Electronic Supplementary Material (ESI) for Chemical Science.

Supporting information for the article: **From mixed group 13 cations $[M(AlCp^*)_3]^+$ (M = Ga/In/Tl) to a novel Al_4^+ cluster**

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Contents

S-1 Supporting experimental data

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%) and Me_3TACN (ChemPUR, 97 %) were used as received. Li[*pf*] ([*pf*]$^-$ = [Al(OR^F)$_4$]$^-$ with OR^F = C(CF$_3$)$_3$),[1] Ga[*pf*],[2] In[*pf*],[3] Tl[*pf*][4] and [(AlCp*)$_4$][5] (Cp* = C_5Me_5) prepared using literature known procedures. Fluorobenzene (fluorochem, PhF), *n*-heptane (Sigma Ahldrich) and 1,2-difluorobenzene (fluorochem, 1,2-DFB) were refluxed over CaH_2, fractionally distilled and stored over activated 3 Å molecular sieves. *n*-Pentane was collected from the solvent-purification system (SPS) and used as received.

NMR spectroscopy: NMR samples were prepared inside an inert atmosphere glovebox in NMR tubes equipped with a gas-tight J. Young valve. ^{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. The graphical representations in the manuscript were created with OriginPro 2021.

IR and Raman spectroscopy:

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

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. The graphical representations in the manuscript were created with OriginPro 2021.

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

Experimental data for $[Ga(AlCp^*)_3][Al(OR^F)_4]$ **1**

Procedure 1: Synthesis of **1** in 1,2-difluorobenzene (1,2-DFB)

$[Ga(PhF)_{2\text{-}3}][Al(OR^F)_4]$ (50 mg, 41 μmol) and $[(AlCp^*)_4]$ (20 mg, 31 μmol, 0.75 equiv.) were weighed into a Schlenk tube and 1,2-difluorobenzene (1 mL) was added at –40°C. The orange solution was stirred for 5 min, layered with *n*-heptane and allowed to crystallize at –31°C. The title compound (48 mg, 32 μmol, 75 %) was isolated as orange crystals.

^{1}H NMR spectrum (300.18 MHz, PhF, 298 K): δ = 1.70 (s, 45 H, $[Ga(Al\mathbf{Cp^*})_3]^+$) ppm.

^{1}H, ^{13}C HMBC spectrum (300.18 MHz, 75.48 MHz, PhF, 298 K): δ(^{13}C) = 8.9 (-**C**H_3), 115.6 (**C**$_5$$Me_5$) ppm.

^{19}F NMR spectrum (282.45 MHz, PhF, 298 K): δ = –75.1 (s, 36 F, $[Al(OC_4\mathbf{F_9})_4]^-$) ppm.

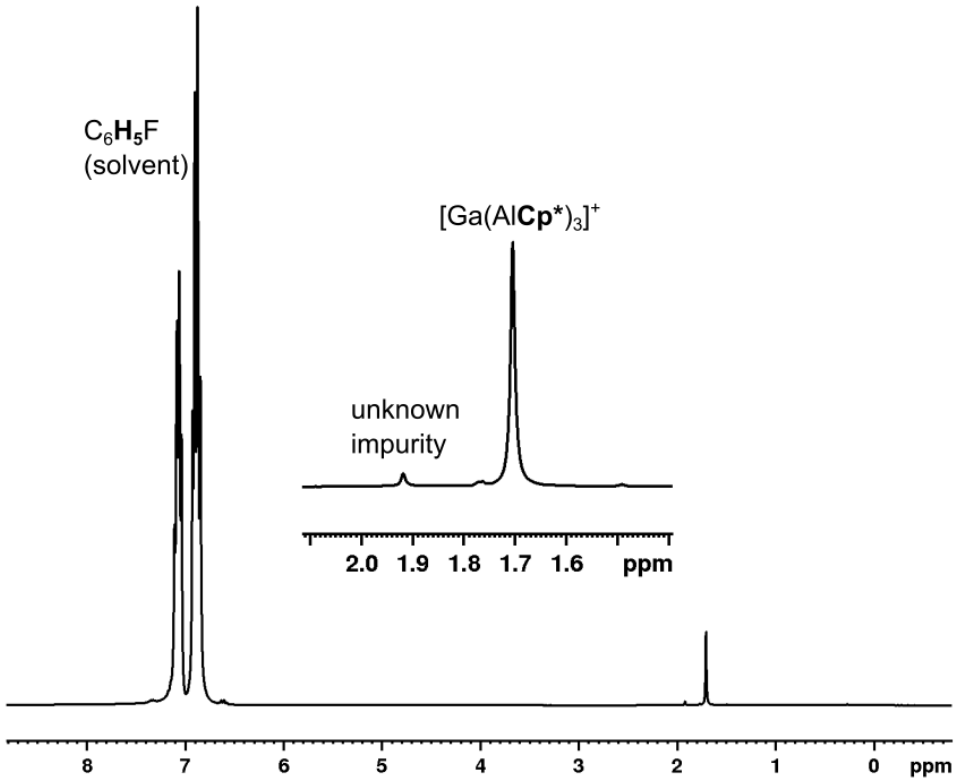
^{27}Al NMR spectrum (78.22 MHz, PhF, 298 K): δ = 35.0 (s, $[\mathbf{Al}(OC_4F_9)_4]^-$), –43.3 (s, $[Ga(\mathbf{Al}Cp^*)_3]^+$ –114.0 (br. s, $[AlCp^*_2]^+$) ppm.

^{71}Ga NMR spectrum (91.54 MHz, 1,2-DFB, 298 K): No signals observed.

