
N1_8–C1_8–H1_8	117.9	C5_10–C4_10–Al2	74.09(11)
C2_8–C1_8–H1_8	117.9	C7_10–C4_10–Al2	119.51(13)
C1_8–C2_8–C3_8	120.56(18)	C1_10–C5_10–C4_10	108.05(16)

C1_10–C5_10–C6_10	125.65(17)	O1_13–C1_13–C4_13	110.7(5)
C4_10–C5_10–C6_10	126.10(18)	O1_13–C1_13–C2_13	111.1(5)
C1_10–C5_10–Al2	75.54(11)	C4_13–C1_13–C2_13	108.9(5)
C4_10–C5_10–Al2	70.79(10)	O1_13–C1_13–C3_13	107.8(5)
C6_10–C5_10–Al2	123.45(13)	C4_13–C1_13–C3_13	109.4(5)
C5_10–C6_10–H6A_10	109.5	C2_13–C1_13–C3_13	108.9(5)
C5_10–C6_10–H6B_10	109.5	F3_13–C2_13–F1_13	107.3(7)
H6A_10–C6_10–H6B_10	109.5	F3_13–C2_13–F2_13	107.0(7)
		F1_13–C2_13–F2_13	107.1(6)
C5_10–C6_10–H6C_10	109.5	F3_13–C2_13–C1_13	111.0(8)
H6A_10–C6_10–H6C_10	109.5	F1_13–C2_13–C1_13	111.4(6)
		F2_13–C2_13–C1_13	112.7(7)
H6B_10–C6_10–H6C_10	109.5	F4_13–C3_13–F5_13	107.8(3)
		F4_13–C3_13–F6_13	107.2(4)
C4_10–C7_10–H7A_10	109.5	F5_13–C3_13–F6_13	107.0(4)
C4_10–C7_10–H7B_10	109.5	F4_13–C3_13–C1_13	111.5(4)
H7A_10–C7_10–H7B_10	109.5	F5_13–C3_13–C1_13	111.0(4)
		F6_13–C3_13–C1_13	112.0(4)
C4_10–C7_10–H7C_10	109.5	F7_13–C4_13–F8_13	107.1(6)
H7A_10–C7_10–H7C_10	109.5	F7_13–C4_13–F9_13	107.6(5)
		F8_13–C4_13–F9_13	107.2(4)
H7B_10–C7_10–H7C_10	109.5	F7_13–C4_13–C1_13	111.7(6)
		F8_13–C4_13–C1_13	113.1(4)
C3_10–C8_10–H8A_10	109.5	F9_13–C4_13–C1_13	109.9(4)
C3_10–C8_10–H8B_10	109.5	C1_14–O1_14–Al5	148.5(5)
H8A_10–C8_10–H8B_10	109.5	O1_14–C1_14–C3_14	110.4(7)
		O1_14–C1_14–C2_14	107.5(6)
C3_10–C8_10–H8C_10	109.5	C3_14–C1_14–C2_14	110.1(8)
H8A_10–C8_10–H8C_10	109.5	O1_14–C1_14–C4_14	111.1(7)
		C3_14–C1_14–C4_14	109.9(7)
H8B_10–C8_10–H8C_10	109.5	C2_14–C1_14–C4_14	107.8(6)
		F3_14–C2_14–F1_14	107.7(7)
C2_10–C9_10–H9A_10	109.5	F3_14–C2_14–F2_14	107.7(6)
C2_10–C9_10–H9B_10	109.5	F1_14–C2_14–F2_14	107.8(7)
H9A_10–C9_10–H9B_10	109.5	F3_14–C2_14–C1_14	110.9(6)
		F1_14–C2_14–C1_14	110.3(9)
C2_10–C9_10–H9C_10	109.5	F2_14–C2_14–C1_14	112.3(6)
H9A_10–C9_10–H9C_10	109.5	F6_14–C3_14–F4_14	107.8(9)
		F6_14–C3_14–F5_14	108.1(8)
H9B_10–C9_10–H9C_10	109.5	F4_14–C3_14–F5_14	107.8(10)
		F6_14–C3_14–C1_14	112.5(8)
C1_10–C10_10–H10A_10	109.5	F4_14–C3_14–C1_14	110.3(10)
		F5_14–C3_14–C1_14	110.1(8)
C1_10–C10_10–H10B_10	109.5	F9_14–C4_14–F7_14	107.5(5)
		F9_14–C4_14–F8_14	107.2(4)
H10A_10–C10_10–H10B_10	109.5	F7_14–C4_14–F8_14	107.4(4)
		F9_14–C4_14–C1_14	111.6(5)
C1_10–C10_10–H10C_10	109.5	F7_14–C4_14–C1_14	110.9(5)
		F8_14–C4_14–C1_14	111.9(5)
H10A_10–C10_10–H10C_10	109.5	C1_15–O1_15–Al5	147.1(4)
		O1_15–C1_15–C4_15	110.4(5)
H10B_10–C10_10–H10C_10	109.5	O1_15–C1_15–C2_15	112.0(5)
		C4_15–C1_15–C2_15	108.7(5)
C1_13–O1_13–Al5	148.7(4)	O1_15–C1_15–C3_15	107.6(5)

C4_15–C1_15–C3_15	109.5(5)
C2_15–C1_15–C3_15	108.6(5)
F3_15–C2_15–F1_15	107.2(3)
F3_15–C2_15–F2_15	107.8(3)
F1_15–C2_15–F2_15	107.4(3)
F3_15–C2_15–C1_15	110.7(4)
F1_15–C2_15–C1_15	111.0(4)
F2_15–C2_15–C1_15	112.6(4)
F5_15–C3_15–F4_15	107.3(3)
F5_15–C3_15–F6_15	107.1(3)
F4_15–C3_15–F6_15	107.4(3)
F5_15–C3_15–C1_15	111.1(4)
F4_15–C3_15–C1_15	111.1(4)
F6_15–C3_15–C1_15	112.7(4)
F8_15–C4_15–F9_15	107.5(7)
F8_15–C4_15–F7_15	107.0(6)
F9_15–C4_15–F7_15	107.0(8)
F8_15–C4_15–C1_15	113.7(6)
F9_15–C4_15–C1_15	109.9(8)
F7_15–C4_15–C1_15	111.4(6)
C1_16–O1_16–Al5	148.6(5)
O1_16–C1_16–C4_16	111.0(8)
O1_16–C1_16–C2_16	108.2(7)
C4_16–C1_16–C2_16	109.2(7)
O1_16–C1_16–C3_16	110.5(7)
C4_16–C1_16–C3_16	109.0(7)
C2_16–C1_16–C3_16	108.9(7)
F2_16–C2_16–F1_16	107.7(5)
F2_16–C2_16–F3_16	107.9(5)
F1_16–C2_16–F3_16	107.6(5)
F2_16–C2_16–C1_16	112.4(6)
F1_16–C2_16–C1_16	110.7(5)
F3_16–C2_16–C1_16	110.4(6)
F6_16–C3_16–F4_16	108.8(6)
F6_16–C3_16–F5_16	108.3(5)
F4_16–C3_16–F5_16	108.1(5)
F6_16–C3_16–C1_16	112.5(6)
F4_16–C3_16–C1_16	109.2(5)
F5_16–C3_16–C1_16	109.9(6)
F7_16–C4_16–F9_16	108.1(11)
F7_16–C4_16–F8_16	107.8(8)
F9_16–C4_16–F8_16	106.7(9)
F7_16–C4_16–C1_16	111.3(8)
F9_16–C4_16–C1_16	110.7(11)
F8_16–C4_16–C1_16	112.1(9)
C1_17–O1_17–Al5	145.6(8)
O1_17–C1_17–C3_17	111.8(7)
O1_17–C1_17–C4_17	108.3(6)
C3_17–C1_17–C4_17	108.6(7)
O1_17–C1_17–C2_17	111.4(6)
C3_17–C1_17–C2_17	107.3(6)
C4_17–C1_17–C2_17	109.4(6)
F2_17–C2_17–F1_17	108.4(5)
F2_17–C2_17–F3_17	107.9(5)
F1_17–C2_17–F3_17	107.7(5)
F2_17–C2_17–C1_17	112.8(6)
F1_17–C2_17–C1_17	109.9(6)
F3_17–C2_17–C1_17	109.9(5)
F5_17–C3_17–F4_17	107.8(10)
F5_17–C3_17–F6_17	107.8(8)
F4_17–C3_17–F6_17	106.9(9)
F5_17–C3_17–C1_17	112.0(9)
F4_17–C3_17–C1_17	109.5(9)
F6_17–C3_17–C1_17	112.6(7)
F9_17–C4_17–F7_17	106.7(8)
F9_17–C4_17–F8_17	106.9(7)
F7_17–C4_17–F8_17	108.3(5)
F9_17–C4_17–C1_17	109.9(8)
F7_17–C4_17–C1_17	111.7(6)
F8_17–C4_17–C1_17	113.0(5)
C1_18–O1_18–Al5	145.6(10)
O1_18–C1_18–C2_18	109.5(8)
O1_18–C1_18–C4_18	110.8(9)
C2_18–C1_18–C4_18	109.7(8)
O1_18–C1_18–C3_18	107.1(8)
C2_18–C1_18–C3_18	108.4(7)
C4_18–C1_18–C3_18	111.3(8)
F1_18–C2_18–F3_18	108.2(9)
F1_18–C2_18–F2_18	108.0(7)
F3_18–C2_18–F2_18	107.2(9)
F1_18–C2_18–C1_18	109.8(7)
F3_18–C2_18–C1_18	112.2(11)
F2_18–C2_18–C1_18	111.4(7)
F5_18–C3_18–F6_18	108.6(6)
F5_18–C3_18–F4_18	107.7(6)
F6_18–C3_18–F4_18	107.4(6)
F5_18–C3_18–C1_18	111.2(7)
F6_18–C3_18–C1_18	111.3(6)
F4_18–C3_18–C1_18	110.5(6)
F9_18–C4_18–F8_18	107.7(12)
F9_18–C4_18–F7_18	107.5(14)
F8_18–C4_18–F7_18	106.8(10)
F9_18–C4_18–C1_18	112.0(12)
F8_18–C4_18–C1_18	112.0(10)
F7_18–C4_18–C1_18	110.7(11)
C2_19–C1_19–C5_19	108.3(4)
C2_19–C1_19–C10_19	127.1(4)
C5_19–C1_19–C10_19	124.6(4)
C2_19–C1_19–Al4	74.8(3)
C5_19–C1_19–Al4	72.4(2)
C10_19–C1_19–Al4	119.9(3)
C1_19–C2_19–C3_19	108.2(4)
C1_19–C2_19–C9_19	125.6(5)
C3_19–C2_19–C9_19	126.0(5)
C1_19–C2_19–Al4	70.3(3)
C3_19–C2_19–Al4	73.9(4)
C9_19–C2_19–Al4	125.3(5)
C2_19–C3_19–C4_19	107.8(4)

C2_19–C3_19–C8_19	125.2(5)
C4_19–C3_19–C8_19	127.0(5)
C2_19–C3_19–Al4	71.7(4)
C4_19–C3_19–Al4	70.9(4)
C8_19–C3_19–Al4	124.1(6)
C5_19–C4_19–C3_19	107.9(4)
C5_19–C4_19–C7_19	126.5(4)
C3_19–C4_19–C7_19	125.5(4)
C5_19–C4_19–Al4	70.9(2)
C3_19–C4_19–Al4	74.4(4)
C7_19–C4_19–Al4	123.2(3)
C1_19–C5_19–C4_19	107.9(3)
C1_19–C5_19–C6_19	125.3(4)
C4_19–C5_19–C6_19	126.9(4)
C1_19–C5_19–Al4	72.2(2)
C4_19–C5_19–Al4	73.8(2)
C6_19–C5_19–Al4	120.1(2)
C5_19–C6_19–H6A_19	109.5
C5_19–C6_19–H6B_19	109.5
H6A_19–C6_19–H6B_19	109.5
C5_19–C6_19–H6C_19	109.5
H6A_19–C6_19–H6C_19	109.5
H6B_19–C6_19–H6C_19	109.5
C4_19–C7_19–H7A_19	109.5
C4_19–C7_19–H7B_19	109.5
H7A_19–C7_19–H7B_19	109.5
C4_19–C7_19–H7C_19	109.5
H7A_19–C7_19–H7C_19	109.5
H7B_19–C7_19–H7C_19	109.5
C3_19–C8_19–H8A_19	109.5
C3_19–C8_19–H8B_19	109.5
H8A_19–C8_19–H8B_19	109.5
C3_19–C8_19–H8C_19	109.5
H8A_19–C8_19–H8C_19	109.5
H8B_19–C8_19–H8C_19	109.5
C2_19–C9_19–H9A_19	109.5
C2_19–C9_19–H9B_19	109.5
H9A_19–C9_19–H9B_19	109.5
C2_19–C9_19–H9C_19	109.5
H9A_19–C9_19–H9C_19	109.5
H9B_19–C9_19–H9C_19	109.5
C1_19–C10_19–H10A_19	109.5
C1_19–C10_19–H10B_19	109.5
H10A_19–C10_19–H10B_19	109.5
C1_19–C10_19–H10C_19	109.5
H10A_19–C10_19–H10C_19	109.5
H10B_19–C10_19–H10C_19	109.5
C5_20–C1_20–C2_20	107.1(7)
C5_20–C1_20–C10_20	126.6(8)
C2_20–C1_20–C10_20	126.1(8)
C3_20–C2_20–C1_20	109.1(6)
C3_20–C2_20–C9_20	126.7(8)
C1_20–C2_20–C9_20	124.1(8)
C3_20–C2_20–Al4	66.7(3)
C1_20–C2_20–Al4	78.3(4)
C9_20–C2_20–Al4	124.4(4)
C2_20–C3_20–C4_20	108.0(6)
C2_20–C3_20–C8_20	126.0(8)
C4_20–C3_20–C8_20	126.0(9)
C2_20–C3_20–Al4	79.1(4)
C4_20–C3_20–Al4	72.3(7)
C8_20–C3_20–Al4	114.7(4)
C3_20–C4_20–C5_20	107.1(8)
C3_20–C4_20–C7_20	127.9(9)
C5_20–C4_20–C7_20	125.0(8)
C3_20–C4_20–Al4	72.0(6)
C5_20–C4_20–Al4	77.8(8)
C7_20–C4_20–Al4	116.8(9)
C1_20–C5_20–C4_20	108.6(8)
C1_20–C5_20–C6_20	125.0(9)
C4_20–C5_20–C6_20	126.1(9)
C1_20–C5_20–Al4	79.0(8)
C4_20–C5_20–Al4	67.3(8)
C6_20–C5_20–Al4	124.4(12)
C5_20–C6_20–H6A_20	109.5
C5_20–C6_20–H6B_20	109.5
H6A_20–C6_20–H6B_20	109.5
C5_20–C6_20–H6C_20	109.5
H6A_20–C6_20–H6C_20	109.5
H6B_20–C6_20–H6C_20	109.5
C4_20–C7_20–H7A_20	109.5
C4_20–C7_20–H7B_20	109.5
H7A_20–C7_20–H7B_20	109.5
C4_20–C7_20–H7C_20	109.5

H7A_20–C7_20–H7C_20	109.5
H7B_20–C7_20–H7C_20	109.5
C3_20–C8_20–H8A_20	109.5
C3_20–C8_20–H8B_20	109.5
H8A_20–C8_20–H8B_20	109.5
C3_20–C8_20–H8C_20	109.5
H8A_20–C8_20–H8C_20	109.5
H8B_20–C8_20–H8C_20	109.5
C2_20–C9_20–H9A_20	109.5
C2_20–C9_20–H9B_20	109.5
H9A_20–C9_20–H9B_20	109.5
C2_20–C9_20–H9C_20	109.5
H9A_20–C9_20–H9C_20	109.5
H9B_20–C9_20–H9C_20	109.5
C1_20–C10_20–H10A_20	109.5
C1_20–C10_20–H10B_20	109.5
H10A_20–C10_20–H10B_20	109.5
C1_20–C10_20–H10C_20	109.5
H10A_20–C10_20–H10C_20	109.5
H10B_20–C10_20–H10C_20	109.5
C5_21–C1_21–C2_21	108.3(5)
C5_21–C1_21–C10_21	124.6(5)
C2_21–C1_21–C10_21	127.0(5)
C5_21–C1_21–Al3	73.8(5)
C2_21–C1_21–Al3	75.2(4)
C10_21–C1_21–Al3	120.9(4)
C3_21–C2_21–C1_21	108.4(6)
C3_21–C2_21–C9_21	127.5(6)
C1_21–C2_21–C9_21	124.0(5)
C3_21–C2_21–Al3	75.5(4)
C1_21–C2_21–Al3	70.2(3)
C9_21–C2_21–Al3	122.4(6)
C2_21–C3_21–C4_21	107.7(6)
C2_21–C3_21–C8_21	125.4(7)
C4_21–C3_21–C8_21	126.7(7)
C2_21–C3_21–Al3	71.0(4)
C4_21–C3_21–Al3	71.6(7)
C8_21–C3_21–Al3	126.8(7)
C3_21–C4_21–C5_21	108.5(6)
C3_21–C4_21–C7_21	123.8(7)
C5_21–C4_21–C7_21	127.5(7)
C3_21–C4_21–Al3	74.8(7)
C5_21–C4_21–Al3	70.8(7)
C7_21–C4_21–Al3	124.1(11)
C1_21–C5_21–C4_21	107.2(5)
C1_21–C5_21–C6_21	127.0(5)
C4_21–C5_21–C6_21	125.8(6)
C1_21–C5_21–Al3	71.4(5)
C4_21–C5_21–Al3	74.8(8)
C6_21–C5_21–Al3	120.0(6)
C5_21–C6_21–H6A_21	109.5
C5_21–C6_21–H6B_21	109.5
H6A_21–C6_21–H6B_21	109.5
C5_21–C6_21–H6C_21	109.5
H6A_21–C6_21–H6C_21	109.5
H6B_21–C6_21–H6C_21	109.5
C4_21–C7_21–H7A_21	109.5
C4_21–C7_21–H7B_21	109.5
H7A_21–C7_21–H7B_21	109.5
C4_21–C7_21–H7C_21	109.5
H7A_21–C7_21–H7C_21	109.5
H7B_21–C7_21–H7C_21	109.5
C3_21–C8_21–H8A_21	109.5
C3_21–C8_21–H8B_21	109.5
H8A_21–C8_21–H8B_21	109.5
C3_21–C8_21–H8C_21	109.5
H8A_21–C8_21–H8C_21	109.5
H8B_21–C8_21–H8C_21	109.5
C2_21–C9_21–H9A_21	109.5
C2_21–C9_21–H9B_21	109.5
H9A_21–C9_21–H9B_21	109.5
C2_21–C9_21–H9C_21	109.5
H9A_21–C9_21–H9C_21	109.5
H9B_21–C9_21–H9C_21	109.5
C1_21–C10_21–H10A_21	109.5
C1_21–C10_21–H10B_21	109.5
H10A_21–C10_21–H10B_21	109.5
C1_21–C10_21–H10C_21	109.5

H10A_21–C10_21–H10C_21	109.5
H10B_21–C10_21–H10C_21	109.5
C5_22–C1_22–C2_22	108.2(8)
C5_22–C1_22–C10_22	125.6(8)
C2_22–C1_22–C10_22	126.2(8)
C5_22–C1_22–Al3	74.7(8)
C2_22–C1_22–Al3	71.9(5)
C10_22–C1_22–Al3	120.6(8)
C1_22–C2_22–C3_22	107.8(8)
C1_22–C2_22–C9_22	125.5(8)
C3_22–C2_22–C9_22	126.7(9)
C1_22–C2_22–Al3	72.1(5)
C3_22–C2_22–Al3	75.0(6)
C9_22–C2_22–Al3	120.7(8)
C4_22–C3_22–C2_22	108.0(9)
C4_22–C3_22–C8_22	126.1(10)
C2_22–C3_22–C8_22	125.9(10)
C4_22–C3_22–Al3	74.2(12)
C2_22–C3_22–Al3	69.6(5)
C8_22–C3_22–Al3	123.1(11)
C5_22–C4_22–C3_22	107.7(9)
C5_22–C4_22–C7_22	123.0(11)
C3_22–C4_22–C7_22	129.2(12)
C5_22–C4_22–Al3	70.7(12)
C3_22–C4_22–Al3	71.2(11)
C7_22–C4_22–Al3	125.5(18)
C1_22–C5_22–C4_22	108.4(8)
C1_22–C5_22–C6_22	125.4(9)
C4_22–C5_22–C6_22	126.1(9)
C1_22–C5_22–Al3	70.2(7)
C4_22–C5_22–Al3	74.6(13)
C6_22–C5_22–Al3	123.1(11)
C5_22–C6_22–H6A_22	109.5
C5_22–C6_22–H6B_22	109.5
H6A_22–C6_22–H6B_22	109.5
C5_22–C6_22–H6C_22	109.5
H6A_22–C6_22–H6C_22	109.5
H6B_22–C6_22–H6C_22	109.5
C4_22–C7_22–H7A_22	109.5
C4_22–C7_22–H7B_22	109.5
H7A_22–C7_22–H7B_22	109.5
C4_22–C7_22–H7C_22	109.5
H7A_22–C7_22–H7C_22	109.5
H7B_22–C7_22–H7C_22	109.5
C3_22–C8_22–H8A_22	109.5
C3_22–C8_22–H8B_22	109.5
H8A_22–C8_22–H8B_22	109.5
C3_22–C8_22–H8C_22	109.5
H8A_22–C8_22–H8C_22	109.5
H8B_22–C8_22–H8C_22	109.5
C2_22–C9_22–H9A_22	109.5
C2_22–C9_22–H9B_22	109.5
H9A_22–C9_22–H9B_22	109.5
C2_22–C9_22–H9C_22	109.5
H9A_22–C9_22–H9C_22	109.5
H9B_22–C9_22–H9C_22	109.5
C1_22–C10_22–H10A_22	109.5
C1_22–C10_22–H10B_22	109.5
H10A_22–C10_22–H10B_22	109.5
C1_22–C10_22–H10C_22	109.5
H10A_22–C10_22–H10C_22	109.5
H10B_22–C10_22–H10C_22	109.5
F1_24–C1_24–C6_24	122.8(12)
F1_24–C1_24–C2_24	115.4(12)
C6_24–C1_24–C2_24	121.6(11)
C3_24–C2_24–F2_24	125.7(13)
C3_24–C2_24–C1_24	119.0(12)
F2_24–C2_24–C1_24	115.2(10)
C2_24–C3_24–C4_24	120.1(14)
C2_24–C3_24–H3_24	119.9
C4_24–C3_24–H3_24	119.9
C5_24–C4_24–C3_24	119.5(15)
C5_24–C4_24–H4_24	120.2
C3_24–C4_24–H4_24	120.2
C6_24–C5_24–C4_24	120.3(14)
C6_24–C5_24–H5_24	119.8
C4_24–C5_24–H5_24	119.8
C1_24–C6_24–C5_24	119.3(13)
C1_24–C6_24–H6_24	120.3
C5_24–C6_24–H6_24	120.3
C1_25–O1_25–Al5	149.4(2)
O1_25–C1_25–C3_25	110.6(2)
O1_25–C1_25–C2_25	110.7(3)
C3_25–C1_25–C2_25	109.5(2)
O1_25–C1_25–C4_25	107.2(2)
C3_25–C1_25–C4_25	109.7(2)
C2_25–C1_25–C4_25	109.1(2)
F3_25–C2_25–F1_25	106.5(3)

F3_25–C2_25–F2_25	109.2(3)	F4_26–C3_26–F6_26	105.5(13)
F1_25–C2_25–F2_25	106.9(3)	F4_26–C3_26–F5_26	104.3(14)
F3_25–C2_25–C1_25	110.5(3)	F6_26–C3_26–F5_26	108.7(14)
F1_25–C2_25–C1_25	111.3(3)	F4_26–C3_26–C1_26	113.7(11)
F2_25–C2_25–C1_25	112.2(3)	F6_26–C3_26–C1_26	112.2(12)
F4_25–C3_25–F5_25	107.1(3)	F5_26–C3_26–C1_26	111.9(11)
F4_25–C3_25–F6_25	106.6(3)	F9_26–C4_26–F8_26	109.5(16)
F5_25–C3_25–F6_25	107.0(3)	F9_26–C4_26–F7_26	100.5(16)
F4_25–C3_25–C1_25	111.7(3)	F8_26–C4_26–F7_26	107.2(15)
F5_25–C3_25–C1_25	112.2(2)	F9_26–C4_26–C1_26	116.5(15)
F6_25–C3_25–C1_25	112.0(3)	F8_26–C4_26–C1_26	110.5(13)
F9_25–C4_25–F8_25	108.9(3)	F7_26–C4_26–C1_26	111.8(13)
F9_25–C4_25–F7_25	106.2(3)	F1_23–C1_23–C6_23	119.0(9)
F8_25–C4_25–F7_25	106.8(3)	F1_23–C1_23–C2_23	120.3(8)
F9_25–C4_25–C1_25	111.3(3)	C6_23–C1_23–C2_23	120.6(8)
F8_25–C4_25–C1_25	113.1(3)	C3_23–C2_23–F2_23	122.1(8)
F7_25–C4_25–C1_25	110.3(2)	C3_23–C2_23–C1_23	119.9(8)
C1_26–O1_26–Al5	142.8(15)	F2_23–C2_23–C1_23	118.0(8)
O1_26–C1_26–C4_26	108.4(13)	C2_23–C3_23–C4_23	121.2(9)
O1_26–C1_26–C2_26	116.1(12)	C2_23–C3_23–H3_23	119.4
C4_26–C1_26–C2_26	108.6(11)	C4_23–C3_23–H3_23	119.4
O1_26–C1_26–C3_26	108.3(11)	C3_23–C4_23–C5_23	120.0(10)
C4_26–C1_26–C3_26	109.1(11)	C3_23–C4_23–H4_23	120.0
C2_26–C1_26–C3_26	106.1(10)	C5_23–C4_23–H4_23	120.0
F1_26–C2_26–F3_26	105.7(15)	C4_23–C5_23–C6_23	119.9(10)
F1_26–C2_26–F2_26	108.3(14)	C4_23–C5_23–H5_23	120.0
F3_26–C2_26–F2_26	108.0(15)	C6_23–C5_23–H5_23	120.0
F1_26–C2_26–C1_26	113.1(11)	C1_23–C6_23–C5_23	118.3(10)
F3_26–C2_26–C1_26	109.5(13)	C1_23–C6_23–H6_23	120.8
F2_26–C2_26–C1_26	112.0(14)	C5_23–C6_23–H6_23	120.8

S-Table 28: Atomic coordinates and U_{eq} [Å^2] for [Cp*{Al(AlCp*)$_3$}$_2$]$^+$[*pf*]$^-$

Atom	***x***	***y***	***z***	U_{eq}
Al1	0.60537(2)	0.63744(2)	0.66735(3)	0.02182(18)
Al3	0.60594(2)	0.61093(3)	0.57308(3)	0.02552(19)
Al4	0.60633(2)	0.69258(3)	0.59669(3)	0.0272(2)
Al5	0.64402(2)	0.61449(2)	0.83169(3)	0.02057(17)
Al6	0.69715(2)	0.60665(3)	0.89511(3)	0.02189(18)
Al7	0.64239(2)	0.63861(2)	0.92695(3)	0.02053(17)
Al8	0.64489(2)	0.55737(2)	0.90021(3)	0.02435(19)
Al9	0.64552(2)	0.88867(2)	0.33213(3)	0.02200(18)
Al10	0.64452(2)	0.94395(3)	0.40260(4)	0.0277(2)
Al11	0.69868(2)	0.89941(3)	0.39473(3)	0.02230(18)
Al12	0.64558(2)	0.86242(3)	0.42677(3)	0.02593(19)
Al13	0.60463(2)	0.86400(2)	0.16827(3)	0.02133(18)
Al14	0.60624(2)	0.88643(3)	0.07240(3)	0.02354(18)
Al15	0.55157(2)	0.85456(3)	0.10466(3)	0.02333(18)
Al16	0.60431(2)	0.80579(3)	0.10150(3)	0.02494(19)
Al17	0.74919(2)	0.63061(2)	0.25207(3)	0.01956(19)
Al2	0.55240(2)	0.64737(3)	0.60461(3)	0.02391(19)
C1_3	0.59712(11)	0.55914(18)	0.5215(2)	0.0330(13)
C2_3	0.61367(17)	0.5473(2)	0.5683(3)	0.0354(16)
C3_3	0.64383(17)	0.5647(2)	0.5735(3)	0.0352(18)

C4_3	0.64554(12)	0.58734(17)	0.5299(2)	0.0314(12)
C5_3	0.61707(14)	0.58454(15)	0.49781(16)	0.0305(11)
C6_3	0.6090(2)	0.60100(19)	0.44618(17)	0.068(3)
H6A_3	0.604891	0.579448	0.421887	0.102
H6B_3	0.626428	0.616948	0.437567	0.102
H6C_3	0.590198	0.617439	0.445102	0.102
C7_3	0.67477(16)	0.6085(2)	0.5188(4)	0.078(3)
H7A_3	0.690949	0.589235	0.513763	0.117
H7B_3	0.682409	0.625634	0.547298	0.117
H7C_3	0.669869	0.624454	0.488268	0.117
C8_3	0.6706(2)	0.5602(4)	0.6151(4)	0.073(4)
H8A_3	0.690024	0.555902	0.600539	0.110
H8B_3	0.666683	0.537589	0.636147	0.110
H8C_3	0.672534	0.584039	0.635774	0.110
C9_3	0.6036(3)	0.5204(3)	0.6075(4)	0.071(3)
H9A_3	0.583369	0.508553	0.594627	0.106
H9B_3	0.601527	0.535483	0.638075	0.106
H9C_3	0.619260	0.499691	0.615299	0.106
C10_3	0.56578(12)	0.5456(2)	0.4977(3)	0.076(3)
H10A_3	0.568292	0.527541	0.469965	0.114
H10B_3	0.553295	0.568321	0.484545	0.114
H10C_3	0.555113	0.532011	0.522857	0.114
C1_4	0.6487(2)	0.7208(3)	0.5656(3)	0.0360(17)
C2_4	0.6231(2)	0.7216(4)	0.5271(4)	0.0318(17)
C3_4	0.5995(3)	0.7449(4)	0.5441(4)	0.0349(19)
C4_4	0.6103(2)	0.7577(3)	0.5938(4)	0.0359(17)
C5_4	0.6411(2)	0.7427(3)	0.6077(3)	0.0374(17)
C6_4	0.6624(3)	0.7516(4)	0.6549(3)	0.071(3)
H6A_4	0.676789	0.729455	0.663022	0.107
H6B_4	0.650014	0.755648	0.682646	0.107
H6C_4	0.674452	0.775378	0.650091	0.107
C7_4	0.5928(3)	0.7841(3)	0.6249(5)	0.060(3)
H7A_4	0.574484	0.794895	0.603865	0.089
H7B_4	0.606540	0.805590	0.638555	0.089
H7C_4	0.586037	0.769028	0.652770	0.089
C8_4	0.5697(3)	0.7546(4)	0.5117(5)	0.044(3)
H8A_4	0.574291	0.767728	0.480963	0.066
H8B_4	0.557113	0.772085	0.530168	0.066
H8C_4	0.557932	0.730361	0.502743	0.066
C9_4	0.6213(3)	0.7025(4)	0.4760(4)	0.040(2)
H9A_4	0.615068	0.722117	0.449756	0.059
H9B_4	0.605698	0.681338	0.473557	0.059
H9C_4	0.641758	0.691616	0.471555	0.059
C10_4	0.6802(2)	0.7016(4)	0.5654(5)	0.058(3)
H10A_4	0.680983	0.688643	0.532902	0.088
H10B_4	0.683566	0.682115	0.592551	0.088
H10C_4	0.696688	0.721680	0.570685	0.088
C1_2	0.5075(3)	0.6586(4)	0.5478(4)	0.032(2)
C2_2	0.5053(3)	0.6216(4)	0.5708(4)	0.033(2)
C3_2	0.5048(4)	0.6273(4)	0.6235(5)	0.032(2)
C4_2	0.5071(7)	0.6682(4)	0.6327(5)	0.028(2)
C5_2	0.5085(4)	0.6877(3)	0.5859(4)	0.0281(19)
C6_2	0.5074(4)	0.7315(4)	0.5789(6)	0.047(3)
H6A_2	0.516374	0.738396	0.548295	0.071

H6B_2	0.519422	0.744179	0.608113	0.071
H6C_2	0.485568	0.740366	0.575685	0.071
C7_2	0.5070(4)	0.6896(6)	0.6819(5)	0.038(3)
H7A_2	0.527271	0.702463	0.691326	0.057
H7B_2	0.503173	0.670875	0.708210	0.057
H7C_2	0.490367	0.709523	0.678171	0.057
C8_2	0.5025(5)	0.5950(5)	0.6616(6)	0.044(3)
H8A_2	0.483196	0.580079	0.652252	0.066
H8B_2	0.502392	0.606627	0.695083	0.066
H8C_2	0.520594	0.577439	0.662139	0.066
C9_2	0.5007(3)	0.5822(4)	0.5452(7)	0.064(4)
H9A_2	0.478207	0.576980	0.536657	0.096
H9B_2	0.510136	0.561608	0.567949	0.096
H9C_2	0.510617	0.582264	0.514313	0.096
C10_2	0.5076(3)	0.6642(6)	0.4920(4)	0.051(3)
H10A_2	0.486587	0.659384	0.474299	0.076
H10B_2	0.522438	0.645773	0.479957	0.076
H10C_2	0.513964	0.691235	0.485474	0.076
C1_6	0.74446(6)	0.62898(10)	0.87342(12)	0.0318(7)
C2_6	0.74323(6)	0.58741(9)	0.86853(11)	0.0280(6)
C3_6	0.74157(7)	0.57147(9)	0.91679(11)	0.0294(6)
C4_6	0.74155(7)	0.60290(10)	0.95199(11)	0.0306(7)
C5_6	0.74335(7)	0.63856(9)	0.92501(12)	0.0329(7)
C6_6	0.74664(9)	0.67932(12)	0.94641(18)	0.0573(11)
H6A_6	0.767651	0.689346	0.943538	0.086
H6B_6	0.743450	0.678720	0.981994	0.086
H6C_6	0.730958	0.696530	0.927674	0.086
C7_6	0.74157(8)	0.59833(14)	1.00772(12)	0.0480(10)
H7A_6	0.730209	0.574345	1.014391	0.072
H7B_6	0.731310	0.621114	1.020833	0.072
H7C_6	0.763200	0.596541	1.024363	0.072
C8_6	0.74237(9)	0.52858(11)	0.92920(15)	0.0451(9)
H8A_6	0.730858	0.513877	0.901148	0.068
H8B_6	0.732613	0.524221	0.959811	0.068
H8C_6	0.764146	0.519530	0.934781	0.068
C9_6	0.74443(8)	0.56367(12)	0.82150(13)	0.0445(9)
H9A_6	0.738740	0.580374	0.791860	0.067
H9B_6	0.729668	0.541694	0.820737	0.067
H9C_6	0.765674	0.553443	0.821223	0.067
C10_6	0.74756(8)	0.65850(12)	0.83262(15)	0.0490(10)
H10A_6	0.745498	0.645148	0.799890	0.074
H10B_6	0.768109	0.671217	0.839028	0.074
H10C_6	0.731080	0.678389	0.832335	0.074
C1_7	0.6523(2)	0.6849(3)	0.9893(3)	0.0253(14)
C2_7	0.6432(2)	0.7031(3)	0.9418(3)	0.0293(16)
C3_7	0.6119(2)	0.6914(3)	0.9248(3)	0.0296(18)
C4_7	0.6020(2)	0.6655(4)	0.9607(4)	0.0277(17)
C5_7	0.6269(2)	0.6618(4)	1.0006(4)	0.0249(16)
C6_7	0.6273(3)	0.6419(4)	1.0510(3)	0.043(2)
H6A_7	0.607803	0.627222	1.051503	0.065
H6B_7	0.629276	0.661819	1.077728	0.065
H6C_7	0.645135	0.623844	1.056504	0.065
C7_7	0.5697(2)	0.6482(4)	0.9601(5)	0.050(3)
H7A_7	0.555453	0.668360	0.969816	0.076