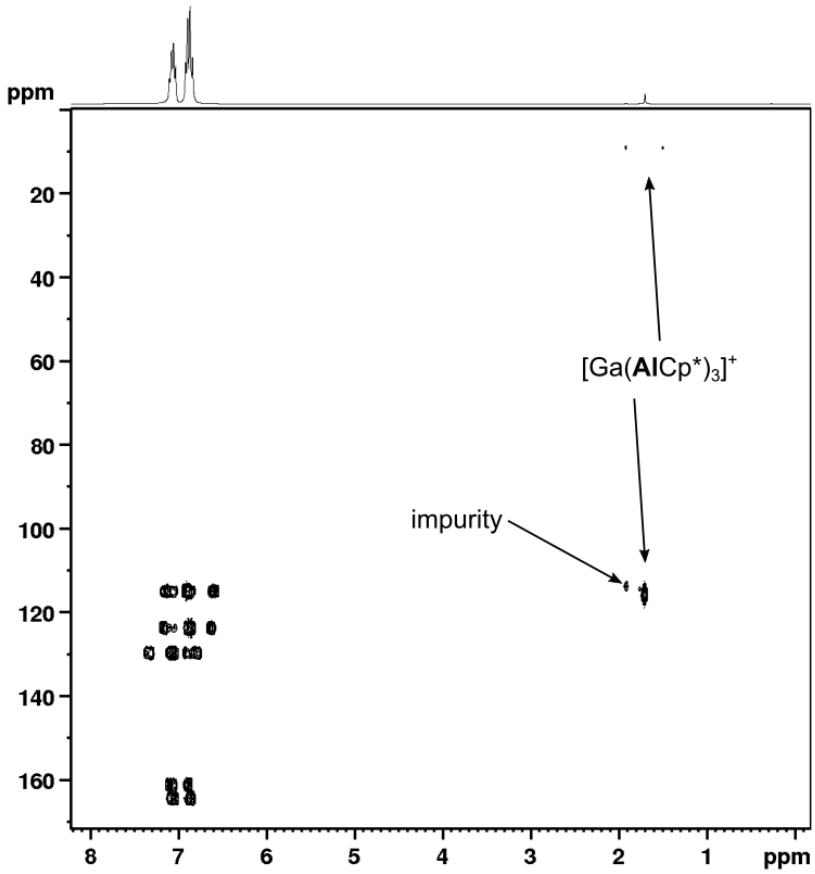
FTIR spectrum (ZnSe-ATR): $\tilde{\nu}$ = 2932 (vw), 1451 (vw), 1418 (vw), 1388 (vw), 1352 (vw), 1298 (w), 1275 (s), 1241 (s), 1212 (vs), 1162 (m), 971 (vs), 830 (vw), 808 (vw), 798 (vw), 755 (vw), 726 (vs), 584 (vw), 570 (vw), 559 (vw) cm^{-1}.

Raman (25 mW, 5000 scans): $\tilde{\nu}$ = 2928 (w), 2757 (vw), 1419 (vw), 1394 (vw), 797 (vw), 746 (vw), 591 (vw), 552 (vw), 519 (vw), 471 (w), 398 (vw), 150 (vs), 81 (s), 322 (vw), 287 (vw), 1471 (vw) cm^{-1}.

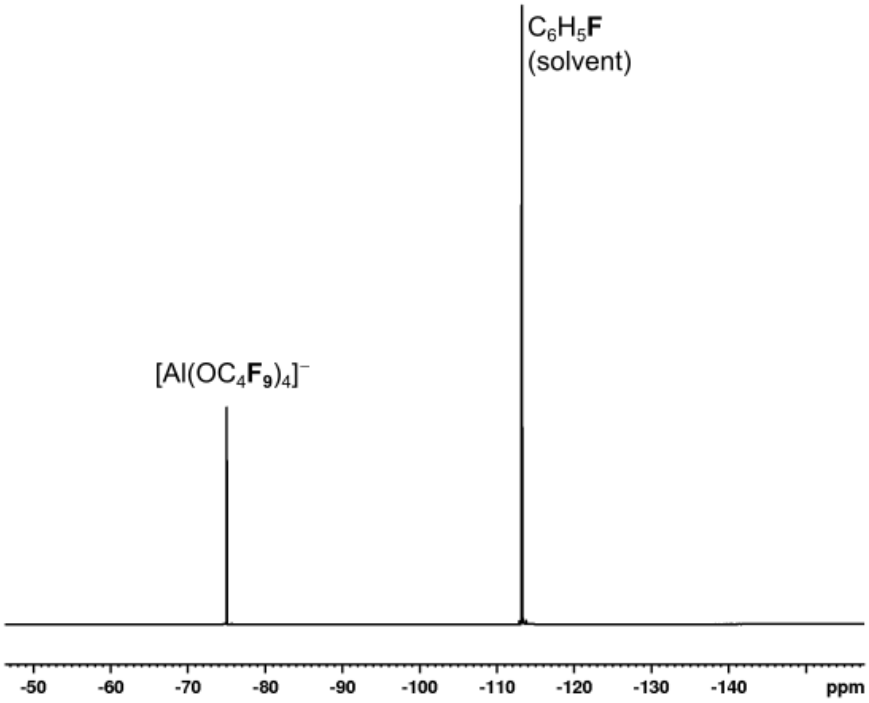
S-Figure 1: Crystals of **1** isolated at low-temperatures via crystallization from 1,2-DFB/*n*-heptane.