H7B_7	0.570665	0.626222	0.983919	0.076
H7C_7	0.562147	0.638709	0.926051	0.076
C8_7	0.5911(3)	0.7052(3)	0.8784(3)	0.054(3)
H8A_7	0.600334	0.697358	0.848346	0.082
H8B_7	0.589211	0.733865	0.879260	0.082
H8C_7	0.570362	0.693242	0.877466	0.082
C9_7	0.6616(3)	0.7302(2)	0.9123(4)	0.052(3)
H9A_7	0.667830	0.716106	0.883242	0.078
H9B_7	0.680410	0.739240	0.933991	0.078
H9C_7	0.648692	0.752902	0.900506	0.078
C10_7	0.68253(18)	0.6906(3)	1.0234(4)	0.045(2)
H10A_7	0.692447	0.665046	1.031205	0.068
H10B_7	0.678354	0.703351	1.054650	0.068
H10C_7	0.696550	0.707251	1.006480	0.068
C1_8	0.6506(3)	0.4885(4)	0.9125(5)	0.028(2)
C2_8	0.6478(2)	0.5079(4)	0.9587(4)	0.0272(18)
C3_8	0.6174(2)	0.5255(3)	0.9540(4)	0.0298(17)
C4_8	0.6023(2)	0.5173(3)	0.9043(4)	0.0309(17)
C5_8	0.6227(3)	0.4949(5)	0.8788(4)	0.0307(17)
C6_8	0.6164(4)	0.4766(5)	0.8274(5)	0.045(3)
H6A_8	0.594748	0.482065	0.812753	0.068
H6B_8	0.619549	0.448102	0.830145	0.068
H6C_8	0.630776	0.487672	0.805608	0.068
C7_8	0.5697(2)	0.5307(4)	0.8845(5)	0.047(3)
H7A_8	0.563439	0.519412	0.850983	0.071
H7B_8	0.569201	0.559448	0.882250	0.071
H7C_8	0.555101	0.521923	0.907433	0.071
C8_8	0.6047(3)	0.5479(3)	0.9951(4)	0.044(2)
H8A_8	0.598906	0.574536	0.983209	0.065
H8B_8	0.620670	0.549460	1.024667	0.065
H8C_8	0.586112	0.534449	1.004204	0.065
C9_8	0.6718(3)	0.5089(5)	1.0049(5)	0.033(2)
H9A_8	0.688616	0.490252	1.000892	0.050
H9B_8	0.661910	0.501768	1.034513	0.050
H9C_8	0.680564	0.535500	1.009311	0.050
C10_8	0.6769(3)	0.4624(6)	0.9000(7)	0.044(3)
H10A_8	0.669489	0.435192	0.896229	0.066
H10B_8	0.694468	0.463858	0.927253	0.066
H10C_8	0.683814	0.471242	0.868400	0.066
C1_1	0.64992(9)	0.63433(14)	0.74329(14)	0.0291(8)
C2_1	0.63844(10)	0.59521(12)	0.74282(14)	0.0287(8)
C3_1	0.60691(9)	0.59657(11)	0.75173(13)	0.0259(7)
C4_1	0.59871(8)	0.63648(11)	0.75856(14)	0.0232(7)
C5_1	0.62535(10)	0.66019(11)	0.75326(17)	0.0248(8)
C6_1	0.62749(13)	0.70394(12)	0.75800(16)	0.0457(11)
H6A_1	0.643346	0.713775	0.738033	0.069
H6B_1	0.633398	0.711064	0.793477	0.069
H6C_1	0.607145	0.715652	0.745580	0.069
C7_1	0.56694(9)	0.65014(14)	0.76887(16)	0.0373(10)
H7A_1	0.566104	0.678921	0.767699	0.056
H7B_1	0.563221	0.641088	0.802338	0.056
H7C_1	0.550823	0.639317	0.743283	0.056
C8_1	0.58506(11)	0.56232(12)	0.75282(17)	0.0426(11)
H8A_1	0.567885	0.564713	0.725051	0.064

H8B_1	0.576532	0.562069	0.785007	0.064
H8C_1	0.596498	0.537817	0.749128	0.064
C9_1	0.65704(12)	0.55851(14)	0.73702(16)	0.0494(13)
H9A_1	0.646843	0.543148	0.708472	0.074
H9B_1	0.658172	0.542799	0.767912	0.074
H9C_1	0.678249	0.565649	0.730886	0.074
C10_1	0.68185(10)	0.64700(17)	0.73321(17)	0.0476(12)
H10A_1	0.682554	0.647391	0.696748	0.071
H10B_1	0.697552	0.628509	0.749234	0.071
H10C_1	0.686296	0.673380	0.747051	0.071
C1_10	0.64284(13)	1.01086(14)	0.4037(2)	0.0442(10)
C2_10	0.61162(13)	0.99682(16)	0.39165(18)	0.0427(10)
C3_10	0.60386(10)	0.97499(13)	0.43305(17)	0.0354(9)
C4_10	0.63015(10)	0.97529(12)	0.47108(15)	0.0329(8)
C5_10	0.65404(11)	0.99735(16)	0.4528(2)	0.0392(10)
C6_10	0.68421(13)	1.0070(2)	0.4846(3)	0.076(2)
H6A_10	0.695468	0.982604	0.494681	0.114
H6B_10	0.679952	1.021284	0.514732	0.114
H6C_10	0.697037	1.023343	0.465206	0.114
C7_10	0.63238(16)	0.95577(15)	0.52185(17)	0.0594(16)
H7A_10	0.611623	0.946424	0.527534	0.089
H7B_10	0.640145	0.974718	0.548165	0.089
H7C_10	0.646836	0.933449	0.522938	0.089
C8_10	0.57264(12)	0.95626(18)	0.4354(3)	0.0663(17)
H8A_10	0.556120	0.972828	0.417655	0.100
H8B_10	0.569244	0.953381	0.470738	0.100
H8C_10	0.572124	0.930310	0.419424	0.100
C9_10	0.58972(16)	1.0060(2)	0.3448(2)	0.078(2)
H9A_10	0.601782	1.014715	0.318284	0.116
H9B_10	0.575320	1.026964	0.352019	0.116
H9C_10	0.577723	0.982437	0.333611	0.116
C10_10	0.66022(18)	1.03610(17)	0.3711(3)	0.080(2)
H10A_10	0.661825	1.022441	0.339298	0.121
H10B_10	0.681266	1.041475	0.388502	0.121
H10C_10	0.648959	1.060946	0.364105	0.121
C1_11	0.7455(3)	0.9139(3)	0.3653(3)	0.0330(19)
C2_11	0.7439(2)	0.9379(2)	0.4081(3)	0.0304(15)
C3_11	0.7436(2)	0.91275(18)	0.4503(2)	0.0256(12)
C4_11	0.7452(2)	0.87321(18)	0.4332(2)	0.0259(12)
C5_11	0.7463(2)	0.8737(2)	0.3808(3)	0.0310(15)
C6_11	0.74751(18)	0.8389(2)	0.3462(3)	0.047(2)
H6A_11	0.748124	0.848124	0.311671	0.070
H6B_11	0.766319	0.823334	0.357287	0.070
H6C_11	0.728872	0.822525	0.347236	0.070
C7_11	0.74813(14)	0.8380(2)	0.4667(3)	0.0446(17)
H7A_11	0.743724	0.814246	0.446303	0.067
H7B_11	0.733171	0.840035	0.491156	0.067
H7C_11	0.769465	0.836642	0.484652	0.067
C8_11	0.74348(18)	0.9231(2)	0.5047(2)	0.0417(17)
H8A_11	0.745819	0.951619	0.508995	0.062
H8B_11	0.760880	0.909770	0.525205	0.062
H8C_11	0.723632	0.914740	0.515436	0.062
C9_11	0.7457(2)	0.98213(19)	0.4096(4)	0.055(2)
H9A_11	0.766812	0.990537	0.404453	0.083

H9B_11	0.741079	0.991521	0.442422	0.083
H9C_11	0.730411	0.993086	0.382833	0.083
C10_11	0.74826(19)	0.9291(3)	0.3135(3)	0.049(2)
H10A_11	0.744846	0.907542	0.289084	0.073
H10B_11	0.769228	0.940129	0.312912	0.073
H10C_11	0.732526	0.949625	0.304566	0.073
C1_12	0.60572(15)	0.8207(2)	0.4343(2)	0.0340(11)
C2_12	0.61505(14)	0.83828(17)	0.4822(2)	0.0362(11)
C3_12	0.64687(13)	0.82544(14)	0.49881(17)	0.0291(10)
C4_12	0.65499(11)	0.80014(14)	0.46052(19)	0.0280(9)
C5_12	0.62997(13)	0.7974(2)	0.4209(2)	0.0318(10)
C6_12	0.63112(17)	0.77292(18)	0.3746(2)	0.0473(15)
H6A_12	0.609749	0.767576	0.358534	0.071
H6B_12	0.641781	0.748038	0.384000	0.071
H6C_12	0.642576	0.787156	0.350966	0.071
C7_12	0.68498(12)	0.77649(16)	0.4623(3)	0.0502(15)
H7A_12	0.680025	0.748370	0.462101	0.075
H7B_12	0.698983	0.782977	0.493098	0.075
H7C_12	0.695301	0.782849	0.432782	0.075
C8_12	0.66604(18)	0.83406(19)	0.5475(2)	0.0590(18)
H8A_12	0.688232	0.834432	0.542860	0.089
H8B_12	0.662530	0.813722	0.572032	0.089
H8C_12	0.660102	0.859751	0.559776	0.089
C9_12	0.59482(18)	0.86111(17)	0.5119(3)	0.0600(17)
H9A_12	0.581655	0.879012	0.489522	0.090
H9B_12	0.607886	0.876358	0.537716	0.090
H9C_12	0.581485	0.843114	0.528146	0.090
C10_12	0.57442(13)	0.8264(2)	0.4016(3)	0.0495(16)
H10A_12	0.576768	0.845521	0.374964	0.074
H10B_12	0.559010	0.836195	0.422494	0.074
H10C_12	0.567272	0.801266	0.386421	0.074
C1_14	0.62425(9)	0.90721(12)	-0.00182(15)	0.0248(8)
C2_14	0.64851(8)	0.91257(11)	0.03877(15)	0.0240(8)
C3_14	0.63801(12)	0.93935(14)	0.07351(17)	0.0286(10)
C4_14	0.60687(12)	0.95051(14)	0.05404(19)	0.0325(10)
C5_14	0.59838(11)	0.93049(16)	0.0081(2)	0.0305(11)
C6_14	0.56933(11)	0.93565(18)	-0.0285(2)	0.0533(15)
H6A_14	0.574740	0.947179	-0.059783	0.080
H6B_14	0.554839	0.953132	-0.013917	0.080
H6C_14	0.559357	0.910026	-0.035801	0.080
C7_14	0.58742(15)	0.97817(14)	0.0806(2)	0.0654(19)
H7A_14	0.570817	0.989419	0.056200	0.098
H7B_14	0.600716	0.999340	0.096375	0.098
H7C_14	0.578019	0.963832	0.106602	0.098
C8_14	0.65722(15)	0.95363(15)	0.12044(17)	0.0570(16)
H8A_14	0.679496	0.951124	0.116984	0.085
H8B_14	0.652524	0.937878	0.149182	0.085
H8C_14	0.652273	0.981270	0.126024	0.085
C9_14	0.68066(9)	0.89407(15)	0.0439(2)	0.0484(13)
H9A_14	0.680966	0.873367	0.018453	0.073
H9B_14	0.685635	0.882676	0.077612	0.073
H9C_14	0.696238	0.914174	0.038796	0.073
C10_14	0.62544(13)	0.88469(15)	-0.04957(16)	0.0475(13)
H10A_14	0.623855	0.902972	-0.078103	0.071

H10B_14	0.607963	0.866041	-0.054487	0.071
H10C_14	0.645280	0.870305	-0.047386	0.071
C1_15	0.50503(7)	0.88094(10)	0.12249(12)	0.0318(6)
C2_15	0.50599(7)	0.88529(11)	0.06987(13)	0.0409(7)
C3_15	0.50673(7)	0.84753(13)	0.04841(12)	0.0449(8)
C4_15	0.50621(7)	0.81974(11)	0.08739(13)	0.0382(7)
C5_15	0.50524(7)	0.84021(10)	0.13342(11)	0.0299(6)
C6_15	0.50336(8)	0.82131(14)	0.18320(14)	0.0534(11)
H6A_15	0.481759	0.813033	0.185040	0.080
H6B_15	0.509918	0.840152	0.210263	0.080
H6C_15	0.517181	0.798319	0.187029	0.080
C7_15	0.50433(10)	0.77610(13)	0.0814(2)	0.0754(15)
H7A_15	0.482316	0.768073	0.074834	0.113
H7B_15	0.514294	0.763454	0.112299	0.113
H7C_15	0.515137	0.768151	0.052974	0.113
C8_15	0.50667(10)	0.8392(2)	-0.00684(14)	0.0799(18)
H8A_15	0.485217	0.841027	-0.024242	0.120
H8B_15	0.514812	0.812672	-0.011089	0.120
H8C_15	0.519923	0.858438	-0.021186	0.120
C9_15	0.50435(10)	0.92372(16)	0.0421(2)	0.0858(19)
H9A_15	0.513829	0.920747	0.010953	0.129
H9B_15	0.515744	0.943848	0.063382	0.129
H9C_15	0.482410	0.931663	0.033741	0.129
C10_15	0.50334(9)	0.91426(12)	0.15876(17)	0.0542(11)
H10A_15	0.521672	0.931267	0.158506	0.081
H10B_15	0.502991	0.903751	0.192790	0.081
H10C_15	0.484240	0.929520	0.148673	0.081
C1_16	0.63161(12)	0.77389(13)	0.04959(17)	0.0334(10)
C2_16	0.64561(10)	0.76443(14)	0.09902(18)	0.0324(10)
C3_16	0.62373(10)	0.74294(11)	0.12292(16)	0.0334(9)
C4_16	0.59579(10)	0.73915(12)	0.08835(17)	0.0314(9)
C5_16	0.60030(12)	0.75807(14)	0.04308(17)	0.0336(10)
C6_16	0.57714(12)	0.76085(15)	-0.00349(17)	0.0492(13)
H6A_16	0.586215	0.749601	-0.031996	0.074
H6B_16	0.571832	0.788500	-0.010478	0.074
H6C_16	0.558156	0.746283	0.001434	0.074
C7_16	0.56876(11)	0.71414(13)	0.1001(2)	0.0495(12)
H7A_16	0.552156	0.714430	0.071262	0.074
H7B_16	0.560607	0.724648	0.129879	0.074
H7C_16	0.575956	0.687081	0.106773	0.074
C8_16	0.62915(13)	0.72491(13)	0.17494(17)	0.0491(12)
H8A_16	0.623004	0.697161	0.172951	0.074
H8B_16	0.616579	0.738888	0.197228	0.074
H8C_16	0.651377	0.726992	0.188410	0.074
C9_16	0.67845(10)	0.77566(15)	0.1201(2)	0.0542(14)
H9A_16	0.692936	0.766891	0.097064	0.081
H9B_16	0.684016	0.763130	0.153061	0.081
H9C_16	0.679833	0.804277	0.123947	0.081
C10_16	0.64665(14)	0.79534(14)	0.0104(2)	0.0564(14)
H10A_16	0.630605	0.803074	-0.017255	0.085
H10B_16	0.661996	0.778162	-0.002539	0.085
H10C_16	0.657219	0.818864	0.025451	0.085
C1_13	0.62488(10)	0.91207(11)	0.24645(13)	0.0271(8)
C2_13	0.65031(8)	0.88634(12)	0.24097(14)	0.0251(8)

C3_13	0.64056(9)	0.84736(11)	0.24829(14)	0.0250(8)
C4_13	0.60890(9)	0.84836(11)	0.25804(14)	0.0262(8)
C5_13	0.59942(8)	0.88843(12)	0.25682(14)	0.0266(8)
C6_13	0.56795(9)	0.90296(14)	0.26701(16)	0.0423(10)
H6A_13	0.563025	0.927667	0.248843	0.063
H6B_13	0.568334	0.907392	0.303287	0.063
H6C_13	0.551947	0.883297	0.255565	0.063
C7_13	0.58904(10)	0.81325(13)	0.26527(15)	0.0411(10)
H7A_13	0.587254	0.796771	0.234974	0.062
H7B_13	0.568153	0.821937	0.271200	0.062
H7C_13	0.598714	0.798054	0.294353	0.062
C8_13	0.66099(10)	0.81172(11)	0.24762(15)	0.0373(9)
H8A_13	0.647968	0.788008	0.245647	0.056
H8B_13	0.676000	0.810985	0.278519	0.056
H8C_13	0.672348	0.812889	0.218253	0.056
C9_13	0.68248(9)	0.89752(15)	0.22917(16)	0.0420(11)
H9A_13	0.685078	0.888306	0.195268	0.063
H9B_13	0.698433	0.885345	0.253886	0.063
H9C_13	0.684813	0.926171	0.230708	0.063
C10_13	0.62450(12)	0.95599(11)	0.24125(16)	0.0421(10)
H10A_13	0.645585	0.965321	0.237480	0.063
H10B_13	0.617720	0.967819	0.271399	0.063
H10C_13	0.609954	0.963514	0.211475	0.063
O1_24	0.7825(2)	0.6076(2)	0.2794(3)	0.0262(13)
C1_24	0.79517(18)	0.5741(2)	0.3011(3)	0.0275(9)
C2_24	0.78700(19)	0.5380(2)	0.2659(3)	0.0314(12)
F1_24	0.75831(16)	0.5248(3)	0.2696(4)	0.0370(14)
F2_24	0.80736(17)	0.50840(19)	0.2773(3)	0.0473(15)
F3_24	0.7884(2)	0.5476(2)	0.2182(3)	0.0438(15)
C3_24	0.83121(18)	0.5798(2)	0.3096(3)	0.0340(12)
F4_24	0.8388(2)	0.6149(2)	0.3294(4)	0.0401(14)
F5_24	0.84348(19)	0.5774(2)	0.2668(3)	0.0463(14)
F6_24	0.8462(2)	0.5524(2)	0.3402(4)	0.0477(17)
C4_24	0.78326(19)	0.5665(2)	0.3521(3)	0.0339(12)
F7_24	0.7957(2)	0.5916(2)	0.3873(3)	0.0442(18)
F8_24	0.79003(17)	0.5300(2)	0.3701(3)	0.0419(13)
F9_24	0.75204(15)	0.5706(2)	0.3465(3)	0.0410(13)
O1_17	0.7579(3)	0.6670(5)	0.2109(5)	0.028(2)
C1_17	0.7785(2)	0.6781(3)	0.1788(4)	0.0304(18)
C2_17	0.8054(3)	0.7031(4)	0.2077(5)	0.046(2)
F1_17	0.7958(3)	0.7390(4)	0.2189(6)	0.071(3)
F2_17	0.8302(3)	0.7075(5)	0.1836(7)	0.050(4)
F3_17	0.8148(6)	0.6868(6)	0.2525(6)	0.078(5)
C3_17	0.7931(2)	0.6426(3)	0.1540(3)	0.0378(18)
F4_17	0.7719(3)	0.6144(2)	0.1431(6)	0.055(2)
F5_17	0.81590(19)	0.6274(3)	0.1842(4)	0.0480(19)
F6_17	0.8042(2)	0.6533(3)	0.1107(3)	0.053(2)
C4_17	0.7597(3)	0.7046(4)	0.1383(5)	0.053(2)
F7_17	0.7407(4)	0.6833(5)	0.1059(6)	0.068(3)
F8_17	0.7783(3)	0.7246(4)	0.1119(5)	0.063(3)
F9_17	0.7414(2)	0.7289(3)	0.1589(4)	0.067(3)
O1_18	0.76513(17)	0.6469(2)	0.1969(2)	0.0277(15)
C1_18	0.7816(3)	0.6738(3)	0.1741(4)	0.0321(19)
C2_18	0.8026(2)	0.6511(3)	0.1412(4)	0.051(2)

F1_18	0.8265(3)	0.6344(4)	0.1693(4)	0.069(3)
F2_18	0.8122(2)	0.6747(3)	0.1060(3)	0.067(2)
F3_18	0.78735(19)	0.6221(2)	0.1160(3)	0.059(2)
C3_18	0.7585(3)	0.7001(4)	0.1393(5)	0.053(3)
F4_18	0.7352(2)	0.7106(3)	0.1636(5)	0.079(3)
F5_18	0.7485(4)	0.6789(7)	0.0982(6)	0.077(5)
F6_18	0.7724(4)	0.7327(5)	0.1250(7)	0.072(4)
C4_18	0.8026(3)	0.6995(4)	0.2125(6)	0.050(3)
F7_18	0.7849(4)	0.7274(3)	0.2299(5)	0.084(3)
F8_18	0.8257(4)	0.7163(6)	0.1910(8)	0.065(4)
F9_18	0.8164(7)	0.6763(7)	0.2494(8)	0.064(5)
O1_19	0.7608(5)	0.6670(8)	0.2187(8)	0.033(3)
C1_19	0.7783(3)	0.6823(4)	0.1849(5)	0.040(2)
C2_19	0.7703(3)	0.6636(4)	0.1322(4)	0.059(2)
F1_19	0.7413(4)	0.6726(7)	0.1114(8)	0.096(6)
F2_19	0.7921(3)	0.6722(5)	0.1030(4)	0.073(3)
F3_19	0.7681(5)	0.6248(4)	0.1377(9)	0.072(4)
C3_19	0.8143(2)	0.6760(3)	0.2021(4)	0.039(2)
F4_19	0.8199(5)	0.6821(6)	0.2523(5)	0.041(3)
F5_19	0.8240(4)	0.6406(4)	0.1976(6)	0.068(4)
F6_19	0.8313(5)	0.7001(7)	0.1779(10)	0.078(6)
C4_19	0.7723(3)	0.7274(3)	0.1834(5)	0.056(2)
F7_19	0.7875(5)	0.7447(5)	0.2244(7)	0.083(5)
F8_19	0.7832(3)	0.7445(4)	0.1447(5)	0.077(4)
F9_19	0.7425(3)	0.7367(6)	0.1824(7)	0.094(5)
O1_22	0.7247(3)	0.5954(5)	0.2204(4)	0.0242(16)
C1_22	0.6951(3)	0.5862(3)	0.1991(4)	0.0288(10)
C2_22	0.6966(2)	0.5718(3)	0.1446(3)	0.0407(14)
F1_22	0.7003(2)	0.6028(3)	0.1142(3)	0.0483(18)
F2_22	0.6711(2)	0.5525(3)	0.1251(4)	0.059(2)
F3_22	0.72141(19)	0.5493(2)	0.1417(4)	0.0590(18)
C3_22	0.6829(2)	0.5520(3)	0.2291(4)	0.0451(15)
F4_22	0.6891(3)	0.5586(3)	0.2775(3)	0.059(2)
F5_22	0.6974(2)	0.5175(3)	0.2195(4)	0.0606(19)
F6_22	0.6518(2)	0.5469(3)	0.2179(4)	0.057(2)
C4_22	0.6728(3)	0.6221(3)	0.1969(4)	0.0344(14)
F7_22	0.6627(2)	0.6274(3)	0.2419(3)	0.0491(18)
F8_22	0.6462(3)	0.6175(4)	0.1645(6)	0.038(2)
F9_22	0.6865(3)	0.6542(3)	0.1841(5)	0.049(2)
O1_25	0.7798(4)	0.6078(4)	0.2906(5)	0.0276(18)
C1_25	0.7974(3)	0.5756(4)	0.3040(5)	0.0301(12)
C2_25	0.8325(3)	0.5888(4)	0.3129(5)	0.0344(15)
F1_25	0.8441(4)	0.5916(4)	0.2692(5)	0.049(2)
F2_25	0.8492(4)	0.5635(4)	0.3442(6)	0.044(2)
F3_25	0.8353(4)	0.6244(4)	0.3342(7)	0.044(2)
C3_25	0.7881(3)	0.5591(4)	0.3540(5)	0.0351(16)
F4_25	0.7570(3)	0.5605(4)	0.3544(6)	0.043(2)
F5_25	0.8006(4)	0.5809(4)	0.3928(5)	0.041(2)
F6_25	0.7976(3)	0.5221(3)	0.3622(5)	0.048(2)
C4_25	0.7934(3)	0.5431(4)	0.2632(5)	0.0362(17)
F7_25	0.7661(3)	0.5237(5)	0.2636(7)	0.042(2)
F8_25	0.8165(3)	0.5161(4)	0.2696(6)	0.057(3)
F9_25	0.7930(4)	0.5590(4)	0.2175(5)	0.047(3)
C1_5	0.6433(3)	0.5650(5)	0.5663(5)	0.028(4)

C2_5	0.6340(3)	0.5823(4)	0.5182(4)	0.029(3)
C3_5	0.6027(3)	0.5706(4)	0.5018(4)	0.027(3)
C4_5	0.5926(3)	0.5468(4)	0.5392(5)	0.026(3)
C5_5	0.6177(3)	0.5420(6)	0.5783(6)	0.025(3)
C6_5	0.6155(6)	0.5178(8)	0.6247(8)	0.060(6)
H6A_5	0.606962	0.491825	0.614799	0.090
H6B_5	0.601638	0.530974	0.645726	0.090
H6C_5	0.636359	0.514835	0.643895	0.090
C7_5	0.5622(3)	0.5244(4)	0.5383(7)	0.053(4)
H7A_5	0.546605	0.535188	0.511974	0.079
H7B_5	0.554681	0.526908	0.571157	0.079
H7C_5	0.565766	0.496586	0.531351	0.079
C8_5	0.5838(4)	0.5808(4)	0.4521(4)	0.052(5)
H8A_5	0.593386	0.568779	0.424579	0.078
H8B_5	0.583229	0.609428	0.447784	0.078
H8C_5	0.562371	0.570866	0.451424	0.078
C9_5	0.6556(4)	0.6047(4)	0.4896(7)	0.064(6)
H9A_5	0.652753	0.596039	0.454404	0.096
H9B_5	0.677254	0.600077	0.504610	0.096
H9C_5	0.650849	0.632877	0.491077	0.096
C10_5	0.6738(4)	0.5691(8)	0.6001(8)	0.045(5)
H10A_5	0.690452	0.575254	0.579800	0.067
H10B_5	0.678659	0.544347	0.618261	0.067
H10C_5	0.672108	0.590285	0.624415	0.067
C1_9	0.5074(4)	0.6125(4)	0.5807(5)	0.035(2)
C2_9	0.5090(4)	0.6460(4)	0.5499(5)	0.031(2)
C3_9	0.5075(5)	0.6798(4)	0.5808(5)	0.031(2)
C4_9	0.5051(9)	0.6668(5)	0.6306(6)	0.029(3)
C5_9	0.5054(5)	0.6253(5)	0.6306(6)	0.032(2)
C6_9	0.5015(6)	0.5992(6)	0.6749(7)	0.044(4)
H6A_9	0.479972	0.589224	0.671400	0.066
H6B_9	0.505827	0.614337	0.706170	0.066
H6C_9	0.516113	0.577064	0.675772	0.066
C7_9	0.5020(5)	0.6938(6)	0.6741(7)	0.030(3)
H7A_9	0.515054	0.717156	0.671623	0.045
H7B_9	0.508950	0.680085	0.705834	0.045
H7C_9	0.480108	0.701721	0.673178	0.045
C8_9	0.5065(6)	0.7221(5)	0.5652(7)	0.044(3)
H8A_9	0.510361	0.724128	0.529982	0.066
H8B_9	0.522583	0.736807	0.586795	0.066
H8C_9	0.485807	0.733052	0.568476	0.066
C9_9	0.5099(4)	0.6468(6)	0.4939(5)	0.048(3)
H9A_9	0.488813	0.651457	0.476384	0.073
H9B_9	0.517761	0.621584	0.483101	0.073
H9C_9	0.523879	0.667985	0.485760	0.073
C10_9	0.5055(4)	0.5705(4)	0.5624(8)	0.057(4)
H10A_9	0.508690	0.569715	0.526840	0.085
H10B_9	0.484777	0.559729	0.566002	0.085
H10C_9	0.521659	0.554814	0.582439	0.085
C1_23	0.59999(16)	0.7612(2)	0.5863(2)	0.0302(13)
C2_23	0.5988(2)	0.7422(3)	0.5392(3)	0.0324(14)
C3_23	0.6278(2)	0.7233(3)	0.5370(3)	0.0374(15)
C4_23	0.64732(15)	0.7301(2)	0.5831(3)	0.0391(14)
C5_23	0.63019(17)	0.7536(2)	0.6134(2)	0.0352(13)

C6_23	0.6421(2)	0.7713(2)	0.6641(3)	0.061(2)
H6A_23	0.644643	0.799780	0.660427	0.091
H6B_23	0.662387	0.759564	0.676914	0.091
H6C_23	0.627111	0.766141	0.687754	0.091
C7_23	0.68009(16)	0.7153(2)	0.5963(4)	0.066(2)
H7A_23	0.680056	0.686517	0.595734	0.099
H7B_23	0.688537	0.724538	0.630069	0.099
H7C_23	0.693136	0.725222	0.571692	0.099
C8_23	0.6357(3)	0.7006(3)	0.4923(4)	0.068(3)
H8A_23	0.620328	0.679512	0.484312	0.102
H8B_23	0.656649	0.689214	0.500128	0.102
H8C_23	0.635198	0.718274	0.463287	0.102
C9_23	0.5727(3)	0.7438(3)	0.4963(3)	0.051(3)
H9A_23	0.581162	0.751249	0.465365	0.077
H9B_23	0.557263	0.763383	0.503674	0.077
H9C_23	0.562739	0.717983	0.491829	0.077
C10_23	0.5760(2)	0.7866(2)	0.6059(3)	0.0503(19)
H10A_23	0.558219	0.790391	0.579439	0.076
H10B_23	0.585310	0.812206	0.615869	0.076
H10C_23	0.568784	0.773991	0.635167	0.076
C1_35	0.6031(4)	0.6657(6)	0.9696(6)	0.027(3)
C2_35	0.6059(3)	0.6889(5)	0.9267(6)	0.024(2)
C3_35	0.6361(3)	0.7059(5)	0.9325(6)	0.028(2)
C4_35	0.6525(3)	0.6915(6)	0.9783(6)	0.033(3)
C5_35	0.6318(4)	0.6670(7)	1.0014(7)	0.031(3)
C6_35	0.6387(6)	0.6488(8)	1.0528(7)	0.065(6)
H6A_35	0.657193	0.631960	1.054105	0.097
H6B_35	0.620682	0.633051	1.059710	0.097
H6C_35	0.642599	0.669631	1.078210	0.097
C7_35	0.6841(3)	0.7034(7)	1.0033(9)	0.064(5)
H7A_35	0.695936	0.679979	1.015722	0.096
H7B_35	0.681854	0.720956	1.031640	0.096
H7C_35	0.695351	0.717142	0.978931	0.096
C8_35	0.6483(4)	0.7320(5)	0.8941(8)	0.052(4)
H8A_35	0.659300	0.716027	0.871570	0.078
H8B_35	0.662819	0.751366	0.911405	0.078
H8C_35	0.630768	0.745707	0.874405	0.078
C9_35	0.5807(4)	0.6953(7)	0.8830(7)	0.055(5)
H9A_35	0.588696	0.712589	0.858255	0.083
H9B_35	0.574578	0.670039	0.867199	0.083
H9C_35	0.562520	0.707632	0.895001	0.083
C10_35	0.5732(4)	0.6448(6)	0.9773(9)	0.048(5)
H10A_35	0.555637	0.663201	0.971603	0.072
H10B_35	0.575011	0.634629	1.011826	0.072
H10C_35	0.569674	0.622900	0.953385	0.072
C1_36	0.6521(3)	0.6146(4)	0.7410(5)	0.027(2)
C2_36	0.6249(3)	0.5924(3)	0.7462(4)	0.0266(19)
C3_36	0.6011(3)	0.6191(4)	0.7552(5)	0.0259(19)
C4_36	0.6137(3)	0.6575(4)	0.7560(7)	0.027(2)
C5_36	0.6450(3)	0.6543(3)	0.7469(6)	0.027(2)
C6_36	0.6680(4)	0.6881(4)	0.7454(7)	0.043(3)
H6A_36	0.672886	0.691338	0.710860	0.064
H6B_36	0.687267	0.682274	0.767956	0.064
H6C_36	0.658645	0.712325	0.756288	0.064

C7_36	0.5970(4)	0.6959(4)	0.7618(6)	0.037(3)
H7A_36	0.594130	0.709767	0.729370	0.055
H7B_36	0.609519	0.712143	0.787117	0.055
H7C_36	0.576511	0.690679	0.772490	0.055
C8_36	0.5686(3)	0.6086(5)	0.7656(6)	0.041(3)
H8A_36	0.553273	0.624866	0.744576	0.061
H8B_36	0.566895	0.613373	0.801263	0.061
H8C_36	0.564581	0.580819	0.757743	0.061
C9_36	0.6214(4)	0.5488(4)	0.7418(6)	0.043(3)
H9A_36	0.605359	0.542384	0.713399	0.065
H9B_36	0.615082	0.538193	0.773001	0.065
H9C_36	0.641397	0.537079	0.736057	0.065
C10_36	0.6840(3)	0.5992(6)	0.7322(6)	0.043(3)
H10A_36	0.693956	0.618152	0.711814	0.065
H10B_36	0.681434	0.573996	0.714274	0.065
H10C_36	0.697088	0.595443	0.764632	0.065
C1_37	0.6045(4)	0.5218(5)	0.9180(7)	0.034(3)
C2_37	0.6241(4)	0.5295(5)	0.9636(6)	0.027(2)
C3_37	0.6535(4)	0.5110(6)	0.9609(6)	0.022(2)
C4_37	0.6519(4)	0.4931(8)	0.9127(7)	0.027(3)
C5_37	0.6212(5)	0.4984(9)	0.8869(8)	0.036(3)
C6_37	0.6091(7)	0.4817(9)	0.8361(8)	0.056(6)
H6A_37	0.587634	0.490843	0.825924	0.084
H6B_37	0.609307	0.452911	0.837975	0.084
H6C_37	0.622462	0.490359	0.811290	0.084
C7_37	0.6765(6)	0.4678(9)	0.8940(12)	0.045(5)
H7A_37	0.666555	0.445179	0.875674	0.068
H7B_37	0.691192	0.458560	0.922679	0.068
H7C_37	0.687880	0.483221	0.871306	0.068
C8_37	0.6803(4)	0.5106(8)	1.0028(7)	0.030(3)
H8A_37	0.695950	0.491353	0.995319	0.046
H8B_37	0.672618	0.503559	1.034497	0.046
H8C_37	0.689898	0.536801	1.006084	0.046
C9_37	0.6165(5)	0.5522(5)	1.0085(7)	0.048(4)
H9A_37	0.633725	0.570278	1.019833	0.072
H9B_37	0.613544	0.533994	1.035815	0.072
H9C_37	0.597206	0.567331	0.999137	0.072
C10_37	0.5712(4)	0.5352(7)	0.9044(10)	0.056(5)
H10A_37	0.568882	0.547821	0.871190	0.084
H10B_37	0.565940	0.554087	0.929661	0.084
H10C_37	0.557158	0.512523	0.903522	0.084
C1_39	0.7432(5)	0.9317(5)	0.4166(5)	0.028(3)
C2_39	0.7439(5)	0.9186(4)	0.3663(5)	0.023(4)
C3_39	0.7440(5)	0.8771(4)	0.3679(6)	0.028(3)
C4_39	0.7426(5)	0.8650(5)	0.4183(7)	0.037(4)
C5_39	0.7426(4)	0.8984(6)	0.4487(5)	0.033(3)
C6_39	0.7418(4)	0.9014(9)	0.5047(5)	0.063(6)
H6A_39	0.732462	0.926532	0.512488	0.095
H6B_39	0.763209	0.899762	0.522359	0.095
H6C_39	0.729293	0.879755	0.515672	0.095
C7_39	0.7444(5)	0.8228(6)	0.4358(12)	0.088(8)
H7A_39	0.731726	0.806304	0.410907	0.132
H7B_39	0.736393	0.820806	0.468321	0.132
H7C_39	0.766218	0.813992	0.439526	0.132