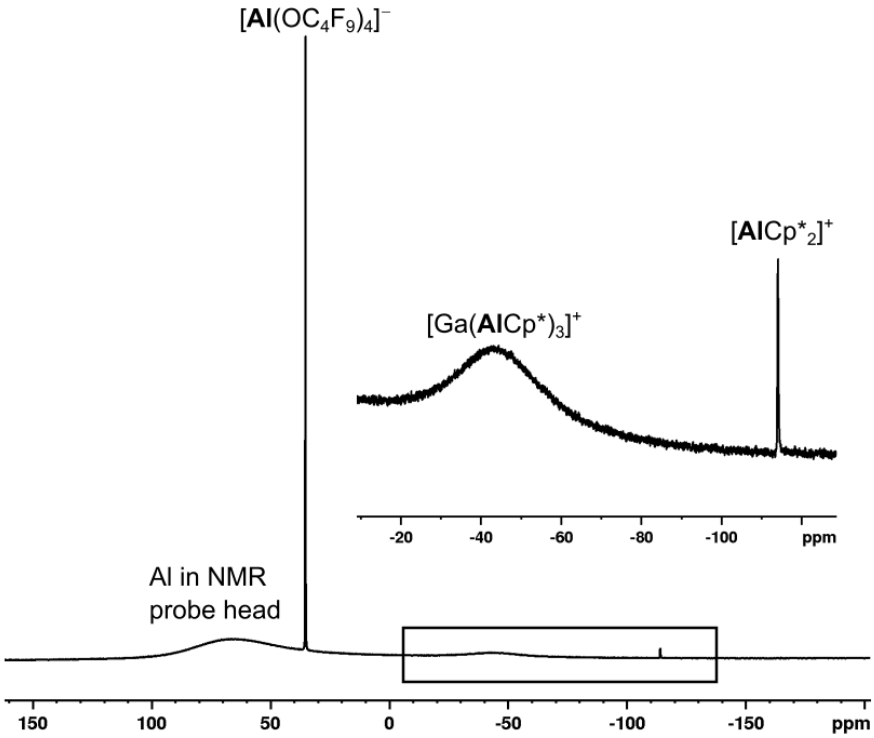
S-Figure 2: ^{1}H NMR spectrum (300.18 MHz, PhF, 300K) of $[Ga(AlCp^*)_3][Al(OR^F)_4]$ **1**.



S-Figure 3: ^{1}H-^{13}C HMBC spectrum (300.18 MHz, 75.48 MHz, PhF, 300K) of $[Ga(AlCp^*)_3][Al(OR^F)_4]$ **1**.

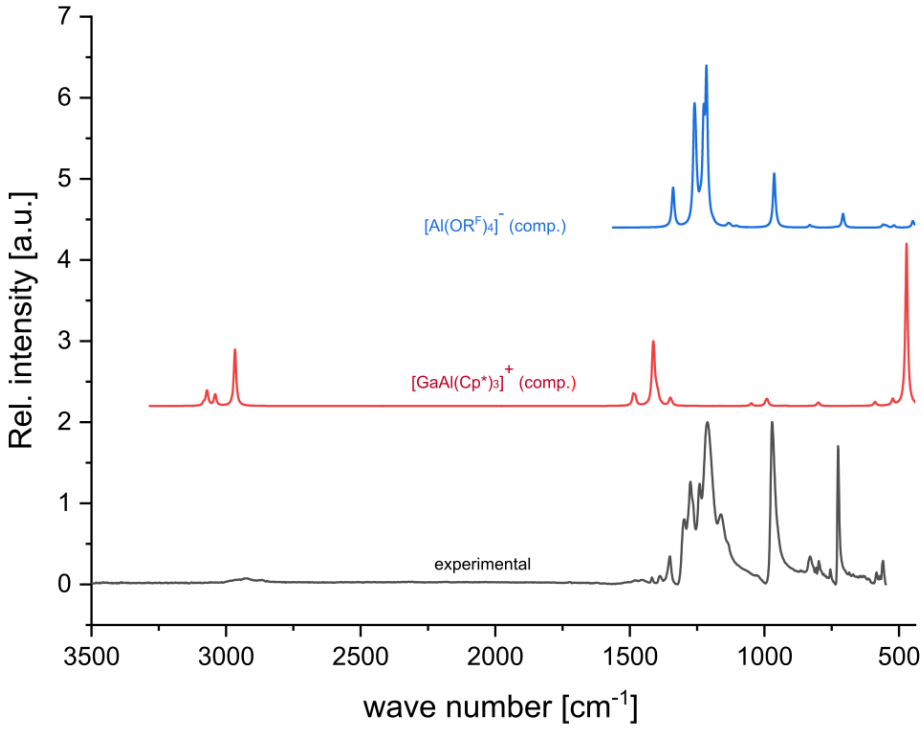


S-Figure 4: ^{19}F NMR spectrum (282.5 MHz, PhF, 300K) of $[Ga(AlCp^*)_3][Al(OR^F)_4]$ **1**.



S-Figure 5: ^{27}Al NMR spectrum (78.2 MHz, PhF, 300K) of $[Ga(AlCp^*)_3][Al(OR^F)_4]$ **1**.

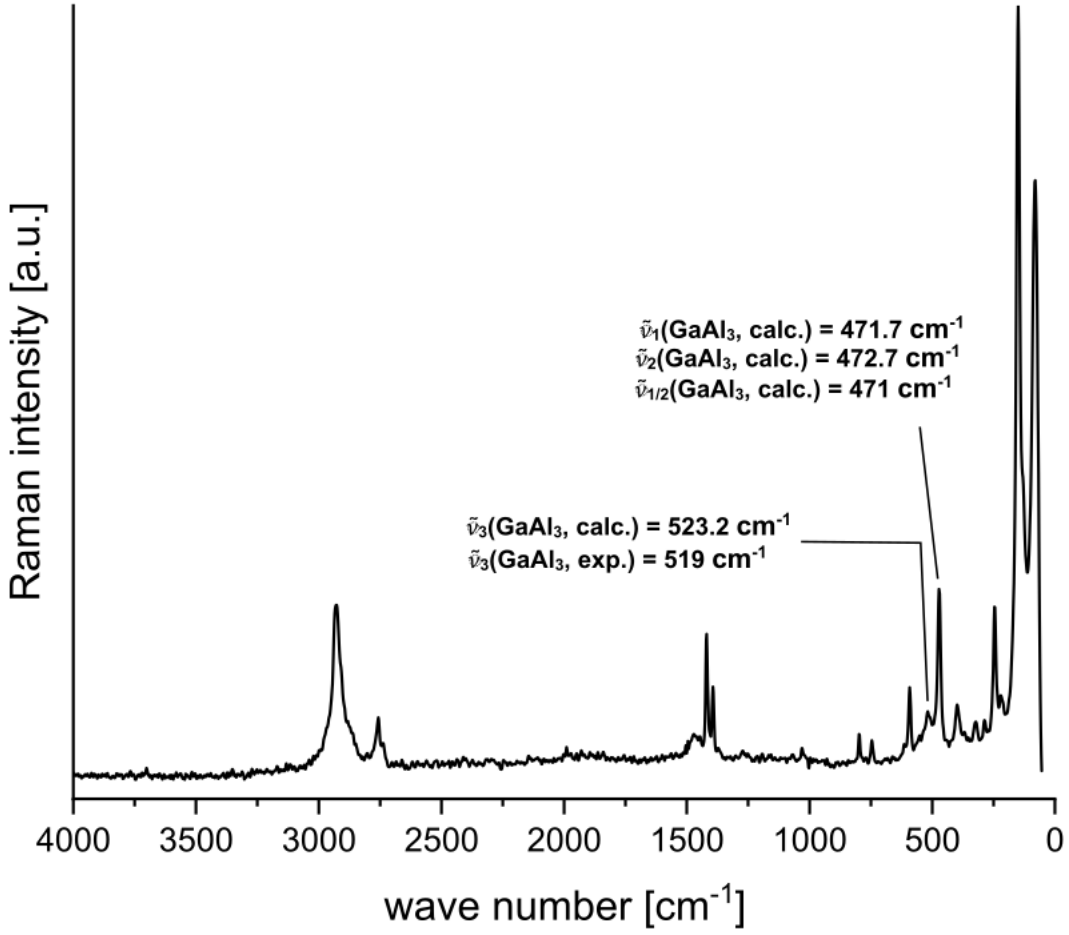
IR spectrum of 1



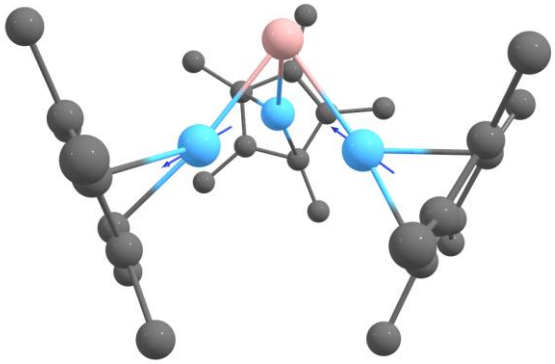
S-Figure 6: Experimental IR spectrum of **1** and computed IR spectra for the $[Ga(AlCp^*)_3]^+$ cation and the $[Al(OR^F)_4]^-$ anion (bp86-d3bj/def2-svp).

Raman spectrum of 1

In the Raman spectrum of $[Ga(AlCp^*)_3]^+[Al(OR^F)_4]$ (S-Figure 7), two degenerate asymmetric stretching vibrations of the In–Al bonds are observed at 471 cm^{-1}. Moreover, the band at 519 cm^{-1} can be assigned to a symmetric stretching vibration. The molecular vibrations were calculated on bp86-d3bj/def2-svp-level of DFT and are visualized in S-Figure 8. 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.[9,10]

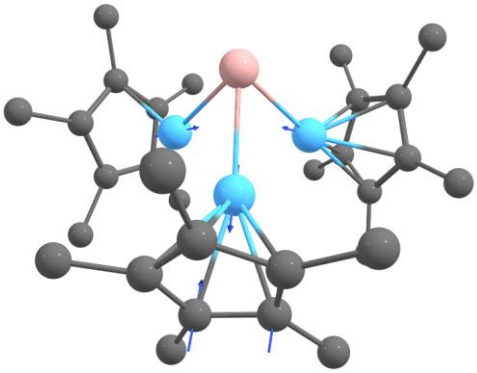


S-Figure 7: Experimental Raman spectrum of **1**.



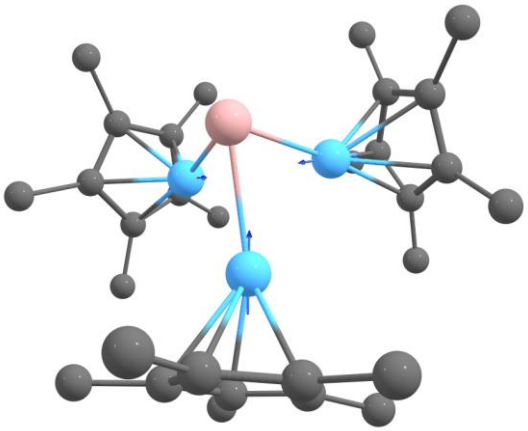
(Threshold for visualization: 0.31)

$\tilde{\nu}_1$(GaAl$_3$, calc.) = 471.7cm^{-1}



(Threshold for visualization: 0.18)

$\tilde{\nu}_2$(GaAl$_3$,calc.) = 472.7 cm^{-1}



(Threshold for visualization: 0.18

$\tilde{\nu}_3$(GaAl$_3$,calc.) = 523.3 cm^{-1}

S-Figure 8: Computed breathing vibrations of the $GaAl_3^+$ unit (at bp86-d3bj/def2-svp level of DFT). The displacement vectors computed for the vibration are displayed as blue arrows.