C8_39	0.7451(5)	0.8497(6)	0.3241(8)	0.058(5)
H8A_39	0.743602	0.864975	0.292813	0.087
H8B_39	0.727606	0.831184	0.322261	0.087
H8C_39	0.764934	0.835167	0.328710	0.087
C9_39	0.7449(4)	0.9459(4)	0.3221(5)	0.028(3)
H9A_39	0.740282	0.931086	0.290564	0.043
H9B_39	0.765854	0.957607	0.323865	0.043
H9C_39	0.729363	0.966806	0.323037	0.043
C10_39	0.7452(5)	0.9743(5)	0.4300(9)	0.054(5)
H10A_39	0.767038	0.982922	0.432564	0.081
H10B_39	0.737449	0.978291	0.462476	0.081
H10C_39	0.732415	0.989523	0.403870	0.081
C1_41	0.6282(3)	1.0097(3)	0.3805(4)	0.042(2)
C2_41	0.6547(3)	1.0117(4)	0.4175(5)	0.043(2)
C3_41	0.6477(3)	0.9917(5)	0.4608(5)	0.040(2)
C4_41	0.6163(3)	0.9781(4)	0.4507(5)	0.0390(18)
C5_41	0.6047(3)	0.9877(5)	0.3999(5)	0.039(2)
C6_41	0.5724(3)	0.9794(5)	0.3736(7)	0.058(3)
H6A_41	0.569515	0.992412	0.340670	0.088
H6B_41	0.556841	0.989410	0.394126	0.088
H6C_41	0.569602	0.950976	0.369014	0.088
C7_41	0.5985(4)	0.9560(5)	0.4858(6)	0.059(3)
H7A_41	0.591449	0.930816	0.470450	0.088
H7B_41	0.580277	0.971439	0.492398	0.088
H7C_41	0.612068	0.951161	0.517586	0.088
C8_41	0.6707(5)	0.9852(6)	0.5072(6)	0.066(4)
H8A_41	0.660101	0.988408	0.537150	0.100
H8B_41	0.687699	1.004470	0.508113	0.100
H8C_41	0.679313	0.958620	0.506569	0.100
C9_41	0.6835(4)	1.0349(5)	0.4087(9)	0.070(4)
H9A_41	0.692022	1.024284	0.379313	0.105
H9B_41	0.699369	1.032849	0.438521	0.105
H9C_41	0.677852	1.062546	0.402735	0.105
C10_41	0.6259(5)	1.0292(5)	0.3295(5)	0.067(4)
H10A_41	0.634455	1.011627	0.305699	0.101
H10B_41	0.637905	1.053798	0.332369	0.101
H10C_41	0.603930	1.034943	0.317210	0.101
C1_42	0.5947(3)	0.9500(4)	0.0396(5)	0.028(3)
C2_42	0.6033(3)	0.9258(4)	0.0013(5)	0.028(3)
C3_42	0.6341(3)	0.9118(4)	0.0166(5)	0.028(2)
C4_42	0.6447(3)	0.9282(5)	0.0648(5)	0.027(3)
C5_42	0.6205(3)	0.9516(3)	0.0787(4)	0.028(2)
C6_42	0.6206(4)	0.9759(4)	0.1262(4)	0.041(4)
H6A_42	0.615732	1.003357	0.117042	0.062
H6B_42	0.641277	0.974481	0.146322	0.062
H6C_42	0.604759	0.965665	0.145912	0.062
C7_42	0.6761(3)	0.9203(5)	0.0950(6)	0.051(4)
H7A_42	0.691235	0.913301	0.072250	0.076
H7B_42	0.674176	0.898591	0.118474	0.076
H7C_42	0.683266	0.943959	0.114099	0.076
C8_42	0.6537(4)	0.8891(5)	-0.0156(6)	0.051(4)
H8A_42	0.648316	0.861148	-0.014558	0.077
H8B_42	0.675890	0.892666	-0.002765	0.077
H8C_42	0.649638	0.898616	-0.050387	0.077

C9_42	0.5832(4)	0.9177(5)	-0.0479(5)	0.045(4)
H9A_42	0.590252	0.934026	-0.074436	0.067
H9B_42	0.561342	0.924043	-0.044730	0.067
H9C_42	0.584842	0.889915	-0.056680	0.067
C10_42	0.5653(3)	0.9740(4)	0.0402(7)	0.047(4)
H10A_42	0.550223	0.967351	0.010673	0.070
H10B_42	0.570390	1.002043	0.039398	0.070
H10C_42	0.556066	0.968179	0.071000	0.070
C1_43	0.6165(3)	0.7735(4)	0.0300(4)	0.033(3)
C2_43	0.5949(3)	0.7508(4)	0.0528(6)	0.038(3)
C3_43	0.6087(3)	0.7392(4)	0.1012(5)	0.034(3)
C4_43	0.6388(4)	0.7559(6)	0.1102(6)	0.034(3)
C5_43	0.6439(3)	0.7761(5)	0.0654(6)	0.033(3)
C6_43	0.6746(3)	0.7951(5)	0.0593(8)	0.049(4)
H6A_43	0.673697	0.805776	0.025119	0.074
H6B_43	0.691401	0.775428	0.064828	0.074
H6C_43	0.678908	0.816344	0.083927	0.074
C7_43	0.6635(4)	0.7480(6)	0.1540(6)	0.053(4)
H7A_43	0.653492	0.740906	0.183558	0.079
H7B_43	0.676234	0.771707	0.161463	0.079
H7C_43	0.676880	0.726379	0.145622	0.079
C8_43	0.5932(5)	0.7143(5)	0.1371(7)	0.058(4)
H8A_43	0.577082	0.697898	0.118044	0.086
H8B_43	0.583539	0.731355	0.160195	0.086
H8C_43	0.608908	0.697491	0.156425	0.086
C9_43	0.5634(4)	0.7388(6)	0.0265(9)	0.065(6)
H9A_43	0.565968	0.724155	-0.004197	0.098
H9B_43	0.550672	0.762335	0.017539	0.098
H9C_43	0.552827	0.722173	0.048958	0.098
C10_43	0.6116(5)	0.7917(6)	-0.0220(5)	0.054(5)
H10A_43	0.629876	0.786410	-0.039189	0.081
H10B_43	0.608832	0.820175	-0.019053	0.081
H10C_43	0.592880	0.780327	-0.041506	0.081
C1_44	0.6414(3)	0.9007(4)	0.2424(5)	0.022(3)
C2_44	0.6103(3)	0.9038(4)	0.2524(5)	0.021(3)
C3_44	0.5998(3)	0.8652(4)	0.2602(5)	0.023(3)
C4_44	0.6245(3)	0.8388(3)	0.2555(6)	0.021(3)
C5_44	0.6499(3)	0.8607(4)	0.2440(7)	0.023(3)
C6_44	0.6815(3)	0.8447(6)	0.2345(7)	0.040(4)
H6A_44	0.682583	0.844208	0.198153	0.060
H6B_44	0.684110	0.817950	0.248053	0.060
H6C_44	0.698198	0.861543	0.251201	0.060
C7_44	0.6228(5)	0.7945(4)	0.2600(7)	0.041(4)
H7A_44	0.602323	0.786942	0.268950	0.062
H7B_44	0.639310	0.785424	0.286290	0.062
H7C_44	0.625821	0.782428	0.227728	0.062
C8_44	0.5680(3)	0.8545(6)	0.2738(8)	0.043(4)
H8A_44	0.553063	0.852042	0.242997	0.065
H8B_44	0.560876	0.875161	0.295250	0.065
H8C_44	0.569353	0.829503	0.292094	0.065
C9_44	0.5914(5)	0.9408(5)	0.2540(7)	0.042(4)
H9A_44	0.575208	0.941750	0.224617	0.063
H9B_44	0.605173	0.963701	0.253635	0.063
H9C_44	0.581447	0.941157	0.284929	0.063

C10_44	0.6630(4)	0.9342(5)	0.2348(7)	0.040(4)
H10A_44	0.683919	0.923854	0.231811	0.060
H10B_44	0.664204	0.952076	0.263655	0.060
H10C_44	0.654989	0.948390	0.203893	0.060
O1_45	0.7233(3)	0.5950(5)	0.2307(4)	0.0292(17)
C1_45	0.6968(3)	0.5849(3)	0.1999(4)	0.0294(10)
C2_45	0.6706(3)	0.6153(3)	0.2022(4)	0.0365(14)
F1_45	0.6596(3)	0.6122(3)	0.2471(4)	0.056(2)
F2_45	0.6470(4)	0.6098(5)	0.1645(6)	0.050(3)
F3_45	0.6818(3)	0.6520(3)	0.1997(4)	0.0434(18)
C3_45	0.7034(2)	0.5808(3)	0.1444(3)	0.0422(14)
F4_45	0.7304(2)	0.5635(3)	0.1421(3)	0.0602(19)
F5_45	0.7042(2)	0.6170(2)	0.1235(3)	0.0562(19)
F6_45	0.6807(2)	0.5599(3)	0.1170(3)	0.065(2)
C4_45	0.6861(2)	0.5445(3)	0.2190(4)	0.0426(14)
F7_45	0.7032(2)	0.5161(2)	0.2017(4)	0.059(2)
F8_45	0.6556(2)	0.5380(3)	0.2020(4)	0.061(2)
F9_45	0.6891(2)	0.5431(2)	0.2689(3)	0.0513(17)
C1_46	0.6322(2)	0.8392(3)	0.5032(3)	0.0362(17)
C2_46	0.6043(2)	0.8415(3)	0.4699(4)	0.0317(16)
C3_46	0.6062(3)	0.8179(4)	0.4279(5)	0.0345(19)
C4_46	0.6357(3)	0.7999(5)	0.4335(5)	0.0362(17)
C5_46	0.6521(2)	0.8122(3)	0.4804(4)	0.0348(16)
C6_46	0.6836(2)	0.7953(4)	0.4990(5)	0.056(3)
H6A_46	0.697144	0.797220	0.472341	0.084
H6B_46	0.681344	0.767632	0.508039	0.084
H6C_46	0.693055	0.809984	0.528672	0.084
C7_46	0.6450(4)	0.7730(4)	0.3933(5)	0.055(3)
H7A_46	0.649755	0.788609	0.364525	0.083
H7B_46	0.627798	0.754840	0.382331	0.083
H7C_46	0.663631	0.757925	0.407056	0.083
C8_46	0.5803(4)	0.8111(6)	0.3848(6)	0.070(4)
H8A_46	0.579792	0.832834	0.360744	0.104
H8B_46	0.560152	0.809548	0.398005	0.104
H8C_46	0.584108	0.786355	0.367821	0.104
C9_46	0.5746(3)	0.8623(4)	0.4798(7)	0.068(3)
H9A_46	0.563676	0.872628	0.448082	0.102
H9B_46	0.579876	0.883973	0.503520	0.102
H9C_46	0.560897	0.843608	0.494360	0.102
C10_46	0.6430(4)	0.8541(4)	0.5554(4)	0.063(3)
H10A_46	0.664009	0.865254	0.556641	0.094
H10B_46	0.643409	0.832309	0.579483	0.094
H10C_46	0.628489	0.874397	0.564167	0.094
Al	0.500000	0.88115(3)	-0.250000	0.0206(2)
O1_32	0.49097(11)	0.91693(14)	-0.21141(18)	0.0364(11)
C1_32	0.47202(16)	0.9298(2)	-0.1774(3)	0.0311(12)
C2_32	0.45635(19)	0.8950(2)	-0.1518(3)	0.0635(16)
F1_32	0.43180(12)	0.88146(16)	-0.1850(2)	0.0764(16)
F2_32	0.44836(17)	0.9074(2)	-0.1091(2)	0.097(2)
F3_32	0.47775(14)	0.86733(16)	-0.14026(19)	0.0764(16)
C3_32	0.49225(18)	0.9543(2)	-0.1374(3)	0.0673(17)
F4_32	0.51028(11)	0.97827(17)	-0.1608(3)	0.0898(19)
F5_32	0.50836(14)	0.9293(2)	-0.1032(2)	0.092(2)
F6_32	0.47274(14)	0.9776(2)	-0.1131(3)	0.111(2)

C4_32	0.44640(15)	0.9567(2)	-0.2050(3)	0.0487(14)
F7_32	0.45794(14)	0.99133(16)	-0.2190(3)	0.0881(19)
F8_32	0.42088(12)	0.95818(19)	-0.1860(3)	0.0809(18)
F9_32	0.43372(12)	0.93717(16)	-0.24947(18)	0.0688(14)
O1_33	0.52323(12)	0.90208(14)	-0.29417(18)	0.0278(10)
C1_33	0.5272(2)	0.9316(3)	-0.3265(4)	0.0448(13)
C2_33	0.5311(2)	0.9732(2)	-0.3024(3)	0.0639(15)
F1_33	0.5012(2)	0.98587(19)	-0.2976(3)	0.096(2)
F2_33	0.54794(13)	0.99676(13)	-0.3294(2)	0.0562(14)
F3_33	0.54717(17)	0.96946(17)	-0.2560(2)	0.0696(18)
C3_33	0.5551(2)	0.9205(3)	-0.3546(3)	0.0687(16)
F4_33	0.55852(18)	0.88356(18)	-0.3615(3)	0.086(2)
F5_33	0.58138(18)	0.9327(3)	-0.3203(4)	0.119(3)
F6_33	0.55561(15)	0.93882(17)	-0.3982(2)	0.0659(16)
C4_33	0.4979(2)	0.9334(3)	-0.3694(4)	0.0617(15)
F7_33	0.5042(2)	0.9017(2)	-0.3993(2)	0.101(2)
F8_33	0.49760(13)	0.96970(15)	-0.3921(2)	0.0583(15)
F9_33	0.47196(11)	0.93022(15)	-0.3497(2)	0.0591(14)
O1_34	0.46806(15)	0.85869(16)	-0.2771(3)	0.0292(14)
C1_34	0.45408(16)	0.8265(2)	-0.2999(3)	0.0288(16)
C2_34	0.46012(16)	0.78962(18)	-0.2656(2)	0.0397(14)
F1_34	0.48867(10)	0.77498(11)	-0.26743(16)	0.0475(11)
F2_34	0.4392(2)	0.7612(3)	-0.2788(4)	0.064(3)
F3_34	0.45782(15)	0.79885(16)	-0.21771(18)	0.0542(14)
C3_34	0.41804(14)	0.8345(2)	-0.3099(2)	0.0438(15)
F4_34	0.41225(14)	0.87043(16)	-0.3276(2)	0.0585(15)
F5_34	0.40506(10)	0.83109(17)	-0.26770(18)	0.0620(14)
F6_34	0.40323(10)	0.80946(14)	-0.34379(18)	0.0596(14)
C4_34	0.46607(19)	0.8183(2)	-0.3513(3)	0.0363(15)
F7_34	0.4544(3)	0.8434(2)	-0.3868(4)	0.050(2)
F8_34	0.45837(13)	0.78222(14)	-0.36851(18)	0.0534(13)
F9_34	0.49702(9)	0.82135(13)	-0.34564(15)	0.0457(10)
O1_30	0.52592(15)	0.84550(17)	-0.2202(3)	0.0258(13)
C1_30	0.55462(17)	0.8346(2)	-0.1980(3)	0.0245(15)
C2_30	0.57890(16)	0.86871(19)	-0.1980(3)	0.0353(15)
F1_30	0.58805(10)	0.87159(16)	-0.24349(17)	0.0563(13)
F2_30	0.60428(12)	0.86347(16)	-0.16432(19)	0.0490(13)
F3_30	0.56570(10)	0.90273(11)	-0.18735(19)	0.0516(12)
C3_30	0.55230(18)	0.8234(2)	-0.1424(3)	0.0409(16)
F4_30	0.52745(15)	0.8008(2)	-0.1395(2)	0.0636(17)
F5_30	0.5495(3)	0.8561(2)	-0.1159(4)	0.053(2)
F6_30	0.57766(12)	0.80370(15)	-0.12093(18)	0.0613(14)
C4_30	0.56586(15)	0.79819(18)	-0.2257(2)	0.0397(15)
F7_30	0.55095(18)	0.7658(2)	-0.2144(4)	0.058(2)
F8_30	0.59652(11)	0.79252(15)	-0.2137(2)	0.0652(15)
F9_30	0.56022(15)	0.8042(2)	-0.2752(2)	0.0628(17)
Al19	0.500000	0.61952(3)	0.250000	0.0221(2)
O1_29	0.51095(10)	0.58087(13)	0.21857(17)	0.0320(10)
C1_29	0.51916(15)	0.56371(18)	0.1769(2)	0.0339(14)
C2_29	0.52608(18)	0.5205(2)	0.1912(3)	0.0516(17)
F1_29	0.50035(13)	0.50042(15)	0.1957(2)	0.0743(16)
F2_29	0.54124(13)	0.50161(14)	0.1584(2)	0.0643(14)
F3_29	0.5441(2)	0.5184(4)	0.2368(4)	0.080(3)
C3_29	0.54686(19)	0.5831(3)	0.1584(3)	0.068(2)

F4_29	0.54361(17)	0.62211(17)	0.1606(3)	0.093(2)
F5_29	0.57371(12)	0.57242(19)	0.1870(3)	0.087(2)
F6_29	0.5485(2)	0.5742(3)	0.1103(3)	0.104(3)
C4_29	0.49027(15)	0.56393(18)	0.1336(2)	0.0387(14)
F7_29	0.48840(15)	0.59860(14)	0.11150(19)	0.0736(16)
F8_29	0.49291(12)	0.53573(15)	0.10010(17)	0.0591(13)
F9_29	0.46401(10)	0.55807(14)	0.15297(16)	0.0528(12)
O1_51	0.46834(11)	0.64162(14)	0.2108(2)	0.0332(11)
C1_51	0.45143(18)	0.6736(2)	0.1972(3)	0.0341(13)
C2_51	0.41605(15)	0.6627(2)	0.1888(3)	0.0493(14)
F1_51	0.41139(13)	0.62830(18)	0.1652(2)	0.0578(14)
F2_51	0.39855(11)	0.68938(17)	0.1611(2)	0.0751(17)
F3_51	0.40533(16)	0.6595(2)	0.2332(2)	0.079(2)
C3_51	0.4570(2)	0.7071(2)	0.2375(3)	0.0607(16)
F4_51	0.48431(14)	0.72554(12)	0.2339(2)	0.0740(15)
F5_51	0.45744(17)	0.69091(16)	0.28319(17)	0.0779(18)
F6_51	0.43369(18)	0.73290(18)	0.2318(2)	0.092(2)
C4_51	0.46030(18)	0.6900(2)	0.1467(3)	0.0449(14)
F7_51	0.49118(18)	0.6905(4)	0.1494(5)	0.068(3)
F8_51	0.45000(13)	0.72616(14)	0.13682(19)	0.0667(15)
F9_51	0.44881(12)	0.66671(16)	0.10802(16)	0.0546(12)
O1_50	0.52510(12)	0.65506(14)	0.26911(19)	0.0281(11)
C1_50	0.55081(19)	0.6665(2)	0.3003(3)	0.0343(14)
C2_50	0.5432(2)	0.6710(3)	0.3548(3)	0.0592(18)
F1_50	0.54244(13)	0.63559(19)	0.37694(18)	0.0686(16)
F2_50	0.56540(18)	0.6920(2)	0.3827(2)	0.094(2)
F3_50	0.5152(3)	0.6869(5)	0.3562(5)	0.079(3)
C3_50	0.56186(19)	0.7063(2)	0.2810(3)	0.0559(16)
F4_50	0.55912(14)	0.70708(19)	0.2311(2)	0.0712(17)
F5_50	0.54411(16)	0.73567(15)	0.2957(3)	0.0864(19)
F6_50	0.59169(13)	0.71345(18)	0.2988(3)	0.088(2)
C4_50	0.57744(17)	0.6350(2)	0.2993(3)	0.0513(15)
F7_50	0.58931(16)	0.6390(3)	0.2557(2)	0.080(2)
F8_50	0.60047(14)	0.6400(2)	0.3373(3)	0.0647(19)
F9_50	0.56573(12)	0.59936(14)	0.3028(2)	0.0752(18)
O1_55	0.7168(6)	0.6085(7)	0.2193(12)	0.032(2)
C1_55	0.6971(4)	0.5797(6)	0.2001(7)	0.0355(14)
C2_55	0.7081(5)	0.5651(7)	0.1501(8)	0.0434(19)
F1_55	0.6986(10)	0.5886(9)	0.1112(11)	0.050(3)
F2_55	0.6960(7)	0.5298(7)	0.1379(11)	0.057(3)
F3_55	0.7393(5)	0.5628(12)	0.1579(12)	0.051(4)
C3_55	0.7018(5)	0.5450(6)	0.2387(8)	0.0421(19)
F4_55	0.7023(8)	0.5598(10)	0.2847(8)	0.051(4)
F5_55	0.7286(5)	0.5267(7)	0.2345(11)	0.052(4)
F6_55	0.6793(6)	0.5180(7)	0.2315(11)	0.053(3)
C4_55	0.6622(4)	0.5912(6)	0.1913(8)	0.0406(18)
F7_55	0.6496(6)	0.5907(9)	0.2345(8)	0.048(3)
F8_55	0.6459(6)	0.5655(7)	0.1603(10)	0.051(4)
F9_55	0.6578(7)	0.6264(7)	0.1692(12)	0.045(3)
O1_56	0.7721(6)	0.5956(9)	0.2737(12)	0.029(2)
C1_56	0.7977(5)	0.5807(5)	0.3021(8)	0.0312(14)
C2_56	0.7898(6)	0.5694(7)	0.3550(9)	0.0365(19)
F1_56	0.7862(9)	0.6014(9)	0.3828(12)	0.036(3)
F2_56	0.8125(7)	0.5467(9)	0.3783(11)	0.044(3)

F3_56	0.7628(7)	0.5490(10)	0.3514(15)	0.040(3)
C3_56	0.8097(5)	0.5446(6)	0.2749(9)	0.0365(18)
F4_56	0.8075(8)	0.5516(10)	0.2254(8)	0.041(3)
F5_56	0.7938(7)	0.5116(7)	0.2821(14)	0.040(3)
F6_56	0.8398(5)	0.5368(9)	0.2906(12)	0.045(3)
C4_56	0.8230(5)	0.6139(6)	0.3072(9)	0.0341(18)
F7_56	0.8350(7)	0.6166(9)	0.2640(9)	0.042(3)
F8_56	0.8460(7)	0.6064(10)	0.3442(12)	0.041(4)
F9_56	0.8106(6)	0.6480(6)	0.3190(11)	0.039(4)
O1_26	0.48333(11)	0.60187(13)	0.30341(17)	0.0284(10)
C1_26	0.46789(16)	0.57506(19)	0.3272(2)	0.0301(12)
C2_26	0.44531(18)	0.5504(2)	0.2895(3)	0.0529(16)
F1_26	0.4629(3)	0.5201(3)	0.2732(5)	0.091(3)
F2_26	0.42214(12)	0.53517(16)	0.31108(18)	0.0594(14)
F3_26	0.43268(12)	0.57162(16)	0.25109(17)	0.0610(15)
C3_26	0.4467(2)	0.5987(3)	0.3620(3)	0.0597(17)
F4_26	0.46261(15)	0.62629(16)	0.3853(2)	0.0691(15)
F5_26	0.42259(15)	0.6132(2)	0.3295(3)	0.098(2)
F6_26	0.4396(2)	0.5725(3)	0.3974(3)	0.081(3)
C4_26	0.49062(18)	0.5482(2)	0.3606(3)	0.0560(16)
F7_26	0.50255(16)	0.5697(2)	0.4028(2)	0.0828(19)
F8_26	0.47611(15)	0.51559(17)	0.3742(3)	0.083(2)
F9_26	0.51323(14)	0.53546(19)	0.3353(3)	0.082(2)
O1_20	0.7272(4)	0.6515(4)	0.2975(5)	0.0286(14)
C1_20	0.7239(2)	0.6802(3)	0.3309(4)	0.0336(11)
C2_20	0.7538(2)	0.6830(3)	0.3706(4)	0.0421(15)
F1_20	0.7536(2)	0.6537(2)	0.4034(3)	0.0519(18)
F2_20	0.7558(4)	0.7165(4)	0.3969(5)	0.049(3)
F3_20	0.7800(3)	0.6802(4)	0.3475(5)	0.049(2)
C3_20	0.7187(2)	0.7206(2)	0.3038(3)	0.0451(14)
F4_20	0.6977(2)	0.7167(4)	0.2629(4)	0.063(2)
F5_20	0.74564(18)	0.7358(2)	0.2927(3)	0.0545(15)
F6_20	0.7069(3)	0.7481(4)	0.3326(5)	0.059(2)
C4_20	0.6954(2)	0.6694(3)	0.3581(4)	0.0491(14)
F7_20	0.66928(17)	0.6771(3)	0.3297(3)	0.0672(19)
F8_20	0.6938(3)	0.6905(4)	0.3997(5)	0.067(3)
F9_20	0.69652(19)	0.6317(2)	0.3703(3)	0.0599(18)
O1_21	0.73817(17)	0.6701(2)	0.2819(2)	0.0281(13)
C1_21	0.7303(2)	0.6873(3)	0.3238(4)	0.0366(12)
C2_21	0.7582(3)	0.6858(4)	0.3668(5)	0.0418(16)
F1_21	0.7617(3)	0.6507(3)	0.3887(4)	0.051(2)
F2_21	0.7571(6)	0.7116(5)	0.4040(6)	0.053(3)
F3_21	0.7851(3)	0.6936(3)	0.3469(5)	0.052(2)
C3_21	0.7233(3)	0.7316(3)	0.3103(4)	0.0439(15)
F4_21	0.7062(3)	0.7344(3)	0.2659(4)	0.055(2)
F5_21	0.7497(2)	0.7514(2)	0.3075(3)	0.0511(17)
F6_21	0.7091(4)	0.7477(5)	0.3472(5)	0.058(3)
C4_21	0.7012(3)	0.6680(3)	0.3403(4)	0.0481(14)
F7_21	0.6752(2)	0.6801(4)	0.3112(4)	0.066(2)
F8_21	0.6987(3)	0.6760(3)	0.3892(4)	0.068(2)
F9_21	0.7043(2)	0.6287(2)	0.3390(3)	0.0587(18)
O1_28	0.7280(8)	0.6537(7)	0.2943(10)	0.034(2)
C1_28	0.7228(3)	0.6817(4)	0.3276(5)	0.0373(13)
C2_28	0.6991(3)	0.7127(3)	0.3017(5)	0.0417(15)

F1_28	0.7067(4)	0.7220(6)	0.2565(5)	0.040(2)
F2_28	0.6981(4)	0.7449(6)	0.3303(9)	0.054(3)
F3_28	0.6702(2)	0.6992(3)	0.2960(5)	0.059(2)
C3_28	0.7083(3)	0.6616(4)	0.3707(5)	0.0510(17)
F4_28	0.7314(3)	0.6420(4)	0.3997(4)	0.074(3)
F5_28	0.6853(3)	0.6370(4)	0.3531(5)	0.057(2)
F6_28	0.6995(6)	0.6874(7)	0.4040(8)	0.065(3)
C4_28	0.7537(3)	0.7038(4)	0.3477(5)	0.0471(16)
F7_28	0.7771(4)	0.6778(6)	0.3585(7)	0.054(3)
F8_28	0.7491(5)	0.7222(6)	0.3906(6)	0.065(3)
F9_28	0.7613(3)	0.7295(3)	0.3145(5)	0.066(2)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

S-Table 29: Bond lengths and angles for $[Cp^*\{Al(AlCp^*)_3\}_2]^+[pf]^-$

Atom–Atom	**Length [Å]**	Al6–C4_6	2.284(3)
Al1–C4_36	2.448(19)	Al6–C2_6	2.291(3)
Al1–C3_36	2.463(13)	Al6–C5_6	2.315(3)
Al1–C5_1	2.469(4)	Al6–C1_6	2.320(3)
Al1–C4_1	2.495(4)	Al6–Al8	2.8249(13)
Al1–Al4	2.6674(13)	Al6–Al7	2.8299(12)
Al1–Al2	2.6690(13)	Al7–C3_7	2.224(11)
Al1–Al3	2.6814(13)	Al7–C2_7	2.228(10)
Al3–C2_3	2.197(8)	Al7–C4_7	2.259(13)
Al3–C1_3	2.239(5)	Al7–C4_35	2.269(19)
Al3–C2_5	2.243(12)	Al7–C1_7	2.291(10)
Al3–C3_3	2.266(8)	Al7–C5_7	2.303(15)
Al3–C1_5	2.268(18)	Al7–C3_35	2.312(17)
Al3–C5_3	2.312(4)	Al7–C5_35	2.31(3)
Al3–C4_3	2.327(6)	Al7–C2_35	2.324(18)
Al3–C3_5	2.338(11)	Al7–C1_35	2.35(2)
Al3–C5_5	2.40(2)	Al8–C1_37	2.224(18)
Al3–C4_5	2.404(13)	Al8–C4_37	2.23(3)
Al3–Al2	2.8438(13)	Al8–C2_37	2.232(16)
Al4–C3_23	2.210(10)	Al8–C5_37	2.26(3)
Al4–C4_4	2.224(11)	Al8–C3_8	2.259(10)
Al4–C4_23	2.248(7)	Al8–C3_37	2.26(2)
Al4–C5_4	2.261(9)	Al8–C2_8	2.290(13)
Al4–C3_4	2.262(14)	Al8–C4_8	2.299(11)
Al4–C2_23	2.278(10)	Al8–C5_8	2.370(17)
Al4–C2_4	2.308(12)	Al8–C1_8	2.375(15)
Al4–C1_4	2.313(9)	Al9–C1_44	2.419(14)
Al4–C5_23	2.334(7)	Al9–C2_13	2.476(4)
Al4–C1_23	2.361(7)	Al9–C1_13	2.478(4)
Al4–Al2	2.8180(13)	Al9–C2_44	2.503(12)
Al5–C2_36	2.445(12)	Al9–Al10	2.6671(13)
Al5–C2_1	2.447(4)	Al9–Al11	2.6768(13)
Al5–C1_36	2.495(13)	Al9–Al12	2.6844(13)
Al5–C1_1	2.505(4)	Al10–C4_41	2.214(14)
Al5–Al8	2.6680(13)	Al10–C3_41	2.243(16)
Al5–Al6	2.6757(12)	Al10–C5_41	2.264(18)
Al5–Al7	2.6870(13)	Al10–C5_10	2.265(6)
Al6–C3_6	2.266(3)	Al10–C4_10	2.275(4)

Al10–C1_10	2.278(5)	Al16–C5_43	2.301(17)
Al10–C2_10	2.285(5)	Al16–C4_16	2.316(4)
Al10–C3_10	2.286(4)	Al16–C1_43	2.324(12)
Al10–C2_41	2.369(13)	Al16–C3_16	2.340(4)
Al10–C1_41	2.395(12)	Al17–O1_56	1.60(2)
Al10–Al11	2.8132(13)	Al17–O1_19	1.643(18)
Al11–C1_39	2.22(2)	Al17–O1_21	1.662(6)
Al11–C5_39	2.222(17)	Al17–O1_45	1.695(13)
Al11–C4_39	2.243(18)	Al17–O1_24	1.714(8)
Al11–C2_39	2.279(19)	Al17–O1_55	1.72(2)
Al11–C3_39	2.30(2)	Al17–O1_17	1.731(12)
Al11–C5_11	2.305(9)	Al17–O1_28	1.73(2)
Al11–C4_11	2.306(8)	Al17–O1_22	1.742(12)
Al11–C1_11	2.312(10)	Al17–O1_25	1.743(13)
Al11–C3_11	2.324(8)	Al17–O1_20	1.785(11)
Al11–C2_11	2.335(9)	Al17–O1_18	1.797(6)
Al12–C4_46	2.181(16)	Al2–C2_9	2.216(14)
Al12–C5_46	2.225(10)	Al2–C3_9	2.245(18)
Al12–C1_12	2.256(8)	Al2–C3_2	2.283(17)
Al12–C2_12	2.262(5)	Al2–C2_2	2.285(12)
Al12–C3_46	2.277(16)	Al2–C1_9	2.292(16)
Al12–C3_12	2.296(4)	Al2–C4_2	2.29(3)
Al12–C5_12	2.311(7)	Al2–C1_2	2.327(12)
Al12–C4_12	2.317(5)	Al2–C4_9	2.33(3)
Al12–C1_46	2.335(9)	Al2–C5_2	2.335(14)
Al12–C2_46	2.355(10)	Al2–C5_9	2.35(2)
Al13–C4_13	2.443(4)	C1_3–C2_3	1.413(7)
Al13–C3_44	2.496(14)	C1_3–C5_3	1.425(7)
Al13–Al16	2.6655(13)	C1_3–C10_3	1.488(6)
Al13–Al15	2.6818(13)	C2_3–C3_3	1.418(8)
Al13–Al14	2.6855(13)	C2_3–C9_3	1.498(7)
Al14–C3_42	2.213(12)	C3_3–C4_3	1.408(7)
Al14–C4_42	2.214(16)	C3_3–C8_3	1.500(8)
Al14–C4_14	2.236(5)	C4_3–C5_3	1.404(6)
Al14–C3_14	2.260(5)	C4_3–C7_3	1.514(6)
Al14–C5_14	2.273(5)	C5_3–C6_3	1.488(6)
Al14–C5_42	2.302(12)	C6_3–H6A_3	0.9800
Al14–C2_14	2.314(4)	C6_3–H6B_3	0.9800
Al14–C2_42	2.315(14)	C6_3–H6C_3	0.9800
Al14–C1_14	2.335(4)	C7_3–H7A_3	0.9800
Al14–C1_42	2.363(13)	C7_3–H7B_3	0.9800
Al14–Al15	2.8296(13)	C7_3–H7C_3	0.9800
Al15–C4_15	2.280(3)	C8_3–H8A_3	0.9800
Al15–C5_15	2.285(3)	C8_3–H8B_3	0.9800
Al15–C3_15	2.298(3)	C8_3–H8C_3	0.9800
Al15–C1_15	2.304(3)	C9_3–H9A_3	0.9800
Al15–C2_15	2.309(3)	C9_3–H9B_3	0.9800
Al15–Al16	2.8235(13)	C9_3–H9C_3	0.9800
Al16–C1_16	2.219(4)	C10_3–H10A_3	0.9800
Al16–C5_16	2.244(5)	C10_3–H10B_3	0.9800
Al16–C4_43	2.25(2)	C10_3–H10C_3	0.9800
Al16–C3_43	2.274(14)	C1_4–C2_4	1.406(9)
Al16–C2_16	2.277(5)	C1_4–C5_4	1.424(10)
Al16–C2_43	2.284(14)	C1_4–C10_4	1.507(10)