Procedure 2: Synthesis of **1** in fluorobenzene (PhF)

$[Ga(PhF)_{2\text{-}3}][Al(OR^F)_4]$ (150 mg, 122 μmol) and $[(AlCp^*)_4]$ (60 mg, 92 μmol, 0.75 equiv.) were dissolved in PhF (3 mL). The yellow solution was stirred for 5 min and layered with *n*-pentane room temperature. The title compound (144 mg, 94.5 μmol, 77 %) was isolated as orange crystals.

Detected NMR signals correspond to the previously observed NMR signals.

S-Figure 9: Crystals of **1** isolated via crystallization from PhF/*n*-pentane at room temperature.

Experimental data for $[In(AlCp^*)_3][Al(OR^F)_4]$ **2**

Procedure: Synthesis of **2** in 1,2-difluorobenzene (1,2-DFB)

$[In(PhF)_{2\text{-}3}][Al(OR^F)_4]$ (47 mg, 37 μmol) and $[(AlCp^*)_4]$ (20 mg, 31 μmol, 0.75 equiv.) were weighed into a Schlenk tube and 1,2-difluorobenzene (1 mL) was added at –30°C. The brown solution was stirred for 30 min, layered with *n*-heptane and allowed to crystallize at –31°C. The title compound (43 mg, 32 μmol, 66 %) was isolated as yellow crystals and could be separated from the black, metallic precipitate formed at the bottom of the Schlenk tube.

^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 298 K): δ = 1.81 (s, 45 H, $[In(Al\mathbf{Cp^*})_3]^+$), 1.97 (s, 30 H, $[Al(Cp^*)_2]^+$, minor impurity) ppm.

^{1}H, ^{13}C HMBC spectrum (300.18 MHz, 75.48 MHz, 1,2-DFB, 298 K): δ(^{13}C) = 8.7 (-**C**H_3), 115.6 (**C$_5$**Me_5) ppm.

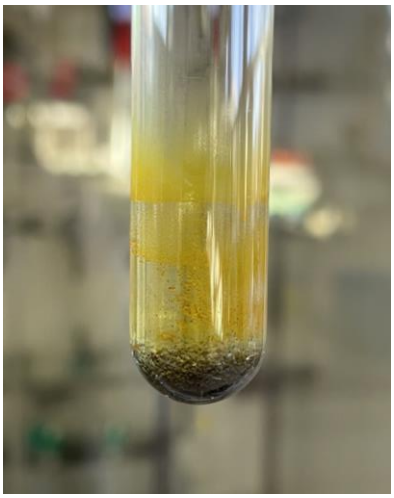
^{19}F NMR spectrum (282.45 MHz, 1,2-DFB, 298 K): δ = –75.0 (s, 36 F, $[Al(OC_4F_9)_4]^-$) ppm.

^{27}Al NMR spectrum (78.22 MHz, PhF, 298 K): δ = 35.0 (s, $[Al(OC_4F_9)_4]^-$), –59.7 (s, $[In(\mathbf{Al}Cp^*)_3]^+$ –114.8 (s, $[AlCp^*_2]^+$) ppm.

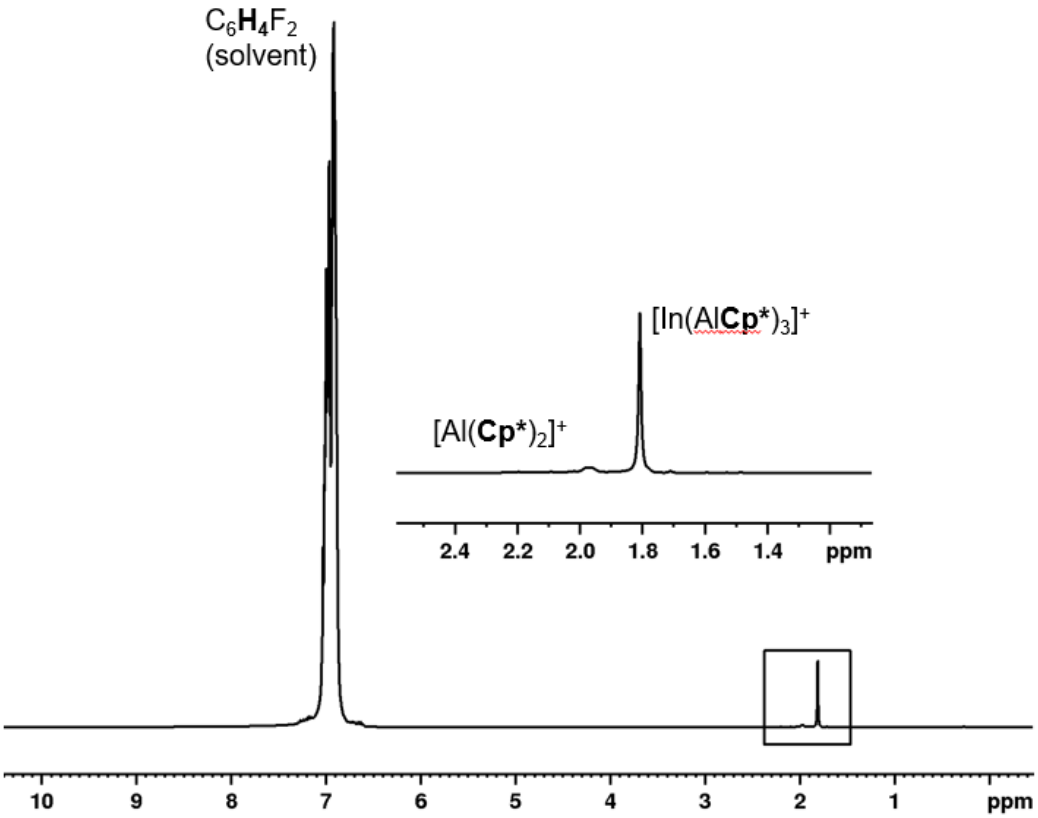
^{115}In NMR spectrum (65.78 MHz, 1,2-DFB, 298 K): No signals observed.