C2_4–C3_4	1.411(11)	C4_6–C5_6	1.419(4)
C2_4–C9_4	1.505(10)	C4_6–C7_6	1.499(4)
C3_4–C4_4	1.418(10)	C5_6–C6_6	1.500(5)
C3_4–C8_4	1.491(11)	C6_6–H6A_6	0.9800
C4_4–C5_4	1.423(10)	C6_6–H6B_6	0.9800
C4_4–C7_4	1.492(10)	C6_6–H6C_6	0.9800
C5_4–C6_4	1.492(9)	C7_6–H7A_6	0.9800
C6_4–H6A_4	0.9800	C7_6–H7B_6	0.9800
C6_4–H6B_4	0.9800	C7_6–H7C_6	0.9800
C6_4–H6C_4	0.9800	C8_6–H8A_6	0.9800
C7_4–H7A_4	0.9800	C8_6–H8B_6	0.9800
C7_4–H7B_4	0.9800	C8_6–H8C_6	0.9800
C7_4–H7C_4	0.9800	C9_6–H9A_6	0.9800
C8_4–H8A_4	0.9800	C9_6–H9B_6	0.9800
C8_4–H8B_4	0.9800	C9_6–H9C_6	0.9800
C8_4–H8C_4	0.9800	C10_6–H10A_6	0.9800
C9_4–H9A_4	0.9800	C10_6–H10B_6	0.9800
C9_4–H9B_4	0.9800	C10_6–H10C_6	0.9800
C9_4–H9C_4	0.9800	C1_7–C5_7	1.413(7)
C10_4–H10A_4	0.9800	C1_7–C2_7	1.420(7)
C10_4–H10B_4	0.9800	C1_7–C10_7	1.501(7)
C10_4–H10C_4	0.9800	C2_7–C3_7	1.421(8)
C1_2–C2_2	1.412(8)	C2_7–C9_7	1.508(8)
C1_2–C5_2	1.415(9)	C3_7–C4_7	1.410(8)
C1_2–C10_2	1.506(9)	C3_7–C8_7	1.504(8)
C2_2–C3_2	1.428(9)	C4_7–C5_7	1.415(8)
C2_2–C9_2	1.506(9)	C4_7–C7_7	1.507(8)
C3_2–C4_2	1.415(9)	C5_7–C6_7	1.505(8)
C3_2–C8_2	1.509(10)	C6_7–H6A_7	0.9800
C4_2–C5_2	1.424(9)	C6_7–H6B_7	0.9800
C4_2–C7_2	1.506(9)	C6_7–H6C_7	0.9800
C5_2–C6_2	1.501(9)	C7_7–H7A_7	0.9800
C6_2–H6A_2	0.9800	C7_7–H7B_7	0.9800
C6_2–H6B_2	0.9800	C7_7–H7C_7	0.9800
C6_2–H6C_2	0.9800	C8_7–H8A_7	0.9800
C7_2–H7A_2	0.9800	C8_7–H8B_7	0.9800
C7_2–H7B_2	0.9800	C8_7–H8C_7	0.9800
C7_2–H7C_2	0.9800	C9_7–H9A_7	0.9800
C8_2–H8A_2	0.9800	C9_7–H9B_7	0.9800
C8_2–H8B_2	0.9800	C9_7–H9C_7	0.9800
C8_2–H8C_2	0.9800	C10_7–H10A_7	0.9800
C9_2–H9A_2	0.9800	C10_7–H10B_7	0.9800
C9_2–H9B_2	0.9800	C10_7–H10C_7	0.9800
C9_2–H9C_2	0.9800	C1_8–C5_8	1.421(8)
C10_2–H10A_2	0.9800	C1_8–C2_8	1.421(8)
C10_2–H10B_2	0.9800	C1_8–C10_8	1.510(9)
C10_2–H10C_2	0.9800	C2_8–C3_8	1.432(8)
C1_6–C2_6	1.421(4)	C2_8–C9_8	1.502(8)
C1_6–C5_6	1.425(4)	C3_8–C4_8	1.425(7)
C1_6–C10_6	1.502(4)	C3_8–C8_8	1.500(8)
C2_6–C3_6	1.411(4)	C4_8–C5_8	1.407(8)
C2_6–C9_6	1.502(4)	C4_8–C7_8	1.506(8)
C3_6–C4_6	1.425(4)	C5_8–C6_8	1.502(8)
C3_6–C8_6	1.496(4)	C6_8–H6A_8	0.9800

C6_8–H6B_8	0.9800	C7_10–H7C_10	0.9800
C6_8–H6C_8	0.9800	C8_10–H8A_10	0.9800
C7_8–H7A_8	0.9800	C8_10–H8B_10	0.9800
C7_8–H7B_8	0.9800	C8_10–H8C_10	0.9800
C7_8–H7C_8	0.9800	C9_10–H9A_10	0.9800
C8_8–H8A_8	0.9800	C9_10–H9B_10	0.9800
C8_8–H8B_8	0.9800	C9_10–H9C_10	0.9800
C8_8–H8C_8	0.9800	C10_10–H10A_10	0.9800
C9_8–H9A_8	0.9800	C10_10–H10B_10	0.9800
C9_8–H9B_8	0.9800	C10_10–H10C_10	0.9800
C9_8–H9C_8	0.9800	C1_11–C2_11	1.415(7)
C10_8–H10A_8	0.9800	C1_11–C5_11	1.427(8)
C10_8–H10B_8	0.9800	C1_11–C10_11	1.501(7)
C10_8–H10C_8	0.9800	C2_11–C3_11	1.416(7)
C1_1–C2_1	1.419(6)	C2_11–C9_11	1.508(7)
C1_1–C5_1	1.429(5)	C3_11–C4_11	1.424(6)
C1_1–C10_1	1.500(5)	C3_11–C8_11	1.499(7)
C2_1–C3_1	1.411(5)	C4_11–C5_11	1.411(7)
C2_1–C9_1	1.503(5)	C4_11–C7_11	1.490(7)
C3_1–C4_1	1.421(5)	C5_11–C6_11	1.508(7)
C3_1–C8_1	1.501(5)	C6_11–H6A_11	0.9800
C4_1–C5_1	1.425(5)	C6_11–H6B_11	0.9800
C4_1–C7_1	1.505(5)	C6_11–H6C_11	0.9800
C5_1–C6_1	1.496(5)	C7_11–H7A_11	0.9800
C6_1–H6A_1	0.9800	C7_11–H7B_11	0.9800
C6_1–H6B_1	0.9800	C7_11–H7C_11	0.9800
C6_1–H6C_1	0.9800	C8_11–H8A_11	0.9800
C7_1–H7A_1	0.9800	C8_11–H8B_11	0.9800
C7_1–H7B_1	0.9800	C8_11–H8C_11	0.9800
C7_1–H7C_1	0.9800	C9_11–H9A_11	0.9800
C8_1–H8A_1	0.9800	C9_11–H9B_11	0.9800
C8_1–H8B_1	0.9800	C9_11–H9C_11	0.9800
C8_1–H8C_1	0.9800	C10_11–H10A_11	0.9800
C9_1–H9A_1	0.9800	C10_11–H10B_11	0.9800
C9_1–H9B_1	0.9800	C10_11–H10C_11	0.9800
C9_1–H9C_1	0.9800	C1_12–C5_12	1.396(7)
C10_1–H10A_1	0.9800	C1_12–C2_12	1.422(7)
C10_1–H10B_1	0.9800	C1_12–C10_12	1.518(7)
C10_1–H10C_1	0.9800	C2_12–C3_12	1.451(7)
C1_10–C5_10	1.415(7)	C2_12–C9_12	1.476(7)
C1_10–C2_10	1.423(7)	C3_12–C4_12	1.417(6)
C1_10–C10_10	1.495(7)	C3_12–C8_12	1.475(6)
C2_10–C3_10	1.410(6)	C4_12–C5_12	1.411(6)
C2_10–C9_10	1.498(6)	C4_12–C7_12	1.517(6)
C3_10–C4_10	1.419(5)	C5_12–C6_12	1.499(7)
C3_10–C8_10	1.497(6)	C6_12–H6A_12	0.9800
C4_10–C5_10	1.412(6)	C6_12–H6B_12	0.9800
C4_10–C7_10	1.503(6)	C6_12–H6C_12	0.9800
C5_10–C6_10	1.492(6)	C7_12–H7A_12	0.9800
C6_10–H6A_10	0.9800	C7_12–H7B_12	0.9800
C6_10–H6B_10	0.9800	C7_12–H7C_12	0.9800
C6_10–H6C_10	0.9800	C8_12–H8A_12	0.9800
C7_10–H7A_10	0.9800	C8_12–H8B_12	0.9800
C7_10–H7B_10	0.9800	C8_12–H8C_12	0.9800

C9_12–H9A_12	0.9800	C10_15–H10B_15	0.9800
C9_12–H9B_12	0.9800	C10_15–H10C_15	0.9800
C9_12–H9C_12	0.9800	C1_16–C2_16	1.416(6)
C10_12–H10A_12	0.9800	C1_16–C5_16	1.441(6)
C10_12–H10B_12	0.9800	C1_16–C10_16	1.493(6)
C10_12–H10C_12	0.9800	C2_16–C3_16	1.411(6)
C1_14–C2_14	1.416(5)	C2_16–C9_16	1.501(6)
C1_14–C5_14	1.420(6)	C3_16–C4_16	1.423(5)
C1_14–C10_14	1.496(5)	C3_16–C8_16	1.511(6)
C2_14–C3_14	1.418(5)	C4_16–C5_16	1.407(6)
C2_14–C9_14	1.511(5)	C4_16–C7_16	1.509(6)
C3_14–C4_14	1.425(6)	C5_16–C6_16	1.492(6)
C3_14–C8_14	1.490(6)	C6_16–H6A_16	0.9800
C4_14–C5_14	1.410(7)	C6_16–H6B_16	0.9800
C4_14–C7_14	1.500(6)	C6_16–H6C_16	0.9800
C5_14–C6_14	1.493(6)	C7_16–H7A_16	0.9800
C6_14–H6A_14	0.9800	C7_16–H7B_16	0.9800
C6_14–H6B_14	0.9800	C7_16–H7C_16	0.9800
C6_14–H6C_14	0.9800	C8_16–H8A_16	0.9800
C7_14–H7A_14	0.9800	C8_16–H8B_16	0.9800
C7_14–H7B_14	0.9800	C8_16–H8C_16	0.9800
C7_14–H7C_14	0.9800	C9_16–H9A_16	0.9800
C8_14–H8A_14	0.9800	C9_16–H9B_16	0.9800
C8_14–H8B_14	0.9800	C9_16–H9C_16	0.9800
C8_14–H8C_14	0.9800	C10_16–H10A_16	0.9800
C9_14–H9A_14	0.9800	C10_16–H10B_16	0.9800
C9_14–H9B_14	0.9800	C10_16–H10C_16	0.9800
C9_14–H9C_14	0.9800	C1_13–C5_13	1.417(5)
C10_14–H10A_14	0.9800	C1_13–C2_13	1.425(5)
C10_14–H10B_14	0.9800	C1_13–C10_13	1.500(5)
C10_14–H10C_14	0.9800	C2_13–C3_13	1.413(5)
C1_15–C5_15	1.416(4)	C2_13–C9_13	1.510(5)
C1_15–C2_15	1.422(4)	C3_13–C4_13	1.423(5)
C1_15–C10_15	1.500(5)	C3_13–C8_13	1.500(5)
C2_15–C3_15	1.409(5)	C4_13–C5_13	1.422(5)
C2_15–C9_15	1.501(5)	C4_13–C7_13	1.497(5)
C3_15–C4_15	1.410(5)	C5_13–C6_13	1.502(5)
C3_15–C8_15	1.505(5)	C6_13–H6A_13	0.9800
C4_15–C5_15	1.420(4)	C6_13–H6B_13	0.9800
C4_15–C7_15	1.494(5)	C6_13–H6C_13	0.9800
C5_15–C6_15	1.491(4)	C7_13–H7A_13	0.9800
C6_15–H6A_15	0.9800	C7_13–H7B_13	0.9800
C6_15–H6B_15	0.9800	C7_13–H7C_13	0.9800
C6_15–H6C_15	0.9800	C8_13–H8A_13	0.9800
C7_15–H7A_15	0.9800	C8_13–H8B_13	0.9800
C7_15–H7B_15	0.9800	C8_13–H8C_13	0.9800
C7_15–H7C_15	0.9800	C9_13–H9A_13	0.9800
C8_15–H8A_15	0.9800	C9_13–H9B_13	0.9800
C8_15–H8B_15	0.9800	C9_13–H9C_13	0.9800
C8_15–H8C_15	0.9800	C10_13–H10A_13	0.9800
C9_15–H9A_15	0.9800	C10_13–H10B_13	0.9800
C9_15–H9B_15	0.9800	C10_13–H10C_13	0.9800
C9_15–H9C_15	0.9800	O1_24–C1_24	1.359(7)
C10_15–H10A_15	0.9800	C1_24–C4_24	1.542(8)

C1_24–C3_24	1.551(8)	C2_22–F3_22	1.325(9)
C1_24–C2_24	1.559(8)	C2_22–F2_22	1.328(8)
C2_24–F3_24	1.326(7)	C2_22–F1_22	1.353(9)
C2_24–F1_24	1.331(7)	C3_22–F4_22	1.305(9)
C2_24–F2_24	1.343(7)	C3_22–F6_22	1.348(9)
C3_24–F5_24	1.327(7)	C3_22–F5_22	1.369(9)
C3_24–F4_24	1.331(7)	C4_22–F9_22	1.309(9)
C3_24–F6_24	1.345(7)	C4_22–F7_22	1.343(9)
C4_24–F7_24	1.332(7)	C4_22–F8_22	1.351(10)
C4_24–F9_24	1.341(7)	O1_25–C1_25	1.353(11)
C4_24–F8_24	1.349(7)	C1_25–C4_25	1.548(11)
O1_17–C1_17	1.364(10)	C1_25–C3_25	1.551(11)
C1_17–C3_17	1.551(10)	C1_25–C2_25	1.566(11)
C1_17–C4_17	1.551(10)	C2_25–F1_25	1.333(11)
C1_17–C2_17	1.559(10)	C2_25–F3_25	1.336(10)
C2_17–F2_17	1.324(11)	C2_25–F2_25	1.341(11)
C2_17–F3_17	1.334(11)	C3_25–F5_25	1.331(11)
C2_17–F1_17	1.337(11)	C3_25–F6_25	1.332(10)
C3_17–F5_17	1.294(9)	C3_25–F4_25	1.341(10)
C3_17–F4_17	1.328(10)	C4_25–F9_25	1.335(11)
C3_17–F6_17	1.360(9)	C4_25–F8_25	1.349(11)
C4_17–F9_17	1.315(11)	C4_25–F7_25	1.351(10)
C4_17–F8_17	1.326(10)	C1_5–C5_5	1.422(12)
C4_17–F7_17	1.327(12)	C1_5–C2_5	1.423(11)
O1_18–C1_18	1.352(10)	C1_5–C10_5	1.498(11)
C1_18–C4_18	1.546(11)	C2_5–C3_5	1.418(11)
C1_18–C2_18	1.549(11)	C2_5–C9_5	1.491(11)
C1_18–C3_18	1.554(11)	C3_5–C4_5	1.400(11)
C2_18–F3_18	1.319(10)	C3_5–C8_5	1.506(10)
C2_18–F1_18	1.321(11)	C4_5–C5_5	1.411(10)
C2_18–F2_18	1.344(11)	C4_5–C7_5	1.511(11)
C3_18–F4_18	1.316(11)	C5_5–C6_5	1.504(12)
C3_18–F5_18	1.338(12)	C6_5–H6A_5	0.9800
C3_18–F6_18	1.340(12)	C6_5–H6B_5	0.9800
C4_18–F9_18	1.339(12)	C6_5–H6C_5	0.9800
C4_18–F8_18	1.341(11)	C7_5–H7A_5	0.9800
C4_18–F7_18	1.341(12)	C7_5–H7B_5	0.9800
O1_19–C1_19	1.355(12)	C7_5–H7C_5	0.9800
C1_19–C2_19	1.543(11)	C8_5–H8A_5	0.9800
C1_19–C4_19	1.555(11)	C8_5–H8B_5	0.9800
C1_19–C3_19	1.571(11)	C8_5–H8C_5	0.9800
C2_19–F2_19	1.332(11)	C9_5–H9A_5	0.9800
C2_19–F3_19	1.334(12)	C9_5–H9B_5	0.9800
C2_19–F1_19	1.334(12)	C9_5–H9C_5	0.9800
C3_19–F5_19	1.285(11)	C10_5–H10A_5	0.9800
C3_19–F6_19	1.326(12)	C10_5–H10B_5	0.9800
C3_19–F4_19	1.349(12)	C10_5–H10C_5	0.9800
C4_19–F9_19	1.318(12)	C1_9–C2_9	1.415(10)
C4_19–F8_19	1.327(11)	C1_9–C5_9	1.418(10)
C4_19–F7_19	1.337(12)	C1_9–C10_9	1.508(10)
O1_22–C1_22	1.359(10)	C2_9–C3_9	1.423(10)
C1_22–C3_22	1.544(9)	C2_9–C9_9	1.505(10)
C1_22–C2_22	1.548(10)	C3_9–C4_9	1.420(10)
C1_22–C4_22	1.551(9)	C3_9–C8_9	1.496(10)

C4_9–C5_9	1.413(11)	C6_35–H6B_35	0.9800
C4_9–C7_9	1.502(11)	C6_35–H6C_35	0.9800
C5_9–C6_9	1.506(10)	C7_35–H7A_35	0.9800
C6_9–H6A_9	0.9800	C7_35–H7B_35	0.9800
C6_9–H6B_9	0.9800	C7_35–H7C_35	0.9800
C6_9–H6C_9	0.9800	C8_35–H8A_35	0.9800
C7_9–H7A_9	0.9800	C8_35–H8B_35	0.9800
C7_9–H7B_9	0.9800	C8_35–H8C_35	0.9800
C7_9–H7C_9	0.9800	C9_35–H9A_35	0.9800
C8_9–H8A_9	0.9800	C9_35–H9B_35	0.9800
C8_9–H8B_9	0.9800	C9_35–H9C_35	0.9800
C8_9–H8C_9	0.9800	C10_35–H10A_35	0.9800
C9_9–H9A_9	0.9800	C10_35–H10B_35	0.9800
C9_9–H9B_9	0.9800	C10_35–H10C_35	0.9800
C9_9–H9C_9	0.9800	C1_36–C5_36	1.398(11)
C10_9–H10A_9	0.9800	C1_36–C2_36	1.415(11)
C10_9–H10B_9	0.9800	C1_36–C10_36	1.518(11)
C10_9–H10C_9	0.9800	C2_36–C3_36	1.415(11)
C1_23–C2_23	1.412(8)	C2_36–C9_36	1.497(12)
C1_23–C5_23	1.426(7)	C3_36–C4_36	1.412(11)
C1_23–C10_23	1.496(8)	C3_36–C8_36	1.503(11)
C2_23–C3_23	1.413(9)	C4_36–C5_36	1.407(11)
C2_23–C9_23	1.495(8)	C4_36–C7_36	1.508(11)
C3_23–C4_23	1.416(8)	C5_36–C6_36	1.522(11)
C3_23–C8_23	1.500(9)	C6_36–H6A_36	0.9800
C4_23–C5_23	1.414(8)	C6_36–H6B_36	0.9800
C4_23–C7_23	1.496(8)	C6_36–H6C_36	0.9800
C5_23–C6_23	1.511(8)	C7_36–H7A_36	0.9800
C6_23–H6A_23	0.9800	C7_36–H7B_36	0.9800
C6_23–H6B_23	0.9800	C7_36–H7C_36	0.9800
C6_23–H6C_23	0.9800	C8_36–H8A_36	0.9800
C7_23–H7A_23	0.9800	C8_36–H8B_36	0.9800
C7_23–H7B_23	0.9800	C8_36–H8C_36	0.9800
C7_23–H7C_23	0.9800	C9_36–H9A_36	0.9800
C8_23–H8A_23	0.9800	C9_36–H9B_36	0.9800
C8_23–H8B_23	0.9800	C9_36–H9C_36	0.9800
C8_23–H8C_23	0.9800	C10_36–H10A_36	0.9800
C9_23–H9A_23	0.9800	C10_36–H10B_36	0.9800
C9_23–H9B_23	0.9800	C10_36–H10C_36	0.9800
C9_23–H9C_23	0.9800	C1_37–C2_37	1.412(10)
C10_23–H10A_23	0.9800	C1_37–C5_37	1.417(11)
C10_23–H10B_23	0.9800	C1_37–C10_37	1.501(11)
C10_23–H10C_23	0.9800	C2_37–C3_37	1.427(11)
C1_35–C5_35	1.405(11)	C2_37–C9_37	1.502(11)
C1_35–C2_35	1.411(11)	C3_37–C4_37	1.420(11)
C1_35–C10_35	1.507(11)	C3_37–C8_37	1.498(11)
C2_35–C3_35	1.415(10)	C4_37–C5_37	1.417(11)
C2_35–C9_35	1.500(11)	C4_37–C7_37	1.503(12)
C3_35–C4_35	1.415(10)	C5_37–C6_37	1.502(11)
C3_35–C8_35	1.506(11)	C6_37–H6A_37	0.9800
C4_35–C5_35	1.419(11)	C6_37–H6B_37	0.9800
C4_35–C7_35	1.494(11)	C6_37–H6C_37	0.9800
C5_35–C6_35	1.502(11)	C7_37–H7A_37	0.9800
C6_35–H6A_35	0.9800	C7_37–H7B_37	0.9800

C7_37–H7C_37	0.9800	C9_41–H9A_41	0.9800
C8_37–H8A_37	0.9800	C9_41–H9B_41	0.9800
C8_37–H8B_37	0.9800	C9_41–H9C_41	0.9800
C8_37–H8C_37	0.9800	C10_41–H10A_41	0.9800
C9_37–H9A_37	0.9800	C10_41–H10B_41	0.9800
C9_37–H9B_37	0.9800	C10_41–H10C_41	0.9800
C9_37–H9C_37	0.9800	C1_42–C2_42	1.405(11)
C10_37–H10A_37	0.9800	C1_42–C5_42	1.423(11)
C10_37–H10B_37	0.9800	C1_42–C10_42	1.509(11)
C10_37–H10C_37	0.9800	C2_42–C3_42	1.418(12)
C1_39–C2_39	1.422(12)	C2_42–C9_42	1.502(12)
C1_39–C5_39	1.424(11)	C3_42–C4_42	1.422(11)
C1_39–C10_39	1.490(12)	C3_42–C8_42	1.496(11)
C2_39–C3_39	1.414(11)	C4_42–C5_42	1.401(11)
C2_39–C9_39	1.510(11)	C4_42–C7_42	1.504(11)
C3_39–C4_39	1.417(11)	C5_42–C6_42	1.516(11)
C3_39–C8_39	1.503(12)	C6_42–H6A_42	0.9800
C4_39–C5_39	1.401(11)	C6_42–H6B_42	0.9800
C4_39–C7_39	1.506(11)	C6_42–H6C_42	0.9800
C5_39–C6_39	1.505(11)	C7_42–H7A_42	0.9800
C6_39–H6A_39	0.9800	C7_42–H7B_42	0.9800
C6_39–H6B_39	0.9800	C7_42–H7C_42	0.9800
C6_39–H6C_39	0.9800	C8_42–H8A_42	0.9800
C7_39–H7A_39	0.9800	C8_42–H8B_42	0.9800
C7_39–H7B_39	0.9800	C8_42–H8C_42	0.9800
C7_39–H7C_39	0.9800	C9_42–H9A_42	0.9800
C8_39–H8A_39	0.9800	C9_42–H9B_42	0.9800
C8_39–H8B_39	0.9800	C9_42–H9C_42	0.9800
C8_39–H8C_39	0.9800	C10_42–H10A_42	0.9800
C9_39–H9A_39	0.9800	C10_42–H10B_42	0.9800
C9_39–H9B_39	0.9800	C10_42–H10C_42	0.9800
C9_39–H9C_39	0.9800	C1_43–C2_43	1.409(12)
C10_39–H10A_39	0.9800	C1_43–C5_43	1.413(11)
C10_39–H10B_39	0.9800	C1_43–C10_43	1.512(12)
C10_39–H10C_39	0.9800	C2_43–C3_43	1.407(12)
C1_41–C2_41	1.410(11)	C2_43–C9_43	1.502(12)
C1_41–C5_41	1.411(11)	C3_43–C4_43	1.409(12)
C1_41–C10_41	1.511(12)	C3_43–C8_43	1.501(12)
C2_41–C3_41	1.408(12)	C4_43–C5_43	1.423(12)
C2_41–C9_41	1.517(12)	C4_43–C7_43	1.497(12)
C3_41–C4_41	1.423(12)	C5_43–C6_43	1.503(12)
C3_41–C8_41	1.497(12)	C6_43–H6A_43	0.9800
C4_41–C5_41	1.422(12)	C6_43–H6B_43	0.9800
C4_41–C7_41	1.493(12)	C6_43–H6C_43	0.9800
C5_41–C6_41	1.502(12)	C7_43–H7A_43	0.9800
C6_41–H6A_41	0.9800	C7_43–H7B_43	0.9800
C6_41–H6B_41	0.9800	C7_43–H7C_43	0.9800
C6_41–H6C_41	0.9800	C8_43–H8A_43	0.9800
C7_41–H7A_41	0.9800	C8_43–H8B_43	0.9800
C7_41–H7B_41	0.9800	C8_43–H8C_43	0.9800
C7_41–H7C_41	0.9800	C9_43–H9A_43	0.9800
C8_41–H8A_41	0.9800	C9_43–H9B_43	0.9800
C8_41–H8B_41	0.9800	C9_43–H9C_43	0.9800
C8_41–H8C_41	0.9800	C10_43–H10A_43	0.9800

C10_43–H10B_43	0.9800	C7_46–H7B_46	0.9800
C10_43–H10C_43	0.9800	C7_46–H7C_46	0.9800
C1_44–C2_44	1.407(12)	C8_46–H8A_46	0.9800
C1_44–C5_44	1.408(12)	C8_46–H8B_46	0.9800
C1_44–C10_44	1.500(12)	C8_46–H8C_46	0.9800
C2_44–C3_44	1.412(12)	C9_46–H9A_46	0.9800
C2_44–C9_44	1.502(12)	C9_46–H9B_46	0.9800
C3_44–C4_44	1.409(12)	C9_46–H9C_46	0.9800
C3_44–C8_44	1.510(12)	C10_46–H10A_46	0.9800
C4_44–C5_44	1.393(11)	C10_46–H10B_46	0.9800
C4_44–C7_44	1.516(12)	C10_46–H10C_46	0.9800
C5_44–C6_44	1.518(12)	Al–O1_34	1.655(6)
C6_44–H6A_44	0.9800	Al–O1_32	1.675(4)
C6_44–H6B_44	0.9800	Al–O1_30	1.766(6)
C6_44–H6C_44	0.9800	Al–O1_33	1.794(5)
C7_44–H7A_44	0.9800	O1_32–C1_32	1.372(8)
C7_44–H7B_44	0.9800	C1_32–C3_32	1.533(9)
C7_44–H7C_44	0.9800	C1_32–C4_32	1.545(8)
C8_44–H8A_44	0.9800	C1_32–C2_32	1.565(9)
C8_44–H8B_44	0.9800	C2_32–F2_32	1.307(9)
C8_44–H8C_44	0.9800	C2_32–F3_32	1.324(8)
C9_44–H9A_44	0.9800	C2_32–F1_32	1.368(9)
C9_44–H9B_44	0.9800	C3_32–F4_32	1.337(9)
C9_44–H9C_44	0.9800	C3_32–F5_32	1.370(9)
C10_44–H10A_44	0.9800	C3_32–F6_32	1.380(8)
C10_44–H10B_44	0.9800	C4_32–F8_32	1.272(8)
C10_44–H10C_44	0.9800	C4_32–F7_32	1.351(8)
O1_45–C1_45	1.357(9)	C4_32–F9_32	1.407(8)
C1_45–C2_45	1.537(9)	O1_33–C1_33	1.350(9)
C1_45–C3_45	1.557(9)	C1_33–C3_33	1.547(10)
C1_45–C4_45	1.558(9)	C1_33–C2_33	1.554(10)
C2_45–F3_45	1.340(8)	C1_33–C4_33	1.592(11)
C2_45–F2_45	1.347(10)	C2_33–F3_33	1.346(9)
C2_45–F1_45	1.353(9)	C2_33–F2_33	1.352(8)
C3_45–F4_45	1.309(9)	C2_33–F1_33	1.383(10)
C3_45–F6_45	1.346(8)	C3_33–F4_33	1.280(9)
C3_45–F5_45	1.354(9)	C3_33–F6_33	1.327(9)
C4_45–F9_45	1.324(9)	C3_33–F5_33	1.421(10)
C4_45–F7_45	1.336(9)	C4_33–F9_33	1.300(9)
C4_45–F8_45	1.354(9)	C4_33–F8_33	1.377(8)
C1_46–C2_46	1.400(10)	C4_33–F7_33	1.391(10)
C1_46–C5_46	1.445(11)	O1_34–C1_34	1.354(8)
C1_46–C10_46	1.500(10)	C1_34–C4_34	1.556(9)
C2_46–C3_46	1.393(11)	C1_34–C2_34	1.557(8)
C2_46–C9_46	1.517(11)	C1_34–C3_34	1.564(8)
C3_46–C4_46	1.401(11)	C2_34–F1_34	1.334(7)
C3_46–C8_46	1.512(11)	C2_34–F3_34	1.336(7)
C4_46–C5_46	1.419(11)	C2_34–F2_34	1.337(8)
C4_46–C7_46	1.506(11)	C3_34–F4_34	1.324(8)
C5_46–C6_46	1.498(10)	C3_34–F5_34	1.329(7)
C6_46–H6A_46	0.9800	C3_34–F6_34	1.342(7)
C6_46–H6B_46	0.9800	C4_34–F7_34	1.326(9)
C6_46–H6C_46	0.9800	C4_34–F9_34	1.326(8)
C7_46–H7A_46	0.9800	C4_34–F8_34	1.337(7)

O1_30–C1_30	1.350(9)	C4_50–F8_50	1.333(8)
C1_30–C3_30	1.552(8)	C4_50–F7_50	1.341(9)
C1_30–C4_30	1.554(8)	O1_55–C1_55	1.353(13)
C1_30–C2_30	1.561(8)	C1_55–C4_55	1.541(12)
C2_30–F1_30	1.332(8)	C1_55–C2_55	1.558(13)
C2_30–F2_30	1.333(7)	C1_55–C3_55	1.565(13)
C2_30–F3_30	1.337(7)	C2_55–F2_55	1.331(14)
C3_30–F4_30	1.328(8)	C2_55–F1_55	1.333(13)
C3_30–F5_30	1.334(9)	C2_55–F3_55	1.336(13)
C3_30–F6_30	1.344(8)	C3_55–F4_55	1.328(13)
C4_30–F7_30	1.329(9)	C3_55–F6_55	1.328(13)
C4_30–F9_30	1.330(8)	C3_55–F5_55	1.331(13)
C4_30–F8_30	1.331(7)	C4_55–F8_55	1.337(13)
Al19–O1_50	1.657(4)	C4_55–F9_55	1.338(13)
Al19–O1_29	1.663(4)	C4_55–F7_55	1.339(13)
Al19–O1_51	1.773(4)	O1_56–C1_56	1.354(14)
Al19–O1_26	1.786(4)	C1_56–C2_56	1.548(13)
O1_29–C1_29	1.346(7)	C1_56–C3_56	1.550(13)
C1_29–C3_29	1.504(9)	C1_56–C4_56	1.561(13)
C1_29–C2_29	1.537(8)	C2_56–F2_56	1.337(14)
C1_29–C4_29	1.584(8)	C2_56–F1_56	1.340(14)
C2_29–F1_29	1.322(8)	C2_56–F3_56	1.343(14)
C2_29–F2_29	1.327(7)	C3_56–F4_56	1.335(14)
C2_29–F3_29	1.359(9)	C3_56–F6_56	1.335(14)
C3_29–F6_29	1.334(10)	C3_56–F5_56	1.341(13)
C3_29–F4_29	1.337(9)	C4_56–F8_56	1.328(14)
C3_29–F5_29	1.350(9)	C4_56–F7_56	1.329(13)
C4_29–F7_29	1.317(7)	C4_56–F9_56	1.333(13)
C4_29–F9_29	1.320(7)	O1_26–C1_26	1.338(7)
C4_29–F8_29	1.328(7)	C1_26–C4_26	1.537(8)
O1_51–C1_51	1.334(8)	C1_26–C2_26	1.550(8)
C1_51–C4_51	1.555(9)	C1_26–C3_26	1.604(9)
C1_51–C2_51	1.556(9)	C2_26–F3_26	1.313(8)
C1_51–C3_51	1.565(9)	C2_26–F2_26	1.324(8)
C2_51–F1_51	1.333(9)	C2_26–F1_26	1.384(11)
C2_51–F3_51	1.335(8)	C3_26–F4_26	1.273(9)
C2_51–F2_51	1.339(7)	C3_26–F5_26	1.357(9)
C3_51–F6_51	1.327(8)	C3_26–F6_26	1.366(10)
C3_51–F5_51	1.337(8)	C4_26–F9_26	1.331(9)
C3_51–F4_51	1.349(9)	C4_26–F8_26	1.346(8)
C4_51–F8_51	1.323(8)	C4_26–F7_26	1.385(9)
C4_51–F7_51	1.323(9)	O1_20–C1_20	1.345(9)
C4_51–F9_51	1.343(8)	C1_20–C3_20	1.553(9)
O1_50–C1_50	1.352(8)	C1_20–C4_20	1.553(10)
C1_50–C2_50	1.546(9)	C1_20–C2_20	1.559(10)
C1_50–C3_50	1.547(9)	C2_20–F1_20	1.327(10)
C1_50–C4_50	1.571(9)	C2_20–F2_20	1.338(10)
C2_50–F3_50	1.326(10)	C2_20–F3_20	1.360(10)
C2_50–F2_50	1.337(9)	C3_20–F4_20	1.330(10)
C2_50–F1_50	1.345(9)	C3_20–F5_20	1.342(10)
C3_50–F4_50	1.326(8)	C3_20–F6_20	1.353(10)
C3_50–F6_50	1.332(8)	C4_20–F7_20	1.297(10)
C3_50–F5_50	1.348(9)	C4_20–F9_20	1.321(9)
C4_50–F9_50	1.321(8)	C4_20–F8_20	1.334(10)

O1_21–C1_21	1.348(10)
C1_21–C4_21	1.527(10)
C1_21–C2_21	1.553(11)
C1_21–C3_21	1.572(10)
C2_21–F1_21	1.327(11)
C2_21–F2_21	1.334(12)
C2_21–F3_21	1.363(11)
C3_21–F4_21	1.316(10)
C3_21–F5_21	1.334(11)
C3_21–F6_21	1.343(11)
C4_21–F7_21	1.342(11)
C4_21–F9_21	1.347(10)
C4_21–F8_21	1.355(10)
O1_28–C1_28	1.344(12)
C1_28–C3_28	1.542(12)
C1_28–C4_28	1.561(11)
C1_28–C2_28	1.566(11)
C2_28–F3_28	1.316(11)
C2_28–F1_28	1.331(12)
C2_28–F2_28	1.340(12)
C3_28–F5_28	1.335(12)
C3_28–F6_28	1.339(12)
C3_28–F4_28	1.354(12)
C4_28–F9_28	1.317(12)
C4_28–F7_28	1.344(12)
C4_28–F8_28	1.345(12)