FTIR spectrum (ZnSe-ATR): $\tilde{\nu}$ = 1391 (vw), 1352 (vw), 1300 (w), 1276 (m), 1242 (s), 1219 (vs), 1164 (vw), 973 (vs), 831 (vw), 806 (vw), 798 (vw), 756 (vw), 728 (s), 583 (vw), 561 (vw) cm^{-1}.

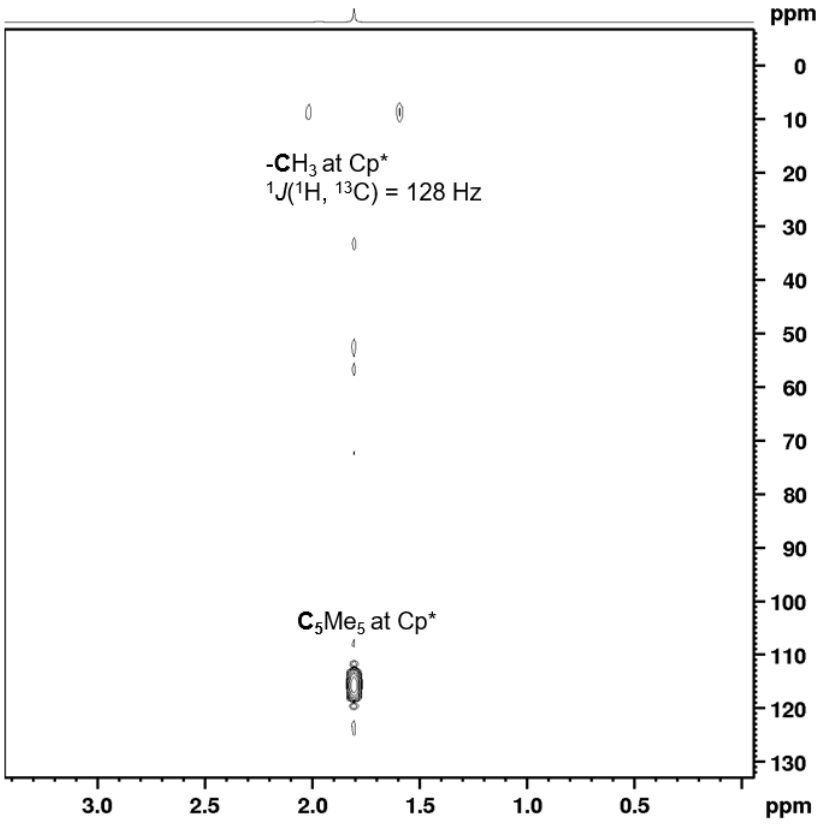
Raman (25 mW, 10000 scans): $\tilde{\nu}$ = 2928 (w), 2758 (vw), 1504 (vw), 1420 (w), 1393 (w), 797 (vw), 592 (vw), 496 (vw), 460 (w), 401 (vw), 1029 (vw), 746 (vw), 554 (vw), 320 (vw), 286 (vw), 201 (vw), 225 (vw), 112 (vs), 81 (vs) cm^{-1}.



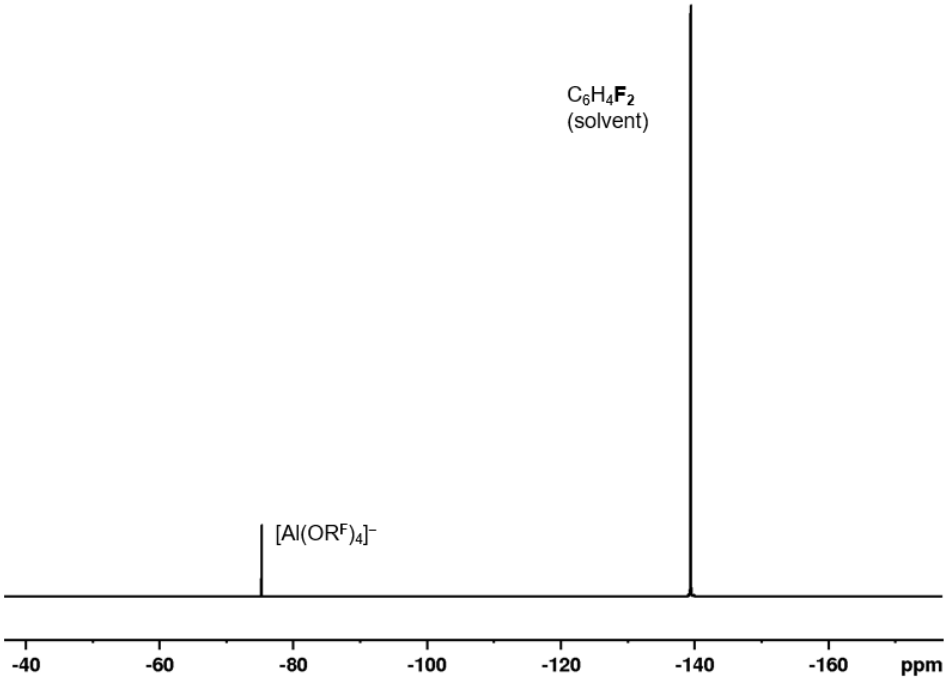
S-Figure 10: Crystals of **2** as well as formed Indium from the decomposition.