Atom–Atom–Atom	**Angle [°]**
C4_36–Al1–C3_36	33.4(3)
C5_1–Al1–C4_1	33.36(12)
C4_36–Al1–Al4	118.5(3)
C3_36–Al1–Al4	149.8(3)
C5_1–Al1–Al4	113.76(10)
C4_1–Al1–Al4	135.81(10)
C4_36–Al1–Al2	125.2(3)
C3_36–Al1–Al2	117.8(3)
C5_1–Al1–Al2	135.15(10)
C4_1–Al1–Al2	114.64(9)
Al4–Al1–Al2	63.75(3)
C4_36–Al1–Al3	170.6(3)
C3_36–Al1–Al3	145.5(3)
C5_1–Al1–Al3	159.27(11)
C4_1–Al1–Al3	158.76(10)
Al4–Al1–Al3	64.35(4)
Al2–Al1–Al3	64.21(3)
C2_3–Al3–C1_3	37.2(2)
C2_3–Al3–C3_3	37.0(2)
C1_3–Al3–C3_3	61.3(2)
C2_5–Al3–C1_5	36.8(4)
C2_3–Al3–C5_3	61.0(2)
C1_3–Al3–C5_3	36.46(17)
C3_3–Al3–C5_3	60.1(2)
C2_3–Al3–C4_3	60.3(2)
C1_3–Al3–C4_3	59.87(17)
C3_3–Al3–C4_3	35.7(2)
C5_3–Al3–C4_3	35.22(16)
C2_5–Al3–C3_5	36.0(3)
C1_5–Al3–C3_5	59.8(4)
C2_5–Al3–C5_5	59.1(5)
C1_5–Al3–C5_5	35.4(4)
C3_5–Al3–C5_5	57.6(4)
C2_5–Al3–C4_5	58.7(4)
C1_5–Al3–C4_5	58.7(4)
C3_5–Al3–C4_5	34.3(3)
C5_5–Al3–C4_5	34.2(3)
C2_3–Al3–Al1	114.02(19)
C1_3–Al3–Al1	145.31(18)
C2_5–Al3–Al1	146.5(3)
C3_3–Al3–Al1	108.99(19)
C1_5–Al3–Al1	113.7(4)
C5_3–Al3–Al1	168.08(14)
C4_3–Al3–Al1	133.01(15)
C3_5–Al3–Al1	163.2(3)
C5_5–Al3–Al1	107.6(4)
C4_5–Al3–Al1	129.0(3)
C2_3–Al3–Al2	125.61(18)
C1_3–Al3–Al2	116.60(13)
C2_5–Al3–Al2	155.8(3)
C3_3–Al3–Al2	156.00(19)
C1_5–Al3–Al2	159.5(4)
C5_3–Al3–Al2	134.24(14)
C4_3–Al3–Al2	167.12(15)
C3_5–Al3–Al2	122.3(3)
C5_5–Al3–Al2	125.6(4)
C4_5–Al3–Al2	110.2(3)
Al1–Al3–Al2	57.68(3)
C3_23–Al4–C4_23	37.0(2)
C4_4–Al4–C5_4	37.0(3)
C4_4–Al4–C3_4	36.8(3)
C5_4–Al4–C3_4	61.1(4)
C3_23–Al4–C2_23	36.7(3)
C4_23–Al4–C2_23	61.0(3)
C4_4–Al4–C2_4	60.8(4)
C5_4–Al4–C2_4	60.6(3)
C3_4–Al4–C2_4	35.9(3)
C4_4–Al4–C1_4	60.5(3)
C5_4–Al4–C1_4	36.3(3)
C3_4–Al4–C1_4	59.6(4)
C2_4–Al4–C1_4	35.4(3)
C3_23–Al4–C5_23	60.1(3)
C4_23–Al4–C5_23	35.9(2)
C2_23–Al4–C5_23	59.3(3)
C3_23–Al4–C1_23	60.1(3)
C4_23–Al4–C1_23	60.0(2)
C2_23–Al4–C1_23	35.4(2)
C5_23–Al4–C1_23	35.35(19)
C3_23–Al4–Al1	153.1(2)
C4_4–Al4–Al1	137.2(3)

C4_23–Al4–Al1	126.91(19)	C5_6–Al6–Al8	156.35(9)
C5_4–Al4–Al1	120.7(2)	C1_6–Al6–Al8	159.84(9)
C3_4–Al4–Al1	168.7(3)	Al5–Al6–Al8	57.95(3)
C2_23–Al4–Al1	170.2(2)	C3_6–Al6–Al7	146.65(9)
C2_4–Al4–Al1	155.4(3)	C4_6–Al6–Al7	118.62(8)
C1_4–Al4–Al1	129.3(2)	C2_6–Al6–Al7	174.00(9)
C5_23–Al4–Al1	122.56(16)	C5_6–Al6–Al7	115.40(9)
C1_23–Al4–Al1	139.99(17)	C1_6–Al6–Al7	138.14(9)
C3_23–Al4–Al2	137.8(2)	Al5–Al6–Al7	58.34(3)
C4_4–Al4–Al2	127.9(3)	Al8–Al6–Al7	60.77(3)
C4_23–Al4–Al2	174.7(2)	C3_7–Al7–C2_7	37.2(3)
C5_4–Al4–Al2	160.0(3)	C3_7–Al7–C4_7	36.7(3)
C3_4–Al4–Al2	115.8(3)	C2_7–Al7–C4_7	61.6(3)
C2_23–Al4–Al2	114.2(2)	C3_7–Al7–C1_7	61.0(3)
C2_4–Al4–Al2	130.1(2)	C2_7–Al7–C1_7	36.6(2)
C1_4–Al4–Al2	162.1(2)	C4_7–Al7–C1_7	60.6(3)
C5_23–Al4–Al2	144.9(2)	C3_7–Al7–C5_7	60.5(4)
C1_23–Al4–Al2	117.68(18)	C2_7–Al7–C5_7	60.6(3)
Al1–Al4–Al2	58.15(3)	C4_7–Al7–C5_7	36.1(3)
C2_36–Al5–C1_36	33.3(3)	C1_7–Al7–C5_7	35.8(2)
C2_1–Al5–C1_1	33.29(13)	C4_35–Al7–C3_35	36.0(4)
C2_36–Al5–Al8	113.1(3)	C4_35–Al7–C5_35	36.1(4)
C2_1–Al5–Al8	117.57(11)	C3_35–Al7–C5_35	59.5(5)
C1_36–Al5–Al8	132.6(3)	C4_35–Al7–C2_35	59.6(5)
C1_1–Al5–Al8	148.32(11)	C3_35–Al7–C2_35	35.6(3)
C2_36–Al5–Al6	135.8(3)	C5_35–Al7–C2_35	58.9(6)
C2_1–Al5–Al6	123.70(10)	C4_35–Al7–C1_35	59.2(5)
C1_36–Al5–Al6	113.5(3)	C3_35–Al7–C1_35	58.8(5)
C1_1–Al5–Al6	116.11(9)	C5_35–Al7–C1_35	35.0(4)
Al8–Al5–Al6	63.83(3)	C2_35–Al7–C1_35	35.1(4)
C2_36–Al5–Al7	158.9(3)	C3_7–Al7–Al5	108.2(2)
C2_1–Al5–Al7	172.60(10)	C2_7–Al7–Al5	117.9(2)
C1_36–Al5–Al7	161.1(3)	C4_7–Al7–Al5	128.4(2)
C1_1–Al5–Al7	146.31(11)	C4_35–Al7–Al5	142.1(4)
Al8–Al5–Al7	64.57(4)	C1_7–Al7–Al5	150.9(2)
Al6–Al5–Al7	63.70(3)	C5_7–Al7–Al5	164.5(2)
C3_6–Al6–C4_6	36.49(10)	C3_35–Al7–Al5	112.4(4)
C3_6–Al6–C2_6	36.06(10)	C5_35–Al7–Al5	167.8(4)
C4_6–Al6–C2_6	60.48(10)	C2_35–Al7–Al5	109.0(4)
C3_6–Al6–C5_6	60.07(12)	C1_35–Al7–Al5	133.7(4)
C4_6–Al6–C5_6	35.93(11)	C3_7–Al7–Al6	144.8(3)
C2_6–Al6–C5_6	60.03(11)	C2_7–Al7–Al6	116.0(2)
C3_6–Al6–C1_6	59.79(11)	C4_7–Al7–Al6	173.6(2)
C4_6–Al6–C1_6	59.94(11)	C4_35–Al7–Al6	112.7(4)
C2_6–Al6–C1_6	35.88(11)	C1_7–Al7–Al6	113.6(2)
C5_6–Al6–C1_6	35.82(11)	C5_7–Al7–Al6	137.5(2)
C3_6–Al6–Al5	146.85(9)	C3_35–Al7–Al6	120.6(3)
C4_6–Al6–Al5	176.64(9)	C5_35–Al7–Al6	133.4(4)
C2_6–Al6–Al5	122.36(8)	C2_35–Al7–Al6	150.9(4)
C5_6–Al6–Al5	142.80(9)	C1_35–Al7–Al6	168.3(4)
C1_6–Al6–Al5	120.99(9)	Al5–Al7–Al6	57.95(3)
C3_6–Al6–Al8	109.01(9)	C1_37–Al8–C4_37	61.8(6)
C4_6–Al6–Al8	122.49(9)	C1_37–Al8–C2_37	36.9(3)
C2_6–Al6–Al8	125.06(9)	C4_37–Al8–C2_37	61.8(6)

C1_37–Al8–C5_37	36.9(4)	Al11–Al9–Al12	64.01(3)
C4_37–Al8–C5_37	36.8(5)	C4_41–Al10–C3_41	37.2(3)
C2_37–Al8–C5_37	61.5(6)	C4_41–Al10–C5_41	37.0(4)
C1_37–Al8–C3_37	61.6(5)	C3_41–Al10–C5_41	61.5(5)
C4_37–Al8–C3_37	36.9(4)	C5_10–Al10–C4_10	36.24(16)
C2_37–Al8–C3_37	37.0(4)	C5_10–Al10–C1_10	36.29(18)
C5_37–Al8–C3_37	61.4(7)	C4_10–Al10–C1_10	60.55(17)
C3_8–Al8–C2_8	36.7(2)	C5_10–Al10–C2_10	60.32(18)
C3_8–Al8–C4_8	36.4(2)	C4_10–Al10–C2_10	60.26(16)
C2_8–Al8–C4_8	60.2(3)	C1_10–Al10–C2_10	36.35(18)
C3_8–Al8–C5_8	59.6(4)	C5_10–Al10–C3_10	60.33(17)
C2_8–Al8–C5_8	59.3(4)	C4_10–Al10–C3_10	36.24(14)
C4_8–Al8–C5_8	35.0(3)	C1_10–Al10–C3_10	60.42(17)
C3_8–Al8–C1_8	59.5(4)	C2_10–Al10–C3_10	35.93(16)
C2_8–Al8–C1_8	35.4(3)	C4_41–Al10–C2_41	59.7(4)
C4_8–Al8–C1_8	58.5(3)	C3_41–Al10–C2_41	35.4(3)
C5_8–Al8–C1_8	34.9(3)	C5_41–Al10–C2_41	59.3(4)
C1_37–Al8–Al5	127.1(4)	C4_41–Al10–C1_41	59.1(4)
C4_37–Al8–Al5	143.9(5)	C3_41–Al10–C1_41	58.9(4)
C2_37–Al8–Al5	149.4(4)	C5_41–Al10–C1_41	35.1(3)
C5_37–Al8–Al5	125.0(6)	C2_41–Al10–C1_41	34.4(3)
C3_8–Al8–Al5	145.7(3)	C4_41–Al10–Al9	147.4(4)
C3_37–Al8–Al5	171.2(4)	C3_41–Al10–Al9	175.3(4)
C2_8–Al8–Al5	177.6(3)	C5_41–Al10–Al9	121.6(4)
C4_8–Al8–Al5	121.7(2)	C5_10–Al10–Al9	165.11(14)
C5_8–Al8–Al5	121.3(3)	C4_10–Al10–Al9	158.61(13)
C1_8–Al8–Al5	143.7(3)	C1_10–Al10–Al9	135.85(14)
C1_37–Al8–Al6	170.1(5)	C2_10–Al10–Al9	122.16(13)
C4_37–Al8–Al6	119.8(5)	C3_10–Al10–Al9	131.49(12)
C2_37–Al8–Al6	133.8(4)	C2_41–Al10–Al9	141.7(3)
C5_37–Al8–Al6	150.0(5)	C1_41–Al10–Al9	121.1(3)
C3_8–Al8–Al6	143.6(3)	C4_41–Al10–Al11	148.4(4)
C3_37–Al8–Al6	113.1(4)	C3_41–Al10–Al11	117.9(4)
C2_8–Al8–Al6	119.8(3)	C5_41–Al10–Al11	169.6(3)
C4_8–Al8–Al6	179.9(3)	C5_10–Al10–Al11	112.94(13)
C5_8–Al8–Al6	145.0(3)	C4_10–Al10–Al11	129.02(11)
C1_8–Al8–Al6	121.6(3)	C1_10–Al10–Al11	124.57(14)
Al5–Al8–Al6	58.22(3)	C2_10–Al10–Al11	157.07(15)
C2_13–Al9–C1_13	33.44(12)	C3_10–Al10–Al11	163.31(13)
C1_44–Al9–C2_44	33.2(3)	C2_41–Al10–Al11	113.6(3)
C1_44–Al9–Al10	125.2(3)	C1_41–Al10–Al11	134.8(3)
C2_13–Al9–Al10	136.89(10)	Al9–Al10–Al11	58.41(3)
C1_13–Al9–Al10	112.96(9)	C1_39–Al11–C5_39	37.4(4)
C2_44–Al9–Al10	113.1(3)	C1_39–Al11–C4_39	61.2(5)
C1_44–Al9–Al11	122.8(3)	C5_39–Al11–C4_39	36.6(4)
C2_13–Al9–Al11	116.38(9)	C1_39–Al11–C2_39	36.8(4)
C1_13–Al9–Al11	135.02(10)	C5_39–Al11–C2_39	62.0(5)
C2_44–Al9–Al11	151.3(3)	C4_39–Al11–C2_39	61.1(5)
Al10–Al9–Al11	63.53(3)	C1_39–Al11–C3_39	60.4(6)
C1_44–Al9–Al12	169.5(3)	C5_39–Al11–C3_39	60.9(5)
C2_13–Al9–Al12	158.22(10)	C4_39–Al11–C3_39	36.4(4)
C1_13–Al9–Al12	159.20(10)	C2_39–Al11–C3_39	36.0(4)
C2_44–Al9–Al12	142.8(3)	C5_11–Al11–C4_11	35.63(19)
Al10–Al9–Al12	64.27(4)	C5_11–Al11–C1_11	36.0(2)

C4_11–Al11–C1_11	59.3(3)	C3_12–Al12–Al9	166.14(14)
C5_11–Al11–C3_11	59.6(2)	C5_12–Al12–Al9	106.89(15)
C4_11–Al11–C3_11	35.84(17)	C4_12–Al12–Al9	130.52(13)
C1_11–Al11–C3_11	59.0(3)	C1_46–Al12–Al9	165.7(3)
C5_11–Al11–C2_11	59.7(3)	C2_46–Al12–Al9	131.0(2)
C4_11–Al11–C2_11	59.4(2)	C4_46–Al12–Al11	129.1(3)
C1_11–Al11–C2_11	35.4(2)	C5_46–Al12–Al11	119.8(3)
C3_11–Al11–C2_11	35.39(19)	C1_12–Al12–Al11	163.31(17)
C1_39–Al11–Al9	150.4(4)	C2_12–Al12–Al11	156.90(16)
C5_39–Al11–Al9	171.2(5)	C3_46–Al12–Al11	158.4(3)
C4_39–Al11–Al9	136.4(5)	C3_12–Al12–Al11	124.41(14)
C2_39–Al11–Al9	121.9(4)	C5_12–Al12–Al11	129.95(16)
C3_39–Al11–Al9	116.9(5)	C4_12–Al12–Al11	114.59(12)
C5_11–Al11–Al9	123.54(19)	C1_46–Al12–Al11	135.8(2)
C4_11–Al11–Al9	147.87(16)	C2_46–Al12–Al11	166.5(3)
C1_11–Al11–Al9	121.9(2)	Al9–Al12–Al11	57.87(3)
C3_11–Al11–Al9	176.28(17)	C4_13–Al13–Al16	119.35(10)
C2_11–Al11–Al9	143.1(2)	C3_44–Al13–Al16	132.8(3)
C1_39–Al11–Al10	114.2(5)	C4_13–Al13–Al15	122.99(10)
C5_39–Al11–Al10	127.0(5)	C3_44–Al13–Al15	116.9(3)
C4_39–Al11–Al10	159.6(5)	Al16–Al13–Al15	63.74(3)
C2_39–Al11–Al10	128.7(4)	C4_13–Al13–Al14	173.06(9)
C3_39–Al11–Al10	161.7(4)	C3_44–Al13–Al14	162.2(3)
C5_11–Al11–Al10	168.8(2)	Al16–Al13–Al14	64.50(4)
C4_11–Al11–Al10	148.70(17)	Al15–Al13–Al14	63.63(3)
C1_11–Al11–Al10	132.9(2)	C3_42–Al14–C4_42	37.5(3)
C3_11–Al11–Al10	118.44(17)	C4_14–Al14–C3_14	36.96(17)
C2_11–Al11–Al10	111.7(2)	C4_14–Al14–C5_14	36.45(18)
Al9–Al11–Al10	58.07(3)	C3_14–Al14–C5_14	60.90(17)
C4_46–Al12–C5_46	37.6(3)	C3_42–Al14–C5_42	60.6(4)
C1_12–Al12–C2_12	36.7(2)	C4_42–Al14–C5_42	36.1(3)
C4_46–Al12–C3_46	36.6(3)	C4_14–Al14–C2_14	60.43(15)
C5_46–Al12–C3_46	60.8(4)	C3_14–Al14–C2_14	36.09(14)
C1_12–Al12–C3_12	61.0(2)	C5_14–Al14–C2_14	59.87(16)
C2_12–Al12–C3_12	37.13(18)	C3_42–Al14–C2_42	36.4(3)
C1_12–Al12–C5_12	35.56(19)	C4_42–Al14–C2_42	60.9(4)
C2_12–Al12–C5_12	60.5(2)	C5_42–Al14–C2_42	59.2(4)
C3_12–Al12–C5_12	60.47(18)	C4_14–Al14–C1_14	60.18(15)
C1_12–Al12–C4_12	59.1(2)	C3_14–Al14–C1_14	60.06(15)
C2_12–Al12–C4_12	59.99(18)	C5_14–Al14–C1_14	35.87(15)
C3_12–Al12–C4_12	35.77(15)	C2_14–Al14–C1_14	35.46(13)
C5_12–Al12–C4_12	35.50(16)	C3_42–Al14–C1_42	59.9(4)
C4_46–Al12–C1_46	61.6(4)	C4_42–Al14–C1_42	60.1(4)
C5_46–Al12–C1_46	36.9(3)	C5_42–Al14–C1_42	35.5(3)
C3_46–Al12–C1_46	59.5(4)	C2_42–Al14–C1_42	34.9(3)
C4_46–Al12–C2_46	59.8(4)	C3_42–Al14–Al13	147.2(3)
C5_46–Al12–C2_46	59.4(3)	C4_42–Al14–Al13	112.7(3)
C3_46–Al12–C2_46	34.9(3)	C4_14–Al14–Al13	119.31(13)
C1_46–Al12–C2_46	34.7(3)	C3_14–Al14–Al13	107.83(12)
C4_46–Al12–Al9	115.2(3)	C5_14–Al14–Al13	152.88(15)
C5_46–Al12–Al9	148.0(3)	C5_42–Al14–Al13	104.2(3)
C1_12–Al12–Al9	112.79(17)	C2_14–Al14–Al13	127.01(11)
C2_12–Al12–Al9	144.17(16)	C2_42–Al14–Al13	160.6(3)
C3_46–Al12–Al9	109.0(3)	C1_14–Al14–Al13	162.11(11)

C1_42–Al14–Al13	125.7(3)	C2_43–Al16–C1_43	35.6(3)
C3_42–Al14–Al15	154.7(3)	C5_43–Al16–C1_43	35.6(3)
C4_42–Al14–Al15	159.7(3)	C1_16–Al16–C3_16	60.27(16)
C4_14–Al14–Al15	118.40(12)	C5_16–Al16–C3_16	60.09(16)
C3_14–Al14–Al15	145.96(13)	C2_16–Al16–C3_16	35.57(15)
C5_14–Al14–Al15	115.92(13)	C4_16–Al16–C3_16	35.60(13)
C5_42–Al14–Al15	124.9(3)	C1_16–Al16–Al13	145.77(13)
C2_14–Al14–Al15	174.86(11)	C5_16–Al16–Al13	175.67(13)
C2_42–Al14–Al15	121.0(3)	C4_43–Al16–Al13	123.1(4)
C1_14–Al14–Al15	139.40(11)	C3_43–Al16–Al13	138.6(4)
C1_42–Al14–Al15	108.7(3)	C2_16–Al16–Al13	122.97(12)
Al13–Al14–Al15	58.12(3)	C2_43–Al16–Al13	167.2(4)
C4_15–Al15–C5_15	36.25(11)	C5_43–Al16–Al13	132.0(4)
C4_15–Al15–C3_15	35.88(13)	C4_16–Al16–Al13	144.64(12)
C5_15–Al15–C3_15	60.16(11)	C1_43–Al16–Al13	157.0(3)
C4_15–Al15–C1_15	59.86(12)	C3_16–Al16–Al13	123.02(11)
C5_15–Al15–C1_15	35.93(11)	C1_16–Al16–Al15	143.28(14)
C3_15–Al15–C1_15	59.81(12)	C5_16–Al16–Al15	117.26(13)
C4_15–Al15–C2_15	59.54(13)	C4_43–Al16–Al15	164.6(4)
C5_15–Al15–C2_15	59.88(11)	C3_43–Al16–Al15	130.8(4)
C3_15–Al15–C2_15	35.62(13)	C2_16–Al16–Al15	177.80(12)
C1_15–Al15–C2_15	35.90(11)	C2_43–Al16–Al15	114.6(4)
C4_15–Al15–Al13	145.74(10)	C5_43–Al16–Al15	156.1(3)
C5_15–Al15–Al13	121.40(8)	C4_16–Al16–Al15	117.89(11)
C3_15–Al15–Al13	178.32(11)	C1_43–Al16–Al15	124.9(3)
C1_15–Al15–Al13	120.93(9)	C3_16–Al16–Al15	142.44(12)
C2_15–Al15–Al13	144.03(11)	Al13–Al16–Al15	58.41(3)
C4_15–Al15–Al16	111.12(10)	O1_56–Al17–O1_19	122.5(15)
C5_15–Al15–Al16	128.83(9)	O1_21–Al17–O1_45	121.4(6)
C3_15–Al15–Al16	121.94(10)	O1_56–Al17–O1_55	106.2(15)
C1_15–Al15–Al16	163.95(9)	O1_19–Al17–O1_55	109.8(13)
C2_15–Al15–Al16	153.99(10)	O1_24–Al17–O1_17	110.9(6)
Al13–Al15–Al16	57.85(3)	O1_56–Al17–O1_28	117.0(17)
C4_15–Al15–Al14	149.68(10)	O1_19–Al17–O1_28	103.8(14)
C5_15–Al15–Al14	169.76(9)	O1_55–Al17–O1_28	93.8(15)
C3_15–Al15–Al14	120.10(10)	O1_24–Al17–O1_22	108.3(6)
C1_15–Al15–Al14	134.15(9)	O1_17–Al17–O1_22	110.5(7)
C2_15–Al15–Al14	113.67(9)	O1_21–Al17–O1_25	108.5(5)
Al13–Al15–Al14	58.25(3)	O1_45–Al17–O1_25	107.2(8)
Al16–Al15–Al14	60.68(3)	O1_24–Al17–O1_20	112.5(6)
C1_16–Al16–C5_16	37.67(17)	O1_17–Al17–O1_20	109.2(7)
C4_43–Al16–C3_43	36.3(4)	O1_22–Al17–O1_20	105.2(7)
C1_16–Al16–C2_16	36.69(16)	O1_21–Al17–O1_18	108.0(4)
C5_16–Al16–C2_16	61.36(16)	O1_45–Al17–O1_18	104.5(5)
C4_43–Al16–C2_43	60.4(5)	O1_25–Al17–O1_18	106.3(6)
C3_43–Al16–C2_43	36.0(3)	C2_9–Al2–C3_9	37.2(3)
C4_43–Al16–C5_43	36.4(4)	C3_2–Al2–C2_2	36.4(3)
C3_43–Al16–C5_43	59.6(4)	C2_9–Al2–C1_9	36.5(3)
C2_43–Al16–C5_43	59.1(4)	C3_9–Al2–C1_9	60.7(4)
C1_16–Al16–C4_16	60.83(16)	C3_2–Al2–C4_2	36.0(4)
C5_16–Al16–C4_16	35.91(16)	C2_2–Al2–C4_2	60.0(5)
C2_16–Al16–C4_16	59.95(15)	C3_2–Al2–C1_2	60.0(4)
C4_43–Al16–C1_43	60.7(5)	C2_2–Al2–C1_2	35.6(3)
C3_43–Al16–C1_43	59.9(4)	C4_2–Al2–C1_2	59.6(5)

C2_9–Al2–C4_9	60.6(6)	C3_3–C4_3–Al3	69.8(4)
C3_9–Al2–C4_9	36.1(4)	C7_3–C4_3–Al3	128.1(4)
C1_9–Al2–C4_9	59.3(6)	C4_3–C5_3–C1_3	107.4(4)
C3_2–Al2–C5_2	59.8(4)	C4_3–C5_3–C6_3	128.3(6)
C2_2–Al2–C5_2	59.3(4)	C1_3–C5_3–C6_3	124.0(6)
C4_2–Al2–C5_2	35.8(3)	C4_3–C5_3–Al3	72.9(3)
C1_2–Al2–C5_2	35.3(3)	C1_3–C5_3–Al3	69.0(3)
C2_9–Al2–C5_9	60.3(5)	C6_3–C5_3–Al3	127.7(3)
C3_9–Al2–C5_9	59.9(5)	C5_3–C6_3–H6A_3	109.5
C1_9–Al2–C5_9	35.5(4)	C5_3–C6_3–H6B_3	109.5
C4_9–Al2–C5_9	35.1(4)	H6A_3–C6_3–H6B_3	109.5
C2_9–Al2–Al1	171.3(4)	C5_3–C6_3–H6C_3	109.5
C3_9–Al2–Al1	150.9(4)	H6A_3–C6_3–H6C_3	109.5
C3_2–Al2–Al1	122.8(3)	H6B_3–C6_3–H6C_3	109.5
C2_2–Al2–Al1	147.2(3)	C4_3–C7_3–H7A_3	109.5
C1_9–Al2–Al1	137.0(4)	C4_3–C7_3–H7B_3	109.5
C4_2–Al2–Al1	121.8(5)	H7A_3–C7_3–H7B_3	109.5
C1_2–Al2–Al1	177.0(3)	C4_3–C7_3–H7C_3	109.5
C4_9–Al2–Al1	123.8(6)	H7A_3–C7_3–H7C_3	109.5
C5_2–Al2–Al1	144.1(3)	H7B_3–C7_3–H7C_3	109.5
C5_9–Al2–Al1	118.1(4)	C3_3–C8_3–H8A_3	109.5
C2_9–Al2–Al4	126.4(4)	C3_3–C8_3–H8B_3	109.5
C3_9–Al2–Al4	113.5(4)	H8A_3–C8_3–H8B_3	109.5
C3_2–Al2–Al4	162.7(3)	C3_3–C8_3–H8C_3	109.5
C2_2–Al2–Al4	151.4(3)	H8A_3–C8_3–H8C_3	109.5
C1_9–Al2–Al4	159.7(4)	H8B_3–C8_3–H8C_3	109.5
C4_2–Al2–Al4	127.0(4)	C2_3–C9_3–H9A_3	109.5
C1_2–Al2–Al4	118.9(3)	C2_3–C9_3–H9B_3	109.5
C4_9–Al2–Al4	129.0(5)	H9A_3–C9_3–H9B_3	109.5
C5_2–Al2–Al4	108.4(3)	C2_3–C9_3–H9C_3	109.5
C5_9–Al2–Al4	161.5(4)	H9A_3–C9_3–H9C_3	109.5
Al1–Al2–Al4	58.10(3)	H9B_3–C9_3–H9C_3	109.5
C2_3–C1_3–C5_3	107.7(4)	C1_3–C10_3–H10A_3	109.5
C2_3–C1_3–C10_3	127.8(6)	C1_3–C10_3–H10B_3	109.5
C5_3–C1_3–C10_3	124.3(6)	H10A_3–C10_3–H10B_3	109.5
C2_3–C1_3–Al3	69.8(4)		
C5_3–C1_3–Al3	74.6(3)	C1_3–C10_3–H10C_3	109.5
C10_3–C1_3–Al3	125.3(4)	H10A_3–C10_3–H10C_3	109.5
C1_3–C2_3–C3_3	108.4(5)		
C1_3–C2_3–C9_3	129.4(7)	H10B_3–C10_3–H10C_3	109.5
C3_3–C2_3–C9_3	122.2(7)		
C1_3–C2_3–Al3	73.0(3)	C2_4–C1_4–C5_4	109.1(8)
C3_3–C2_3–Al3	74.1(4)	C2_4–C1_4–C10_4	128.7(8)
C9_3–C2_3–Al3	120.0(5)	C5_4–C1_4–C10_4	122.2(8)
C4_3–C3_3–C2_3	107.1(5)	C2_4–C1_4–Al4	72.1(5)
C4_3–C3_3–C8_3	123.5(7)	C5_4–C1_4–Al4	69.9(5)
C2_3–C3_3–C8_3	129.4(7)	C10_4–C1_4–Al4	125.2(7)
C4_3–C3_3–Al3	74.5(3)	C1_4–C2_4–C3_4	107.6(8)
C2_3–C3_3–Al3	68.8(4)	C1_4–C2_4–C9_4	126.8(9)
C8_3–C3_3–Al3	123.9(6)	C3_4–C2_4–C9_4	125.5(9)
C5_3–C4_3–C3_3	109.4(5)	C1_4–C2_4–Al4	72.5(5)
C5_3–C4_3–C7_3	126.5(6)	C3_4–C2_4–Al4	70.2(5)
C3_3–C4_3–C7_3	123.9(6)	C9_4–C2_4–Al4	124.2(8)
C5_3–C4_3–Al3	71.8(3)	C2_4–C3_4–C4_4	108.4(9)

C2_4–C3_4–C8_4	122.7(9)
C4_4–C3_4–C8_4	128.8(10)
C2_4–C3_4–Al4	73.8(5)
C4_4–C3_4–Al4	70.1(6)
C8_4–C3_4–Al4	124.5(9)
C3_4–C4_4–C5_4	108.1(8)
C3_4–C4_4–C7_4	125.6(9)
C5_4–C4_4–C7_4	126.3(9)
C3_4–C4_4–Al4	73.0(7)
C5_4–C4_4–Al4	72.9(6)
C7_4–C4_4–Al4	122.2(7)
C4_4–C5_4–C1_4	106.7(7)
C4_4–C5_4–C6_4	126.6(10)
C1_4–C5_4–C6_4	126.4(9)
C4_4–C5_4–Al4	70.1(6)
C1_4–C5_4–Al4	73.8(5)
C6_4–C5_4–Al4	125.8(7)
C5_4–C6_4–H6A_4	109.5
C5_4–C6_4–H6B_4	109.5
H6A_4–C6_4–H6B_4	109.5
C5_4–C6_4–H6C_4	109.5
H6A_4–C6_4–H6C_4	109.5
H6B_4–C6_4–H6C_4	109.5
C4_4–C7_4–H7A_4	109.5
C4_4–C7_4–H7B_4	109.5
H7A_4–C7_4–H7B_4	109.5
C4_4–C7_4–H7C_4	109.5
H7A_4–C7_4–H7C_4	109.5
H7B_4–C7_4–H7C_4	109.5
C3_4–C8_4–H8A_4	109.5
C3_4–C8_4–H8B_4	109.5
H8A_4–C8_4–H8B_4	109.5
C3_4–C8_4–H8C_4	109.5
H8A_4–C8_4–H8C_4	109.5
H8B_4–C8_4–H8C_4	109.5
C2_4–C9_4–H9A_4	109.5
C2_4–C9_4–H9B_4	109.5
H9A_4–C9_4–H9B_4	109.5
C2_4–C9_4–H9C_4	109.5
H9A_4–C9_4–H9C_4	109.5
H9B_4–C9_4–H9C_4	109.5
C1_4–C10_4–H10A_4	109.5
C1_4–C10_4–H10B_4	109.5
H10A_4–C10_4–H10B_4	109.5
C1_4–C10_4–H10C_4	109.5
H10A_4–C10_4–H10C_4	109.5
H10B_4–C10_4–H10C_4	109.5
C2_2–C1_2–C5_2	107.9(7)
C2_2–C1_2–C10_2	123.6(8)
C5_2–C1_2–C10_2	128.4(8)
C2_2–C1_2–Al2	70.6(5)
C5_2–C1_2–Al2	72.6(6)
C10_2–C1_2–Al2	123.8(7)
C1_2–C2_2–C3_2	108.6(7)
C1_2–C2_2–C9_2	127.6(8)
C3_2–C2_2–C9_2	123.5(9)
C1_2–C2_2–Al2	73.8(5)
C3_2–C2_2–Al2	71.7(6)
C9_2–C2_2–Al2	125.4(7)
C4_2–C3_2–C2_2	107.2(8)
C4_2–C3_2–C8_2	127.4(10)
C2_2–C3_2–C8_2	125.4(9)
C4_2–C3_2–Al2	72.4(12)
C2_2–C3_2–Al2	71.9(5)
C8_2–C3_2–Al2	120.4(10)
C3_2–C4_2–C5_2	108.4(8)
C3_2–C4_2–C7_2	128.3(10)
C5_2–C4_2–C7_2	123.3(10)
C3_2–C4_2–Al2	71.6(10)
C5_2–C4_2–Al2	73.7(10)
C7_2–C4_2–Al2	122.6(17)
C1_2–C5_2–C4_2	107.9(7)
C1_2–C5_2–C6_2	127.2(8)
C4_2–C5_2–C6_2	124.5(9)
C1_2–C5_2–Al2	72.0(6)
C4_2–C5_2–Al2	70.5(11)
C6_2–C5_2–Al2	128.4(10)
C5_2–C6_2–H6A_2	109.5
C5_2–C6_2–H6B_2	109.5
H6A_2–C6_2–H6B_2	109.5
C5_2–C6_2–H6C_2	109.5
H6A_2–C6_2–H6C_2	109.5
H6B_2–C6_2–H6C_2	109.5
C4_2–C7_2–H7A_2	109.5
C4_2–C7_2–H7B_2	109.5
H7A_2–C7_2–H7B_2	109.5
C4_2–C7_2–H7C_2	109.5
H7A_2–C7_2–H7C_2	109.5
H7B_2–C7_2–H7C_2	109.5
C3_2–C8_2–H8A_2	109.5
C3_2–C8_2–H8B_2	109.5
H8A_2–C8_2–H8B_2	109.5
C3_2–C8_2–H8C_2	109.5
H8A_2–C8_2–H8C_2	109.5
H8B_2–C8_2–H8C_2	109.5
C2_2–C9_2–H9A_2	109.5
C2_2–C9_2–H9B_2	109.5
H9A_2–C9_2–H9B_2	109.5
C2_2–C9_2–H9C_2	109.5
H9A_2–C9_2–H9C_2	109.5
H9B_2–C9_2–H9C_2	109.5
C1_2–C10_2–H10A_2	109.5
C1_2–C10_2–H10B_2	109.5
H10A_2–C10_2–H10B_2	109.5

C1_2–C10_2–H10C_2	109.5	C2_6–C9_6–H9B_6	109.5
H10A_2–C10_2–H10C_2	109.5	H9A_6–C9_6–H9B_6	109.5
		C2_6–C9_6–H9C_6	109.5
H10B_2–C10_2–H10C_2	109.5	H9A_6–C9_6–H9C_6	109.5
		H9B_6–C9_6–H9C_6	109.5
C2_6–C1_6–C5_6	108.1(3)	C1_6–C10_6–H10A_6	109.5
C2_6–C1_6–C10_6	127.2(3)	C1_6–C10_6–H10B_6	109.5
C5_6–C1_6–C10_6	124.7(3)	H10A_6–C10_6–H10B_6	109.5
C2_6–C1_6–Al6	70.95(16)		
C5_6–C1_6–Al6	71.88(17)	C1_6–C10_6–H10C_6	109.5
C10_6–C1_6–Al6	124.5(2)	H10A_6–C10_6–H10C_6	109.5
C3_6–C2_6–C1_6	107.7(3)		
C3_6–C2_6–C9_6	124.8(3)	H10B_6–C10_6–H10C_6	109.5
C1_6–C2_6–C9_6	127.4(3)		
C3_6–C2_6–Al6	71.01(16)	C5_7–C1_7–C2_7	107.8(6)
C1_6–C2_6–Al6	73.17(16)	C5_7–C1_7–C10_7	125.2(6)
C9_6–C2_6–Al6	122.8(2)	C2_7–C1_7–C10_7	127.0(6)
C2_6–C3_6–C4_6	108.7(3)	C5_7–C1_7–Al7	72.5(7)
C2_6–C3_6–C8_6	125.2(3)	C2_7–C1_7–Al7	69.3(4)
C4_6–C3_6–C8_6	126.0(3)	C10_7–C1_7–Al7	126.4(7)
C2_6–C3_6–Al6	72.93(16)	C1_7–C2_7–C3_7	107.6(6)
C4_6–C3_6–Al6	72.44(17)	C1_7–C2_7–C9_7	129.2(7)
C8_6–C3_6–Al6	124.4(2)	C3_7–C2_7–C9_7	123.2(7)
C5_6–C4_6–C3_6	107.5(3)	C1_7–C2_7–Al7	74.1(4)
C5_6–C4_6–C7_6	127.0(3)	C3_7–C2_7–Al7	71.2(4)
C3_6–C4_6–C7_6	125.4(3)	C9_7–C2_7–Al7	120.4(6)
C5_6–C4_6–Al6	73.19(17)	C4_7–C3_7–C2_7	108.5(6)
C3_6–C4_6–Al6	71.07(16)	C4_7–C3_7–C8_7	123.8(7)
C7_6–C4_6–Al6	123.9(2)	C2_7–C3_7–C8_7	127.7(7)
C4_6–C5_6–C1_6	108.0(3)	C4_7–C3_7–Al7	73.1(5)
C4_6–C5_6–C6_6	127.2(3)	C2_7–C3_7–Al7	71.6(4)
C1_6–C5_6–C6_6	124.6(3)	C8_7–C3_7–Al7	123.8(7)
C4_6–C5_6–Al6	70.88(17)	C3_7–C4_7–C5_7	107.6(6)
C1_6–C5_6–Al6	72.31(17)	C3_7–C4_7–C7_7	126.7(7)
C6_6–C5_6–Al6	126.8(2)	C5_7–C4_7–C7_7	125.4(7)
C5_6–C6_6–H6A_6	109.5	C3_7–C4_7–Al7	70.3(5)
C5_6–C6_6–H6B_6	109.5	C5_7–C4_7–Al7	73.6(7)
H6A_6–C6_6–H6B_6	109.5	C7_7–C4_7–Al7	126.5(8)
C5_6–C6_6–H6C_6	109.5	C1_7–C5_7–C4_7	108.6(6)
H6A_6–C6_6–H6C_6	109.5	C1_7–C5_7–C6_7	121.7(7)
H6B_6–C6_6–H6C_6	109.5	C4_7–C5_7–C6_7	129.3(7)
C4_6–C7_6–H7A_6	109.5	C1_7–C5_7–Al7	71.6(6)
C4_6–C7_6–H7B_6	109.5	C4_7–C5_7–Al7	70.2(7)
H7A_6–C7_6–H7B_6	109.5	C6_7–C5_7–Al7	129.9(10)
C4_6–C7_6–H7C_6	109.5	C5_7–C6_7–H6A_7	109.5
H7A_6–C7_6–H7C_6	109.5	C5_7–C6_7–H6B_7	109.5
H7B_6–C7_6–H7C_6	109.5	H6A_7–C6_7–H6B_7	109.5
C3_6–C8_6–H8A_6	109.5	C5_7–C6_7–H6C_7	109.5
C3_6–C8_6–H8B_6	109.5	H6A_7–C6_7–H6C_7	109.5
H8A_6–C8_6–H8B_6	109.5	H6B_7–C6_7–H6C_7	109.5
C3_6–C8_6–H8C_6	109.5	C4_7–C7_7–H7A_7	109.5
H8A_6–C8_6–H8C_6	109.5	C4_7–C7_7–H7B_7	109.5
H8B_6–C8_6–H8C_6	109.5	H7A_7–C7_7–H7B_7	109.5
C2_6–C9_6–H9A_6	109.5	C4_7–C7_7–H7C_7	109.5

H7A_7–C7_7–H7C_7	109.5	C5_8–C6_8–H6B_8	109.5
H7B_7–C7_7–H7C_7	109.5	H6A_8–C6_8–H6B_8	109.5
C3_7–C8_7–H8A_7	109.5	C5_8–C6_8–H6C_8	109.5
C3_7–C8_7–H8B_7	109.5	H6A_8–C6_8–H6C_8	109.5
H8A_7–C8_7–H8B_7	109.5	H6B_8–C6_8–H6C_8	109.5
C3_7–C8_7–H8C_7	109.5	C4_8–C7_8–H7A_8	109.5
H8A_7–C8_7–H8C_7	109.5	C4_8–C7_8–H7B_8	109.5
H8B_7–C8_7–H8C_7	109.5	H7A_8–C7_8–H7B_8	109.5
C2_7–C9_7–H9A_7	109.5	C4_8–C7_8–H7C_8	109.5
C2_7–C9_7–H9B_7	109.5	H7A_8–C7_8–H7C_8	109.5
H9A_7–C9_7–H9B_7	109.5	H7B_8–C7_8–H7C_8	109.5
C2_7–C9_7–H9C_7	109.5	C3_8–C8_8–H8A_8	109.5
H9A_7–C9_7–H9C_7	109.5	C3_8–C8_8–H8B_8	109.5
H9B_7–C9_7–H9C_7	109.5	H8A_8–C8_8–H8B_8	109.5
C1_7–C10_7–H10A_7	109.5	C3_8–C8_8–H8C_8	109.5
C1_7–C10_7–H10B_7	109.5	H8A_8–C8_8–H8C_8	109.5
H10A_7–C10_7–H10B_7	109.5	H8B_8–C8_8–H8C_8	109.5
C1_7–C10_7–H10C_7	109.5	C2_8–C9_8–H9A_8	109.5
H10A_7–C10_7–H10C_7	109.5	C2_8–C9_8–H9B_8	109.5
H10B_7–C10_7–H10C_7	109.5	H9A_8–C9_8–H9B_8	109.5
C5_8–C1_8–C2_8	108.5(7)	C2_8–C9_8–H9C_8	109.5
C5_8–C1_8–C10_8	123.1(9)	H9A_8–C9_8–H9C_8	109.5
C2_8–C1_8–C10_8	128.2(9)	H9B_8–C9_8–H9C_8	109.5
C5_8–C1_8–Al8	72.4(8)	C1_8–C10_8–H10A_8	109.5
C2_8–C1_8–Al8	69.0(5)	C1_8–C10_8–H10B_8	109.5
C10_8–C1_8–Al8	128.0(10)	H10A_8–C10_8–H10B_8	109.5
C1_8–C2_8–C3_8	107.5(6)	C1_8–C10_8–H10C_8	109.5
C1_8–C2_8–C9_8	126.7(8)	H10A_8–C10_8–H10C_8	109.5
C3_8–C2_8–C9_8	125.8(8)	H10B_8–C10_8–H10C_8	109.5
C1_8–C2_8–Al8	75.6(6)	C2_1–C1_1–C5_1	108.2(3)
C3_8–C2_8–Al8	70.5(4)	C2_1–C1_1–C10_1	126.5(4)
C9_8–C2_8–Al8	120.9(8)	C5_1–C1_1–C10_1	125.2(4)
C4_8–C3_8–C2_8	107.4(6)	C2_1–C1_1–Al5	71.1(2)
C4_8–C3_8–C8_8	128.1(6)	C5_1–C1_1–Al5	79.6(2)
C2_8–C3_8–C8_8	124.5(7)	C10_1–C1_1–Al5	117.2(3)
C4_8–C3_8–Al8	73.3(5)	C3_1–C2_1–C1_1	108.1(3)
C2_8–C3_8–Al8	72.8(5)	C3_1–C2_1–C9_1	125.7(4)
C8_8–C3_8–Al8	119.7(6)	C1_1–C2_1–C9_1	126.1(4)
C5_8–C4_8–C3_8	108.8(6)	C3_1–C2_1–Al5	78.5(2)
C5_8–C4_8–C7_8	127.3(7)	C1_1–C2_1–Al5	75.6(2)
C3_8–C4_8–C7_8	123.9(7)	C9_1–C2_1–Al5	109.8(2)
C5_8–C4_8–Al8	75.2(7)	C2_1–C3_1–C4_1	108.3(3)
C3_8–C4_8–Al8	70.3(4)	C2_1–C3_1–C8_1	126.8(4)
C7_8–C4_8–Al8	121.2(7)	C4_1–C3_1–C8_1	124.9(4)
C4_8–C5_8–C1_8	107.8(6)	C3_1–C4_1–C5_1	108.1(3)
C4_8–C5_8–C6_8	128.4(7)	C3_1–C4_1–C7_1	124.5(4)
C1_8–C5_8–C6_8	123.5(8)	C5_1–C4_1–C7_1	127.4(4)
C4_8–C5_8–Al8	69.7(6)	C3_1–C4_1–Al1	79.8(2)
C1_8–C5_8–Al8	72.8(7)	C5_1–C4_1–Al1	72.3(2)
C6_8–C5_8–Al8	127.6(11)	C7_1–C4_1–Al1	113.6(2)
C5_8–C6_8–H6A_8	109.5	C4_1–C5_1–C1_1	107.3(3)

C4_1–C5_1–C6_1	126.6(4)
C1_1–C5_1–C6_1	126.1(4)
C4_1–C5_1–Al1	74.3(2)
C1_1–C5_1–Al1	79.0(2)
C6_1–C5_1–Al1	113.6(3)
C5_1–C6_1–H6A_1	109.5
C5_1–C6_1–H6B_1	109.5
H6A_1–C6_1–H6B_1	109.5
C5_1–C6_1–H6C_1	109.5
H6A_1–C6_1–H6C_1	109.5
H6B_1–C6_1–H6C_1	109.5
C4_1–C7_1–H7A_1	109.5
C4_1–C7_1–H7B_1	109.5
H7A_1–C7_1–H7B_1	109.5
C4_1–C7_1–H7C_1	109.5
H7A_1–C7_1–H7C_1	109.5
H7B_1–C7_1–H7C_1	109.5
C3_1–C8_1–H8A_1	109.5
C3_1–C8_1–H8B_1	109.5
H8A_1–C8_1–H8B_1	109.5
C3_1–C8_1–H8C_1	109.5
H8A_1–C8_1–H8C_1	109.5
H8B_1–C8_1–H8C_1	109.5
C2_1–C9_1–H9A_1	109.5
C2_1–C9_1–H9B_1	109.5
H9A_1–C9_1–H9B_1	109.5
C2_1–C9_1–H9C_1	109.5
H9A_1–C9_1–H9C_1	109.5
H9B_1–C9_1–H9C_1	109.5
C1_1–C10_1–H10A_1	109.5
C1_1–C10_1–H10B_1	109.5
H10A_1–C10_1–H10B_1	109.5
C1_1–C10_1–H10C_1	109.5
H10A_1–C10_1–H10C_1	109.5
H10B_1–C10_1–H10C_1	109.5
C5_10–C1_10–C2_10	107.3(4)
C5_10–C1_10–C10_10	126.4(6)
C2_10–C1_10–C10_10	126.3(6)
C5_10–C1_10–Al10	71.3(3)
C2_10–C1_10–Al10	72.1(3)
C10_10–C1_10–Al10	123.2(3)
C3_10–C2_10–C1_10	108.3(4)
C3_10–C2_10–C9_10	125.3(6)
C1_10–C2_10–C9_10	126.3(6)
C3_10–C2_10–Al10	72.1(3)
C1_10–C2_10–Al10	71.6(3)
C9_10–C2_10–Al10	125.7(4)
C2_10–C3_10–C4_10	108.0(4)
C2_10–C3_10–C8_10	124.4(5)
C4_10–C3_10–C8_10	127.5(5)
C2_10–C3_10–Al10	72.0(3)
C4_10–C3_10–Al10	71.5(2)
C8_10–C3_10–Al10	123.6(3)
C5_10–C4_10–C3_10	107.8(4)
C5_10–C4_10–C7_10	125.8(5)
C3_10–C4_10–C7_10	126.4(5)
C5_10–C4_10–Al10	71.5(3)
C3_10–C4_10–Al10	72.3(2)
C7_10–C4_10–Al10	121.9(3)
C4_10–C5_10–C1_10	108.6(4)
C4_10–C5_10–C6_10	122.7(5)
C1_10–C5_10–C6_10	128.4(5)
C4_10–C5_10–Al10	72.3(3)
C1_10–C5_10–Al10	72.4(3)
C6_10–C5_10–Al10	126.1(4)
C5_10–C6_10–H6A_10	109.5
C5_10–C6_10–H6B_10	109.5
H6A_10–C6_10–H6B_10	109.5
C5_10–C6_10–H6C_10	109.5
H6A_10–C6_10–H6C_10	109.5
H6B_10–C6_10–H6C_10	109.5
C4_10–C7_10–H7A_10	109.5
C4_10–C7_10–H7B_10	109.5
H7A_10–C7_10–H7B_10	109.5
C4_10–C7_10–H7C_10	109.5
H7A_10–C7_10–H7C_10	109.5
H7B_10–C7_10–H7C_10	109.5
C3_10–C8_10–H8A_10	109.5
C3_10–C8_10–H8B_10	109.5
H8A_10–C8_10–H8B_10	109.5
C3_10–C8_10–H8C_10	109.5
H8A_10–C8_10–H8C_10	109.5
H8B_10–C8_10–H8C_10	109.5
C2_10–C9_10–H9A_10	109.5
C2_10–C9_10–H9B_10	109.5
H9A_10–C9_10–H9B_10	109.5
C2_10–C9_10–H9C_10	109.5
H9A_10–C9_10–H9C_10	109.5
H9B_10–C9_10–H9C_10	109.5
C1_10–C10_10–H10A_10	109.5
C1_10–C10_10–H10B_10	109.5

H10A_10–C10_10–H10B_10	109.5
C1_10–C10_10–H10C_10	109.5
H10A_10–C10_10–H10C_10	109.5
H10B_10–C10_10–H10C_10	109.5
C2_11–C1_11–C5_11	108.7(6)
C2_11–C1_11–C10_11	124.5(7)
C5_11–C1_11–C10_11	126.6(7)
C2_11–C1_11–Al11	73.2(4)
C5_11–C1_11–Al11	71.7(4)
C10_11–C1_11–Al11	124.6(6)
C1_11–C2_11–C3_11	107.6(5)
C1_11–C2_11–C9_11	126.2(6)
C3_11–C2_11–C9_11	126.0(6)
C1_11–C2_11–Al11	71.4(4)
C3_11–C2_11–Al11	71.9(4)
C9_11–C2_11–Al11	127.1(6)
C2_11–C3_11–C4_11	108.0(5)
C2_11–C3_11–C8_11	129.3(5)
C4_11–C3_11–C8_11	122.6(5)
C2_11–C3_11–Al11	72.7(4)
C4_11–C3_11–Al11	71.4(4)
C8_11–C3_11–Al11	123.8(5)
C5_11–C4_11–C3_11	108.4(5)
C5_11–C4_11–C7_11	126.6(6)
C3_11–C4_11–C7_11	124.8(5)
C5_11–C4_11–Al11	72.2(4)
C3_11–C4_11–Al11	72.8(4)
C7_11–C4_11–Al11	125.4(5)
C4_11–C5_11–C1_11	107.2(5)
C4_11–C5_11–C6_11	127.5(6)
C1_11–C5_11–C6_11	125.2(6)
C4_11–C5_11–Al11	72.2(4)
C1_11–C5_11–Al11	72.3(4)
C6_11–C5_11–Al11	120.1(6)
C5_11–C6_11–H6A_11	109.5
C5_11–C6_11–H6B_11	109.5
H6A_11–C6_11–H6B_11	109.5
C5_11–C6_11–H6C_11	109.5
H6A_11–C6_11–H6C_11	109.5
H6B_11–C6_11–H6C_11	109.5
C4_11–C7_11–H7A_11	109.5
C4_11–C7_11–H7B_11	109.5
H7A_11–C7_11–H7B_11	109.5
C4_11–C7_11–H7C_11	109.5
H7A_11–C7_11–H7C_11	109.5
H7B_11–C7_11–H7C_11	109.5
C3_11–C8_11–H8A_11	109.5
C3_11–C8_11–H8B_11	109.5
H8A_11–C8_11–H8B_11	109.5
C3_11–C8_11–H8C_11	109.5
H8A_11–C8_11–H8C_11	109.5
H8B_11–C8_11–H8C_11	109.5
C2_11–C9_11–H9A_11	109.5
C2_11–C9_11–H9B_11	109.5
H9A_11–C9_11–H9B_11	109.5
C2_11–C9_11–H9C_11	109.5
H9A_11–C9_11–H9C_11	109.5
H9B_11–C9_11–H9C_11	109.5
C1_11–C10_11–H10A_11	109.5
C1_11–C10_11–H10B_11	109.5
H10A_11–C10_11–H10B_11	109.5
C1_11–C10_11–H10C_11	109.5
H10A_11–C10_11–H10C_11	109.5
H10B_11–C10_11–H10C_11	109.5
C5_12–C1_12–C2_12	109.7(5)
C5_12–C1_12–C10_12	124.3(6)
C2_12–C1_12–C10_12	126.0(6)
C5_12–C1_12–Al12	74.4(4)
C2_12–C1_12–Al12	71.9(3)
C10_12–C1_12–Al12	119.8(5)
C1_12–C2_12–C3_12	107.0(5)
C1_12–C2_12–C9_12	126.1(6)
C3_12–C2_12–C9_12	126.5(6)
C1_12–C2_12–Al12	71.4(3)
C3_12–C2_12–Al12	72.7(3)
C9_12–C2_12–Al12	126.7(4)
C4_12–C3_12–C2_12	105.9(4)
C4_12–C3_12–C8_12	126.5(5)
C2_12–C3_12–C8_12	127.3(6)
C4_12–C3_12–Al12	72.9(3)
C2_12–C3_12–Al12	70.2(3)
C8_12–C3_12–Al12	125.4(3)
C5_12–C4_12–C3_12	110.2(4)
C5_12–C4_12–C7_12	123.4(5)
C3_12–C4_12–C7_12	126.2(5)
C5_12–C4_12–Al12	72.0(3)

C3_12–C4_12–Al12	71.3(3)
C7_12–C4_12–Al12	127.0(3)
C1_12–C5_12–C4_12	107.1(5)
C1_12–C5_12–C6_12	129.4(5)
C4_12–C5_12–C6_12	123.5(5)
C1_12–C5_12–Al12	70.1(4)
C4_12–C5_12–Al12	72.5(3)
C6_12–C5_12–Al12	123.1(5)
C5_12–C6_12–H6A_12	109.5
C5_12–C6_12–H6B_12	109.5
H6A_12–C6_12–H6B_12	109.5
C5_12–C6_12–H6C_12	109.5
H6A_12–C6_12–H6C_12	109.5
H6B_12–C6_12–H6C_12	109.5
C4_12–C7_12–H7A_12	109.5
C4_12–C7_12–H7B_12	109.5
H7A_12–C7_12–H7B_12	109.5
C4_12–C7_12–H7C_12	109.5
H7A_12–C7_12–H7C_12	109.5
H7B_12–C7_12–H7C_12	109.5
C3_12–C8_12–H8A_12	109.5
C3_12–C8_12–H8B_12	109.5
H8A_12–C8_12–H8B_12	109.5
C3_12–C8_12–H8C_12	109.5
H8A_12–C8_12–H8C_12	109.5
H8B_12–C8_12–H8C_12	109.5
C2_12–C9_12–H9A_12	109.5
C2_12–C9_12–H9B_12	109.5
H9A_12–C9_12–H9B_12	109.5
C2_12–C9_12–H9C_12	109.5
H9A_12–C9_12–H9C_12	109.5
H9B_12–C9_12–H9C_12	109.5
C1_12–C10_12–H10A_12	109.5
C1_12–C10_12–H10B_12	109.5
H10A_12–C10_12–H10B_12	109.5
C1_12–C10_12–H10C_12	109.5
H10A_12–C10_12–H10C_12	109.5
H10B_12–C10_12–H10C_12	109.5
C2_14–C1_14–C5_14	107.6(4)
C2_14–C1_14–C10_14	128.0(4)
C5_14–C1_14–C10_14	124.2(4)
C2_14–C1_14–Al14	71.4(2)
C5_14–C1_14–Al14	69.7(3)
C10_14–C1_14–Al14	128.6(3)
C1_14–C2_14–C3_14	108.5(4)
C1_14–C2_14–C9_14	126.2(4)
C3_14–C2_14–C9_14	125.2(4)
C1_14–C2_14–Al14	73.1(2)
C3_14–C2_14–Al14	69.9(2)
C9_14–C2_14–Al14	124.4(3)
C2_14–C3_14–C4_14	107.4(4)
C2_14–C3_14–C8_14	124.9(5)
C4_14–C3_14–C8_14	127.7(5)
C2_14–C3_14–Al14	74.0(2)
C4_14–C3_14–Al14	70.6(3)
C8_14–C3_14–Al14	122.6(3)
C5_14–C4_14–C3_14	108.2(4)
C5_14–C4_14–C7_14	128.3(5)
C3_14–C4_14–C7_14	123.5(5)
C5_14–C4_14–Al14	73.2(3)
C3_14–C4_14–Al14	72.4(3)
C7_14–C4_14–Al14	118.9(3)
C4_14–C5_14–C1_14	108.2(4)
C4_14–C5_14–C6_14	127.8(5)
C1_14–C5_14–C6_14	123.6(5)
C4_14–C5_14–Al14	70.3(3)
C1_14–C5_14–Al14	74.5(3)
C6_14–C5_14–Al14	127.0(4)
C5_14–C6_14–H6A_14	109.5
C5_14–C6_14–H6B_14	109.5
H6A_14–C6_14–H6B_14	109.5
C5_14–C6_14–H6C_14	109.5
H6A_14–C6_14–H6C_14	109.5
H6B_14–C6_14–H6C_14	109.5
C4_14–C7_14–H7A_14	109.5
C4_14–C7_14–H7B_14	109.5
H7A_14–C7_14–H7B_14	109.5
C4_14–C7_14–H7C_14	109.5
H7A_14–C7_14–H7C_14	109.5
H7B_14–C7_14–H7C_14	109.5
C3_14–C8_14–H8A_14	109.5
C3_14–C8_14–H8B_14	109.5
H8A_14–C8_14–H8B_14	109.5

C3_14–C8_14–H8C_14	109.5
H8A_14–C8_14–H8C_14	109.5
H8B_14–C8_14–H8C_14	109.5
C2_14–C9_14–H9A_14	109.5
C2_14–C9_14–H9B_14	109.5
H9A_14–C9_14–H9B_14	109.5
C2_14–C9_14–H9C_14	109.5
H9A_14–C9_14–H9C_14	109.5
H9B_14–C9_14–H9C_14	109.5
C1_14–C10_14–H10A_14	109.5
C1_14–C10_14–H10B_14	109.5
H10A_14–C10_14–H10B_14	109.5
C1_14–C10_14–H10C_14	109.5
H10A_14–C10_14–H10C_14	109.5
H10B_14–C10_14–H10C_14	109.5
C5_15–C1_15–C2_15	107.8(3)
C5_15–C1_15–C10_15	127.3(3)
C2_15–C1_15–C10_15	124.9(3)
C5_15–C1_15–Al15	71.30(17)
C2_15–C1_15–Al15	72.23(17)
C10_15–C1_15–Al15	123.1(2)
C3_15–C2_15–C1_15	108.3(3)
C3_15–C2_15–C9_15	126.5(4)
C1_15–C2_15–C9_15	125.1(4)
C3_15–C2_15–Al15	71.78(18)
C1_15–C2_15–Al15	71.86(17)
C9_15–C2_15–Al15	125.1(2)
C2_15–C3_15–C4_15	107.8(3)
C2_15–C3_15–C8_15	125.1(4)
C4_15–C3_15–C8_15	127.0(4)
C2_15–C3_15–Al15	72.60(18)
C4_15–C3_15–Al15	71.34(18)
C8_15–C3_15–Al15	123.7(2)
C3_15–C4_15–C5_15	108.5(3)
C3_15–C4_15–C7_15	126.3(4)
C5_15–C4_15–C7_15	125.0(4)
C3_15–C4_15–Al15	72.78(19)
C5_15–C4_15–Al15	72.08(17)
C7_15–C4_15–Al15	124.8(2)
C1_15–C5_15–C4_15	107.5(3)
C1_15–C5_15–C6_15	127.4(3)
C4_15–C5_15–C6_15	125.0(3)
C1_15–C5_15–Al15	72.77(17)
C4_15–C5_15–Al15	71.67(17)
C6_15–C5_15–Al15	123.1(2)
C5_15–C6_15–H6A_15	109.5
C5_15–C6_15–H6B_15	109.5
H6A_15–C6_15–H6B_15	109.5
C5_15–C6_15–H6C_15	109.5
H6A_15–C6_15–H6C_15	109.5
H6B_15–C6_15–H6C_15	109.5
C4_15–C7_15–H7A_15	109.5
C4_15–C7_15–H7B_15	109.5
H7A_15–C7_15–H7B_15	109.5
C4_15–C7_15–H7C_15	109.5
H7A_15–C7_15–H7C_15	109.5
H7B_15–C7_15–H7C_15	109.5
C3_15–C8_15–H8A_15	109.5
C3_15–C8_15–H8B_15	109.5
H8A_15–C8_15–H8B_15	109.5
C3_15–C8_15–H8C_15	109.5
H8A_15–C8_15–H8C_15	109.5
H8B_15–C8_15–H8C_15	109.5
C2_15–C9_15–H9A_15	109.5
C2_15–C9_15–H9B_15	109.5
H9A_15–C9_15–H9B_15	109.5
C2_15–C9_15–H9C_15	109.5
H9A_15–C9_15–H9C_15	109.5
H9B_15–C9_15–H9C_15	109.5
C1_15–C10_15–H10A_15	109.5
C1_15–C10_15–H10B_15	109.5
H10A_15–C10_15–H10B_15	109.5
C1_15–C10_15–H10C_15	109.5
H10A_15–C10_15–H10C_15	109.5
H10B_15–C10_15–H10C_15	109.5
C2_16–C1_16–C5_16	107.7(4)
C2_16–C1_16–C10_16	126.5(5)
C5_16–C1_16–C10_16	125.8(5)
C2_16–C1_16–Al16	73.9(2)

C5_16–C1_16–Al16	72.1(3)	C2_16–C9_16–H9B_16	109.5
C10_16–C1_16–Al16	121.0(3)	H9A_16–C9_16–H9B_16	109.5
C3_16–C2_16–C1_16	108.3(4)	C2_16–C9_16–H9C_16	109.5
C3_16–C2_16–C9_16	127.9(5)	H9A_16–C9_16–H9C_16	109.5
C1_16–C2_16–C9_16	123.8(5)	H9B_16–C9_16–H9C_16	109.5
C3_16–C2_16–Al16	74.7(2)	C1_16–C10_16–H10A_16	109.5
C1_16–C2_16–Al16	69.4(2)	C1_16–C10_16–H10B_16	109.5
C9_16–C2_16–Al16	122.2(3)	H10A_16–C10_16–H10B_16	109.5
C2_16–C3_16–C4_16	108.1(4)	C1_16–C10_16–H10C_16	109.5
C2_16–C3_16–C8_16	126.7(4)	H10A_16–C10_16–H10C_16	109.5
C4_16–C3_16–C8_16	125.2(4)	H10B_16–C10_16–H10C_16	109.5
C2_16–C3_16–Al16	69.8(2)	C5_13–C1_13–C2_13	107.3(3)
C4_16–C3_16–Al16	71.3(2)	C5_13–C1_13–C10_13	125.7(4)
C8_16–C3_16–Al16	127.1(3)	C2_13–C1_13–C10_13	126.9(4)
C5_16–C4_16–C3_16	108.4(4)	C5_13–C1_13–Al9	80.1(2)
C5_16–C4_16–C7_16	129.5(4)	C2_13–C1_13–Al9	73.2(2)
C3_16–C4_16–C7_16	121.7(4)	C10_13–C1_13–Al9	113.8(3)
C5_16–C4_16–Al16	69.3(2)	C3_13–C2_13–C1_13	108.4(3)
C3_16–C4_16–Al16	73.1(2)	C3_13–C2_13–C9_13	124.3(4)
C7_16–C4_16–Al16	129.2(3)	C1_13–C2_13–C9_13	127.3(4)
C4_16–C5_16–C1_16	107.5(4)	C3_13–C2_13–Al9	80.1(2)
C4_16–C5_16–C6_16	126.4(5)	C1_13–C2_13–Al9	73.3(2)
C1_16–C5_16–C6_16	126.1(5)	C9_13–C2_13–Al9	113.4(2)
C4_16–C5_16–Al16	74.8(3)	C2_13–C3_13–C4_13	108.3(3)
C1_16–C5_16–Al16	70.2(2)	C2_13–C3_13–C8_13	124.8(4)
C6_16–C5_16–Al16	121.1(3)	C4_13–C3_13–C8_13	126.9(4)
C5_16–C6_16–H6A_16	109.5	C5_13–C4_13–C3_13	107.4(3)
C5_16–C6_16–H6B_16	109.5	C5_13–C4_13–C7_13	126.9(4)
H6A_16–C6_16–H6B_16	109.5	C3_13–C4_13–C7_13	125.7(4)
C5_16–C6_16–H6C_16	109.5	C5_13–C4_13–Al13	77.6(2)
H6A_16–C6_16–H6C_16	109.5	C3_13–C4_13–Al13	76.9(2)
H6B_16–C6_16–H6C_16	109.5	C7_13–C4_13–Al13	109.3(2)
C4_16–C7_16–H7A_16	109.5	C1_13–C5_13–C4_13	108.7(3)
C4_16–C7_16–H7B_16	109.5	C1_13–C5_13–C6_13	126.2(4)
H7A_16–C7_16–H7B_16	109.5	C4_13–C5_13–C6_13	125.1(4)
C4_16–C7_16–H7C_16	109.5	C5_13–C6_13–H6A_13	109.5
H7A_16–C7_16–H7C_16	109.5	C5_13–C6_13–H6B_13	109.5
H7B_16–C7_16–H7C_16	109.5	H6A_13–C6_13–H6B_13	109.5
C3_16–C8_16–H8A_16	109.5	C5_13–C6_13–H6C_13	109.5
C3_16–C8_16–H8B_16	109.5	H6A_13–C6_13–H6C_13	109.5
H8A_16–C8_16–H8B_16	109.5	H6B_13–C6_13–H6C_13	109.5
C3_16–C8_16–H8C_16	109.5	C4_13–C7_13–H7A_13	109.5
H8A_16–C8_16–H8C_16	109.5		
H8B_16–C8_16–H8C_16	109.5		
C2_16–C9_16–H9A_16	109.5		

C4_13–C7_13–H7B_13	109.5
H7A_13–C7_13–H7B_13	109.5
C4_13–C7_13–H7C_13	109.5
H7A_13–C7_13–H7C_13	109.5
H7B_13–C7_13–H7C_13	109.5
C3_13–C8_13–H8A_13	109.5
C3_13–C8_13–H8B_13	109.5
H8A_13–C8_13–H8B_13	109.5
C3_13–C8_13–H8C_13	109.5
H8A_13–C8_13–H8C_13	109.5
H8B_13–C8_13–H8C_13	109.5
C2_13–C9_13–H9A_13	109.5
C2_13–C9_13–H9B_13	109.5
H9A_13–C9_13–H9B_13	109.5
C2_13–C9_13–H9C_13	109.5
H9A_13–C9_13–H9C_13	109.5
H9B_13–C9_13–H9C_13	109.5
C1_13–C10_13–H10A_13	109.5
C1_13–C10_13–H10B_13	109.5
H10A_13–C10_13–H10B_13	109.5
C1_13–C10_13–H10C_13	109.5
H10A_13–C10_13–H10C_13	109.5
H10B_13–C10_13–H10C_13	109.5
C1_24–O1_24–Al17	146.2(8)
O1_24–C1_24–C4_24	110.9(6)
O1_24–C1_24–C3_24	107.1(7)
C4_24–C1_24–C3_24	109.6(6)
O1_24–C1_24–C2_24	110.9(6)
C4_24–C1_24–C2_24	109.1(6)
C3_24–C1_24–C2_24	109.2(5)
F3_24–C2_24–F1_24	108.4(6)
F3_24–C2_24–F2_24	107.0(6)
F1_24–C2_24–F2_24	108.3(6)
F3_24–C2_24–C1_24	110.6(6)
F1_24–C2_24–C1_24	111.0(6)
F2_24–C2_24–C1_24	111.4(6)
F5_24–C3_24–F4_24	107.0(6)
F5_24–C3_24–F6_24	105.6(7)
F4_24–C3_24–F6_24	107.9(6)
F5_24–C3_24–C1_24	111.8(6)
F4_24–C3_24–C1_24	111.1(6)
F6_24–C3_24–C1_24	113.1(6)
F7_24–C4_24–F9_24	108.4(7)
F7_24–C4_24–F8_24	106.8(6)
F9_24–C4_24–F8_24	107.6(5)
F7_24–C4_24–C1_24	111.6(7)
F9_24–C4_24–C1_24	109.3(6)
F8_24–C4_24–C1_24	112.9(6)
C1_17–O1_17–Al17	144.4(13)
O1_17–C1_17–C3_17	112.7(10)
O1_17–C1_17–C4_17	106.3(10)
C3_17–C1_17–C4_17	110.8(8)
O1_17–C1_17–C2_17	110.1(10)
C3_17–C1_17–C2_17	108.5(8)
C4_17–C1_17–C2_17	108.3(9)
F2_17–C2_17–F3_17	108.5(13)
F2_17–C2_17–F1_17	107.4(12)
F3_17–C2_17–F1_17	104.1(13)
F2_17–C2_17–C1_17	114.6(11)
F3_17–C2_17–C1_17	109.7(12)
F1_17–C2_17–C1_17	112.0(9)
F5_17–C3_17–F4_17	106.8(9)
F5_17–C3_17–F6_17	108.3(8)
F4_17–C3_17–F6_17	108.3(9)
F5_17–C3_17–C1_17	111.3(8)
F4_17–C3_17–C1_17	110.5(8)
F6_17–C3_17–C1_17	111.4(8)
F9_17–C4_17–F8_17	109.8(10)
F9_17–C4_17–F7_17	105.3(12)
F8_17–C4_17–F7_17	107.4(12)
F9_17–C4_17–C1_17	111.0(9)
F8_17–C4_17–C1_17	112.1(10)
F7_17–C4_17–C1_17	111.0(10)
C1_18–O1_18–Al17	149.4(7)
O1_18–C1_18–C4_18	112.3(9)
O1_18–C1_18–C2_18	107.5(8)
C4_18–C1_18–C2_18	109.0(9)
O1_18–C1_18–C3_18	108.9(9)
C4_18–C1_18–C3_18	110.2(9)
C2_18–C1_18–C3_18	108.9(9)
F3_18–C2_18–F1_18	105.5(10)
F3_18–C2_18–F2_18	105.6(9)
F1_18–C2_18–F2_18	111.6(11)
F3_18–C2_18–C1_18	112.1(9)
F1_18–C2_18–C1_18	111.1(9)
F2_18–C2_18–C1_18	110.8(9)
F4_18–C3_18–F5_18	111.8(13)
F4_18–C3_18–F6_18	108.5(12)
F5_18–C3_18–F6_18	108.5(14)
F4_18–C3_18–C1_18	109.4(10)
F5_18–C3_18–C1_18	107.0(12)
F6_18–C3_18–C1_18	111.8(12)
F9_18–C4_18–F8_18	106.6(15)