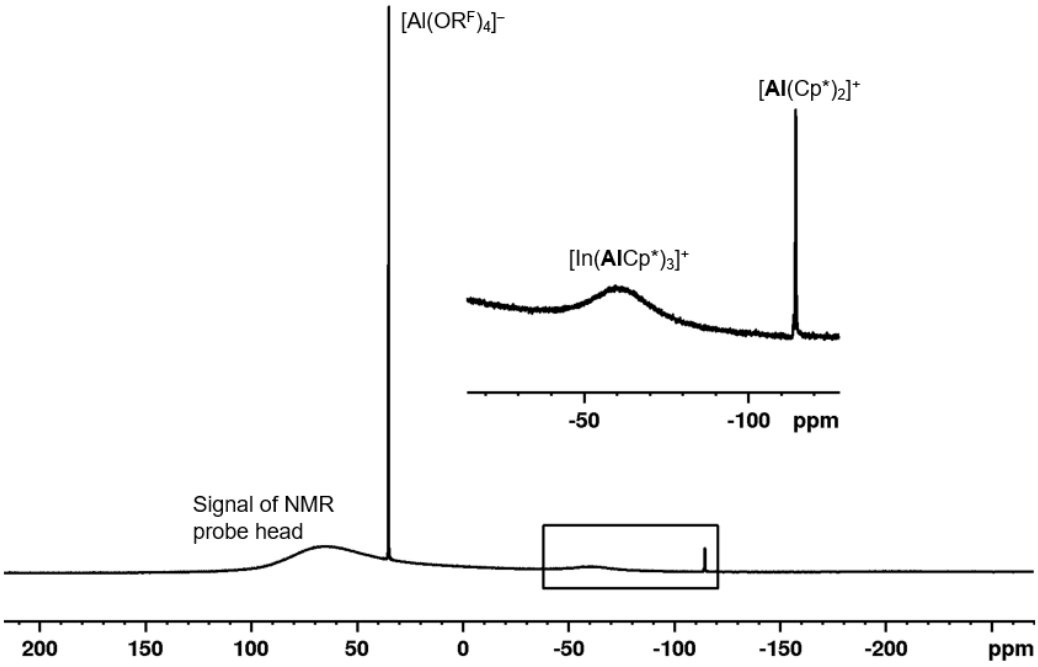
S-Figure 11: ^{1}H NMR spectrum (300.18 MHz, 1,2-DFB, 300K) of [In(AlCp*)$_3$][Al(OR^F)$_4$] **2**.



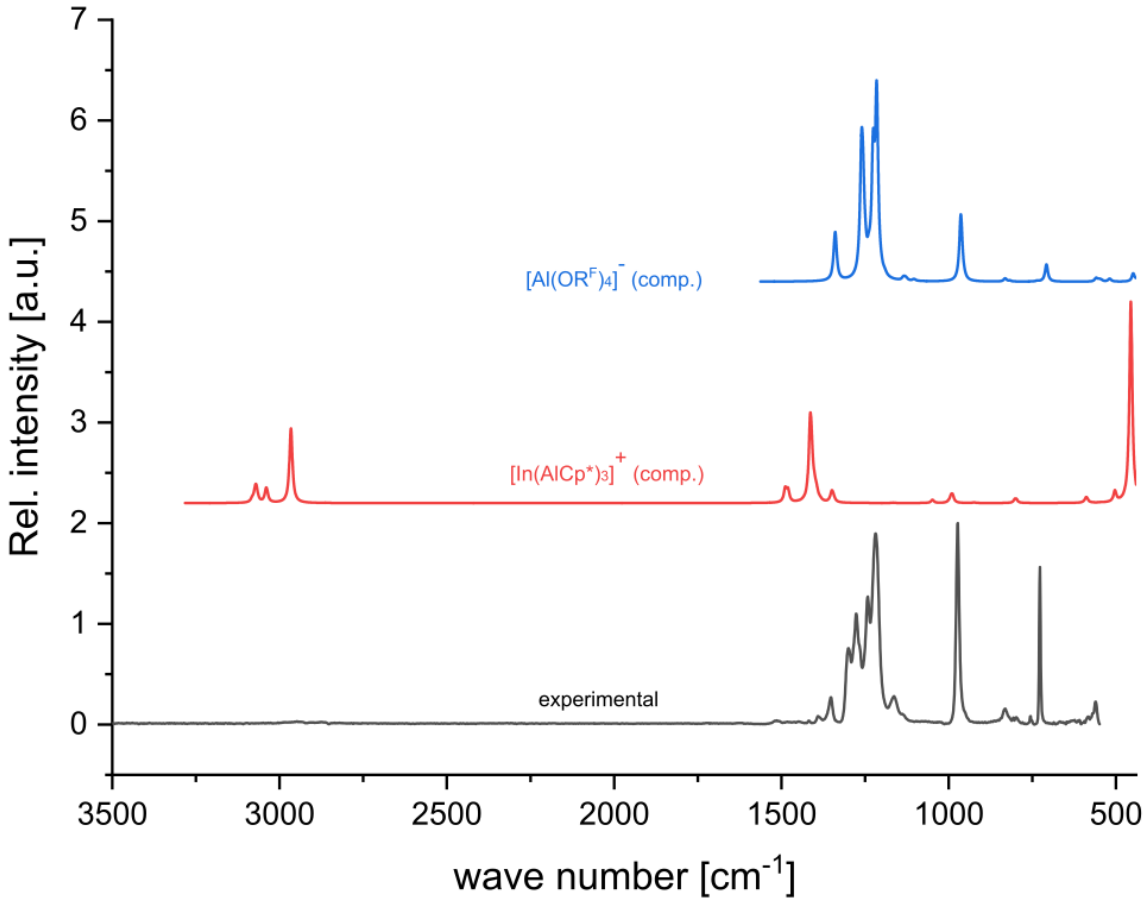
S-Figure 12: ^{1}H-^{13}C HMBC spectrum (300.18 MHz, 75.48 MHz, 1,2-DFB, 300K) of [In(AlCp*)$_3$][Al(OR^F)$_4$] **2**.