F9_18–C4_18–F7_18	112.2(14)	F8_22–C4_22–C1_22	113.8(9)
F8_18–C4_18–F7_18	109.5(12)	C1_25–O1_25–Al17	150.5(13)
F9_18–C4_18–C1_18	108.7(13)	O1_25–C1_25–C4_25	112.6(10)
F8_18–C4_18–C1_18	111.1(12)	O1_25–C1_25–C3_25	108.9(9)
F7_18–C4_18–C1_18	108.7(10)	C4_25–C1_25–C3_25	109.3(9)
C1_19–O1_19–Al17	153(2)	O1_25–C1_25–C2_25	107.8(11)
O1_19–C1_19–C2_19	111.9(13)	C4_25–C1_25–C2_25	109.0(9)
O1_19–C1_19–C4_19	106.9(14)	C3_25–C1_25–C2_25	109.2(9)
C2_19–C1_19–C4_19	111.5(10)	F1_25–C2_25–F3_25	106.6(10)
O1_19–C1_19–C3_19	111.4(13)	F1_25–C2_25–F2_25	111.3(12)
C2_19–C1_19–C3_19	107.6(9)	F3_25–C2_25–F2_25	107.7(10)
C4_19–C1_19–C3_19	107.4(9)	F1_25–C2_25–C1_25	110.8(10)
F2_19–C2_19–F3_19	110.1(14)	F3_25–C2_25–C1_25	110.6(10)
F2_19–C2_19–F1_19	113.5(14)	F2_25–C2_25–C1_25	109.7(10)
F3_19–C2_19–F1_19	101.3(14)	F5_25–C3_25–F6_25	108.3(10)
F2_19–C2_19–C1_19	110.9(10)	F5_25–C3_25–F4_25	106.1(11)
F3_19–C2_19–C1_19	108.6(12)	F6_25–C3_25–F4_25	108.6(9)
F1_19–C2_19–C1_19	111.9(13)	F5_25–C3_25–C1_25	110.1(10)
F5_19–C3_19–F6_19	108.9(15)	F6_25–C3_25–C1_25	112.1(10)
F5_19–C3_19–F4_19	102.7(12)	F4_25–C3_25–C1_25	111.5(10)
F6_19–C3_19–F4_19	110.7(15)	F9_25–C4_25–F8_25	108.2(11)
F5_19–C3_19–C1_19	115.1(10)	F9_25–C4_25–F7_25	107.4(10)
F6_19–C3_19–C1_19	111.1(13)	F8_25–C4_25–F7_25	107.0(10)
F4_19–C3_19–C1_19	108.0(10)	F9_25–C4_25–C1_25	110.2(10)
F9_19–C4_19–F8_19	109.0(11)	F8_25–C4_25–C1_25	112.7(10)
F9_19–C4_19–F7_19	106.5(14)	F7_25–C4_25–C1_25	111.0(10)
F8_19–C4_19–F7_19	105.0(13)	C5_5–C1_5–C2_5	107.2(9)
F9_19–C4_19–C1_19	113.3(11)	C5_5–C1_5–C10_5	123.9(12)
F8_19–C4_19–C1_19	112.1(11)	C2_5–C1_5–C10_5	128.9(13)
F7_19–C4_19–C1_19	110.4(11)	C5_5–C1_5–Al3	77.3(10)
C1_22–O1_22–Al17	146.7(12)	C2_5–C1_5–Al3	70.6(6)
O1_22–C1_22–C3_22	108.7(9)	C10_5–C1_5–Al3	117.6(12)
O1_22–C1_22–C2_22	108.3(8)	C3_5–C2_5–C1_5	107.9(8)
C3_22–C1_22–C2_22	108.1(7)	C3_5–C2_5–C9_5	128.0(12)
O1_22–C1_22–C4_22	112.1(10)	C1_5–C2_5–C9_5	123.7(12)
C3_22–C1_22–C4_22	111.1(7)	C3_5–C2_5–Al3	75.7(6)
C2_22–C1_22–C4_22	108.4(8)	C1_5–C2_5–Al3	72.6(7)
F3_22–C2_22–F2_22	108.9(7)	C9_5–C2_5–Al3	122.7(8)
F3_22–C2_22–F1_22	104.7(8)	C4_5–C3_5–C2_5	108.2(8)
F2_22–C2_22–F1_22	107.8(8)	C4_5–C3_5–C8_5	125.6(11)
F3_22–C2_22–C1_22	111.9(8)	C2_5–C3_5–C8_5	126.2(11)
F2_22–C2_22–C1_22	113.1(8)	C4_5–C3_5–Al3	75.4(8)
F1_22–C2_22–C1_22	110.1(7)	C2_5–C3_5–Al3	68.3(5)
F4_22–C3_22–F6_22	107.9(8)	C8_5–C3_5–Al3	123.5(7)
F4_22–C3_22–F5_22	107.1(8)	C3_5–C4_5–C5_5	108.4(9)
F6_22–C3_22–F5_22	108.1(8)	C3_5–C4_5–C7_5	129.1(11)
F4_22–C3_22–C1_22	110.4(8)	C5_5–C4_5–C7_5	122.0(10)
F6_22–C3_22–C1_22	112.2(8)	C3_5–C4_5–Al3	70.3(7)
F5_22–C3_22–C1_22	110.8(8)	C5_5–C4_5–Al3	72.7(10)
F9_22–C4_22–F7_22	109.5(8)	C7_5–C4_5–Al3	128.7(10)
F9_22–C4_22–F8_22	107.5(10)	C4_5–C5_5–C1_5	108.1(9)
F7_22–C4_22–F8_22	104.0(10)	C4_5–C5_5–C6_5	123.2(12)
F9_22–C4_22–C1_22	111.5(9)	C1_5–C5_5–C6_5	128.6(13)
F7_22–C4_22–C1_22	110.2(8)	C4_5–C5_5–Al3	73.1(9)

C1_5–C5_5–Al3	67.3(9)
C6_5–C5_5–Al3	123.2(16)
C5_5–C6_5–H6A_5	109.5
C5_5–C6_5–H6B_5	109.5
H6A_5–C6_5–H6B_5	109.5
C5_5–C6_5–H6C_5	109.5
H6A_5–C6_5–H6C_5	109.5
H6B_5–C6_5–H6C_5	109.5
C4_5–C7_5–H7A_5	109.5
C4_5–C7_5–H7B_5	109.5
H7A_5–C7_5–H7B_5	109.5
C4_5–C7_5–H7C_5	109.5
H7A_5–C7_5–H7C_5	109.5
H7B_5–C7_5–H7C_5	109.5
C3_5–C8_5–H8A_5	109.5
C3_5–C8_5–H8B_5	109.5
H8A_5–C8_5–H8B_5	109.5
C3_5–C8_5–H8C_5	109.5
H8A_5–C8_5–H8C_5	109.5
H8B_5–C8_5–H8C_5	109.5
C2_5–C9_5–H9A_5	109.5
C2_5–C9_5–H9B_5	109.5
H9A_5–C9_5–H9B_5	109.5
C2_5–C9_5–H9C_5	109.5
H9A_5–C9_5–H9C_5	109.5
H9B_5–C9_5–H9C_5	109.5
C1_5–C10_5–H10A_5	109.5
C1_5–C10_5–H10B_5	109.5
H10A_5–C10_5–H10B_5	109.5
C1_5–C10_5–H10C_5	109.5
H10A_5–C10_5–H10C_5	109.5
H10B_5–C10_5–H10C_5	109.5
C2_9–C1_9–C5_9	108.3(8)
C2_9–C1_9–C10_9	125.4(10)
C5_9–C1_9–C10_9	126.2(10)
C2_9–C1_9–Al2	68.8(6)
C5_9–C1_9–Al2	74.5(8)
C10_9–C1_9–Al2	126.1(10)
C1_9–C2_9–C3_9	107.8(8)
C1_9–C2_9–C9_9	127.2(9)
C3_9–C2_9–C9_9	124.9(9)
C1_9–C2_9–Al2	74.6(6)
C3_9–C2_9–Al2	72.5(7)
C9_9–C2_9–Al2	121.7(10)
C4_9–C3_9–C2_9	107.8(9)
C4_9–C3_9–C8_9	123.9(10)
C2_9–C3_9–C8_9	128.1(10)
C4_9–C3_9–Al2	75.3(14)
C2_9–C3_9–Al2	70.3(6)
C8_9–C3_9–Al2	123.0(12)
C5_9–C4_9–C3_9	108.1(9)
C5_9–C4_9–C7_9	127.7(12)
C3_9–C4_9–C7_9	124.1(12)
C5_9–C4_9–Al2	73.1(13)
C3_9–C4_9–Al2	68.6(12)
C7_9–C4_9–Al2	125(2)
C4_9–C5_9–C1_9	107.9(9)
C4_9–C5_9–C6_9	126.0(11)
C1_9–C5_9–C6_9	125.8(11)
C4_9–C5_9–Al2	71.8(14)
C1_9–C5_9–Al2	70.0(7)
C6_9–C5_9–Al2	127.8(14)
C5_9–C6_9–H6A_9	109.5
C5_9–C6_9–H6B_9	109.5
H6A_9–C6_9–H6B_9	109.5
C5_9–C6_9–H6C_9	109.5
H6A_9–C6_9–H6C_9	109.5
H6B_9–C6_9–H6C_9	109.5
C4_9–C7_9–H7A_9	109.5
C4_9–C7_9–H7B_9	109.5
H7A_9–C7_9–H7B_9	109.5
C4_9–C7_9–H7C_9	109.5
H7A_9–C7_9–H7C_9	109.5
H7B_9–C7_9–H7C_9	109.5
C3_9–C8_9–H8A_9	109.5
C3_9–C8_9–H8B_9	109.5
H8A_9–C8_9–H8B_9	109.5
C3_9–C8_9–H8C_9	109.5
H8A_9–C8_9–H8C_9	109.5
H8B_9–C8_9–H8C_9	109.5
C2_9–C9_9–H9A_9	109.5
C2_9–C9_9–H9B_9	109.5
H9A_9–C9_9–H9B_9	109.5
C2_9–C9_9–H9C_9	109.5
H9A_9–C9_9–H9C_9	109.5
H9B_9–C9_9–H9C_9	109.5
C1_9–C10_9–H10A_9	109.5
C1_9–C10_9–H10B_9	109.5
H10A_9–C10_9–H10B_9	109.5
C1_9–C10_9–H10C_9	109.5
H10A_9–C10_9–H10C_9	109.5
H10B_9–C10_9–H10C_9	109.5
C2_23–C1_23–C5_23	107.1(6)
C2_23–C1_23–C10_23	129.2(6)
C5_23–C1_23–C10_23	123.5(6)
C2_23–C1_23–Al4	69.1(4)
C5_23–C1_23–Al4	71.3(4)
C10_23–C1_23–Al4	127.3(5)
C1_23–C2_23–C3_23	108.4(7)
C1_23–C2_23–C9_23	127.1(7)
C3_23–C2_23–C9_23	124.3(7)
C1_23–C2_23–Al4	75.5(4)

C3_23–C2_23–Al4	69.1(4)
C9_23–C2_23–Al4	124.8(6)
C2_23–C3_23–C4_23	108.5(6)
C2_23–C3_23–C8_23	124.1(7)
C4_23–C3_23–C8_23	127.4(8)
C2_23–C3_23–Al4	74.3(4)
C4_23–C3_23–Al4	72.9(4)
C8_23–C3_23–Al4	119.6(6)
C5_23–C4_23–C3_23	107.2(6)
C5_23–C4_23–C7_23	127.1(7)
C3_23–C4_23–C7_23	125.7(7)
C5_23–C4_23–Al4	75.4(4)
C3_23–C4_23–Al4	70.1(4)
C7_23–C4_23–Al4	120.5(5)
C4_23–C5_23–C1_23	108.7(5)
C4_23–C5_23–C6_23	126.8(7)
C1_23–C5_23–C6_23	124.3(6)
C4_23–C5_23–Al4	68.7(4)
C1_23–C5_23–Al4	73.4(4)
C6_23–C5_23–Al4	128.0(5)
C5_23–C6_23–H6A_23	109.5
C5_23–C6_23–H6B_23	109.5
H6A_23–C6_23–H6B_23	109.5
C5_23–C6_23–H6C_23	109.5
H6A_23–C6_23–H6C_23	109.5
H6B_23–C6_23–H6C_23	109.5
C4_23–C7_23–H7A_23	109.5
C4_23–C7_23–H7B_23	109.5
H7A_23–C7_23–H7B_23	109.5
C4_23–C7_23–H7C_23	109.5
H7A_23–C7_23–H7C_23	109.5
H7B_23–C7_23–H7C_23	109.5
C3_23–C8_23–H8A_23	109.5
C3_23–C8_23–H8B_23	109.5
H8A_23–C8_23–H8B_23	109.5
C3_23–C8_23–H8C_23	109.5
H8A_23–C8_23–H8C_23	109.5
H8B_23–C8_23–H8C_23	109.5
C2_23–C9_23–H9A_23	109.5
C2_23–C9_23–H9B_23	109.5
H9A_23–C9_23–H9B_23	109.5
C2_23–C9_23–H9C_23	109.5
H9A_23–C9_23–H9C_23	109.5
H9B_23–C9_23–H9C_23	109.5
C1_23–C10_23–H10A_23	109.5
C1_23–C10_23–H10B_23	109.5
H10A_23–C10_23–H10B_23	109.5
C1_23–C10_23–H10C_23	109.5
H10A_23–C10_23–H10C_23	109.5
H10B_23–C10_23–H10C_23	109.5
C5_35–C1_35–C2_35	108.2(10)
C5_35–C1_35–C10_35	129.1(12)
C2_35–C1_35–C10_35	122.7(11)
C5_35–C1_35–Al7	70.9(12)
C2_35–C1_35–Al7	71.3(7)
C10_35–C1_35–Al7	124.2(12)
C1_35–C2_35–C3_35	108.3(10)
C1_35–C2_35–C9_35	125.9(11)
C3_35–C2_35–C9_35	125.7(11)
C1_35–C2_35–Al7	73.6(7)
C3_35–C2_35–Al7	71.8(7)
C9_35–C2_35–Al7	121.9(12)
C2_35–C3_35–C4_35	107.4(9)
C2_35–C3_35–C8_35	124.5(10)
C4_35–C3_35–C8_35	127.9(10)
C2_35–C3_35–Al7	72.7(7)
C4_35–C3_35–Al7	70.4(8)
C8_35–C3_35–Al7	119.1(11)
C3_35–C4_35–C5_35	108.1(9)
C3_35–C4_35–C7_35	127.9(11)
C5_35–C4_35–C7_35	123.5(11)
C3_35–C4_35–Al7	73.6(8)
C5_35–C4_35–Al7	73.6(12)
C7_35–C4_35–Al7	125.2(12)
C1_35–C5_35–C4_35	107.9(10)
C1_35–C5_35–C6_35	126.2(12)
C4_35–C5_35–C6_35	125.6(11)
C1_35–C5_35–Al7	74.1(11)
C4_35–C5_35–Al7	70.3(11)
C6_35–C5_35–Al7	125.5(17)
C5_35–C6_35–H6A_35	109.5
C5_35–C6_35–H6B_35	109.5
H6A_35–C6_35–H6B_35	109.5
C5_35–C6_35–H6C_35	109.5
H6A_35–C6_35–H6C_35	109.5
H6B_35–C6_35–H6C_35	109.5
C4_35–C7_35–H7A_35	109.5

C4_35–C7_35–H7B_35	109.5
H7A_35–C7_35–H7B_35	109.5
C4_35–C7_35–H7C_35	109.5
H7A_35–C7_35–H7C_35	109.5
H7B_35–C7_35–H7C_35	109.5
C3_35–C8_35–H8A_35	109.5
C3_35–C8_35–H8B_35	109.5
H8A_35–C8_35–H8B_35	109.5
C3_35–C8_35–H8C_35	109.5
H8A_35–C8_35–H8C_35	109.5
H8B_35–C8_35–H8C_35	109.5
C2_35–C9_35–H9A_35	109.5
C2_35–C9_35–H9B_35	109.5
H9A_35–C9_35–H9B_35	109.5
C2_35–C9_35–H9C_35	109.5
H9A_35–C9_35–H9C_35	109.5
H9B_35–C9_35–H9C_35	109.5
C1_35–C10_35–H10A_35	109.5
C1_35–C10_35–H10B_35	109.5
H10A_35–C10_35–H10B_35	109.5
C1_35–C10_35–H10C_35	109.5
H10A_35–C10_35–H10C_35	109.5
H10B_35–C10_35–H10C_35	109.5
C5_36–C1_36–C2_36	107.9(9)
C5_36–C1_36–C10_36	124.5(12)
C2_36–C1_36–C10_36	127.6(12)
C5_36–C1_36–Al5	80.3(8)
C2_36–C1_36–Al5	71.4(6)
C10_36–C1_36–Al5	113.4(9)
C1_36–C2_36–C3_36	107.7(9)
C1_36–C2_36–C9_36	126.6(12)
C3_36–C2_36–C9_36	125.7(12)
C1_36–C2_36–Al5	75.3(6)
C3_36–C2_36–Al5	78.8(6)
C9_36–C2_36–Al5	113.3(8)
C4_36–C3_36–C2_36	108.0(9)
C4_36–C3_36–C8_36	125.6(12)
C2_36–C3_36–C8_36	126.3(12)
C4_36–C3_36–Al1	72.7(9)
C2_36–C3_36–Al1	81.4(6)
C8_36–C3_36–Al1	115.2(9)
C5_36–C4_36–C3_36	107.6(9)
C5_36–C4_36–C7_36	124.5(12)
C3_36–C4_36–C7_36	127.8(12)
C5_36–C4_36–Al1	80.2(10)
C3_36–C4_36–Al1	73.9(9)
C7_36–C4_36–Al1	109.2(11)
C1_36–C5_36–C4_36	108.9(9)
C1_36–C5_36–C6_36	125.0(12)
C4_36–C5_36–C6_36	126.1(11)
C5_36–C6_36–H6A_36	109.5
C5_36–C6_36–H6B_36	109.5
H6A_36–C6_36–H6B_36	109.5
C5_36–C6_36–H6C_36	109.5
H6A_36–C6_36–H6C_36	109.5
H6B_36–C6_36–H6C_36	109.5
C4_36–C7_36–H7A_36	109.5
C4_36–C7_36–H7B_36	109.5
H7A_36–C7_36–H7B_36	109.5
C4_36–C7_36–H7C_36	109.5
H7A_36–C7_36–H7C_36	109.5
H7B_36–C7_36–H7C_36	109.5
C3_36–C8_36–H8A_36	109.5
C3_36–C8_36–H8B_36	109.5
H8A_36–C8_36–H8B_36	109.5
C3_36–C8_36–H8C_36	109.5
H8A_36–C8_36–H8C_36	109.5
H8B_36–C8_36–H8C_36	109.5
C2_36–C9_36–H9A_36	109.5
C2_36–C9_36–H9B_36	109.5
H9A_36–C9_36–H9B_36	109.5
C2_36–C9_36–H9C_36	109.5
H9A_36–C9_36–H9C_36	109.5
H9B_36–C9_36–H9C_36	109.5
C1_36–C10_36–H10A_36	109.5
C1_36–C10_36–H10B_36	109.5
H10A_36–C10_36–H10B_36	109.5

C1_36–C10_36–H10C_36	109.5
H10A_36–C10_36–H10C_36	109.5
H10B_36–C10_36–H10C_36	109.5
C2_37–C1_37–C5_37	108.5(9)
C2_37–C1_37–C10_37	126.6(11)
C5_37–C1_37–C10_37	124.9(11)
C2_37–C1_37–Al8	71.8(7)
C5_37–C1_37–Al8	72.8(13)
C10_37–C1_37–Al8	122.1(12)
C1_37–C2_37–C3_37	108.1(9)
C1_37–C2_37–C9_37	128.0(10)
C3_37–C2_37–C9_37	123.9(10)
C1_37–C2_37–Al8	71.2(7)
C3_37–C2_37–Al8	72.6(7)
C9_37–C2_37–Al8	122.7(10)
C4_37–C3_37–C2_37	107.2(9)
C4_37–C3_37–C8_37	128.2(12)
C2_37–C3_37–C8_37	124.6(12)
C4_37–C3_37–Al8	70.3(10)
C2_37–C3_37–Al8	70.4(7)
C8_37–C3_37–Al8	125.5(12)
C5_37–C4_37–C3_37	108.6(10)
C5_37–C4_37–C7_37	124.4(14)
C3_37–C4_37–C7_37	126.5(14)
C5_37–C4_37–Al8	72.7(14)
C3_37–C4_37–Al8	72.8(9)
C7_37–C4_37–Al8	126.8(17)
C4_37–C5_37–C1_37	107.5(10)
C4_37–C5_37–C6_37	125.6(13)
C1_37–C5_37–C6_37	127.0(13)
C4_37–C5_37–Al8	70.5(14)
C1_37–C5_37–Al8	70.3(11)
C6_37–C5_37–Al8	125(2)
C5_37–C6_37–H6A_37	109.5
C5_37–C6_37–H6B_37	109.5
H6A_37–C6_37–H6B_37	109.5
C5_37–C6_37–H6C_37	109.5
H6A_37–C6_37–H6C_37	109.5
H6B_37–C6_37–H6C_37	109.5
C4_37–C7_37–H7A_37	109.5
C4_37–C7_37–H7B_37	109.5
H7A_37–C7_37–H7B_37	109.5
C4_37–C7_37–H7C_37	109.5
H7A_37–C7_37–H7C_37	109.5
H7B_37–C7_37–H7C_37	109.5
C3_37–C8_37–H8A_37	109.5
C3_37–C8_37–H8B_37	109.5
H8A_37–C8_37–H8B_37	109.5
C3_37–C8_37–H8C_37	109.5
H8A_37–C8_37–H8C_37	109.5
H8B_37–C8_37–H8C_37	109.5
C2_37–C9_37–H9A_37	109.5
C2_37–C9_37–H9B_37	109.5
H9A_37–C9_37–H9B_37	109.5
C2_37–C9_37–H9C_37	109.5
H9A_37–C9_37–H9C_37	109.5
H9B_37–C9_37–H9C_37	109.5
C1_37–C10_37–H10A_37	109.5
C1_37–C10_37–H10B_37	109.5
H10A_37–C10_37–H10B_37	109.5
C1_37–C10_37–H10C_37	109.5
H10A_37–C10_37–H10C_37	109.5
H10B_37–C10_37–H10C_37	109.5
C2_39–C1_39–C5_39	109.0(10)
C2_39–C1_39–C10_39	121.6(11)
C5_39–C1_39–C10_39	129.2(12)
C2_39–C1_39–Al11	73.9(7)
C5_39–C1_39–Al11	71.4(9)
C10_39–C1_39–Al11	124.4(13)
C3_39–C2_39–C1_39	106.5(10)
C3_39–C2_39–C9_39	129.7(11)
C1_39–C2_39–C9_39	123.8(11)
C3_39–C2_39–Al11	72.6(7)
C1_39–C2_39–Al11	69.3(7)
C9_39–C2_39–Al11	123.6(12)
C2_39–C3_39–C4_39	108.7(10)
C2_39–C3_39–C8_39	126.5(12)
C4_39–C3_39–C8_39	124.8(11)
C2_39–C3_39–Al11	71.4(7)
C4_39–C3_39–Al11	69.8(9)
C8_39–C3_39–Al11	124.4(12)
C5_39–C4_39–C3_39	108.6(9)
C5_39–C4_39–C7_39	126.6(12)
C3_39–C4_39–C7_39	124.4(12)
C5_39–C4_39–Al11	70.9(9)
C3_39–C4_39–Al11	73.9(9)
C7_39–C4_39–Al11	126.3(13)

C4_39–C5_39–C1_39	107.1(9)
C4_39–C5_39–C6_39	129.4(12)
C1_39–C5_39–C6_39	123.5(12)
C4_39–C5_39–Al11	72.5(9)
C1_39–C5_39–Al11	71.2(9)
C6_39–C5_39–Al11	121.2(12)
C5_39–C6_39–H6A_39	109.5
C5_39–C6_39–H6B_39	109.5
H6A_39–C6_39–H6B_39	109.5
C5_39–C6_39–H6C_39	109.5
H6A_39–C6_39–H6C_39	109.5
H6B_39–C6_39–H6C_39	109.5
C4_39–C7_39–H7A_39	109.5
C4_39–C7_39–H7B_39	109.5
H7A_39–C7_39–H7B_39	109.5
C4_39–C7_39–H7C_39	109.5
H7A_39–C7_39–H7C_39	109.5
H7B_39–C7_39–H7C_39	109.5
C3_39–C8_39–H8A_39	109.5
C3_39–C8_39–H8B_39	109.5
H8A_39–C8_39–H8B_39	109.5
C3_39–C8_39–H8C_39	109.5
H8A_39–C8_39–H8C_39	109.5
H8B_39–C8_39–H8C_39	109.5
C2_39–C9_39–H9A_39	109.5
C2_39–C9_39–H9B_39	109.5
H9A_39–C9_39–H9B_39	109.5
C2_39–C9_39–H9C_39	109.5
H9A_39–C9_39–H9C_39	109.5
H9B_39–C9_39–H9C_39	109.5
C1_39–C10_39–H10A_39	109.5
C1_39–C10_39–H10B_39	109.5
H10A_39–C10_39–H10B_39	109.5
C1_39–C10_39–H10C_39	109.5
H10A_39–C10_39–H10C_39	109.5
H10B_39–C10_39–H10C_39	109.5
C2_41–C1_41–C5_41	108.7(10)
C2_41–C1_41–C10_41	124.3(12)
C5_41–C1_41–C10_41	127.0(12)
C2_41–C1_41–Al10	71.8(6)
C5_41–C1_41–Al10	67.4(9)
C10_41–C1_41–Al10	128.0(9)
C3_41–C2_41–C1_41	108.2(10)
C3_41–C2_41–C9_41	130.3(13)
C1_41–C2_41–C9_41	121.3(12)
C3_41–C2_41–Al10	67.4(6)
C1_41–C2_41–Al10	73.8(6)
C9_41–C2_41–Al10	128.1(10)
C2_41–C3_41–C4_41	107.5(10)
C2_41–C3_41–C8_41	124.2(13)
C4_41–C3_41–C8_41	128.2(13)
C2_41–C3_41–Al10	77.2(6)
C4_41–C3_41–Al10	70.3(8)
C8_41–C3_41–Al10	116.2(10)
C5_41–C4_41–C3_41	108.2(9)
C5_41–C4_41–C7_41	124.9(12)
C3_41–C4_41–C7_41	126.8(12)
C5_41–C4_41–Al10	73.4(9)
C3_41–C4_41–Al10	72.5(8)
C7_41–C4_41–Al10	117.9(11)
C1_41–C5_41–C4_41	107.1(9)
C1_41–C5_41–C6_41	126.5(13)
C4_41–C5_41–C6_41	126.1(12)
C1_41–C5_41–Al10	77.5(8)
C4_41–C5_41–Al10	69.6(9)
C6_41–C5_41–Al10	123.0(12)
C5_41–C6_41–H6A_41	109.5
C5_41–C6_41–H6B_41	109.5
H6A_41–C6_41–H6B_41	109.5
C5_41–C6_41–H6C_41	109.5
H6A_41–C6_41–H6C_41	109.5
H6B_41–C6_41–H6C_41	109.5
C4_41–C7_41–H7A_41	109.5
C4_41–C7_41–H7B_41	109.5
H7A_41–C7_41–H7B_41	109.5
C4_41–C7_41–H7C_41	109.5
H7A_41–C7_41–H7C_41	109.5
H7B_41–C7_41–H7C_41	109.5
C3_41–C8_41–H8A_41	109.5
C3_41–C8_41–H8B_41	109.5
H8A_41–C8_41–H8B_41	109.5
C3_41–C8_41–H8C_41	109.5

H8A_41–C8_41–H8C_41	109.5
H8B_41–C8_41–H8C_41	109.5
C2_41–C9_41–H9A_41	109.5
C2_41–C9_41–H9B_41	109.5
H9A_41–C9_41–H9B_41	109.5
C2_41–C9_41–H9C_41	109.5
H9A_41–C9_41–H9C_41	109.5
H9B_41–C9_41–H9C_41	109.5
C1_41–C10_41–H10A_41	109.5
C1_41–C10_41–H10B_41	109.5
H10A_41–C10_41–H10B_41	109.5
C1_41–C10_41–H10C_41	109.5
H10A_41–C10_41–H10C_41	109.5
H10B_41–C10_41–H10C_41	109.5
C2_42–C1_42–C5_42	107.5(9)
C2_42–C1_42–C10_42	129.0(11)
C5_42–C1_42–C10_42	123.3(11)
C2_42–C1_42–Al14	70.7(6)
C5_42–C1_42–Al14	69.9(7)
C10_42–C1_42–Al14	128.8(9)
C1_42–C2_42–C3_42	108.3(9)
C1_42–C2_42–C9_42	124.7(12)
C3_42–C2_42–C9_42	127.0(12)
C1_42–C2_42–Al14	74.4(6)
C3_42–C2_42–Al14	67.9(6)
C9_42–C2_42–Al14	125.3(9)
C2_42–C3_42–C4_42	107.8(9)
C2_42–C3_42–C8_42	125.7(12)
C4_42–C3_42–C8_42	125.9(12)
C2_42–C3_42–Al14	75.7(6)
C4_42–C3_42–Al14	71.3(8)
C8_42–C3_42–Al14	125.7(9)
C5_42–C4_42–C3_42	107.6(9)
C5_42–C4_42–C7_42	127.2(12)
C3_42–C4_42–C7_42	125.1(12)
C5_42–C4_42–Al14	75.4(8)
C3_42–C4_42–Al14	71.2(8)
C7_42–C4_42–Al14	117.8(11)
C4_42–C5_42–C1_42	108.7(9)
C4_42–C5_42–C6_42	127.9(11)
C1_42–C5_42–C6_42	123.3(11)
C4_42–C5_42–Al14	68.5(8)
C1_42–C5_42–Al14	74.6(7)
C6_42–C5_42–Al14	123.9(9)
C5_42–C6_42–H6A_42	109.5
C5_42–C6_42–H6B_42	109.5
H6A_42–C6_42–H6B_42	109.5
C5_42–C6_42–H6C_42	109.5
H6A_42–C6_42–H6C_42	109.5
H6B_42–C6_42–H6C_42	109.5
C4_42–C7_42–H7A_42	109.5
C4_42–C7_42–H7B_42	109.5
H7A_42–C7_42–H7B_42	109.5
C4_42–C7_42–H7C_42	109.5
H7A_42–C7_42–H7C_42	109.5
H7B_42–C7_42–H7C_42	109.5
C3_42–C8_42–H8A_42	109.5
C3_42–C8_42–H8B_42	109.5
H8A_42–C8_42–H8B_42	109.5
C3_42–C8_42–H8C_42	109.5
H8A_42–C8_42–H8C_42	109.5
H8B_42–C8_42–H8C_42	109.5
C2_42–C9_42–H9A_42	109.5
C2_42–C9_42–H9B_42	109.5
H9A_42–C9_42–H9B_42	109.5
C2_42–C9_42–H9C_42	109.5
H9A_42–C9_42–H9C_42	109.5
H9B_42–C9_42–H9C_42	109.5
C1_42–C10_42–H10A_42	109.5
C1_42–C10_42–H10B_42	109.5
H10A_42–C10_42–H10B_42	109.5
C1_42–C10_42–H10C_42	109.5
H10A_42–C10_42–H10C_42	109.5
H10B_42–C10_42–H10C_42	109.5
C2_43–C1_43–C5_43	106.5(10)
C2_43–C1_43–C10_43	127.0(13)
C5_43–C1_43–C10_43	126.5(13)
C2_43–C1_43–Al16	70.7(6)
C5_43–C1_43–Al16	71.3(9)

C10_43–C1_43–Al16	123.0(9)
C3_43–C2_43–C1_43	109.3(10)
C3_43–C2_43–C9_43	126.8(14)
C1_43–C2_43–C9_43	123.7(14)
C3_43–C2_43–Al16	71.6(6)
C1_43–C2_43–Al16	73.8(6)
C9_43–C2_43–Al16	124.8(10)
C2_43–C3_43–C4_43	108.1(10)
C2_43–C3_43–C8_43	125.3(13)
C4_43–C3_43–C8_43	126.5(13)
C2_43–C3_43–Al16	72.4(6)
C4_43–C3_43–Al16	70.9(10)
C8_43–C3_43–Al16	121.0(10)
C3_43–C4_43–C5_43	106.9(10)
C3_43–C4_43–C7_43	127.2(13)
C5_43–C4_43–C7_43	125.0(13)
C3_43–C4_43–Al16	72.8(9)
C5_43–C4_43–Al16	73.8(10)
C7_43–C4_43–Al16	127.3(14)
C1_43–C5_43–C4_43	109.1(10)
C1_43–C5_43–C6_43	128.5(13)
C4_43–C5_43–C6_43	122.3(12)
C1_43–C5_43–Al16	73.1(8)
C4_43–C5_43–Al16	69.8(10)
C6_43–C5_43–Al16	124.8(12)
C5_43–C6_43–H6A_43	109.5
C5_43–C6_43–H6B_43	109.5
H6A_43–C6_43–H6B_43	109.5
C5_43–C6_43–H6C_43	109.5
H6A_43–C6_43–H6C_43	109.5
H6B_43–C6_43–H6C_43	109.5
C4_43–C7_43–H7A_43	109.5
C4_43–C7_43–H7B_43	109.5
H7A_43–C7_43–H7B_43	109.5
C4_43–C7_43–H7C_43	109.5
H7A_43–C7_43–H7C_43	109.5
H7B_43–C7_43–H7C_43	109.5
C3_43–C8_43–H8A_43	109.5
C3_43–C8_43–H8B_43	109.5
H8A_43–C8_43–H8B_43	109.5
C3_43–C8_43–H8C_43	109.5
H8A_43–C8_43–H8C_43	109.5
H8B_43–C8_43–H8C_43	109.5
C2_43–C9_43–H9A_43	109.5
C2_43–C9_43–H9B_43	109.5
H9A_43–C9_43–H9B_43	109.5
C2_43–C9_43–H9C_43	109.5
H9A_43–C9_43–H9C_43	109.5
H9B_43–C9_43–H9C_43	109.5
C1_43–C10_43–H10A_43	109.5
C1_43–C10_43–H10B_43	109.5
H10A_43–C10_43–H10B_43	109.5
C1_43–C10_43–H10C_43	109.5
H10A_43–C10_43–H10C_43	109.5
H10B_43–C10_43–H10C_43	109.5
C2_44–C1_44–C5_44	108.5(9)
C2_44–C1_44–C10_44	126.4(13)
C5_44–C1_44–C10_44	124.9(13)
C2_44–C1_44–Al9	76.7(6)
C5_44–C1_44–Al9	79.7(9)
C10_44–C1_44–Al9	107.4(9)
C1_44–C2_44–C3_44	106.8(9)
C1_44–C2_44–C9_44	127.0(13)
C3_44–C2_44–C9_44	126.2(13)
C1_44–C2_44–Al9	70.1(6)
C3_44–C2_44–Al9	81.4(6)
C9_44–C2_44–Al9	114.7(9)
C4_44–C3_44–C2_44	108.7(9)
C4_44–C3_44–C8_44	126.0(13)
C2_44–C3_44–C8_44	125.2(12)
C4_44–C3_44–Al13	74.9(8)
C2_44–C3_44–Al13	78.5(6)
C8_44–C3_44–Al13	115.5(10)
C5_44–C4_44–C3_44	107.7(10)
C5_44–C4_44–C7_44	126.6(12)
C3_44–C4_44–C7_44	125.7(12)
C4_44–C5_44–C1_44	108.3(10)
C4_44–C5_44–C6_44	126.4(12)
C1_44–C5_44–C6_44	125.3(12)
C5_44–C6_44–H6A_44	109.5
C5_44–C6_44–H6B_44	109.5
H6A_44–C6_44–H6B_44	109.5
C5_44–C6_44–H6C_44	109.5
H6A_44–C6_44–H6C_44	109.5
H6B_44–C6_44–H6C_44	109.5
C4_44–C7_44–H7A_44	109.5
C4_44–C7_44–H7B_44	109.5

H7A_44–C7_44–H7B_44	109.5
C4_44–C7_44–H7C_44	109.5
H7A_44–C7_44–H7C_44	109.5
H7B_44–C7_44–H7C_44	109.5
C3_44–C8_44–H8A_44	109.5
C3_44–C8_44–H8B_44	109.5
H8A_44–C8_44–H8B_44	109.5
C3_44–C8_44–H8C_44	109.5
H8A_44–C8_44–H8C_44	109.5
H8B_44–C8_44–H8C_44	109.5
C2_44–C9_44–H9A_44	109.5
C2_44–C9_44–H9B_44	109.5
H9A_44–C9_44–H9B_44	109.5
C2_44–C9_44–H9C_44	109.5
H9A_44–C9_44–H9C_44	109.5
H9B_44–C9_44–H9C_44	109.5
C1_44–C10_44–H10A_44	109.5
C1_44–C10_44–H10B_44	109.5
H10A_44–C10_44–H10B_44	109.5
C1_44–C10_44–H10C_44	109.5
H10A_44–C10_44–H10C_44	109.5
H10B_44–C10_44–H10C_44	109.5
C1_45–O1_45–Al7	148.0(12)
O1_45–C1_45–C2_45	111.6(10)
O1_45–C1_45–C3_45	110.8(8)
C2_45–C1_45–C3_45	109.0(7)
O1_45–C1_45–C4_45	106.6(9)
C2_45–C1_45–C4_45	109.4(7)
C3_45–C1_45–C4_45	109.4(7)
F3_45–C2_45–F2_45	109.5(9)
F3_45–C2_45–F1_45	106.7(8)
F2_45–C2_45–F1_45	109.4(11)
F3_45–C2_45–C1_45	110.7(8)
F2_45–C2_45–C1_45	111.3(10)
F1_45–C2_45–C1_45	109.0(8)
F4_45–C3_45–F6_45	108.9(8)
F4_45–C3_45–F5_45	108.5(8)
F6_45–C3_45–F5_45	108.2(7)
F4_45–C3_45–C1_45	111.1(7)
F6_45–C3_45–C1_45	110.9(7)
F5_45–C3_45–C1_45	109.2(7)
F9_45–C4_45–F7_45	109.8(8)
F9_45–C4_45–F8_45	107.0(8)
F7_45–C4_45–F8_45	108.8(7)
F9_45–C4_45–C1_45	111.7(7)
F7_45–C4_45–C1_45	109.0(7)
F8_45–C4_45–C1_45	110.6(8)
C2_46–C1_46–C5_46	106.0(8)
C2_46–C1_46–C10_46	134.9(11)
C5_46–C1_46–C10_46	118.7(10)
C2_46–C1_46–Al12	73.4(5)
C5_46–C1_46–Al12	67.4(5)
C10_46–C1_46–Al12	128.2(7)
C3_46–C2_46–C1_46	110.1(9)
C3_46–C2_46–C9_46	123.5(10)
C1_46–C2_46–C9_46	126.1(10)
C3_46–C2_46–Al12	69.4(6)
C1_46–C2_46–Al12	71.8(5)
C9_46–C2_46–Al12	131.0(8)
C2_46–C3_46–C4_46	108.4(9)
C2_46–C3_46–C8_46	126.0(11)
C4_46–C3_46–C8_46	125.5(11)
C2_46–C3_46–Al12	75.6(6)
C4_46–C3_46–Al12	68.0(9)
C8_46–C3_46–Al12	124.7(10)
C3_46–C4_46–C5_46	107.7(9)
C3_46–C4_46–C7_46	121.0(10)
C5_46–C4_46–C7_46	131.4(10)
C3_46–C4_46–Al12	75.4(9)
C5_46–C4_46–Al12	72.9(7)
C7_46–C4_46–Al12	117.5(11)
C4_46–C5_46–C1_46	107.9(8)
C4_46–C5_46–C6_46	120.3(10)
C1_46–C5_46–C6_46	131.8(10)
C4_46–C5_46–Al12	69.5(8)
C1_46–C5_46–Al12	75.7(5)
C6_46–C5_46–Al12	122.6(8)
C5_46–C6_46–H6A_46	109.5
C5_46–C6_46–H6B_46	109.5
H6A_46–C6_46–H6B_46	109.5
C5_46–C6_46–H6C_46	109.5
H6A_46–C6_46–H6C_46	109.5
H6B_46–C6_46–H6C_46	109.5
C4_46–C7_46–H7A_46	109.5
C4_46–C7_46–H7B_46	109.5
H7A_46–C7_46–H7B_46	109.5
C4_46–C7_46–H7C_46	109.5
H7A_46–C7_46–H7C_46	109.5

H7B_46–C7_46–H7C_46	109.5
C3_46–C8_46–H8A_46	109.5
C3_46–C8_46–H8B_46	109.5
H8A_46–C8_46–H8B_46	109.5
C3_46–C8_46–H8C_46	109.5
H8A_46–C8_46–H8C_46	109.5
H8B_46–C8_46–H8C_46	109.5
C2_46–C9_46–H9A_46	109.5
C2_46–C9_46–H9B_46	109.5
H9A_46–C9_46–H9B_46	109.5
C2_46–C9_46–H9C_46	109.5
H9A_46–C9_46–H9C_46	109.5
H9B_46–C9_46–H9C_46	109.5
C1_46–C10_46–H10A_46	109.5
C1_46–C10_46–H10B_46	109.5
H10A_46–C10_46–H10B_46	109.5
C1_46–C10_46–H10C_46	109.5
H10A_46–C10_46–H10C_46	109.5
H10B_46–C10_46–H10C_46	109.5
O1_34–Al–O1_32	111.0(3)
O1_34–Al–O1_33	113.5(3)
O1_32–Al–O1_33	108.2(3)
C1_32–O1_32–Al	147.9(5)
O1_32–C1_32–C3_32	107.6(6)
O1_32–C1_32–C4_32	108.7(6)
C3_32–C1_32–C4_32	108.4(6)
O1_32–C1_32–C2_32	112.3(6)
C3_32–C1_32–C2_32	110.1(6)
C4_32–C1_32–C2_32	109.6(6)
F2_32–C2_32–F3_32	106.4(7)
F2_32–C2_32–F1_32	114.0(7)
F3_32–C2_32–F1_32	111.5(7)
F2_32–C2_32–C1_32	108.5(7)
F3_32–C2_32–C1_32	108.1(6)
F1_32–C2_32–C1_32	108.1(6)
F4_32–C3_32–F5_32	114.6(7)
F4_32–C3_32–F6_32	107.3(7)
F5_32–C3_32–F6_32	109.1(7)
F4_32–C3_32–C1_32	108.6(7)
F5_32–C3_32–C1_32	108.7(6)
F6_32–C3_32–C1_32	108.4(6)
F8_32–C4_32–F7_32	116.4(6)
F8_32–C4_32–F9_32	95.6(6)
F7_32–C4_32–F9_32	107.1(6)
F8_32–C4_32–C1_32	115.6(6)
F7_32–C4_32–C1_32	112.5(6)
F9_32–C4_32–C1_32	107.3(5)
C1_33–O1_33–Al	147.7(6)
O1_33–C1_33–C3_33	107.6(7)
O1_33–C1_33–C2_33	115.4(7)
C3_33–C1_33–C2_33	112.0(8)
O1_33–C1_33–C4_33	109.5(7)
C3_33–C1_33–C4_33	104.6(7)
C2_33–C1_33–C4_33	107.2(7)
F3_33–C2_33–F2_33	107.6(7)
F3_33–C2_33–F1_33	108.4(8)
F2_33–C2_33–F1_33	115.9(7)
F3_33–C2_33–C1_33	108.1(7)
F2_33–C2_33–C1_33	110.9(7)
F1_33–C2_33–C1_33	105.7(7)
F4_33–C3_33–F6_33	108.6(8)
F4_33–C3_33–F5_33	106.4(9)
F6_33–C3_33–F5_33	109.0(8)
F4_33–C3_33–C1_33	114.9(7)
F6_33–C3_33–C1_33	114.7(7)
F5_33–C3_33–C1_33	102.7(8)
F9_33–C4_33–F8_33	107.2(7)
F9_33–C4_33–F7_33	114.3(8)
F8_33–C4_33–F7_33	115.6(7)
F9_33–C4_33–C1_33	110.3(7)
F8_33–C4_33–C1_33	108.2(7)
F7_33–C4_33–C1_33	100.9(7)
C1_34–O1_34–Al	149.9(5)
O1_34–C1_34–C4_34	111.3(6)
O1_34–C1_34–C2_34	110.9(6)
C4_34–C1_34–C2_34	109.0(6)
O1_34–C1_34–C3_34	108.0(6)
C4_34–C1_34–C3_34	108.7(6)
C2_34–C1_34–C3_34	108.9(6)
F1_34–C2_34–F3_34	108.0(6)
F1_34–C2_34–F2_34	108.2(6)
F3_34–C2_34–F2_34	106.9(7)
F1_34–C2_34–C1_34	111.2(5)
F3_34–C2_34–C1_34	110.4(6)
F2_34–C2_34–C1_34	111.9(7)
F4_34–C3_34–F5_34	107.7(6)
F4_34–C3_34–F6_34	107.0(6)
F5_34–C3_34–F6_34	107.7(5)
F4_34–C3_34–C1_34	110.9(6)
F5_34–C3_34–C1_34	111.2(5)
F6_34–C3_34–C1_34	112.2(6)
F7_34–C4_34–F9_34	108.2(8)
F7_34–C4_34–F8_34	106.9(7)
F9_34–C4_34–F8_34	108.1(7)
F7_34–C4_34–C1_34	112.2(8)

F9_34–C4_34–C1_34	109.4(5)	F8_29–C4_29–C1_29	111.2(5)
F8_34–C4_34–C1_34	111.9(6)	C1_51–O1_51–Al19	149.0(5)
C1_30–O1_30–Al	150.9(5)	O1_51–C1_51–C4_51	110.0(6)
O1_30–C1_30–C3_30	108.5(6)	O1_51–C1_51–C2_51	109.5(6)
O1_30–C1_30–C4_30	109.5(6)	C4_51–C1_51–C2_51	108.0(6)
C3_30–C1_30–C4_30	108.8(6)	O1_51–C1_51–C3_51	112.1(6)
O1_30–C1_30–C2_30	111.8(6)	C4_51–C1_51–C3_51	107.9(6)
C3_30–C1_30–C2_30	108.1(6)	C2_51–C1_51–C3_51	109.3(6)
C4_30–C1_30–C2_30	110.0(6)	F1_51–C2_51–F3_51	107.5(7)
F1_30–C2_30–F2_30	108.1(6)	F1_51–C2_51–F2_51	107.1(6)
F1_30–C2_30–F3_30	108.5(6)	F3_51–C2_51–F2_51	108.3(6)
F2_30–C2_30–F3_30	107.8(6)	F1_51–C2_51–C1_51	111.2(6)
F1_30–C2_30–C1_30	109.5(6)	F3_51–C2_51–C1_51	109.8(6)
F2_30–C2_30–C1_30	113.0(6)	F2_51–C2_51–C1_51	112.8(6)
F3_30–C2_30–C1_30	109.8(6)	F6_51–C3_51–F5_51	107.3(7)
F4_30–C3_30–F5_30	108.6(8)	F6_51–C3_51–F4_51	109.7(7)
F4_30–C3_30–F6_30	107.6(6)	F5_51–C3_51–F4_51	110.5(7)
F5_30–C3_30–F6_30	108.4(8)	F6_51–C3_51–C1_51	110.9(7)
F4_30–C3_30–C1_30	110.8(6)	F5_51–C3_51–C1_51	108.3(6)
F5_30–C3_30–C1_30	109.0(7)	F4_51–C3_51–C1_51	110.1(6)
F6_30–C3_30–C1_30	112.4(6)	F8_51–C4_51–F7_51	107.8(8)
F7_30–C4_30–F9_30	108.8(7)	F8_51–C4_51–F9_51	108.4(6)
F7_30–C4_30–F8_30	108.6(6)	F7_51–C4_51–F9_51	108.4(8)
F9_30–C4_30–F8_30	107.9(6)	F8_51–C4_51–C1_51	113.0(6)
F7_30–C4_30–C1_30	111.3(6)	F7_51–C4_51–C1_51	108.6(8)
F9_30–C4_30–C1_30	108.9(6)	F9_51–C4_51–C1_51	110.5(6)
F8_30–C4_30–C1_30	111.3(5)	C1_50–O1_50–Al19	147.9(5)
O1_50–Al19–O1_29	121.0(2)	O1_50–C1_50–C2_50	110.6(7)
O1_50–Al19–O1_26	108.3(2)	O1_50–C1_50–C3_50	108.0(6)
O1_29–Al19–O1_26	108.1(3)	C2_50–C1_50–C3_50	109.8(6)
C1_29–O1_29–Al19	152.3(5)	O1_50–C1_50–C4_50	109.6(6)
O1_29–C1_29–C3_29	113.0(6)	C2_50–C1_50–C4_50	109.3(7)
O1_29–C1_29–C2_29	105.8(5)	C3_50–C1_50–C4_50	109.5(7)
C3_29–C1_29–C2_29	111.4(6)	F3_50–C2_50–F2_50	110.8(10)
O1_29–C1_29–C4_29	109.6(5)	F3_50–C2_50–F1_50	106.1(9)
C3_29–C1_29–C4_29	109.7(6)	F2_50–C2_50–F1_50	106.9(7)
C2_29–C1_29–C4_29	107.1(5)	F3_50–C2_50–C1_50	112.0(8)
F1_29–C2_29–F2_29	107.5(6)	F2_50–C2_50–C1_50	110.7(7)
F1_29–C2_29–F3_29	106.0(8)	F1_50–C2_50–C1_50	110.2(7)
F2_29–C2_29–F3_29	107.1(8)	F4_50–C3_50–F6_50	107.9(7)
F1_29–C2_29–C1_29	112.4(6)	F4_50–C3_50–F5_50	107.5(7)
F2_29–C2_29–C1_29	113.3(6)	F6_50–C3_50–F5_50	108.6(7)
F3_29–C2_29–C1_29	110.1(7)	F4_50–C3_50–C1_50	111.3(6)
F6_29–C3_29–F4_29	106.6(9)	F6_50–C3_50–C1_50	111.5(6)
F6_29–C3_29–F5_29	109.6(8)	F5_50–C3_50–C1_50	109.9(7)
F4_29–C3_29–F5_29	109.2(7)	F9_50–C4_50–F8_50	108.4(7)
F6_29–C3_29–C1_29	111.5(7)	F9_50–C4_50–F7_50	110.2(7)
F4_29–C3_29–C1_29	109.2(7)	F8_50–C4_50–F7_50	108.6(7)
F5_29–C3_29–C1_29	110.7(7)	F9_50–C4_50–C1_50	109.7(6)
F7_29–C4_29–F9_29	107.9(6)	F8_50–C4_50–C1_50	111.9(7)
F7_29–C4_29–F8_29	110.4(6)	F7_50–C4_50–C1_50	108.0(7)
F9_29–C4_29–F8_29	108.1(5)	C1_55–O1_55–Al17	159(2)
F7_29–C4_29–C1_29	109.2(5)	O1_55–C1_55–C4_55	115.1(16)
F9_29–C4_29–C1_29	110.1(5)	O1_55–C1_55–C2_55	108.0(16)

C4_55–C1_55–C2_55	110.7(13)	F3_26–C2_26–F2_26	107.4(6)
O1_55–C1_55–C3_55	106.1(15)	F3_26–C2_26–F1_26	110.5(8)
C4_55–C1_55–C3_55	109.3(13)	F2_26–C2_26–F1_26	108.8(8)
C2_55–C1_55–C3_55	107.3(13)	F3_26–C2_26–C1_26	111.8(6)
F2_55–C2_55–F1_55	106.3(18)	F2_26–C2_26–C1_26	111.9(6)
F2_55–C2_55–F3_55	109.9(19)	F1_26–C2_26–C1_26	106.5(7)
F1_55–C2_55–F3_55	110.6(19)	F4_26–C3_26–F5_26	111.4(8)
F2_55–C2_55–C1_55	110.1(16)	F4_26–C3_26–F6_26	107.3(8)
F1_55–C2_55–C1_55	112.5(18)	F5_26–C3_26–F6_26	117.2(8)
F3_55–C2_55–C1_55	107.5(16)	F4_26–C3_26–C1_26	110.1(7)
F4_55–C3_55–F6_55	108.7(18)	F5_26–C3_26–C1_26	104.8(7)
F4_55–C3_55–F5_55	110.2(18)	F6_26–C3_26–C1_26	105.8(7)
F6_55–C3_55–F5_55	106.8(18)	F9_26–C4_26–F8_26	105.5(7)
F4_55–C3_55–C1_55	108.0(16)	F9_26–C4_26–F7_26	111.7(7)
F6_55–C3_55–C1_55	113.4(16)	F8_26–C4_26–F7_26	110.5(7)
F5_55–C3_55–C1_55	109.7(15)	F9_26–C4_26–C1_26	110.5(6)
F8_55–C4_55–F9_55	106.2(17)	F8_26–C4_26–C1_26	111.3(6)
F8_55–C4_55–F7_55	106.8(17)	F7_26–C4_26–C1_26	107.4(6)
F9_55–C4_55–F7_55	110.1(18)	C1_20–O1_20–Al17	148.7(12)
F8_55–C4_55–C1_55	110.3(15)	O1_20–C1_20–C3_20	110.8(9)
F9_55–C4_55–C1_55	111.8(16)	O1_20–C1_20–C4_20	107.3(9)
F7_55–C4_55–C1_55	111.3(15)	C3_20–C1_20–C4_20	110.8(7)
C1_56–O1_56–Al17	154(2)	O1_20–C1_20–C2_20	110.2(10)
O1_56–C1_56–C2_56	110.0(16)	C3_20–C1_20–C2_20	108.7(7)
O1_56–C1_56–C3_56	109.2(16)	C4_20–C1_20–C2_20	109.1(7)
C2_56–C1_56–C3_56	111.1(13)	F1_20–C2_20–F2_20	107.3(10)
O1_56–C1_56–C4_56	106.6(16)	F1_20–C2_20–F3_20	108.9(9)
C2_56–C1_56–C4_56	109.7(13)	F2_20–C2_20–F3_20	107.3(11)
C3_56–C1_56–C4_56	110.0(13)	F1_20–C2_20–C1_20	109.3(8)
F2_56–C2_56–F1_56	110.0(19)	F2_20–C2_20–C1_20	113.6(10)
F2_56–C2_56–F3_56	108.0(19)	F3_20–C2_20–C1_20	110.3(9)
F1_56–C2_56–F3_56	107.3(19)	F4_20–C3_20–F5_20	111.6(8)
F2_56–C2_56–C1_56	109.4(16)	F4_20–C3_20–F6_20	105.8(10)
F1_56–C2_56–C1_56	111.1(17)	F5_20–C3_20–F6_20	105.1(9)
F3_56–C2_56–C1_56	111.0(18)	F4_20–C3_20–C1_20	109.8(8)
F4_56–C3_56–F6_56	106.6(18)	F5_20–C3_20–C1_20	111.7(7)
F4_56–C3_56–F5_56	108.7(19)	F6_20–C3_20–C1_20	112.8(10)
F6_56–C3_56–F5_56	106.4(18)	F7_20–C4_20–F9_20	110.1(9)
F4_56–C3_56–C1_56	109.9(16)	F7_20–C4_20–F8_20	103.9(9)
F6_56–C3_56–C1_56	112.1(16)	F9_20–C4_20–F8_20	108.7(10)
F5_56–C3_56–C1_56	112.8(16)	F7_20–C4_20–C1_20	110.8(8)
F8_56–C4_56–F7_56	108.9(19)	F9_20–C4_20–C1_20	109.9(7)
F8_56–C4_56–F9_56	105.7(18)	F8_20–C4_20–C1_20	113.2(9)
F7_56–C4_56–F9_56	111.1(18)	C1_21–O1_21–Al17	150.4(7)
F8_56–C4_56–C1_56	111.7(17)	O1_21–C1_21–C4_21	111.2(8)
F7_56–C4_56–C1_56	108.8(16)	O1_21–C1_21–C2_21	110.2(8)
F9_56–C4_56–C1_56	110.6(16)	C4_21–C1_21–C2_21	110.9(8)
C1_26–O1_26–Al19	152.5(5)	O1_21–C1_21–C3_21	106.8(7)
O1_26–C1_26–C4_26	111.3(6)	C4_21–C1_21–C3_21	109.7(8)
O1_26–C1_26–C2_26	111.6(5)	C2_21–C1_21–C3_21	107.9(8)
C4_26–C1_26–C2_26	110.7(6)	F1_21–C2_21–F2_21	106.0(12)
O1_26–C1_26–C3_26	106.9(6)	F1_21–C2_21–F3_21	107.3(10)
C4_26–C1_26–C3_26	109.2(6)	F2_21–C2_21–F3_21	106.1(14)
C2_26–C1_26–C3_26	107.0(6)	F1_21–C2_21–C1_21	112.7(10)

F2_21–C2_21–C1_21	115.5(13)
F3_21–C2_21–C1_21	108.7(9)
F4_21–C3_21–F5_21	106.9(10)
F4_21–C3_21–F6_21	112.3(10)
F5_21–C3_21–F6_21	108.2(10)
F4_21–C3_21–C1_21	110.1(8)
F5_21–C3_21–C1_21	111.0(8)
F6_21–C3_21–C1_21	108.4(10)
F7_21–C4_21–F9_21	111.6(10)
F7_21–C4_21–F8_21	109.3(10)
F9_21–C4_21–F8_21	104.2(9)
F7_21–C4_21–C1_21	110.7(9)
F9_21–C4_21–C1_21	109.3(8)
F8_21–C4_21–C1_21	111.6(8)
C1_28–O1_28–Al17	154(2)
O1_28–C1_28–C3_28	107.6(15)
O1_28–C1_28–C4_28	111.1(16)
C3_28–C1_28–C4_28	111.6(10)
O1_28–C1_28–C2_28	109.9(15)
C3_28–C1_28–C2_28	109.0(10)
C4_28–C1_28–C2_28	107.6(9)
F3_28–C2_28–F1_28	108.7(11)
F3_28–C2_28–F2_28	104.5(12)
F1_28–C2_28–F2_28	110.9(14)
F3_28–C2_28–C1_28	111.5(10)
F1_28–C2_28–C1_28	109.7(11)
F2_28–C2_28–C1_28	111.5(12)
F5_28–C3_28–F6_28	112.5(15)
F5_28–C3_28–F4_28	110.4(12)
F6_28–C3_28–F4_28	101.1(14)
F5_28–C3_28–C1_28	111.7(11)
F6_28–C3_28–C1_28	112.6(15)
F4_28–C3_28–C1_28	107.9(10)
F9_28–C4_28–F7_28	109.6(13)
F9_28–C4_28–F8_28	110.0(13)
F7_28–C4_28–F8_28	108.3(13)
F9_28–C4_28–C1_28	111.5(10)
F7_28–C4_28–C1_28	109.7(12)
F8_28–C4_28–C1_28	107.7(12)

Literature

S-5 References

1. Purath, A., Köppe, R. & Schnöckel, H. [Al7{N(SiMe3)2}6]−: A First Step towards Aluminum Metal Formation by Disproportionation. *Angew. Chem. Int. Ed.* **38,** 2926–2928; 10.1002/(SICI)1521-3773(19991004)38:19<2926::AID-ANIE2926>3.0.CO;2-B (1999).

2. Yang, P. *et al.* Al(Al3R3)2: prototype of a metalloid Al cluster or a sandwich-stabilized Al atom? *Angew. Chem. Int. Ed.* **46,** 3579–3583; 10.1002/anie.200604567 (2007).

3. Purath, A. & Schnöckel, H. Tetrakis[tris(trimethylsilyl)silylaluminium(I)] Al4[Si(SiMe3)3]4—eine siliziumreicheVerbindung mit zentralem tetraedrischem Al4-Kern. *J. Organomet. Chem.* **579,** 373–375; 10.1016/S0022-328X(99)00027-3 (1999).

4. Purath, A. *et al.* Synthesis and Crystal Structure of the Tetraaluminatetrahedrane Al 4 [Si(t -Bu) 3] 4 , the Second Al 4 R 4 Compound. *Organometallics* **17,** 1894–1896; 10.1021/om971015h (1998).

5. Schiefer, M., Reddy, N. D., Roesky, H. W. & Vidovic, D. Synthesis and Structural Characterization of an Exclusively N-Based Tetrameric Aluminum(I) Compound. *Organometallics* **22,** 3637–3638; 10.1021/om0302793 (2003).

6. Sitzmann, H., Lappert, M. F., Dohmeier, C., Üffing, C. & Schnöckel, H. Cyclopentadienylderivate von Aluminium(I). *J. Organomet. Chem.* **561,** 203–208; 10.1016/S0022-328X(98)00555-5 (1998).

7. Schnitter, C. *et al.* The Behavior of [RAlX2·THF] Compounds under Reductive Conditions: Tetrakis[tris(trimethylsilyl)methylaluminum(I)]—A Neutral Aluminum(I) Compound with σ-Bound Alkyl Groups and a Tetrahedral Structure. *Angew. Chem. Int. Ed.* **37,** 1952–1955; 10.1002/(SICI)1521-3773(19980803)37:13/14<1952::AID-ANIE1952>3.0.CO;2-U (1998).

8. Dohmeier, C., Robl, C., Tacke, M. & Schnöckel, H. The Tetrameric Aluminum(I) Compound[{Al(η5-C5Me5)}4]. *Angew. Chem. Int. Ed.* **30,** 564–565; 10.1002/anie.199105641 (1991).

9. Roesky, H. W. & Kennepohl, D. K. *Experiments in green and sustainable chemistry* (Wiley-VCH, Weinheim, 2009).

10. Gruber, M., Bauer, W., Maid, H., Schöll, K. & Tykwinski, R. R. Synthetic and NMR studies on hexaphenylcarbodiphosphorane (Ph3P C PPh3). *Inorganica Chimica Acta* **468,** 152–158; 10.1016/j.ica.2017.04.018 (2017).

11. Pranckevicius, C., Iovan, D. A. & Stephan, D. W. Three and four coordinate Fe carbodiphosphorane complexes. *Dalton Trans.* **45,** 16820–16825; 10.1039/c6dt03453e (2016).

12. Ganesamoorthy, C. *et al.* Reductive elimination: a pathway to low-valent aluminium species. *Chem. Commun.* **49,** 2858–2860; 10.1039/c3cc38584a (2013).

13. Cosier, J. & Glazer, A. M. A nitrogen-gas-stream cryostat for general X-ray diffraction studies. *J. Appl. Crystallogr.* **19,** 105–107; 10.1107/S0021889886089835 (1986).

14. Sheldrick, G. M. A short history of SHELX. *Acta crystallographica. Section A, Foundations of crystallography* **64,** 112–122; 10.1107/S0108767307043930 (2008).

15. Kratzert, D., Holstein, J. J. & Krossing, I. DSR: enhanced modelling and refinement of disordered structures with SHELXL. *J. Appl. Crystallogr.* **48,** 933–938; 10.1107/S1600576715005580 (2015).

16. Daniel Kratzert, can be found under https://www.xs3.uni-freiburg.de/research/finalcif. ,

17. Del Rio, D. *et al.* IR and Raman characterization of the zincocenes (eta(5)-C5Me5)2Zn2 and (eta(5)-C5Me5)(eta(1)-C5Me5)Zn. *J. Phys. Chem. A* **112,** 10516–10525; 10.1021/jp805291e (2008).

18. Bencze, É., Lokshin, B. V., Mink*, J., Herrmann, W. A. & Kühn*, F. E. Vibrational spectra and structure of the cyclopentadienyl-anion (Cp−), the pentamethylcyclopentadienyl-anion (Cp*−) and of alkali metal cyclopentadienyls CpM and Cp*M (M=Li, Na, K). *J. Organomet. Chem.* **627,** 55–66; 10.1016/S0022-328X(01)00710-0 (2001).

19. Hansgerorg Schnöckel. Decamethylaluminocenium, a π-Stabilized R2Al+ Cation. *Angew. Chem. Int. Ed.* **32,** 1655–1657 (1993).

20. Akitt, J. W. Multinuclear studies of aluminium compounds. *Prog. Nucl. Magn. Reson. Spectrosc.* **21,** 1–149; 10.1016/0079-6565(89)80001-9 (1989).

21. Raabe, I. *et al.* Tetraalkylammonium salts of weakly coordinating aluminates: ionic liquids, materials for electrochemical applications and useful compounds for anion investigation. *Chem. Eur. J.* **15,** 1966–1976; 10.1002/chem.200800417 (2009).

22. Arnim, M. von & Ahlrichs, R. Performance of parallel TURBOMOLE for density functional calculations. *J. Comput. Chem.* **19,** 1746–1757; 10.1002/(SICI)1096-987X(19981130)19:15<1746::AID-JCC7>3.0.CO;2-N (1998).

23. Treutler, O. & Ahlrichs, R. Efficient molecular numerical integration schemes. *J. Chem. Phys.* **102,** 346–354; 10.1063/1.469408 (1995).

24. Perdew. Density-functional approximation for the correlation energy of the inhomogeneous electron gas. *Physical review. B, Condensed matter* **33,** 8822–8824; 10.1103/PhysRevB.33.8822 (1986).

25. Perdew, J. P. Erratum: Density-functional approximation for the correlation energy of the inhomogeneous electron gas. *Physical review. B, Condensed matter* **34,** 7406; 10.1103/PhysRevB.34.7406 (1986).

26. Weigend, F. & Ahlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.* **7,** 3297–3305; 10.1039/B508541A (2005).

27. Sierka, M., Hogekamp, A. & Ahlrichs, R. Fast evaluation of the Coulomb potential for electron densities using multipole accelerated resolution of identity approximation. *J. Chem. Phys.* **118,** 9136–9148; 10.1063/1.1567253 (2003).

28. Ahlrichs, R. Efficient evaluation of three-center two-electron integrals over Gaussian functions. *Phys. Chem. Chem. Phys.* **6,** 5119; 10.1039/B413539C (2004).

29. Weigend, F. Accurate Coulomb-fitting basis sets for H to Rn. *Phys. Chem. Chem. Phys.* **8,** 1057–1065; 10.1039/B515623H (2006).

30. Grimme, S., Antony, J., Ehrlich, S. & Krieg, H. A consistent and accurate ab initio parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **132,** 154104; 10.1063/1.3382344 (2010).

31. Grimme, S., Ehrlich, S. & Goerigk, L. Effect of the damping function in dispersion corrected density functional theory. *J. Comput. Chem.* **32,** 1456–1465; 10.1002/jcc.21759 (2011).

32. Deglmann, P., Furche, F. & Ahlrichs, R. An efficient implementation of second analytical derivatives for density functional methods. *Chem. Phys. Let.* **362,** 511–518; 10.1016/S0009-2614(02)01084-9 (2002).

33. Furche, F. & Ahlrichs, R. Adiabatic time-dependent density functional methods for excited state properties. *J. Chem. Phys.* **117,** 7433–7447; 10.1063/1.1508368 (2002).

34. Klamt, A. Conductor-like Screening Model for Real Solvents: A New Approach to the Quantitative Calculation of Solvation Phenomena. *J. Phys. Chem.* **99,** 2224–2235; 10.1021/j100007a062 (1995).

35. Klamt, A., Jonas, V., Bürger, T. & Lohrenz, J. C. W. Refinement and Parametrization of COSMO-RS. *J. Phys. Chem. A* **102,** 5074–5085; 10.1021/jp980017s (1998).

36. Rappoport, D. & Furche, F. Property-optimized gaussian basis sets for molecular response calculations. *J. Chem. Phys.* **133,** 134105; 10.1063/1.3484283 (2010).

37. F. Eckert, A. K. COSMOtherm. *VersionC3.0, Release 15.01* **COSMOlogic GMBH & Co. KG, Leverkusen, Germany** (2014).

38. Adamo, C. & Barone, V. Toward reliable density functional methods without adjustable parameters: The PBE0 model. *J. Chem. Phys.* **110,** 6158–6170; 10.1063/1.478522 (1999).

39. Perdew, J. P., Ernzerhof, M. & Burke, K. Rationale for mixing exact exchange with density functional approximations. *J. Chem. Phys.* **105,** 9982–9985; 10.1063/1.472933 (1996).

40. Lu, T. & Chen, F. Multiwfn: a multifunctional wavefunction analyzer. *J. Comput. Chem.* **33,** 580–592; 10.1002/jcc.22885 (2012).

41. Mitoraj, M. P., Michalak, A. & Ziegler, T. A Combined Charge and Energy Decomposition Scheme for Bond Analysis. *J. Chem. Theory Comput.* **5,** 962–975; 10.1021/ct800503d (2009).

42. te Velde, G. *et al.* Chemistry with ADF. *J. Comput. Chem.* **22,** 931–967; 10.1002/jcc.1056 (2001).