S-Figure 13: ^{19}F NMR spectrum (282.5 MHz, 1,2-DFB, 300K) of [In(AlCp*)$_3$][Al(OR^F)$_4$] **2**.



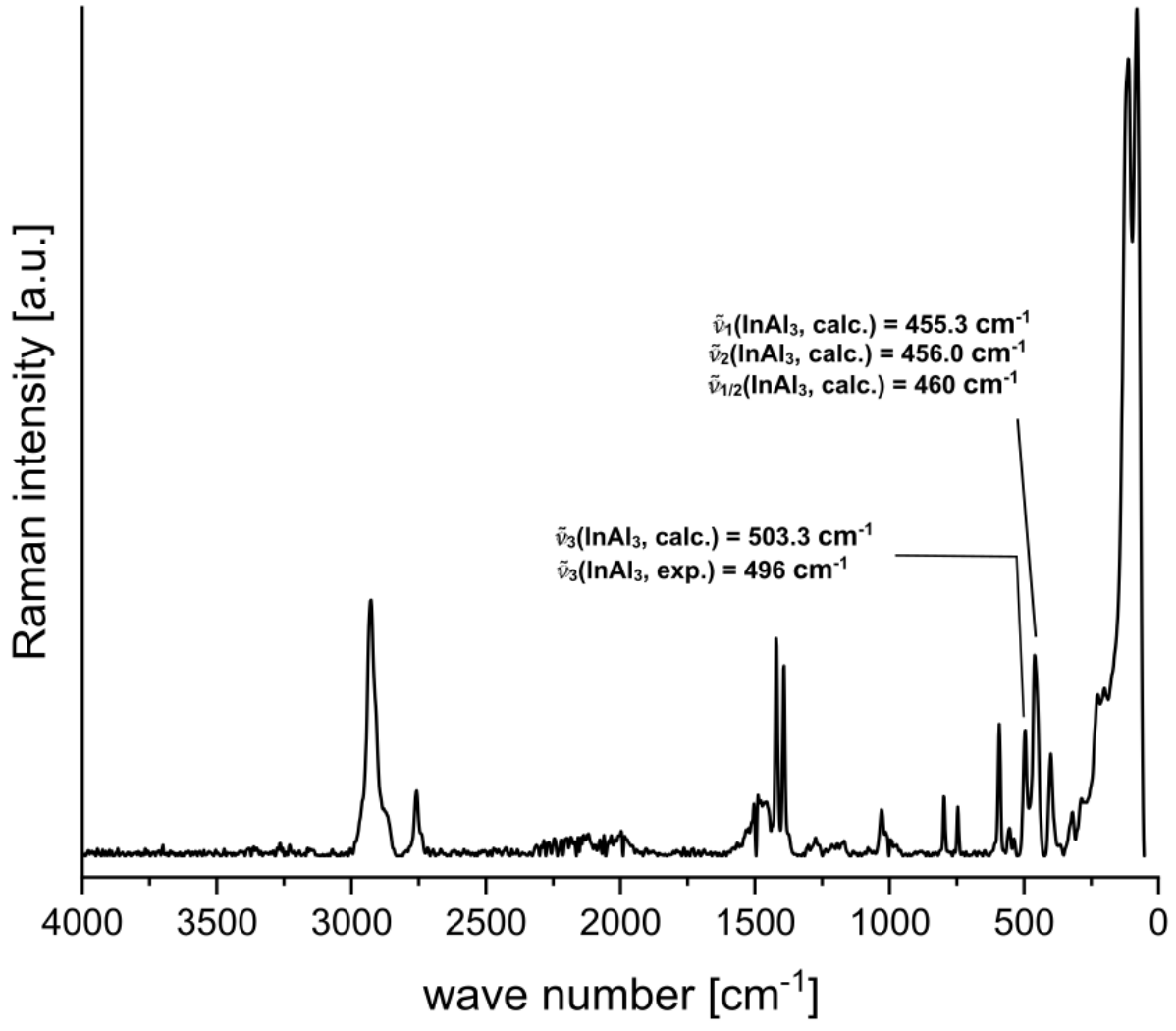
S-Figure 14: ^{27}Al NMR spectrum (78.2 MHz, 1,2-DFB, 300K) of [In(AlCp*)$_3$][Al(OR^F)$_4$] **2**.



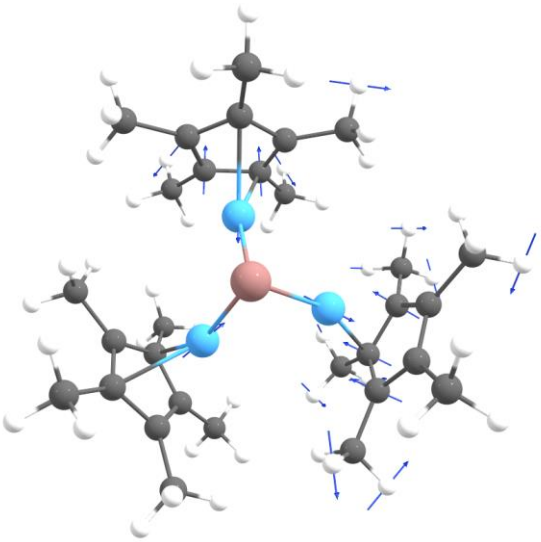
S-Figure 15: Experimental IR spectrum of **2** and computed IR spectra for the $[In(AlCp^*)_3]^+$ cation and the $[Al(OR^F)_4]^-$ anion (bp86-d3bj/def2-svp).

Raman spectrum of 2

In the Raman spectrum of $[In(AlCp^*)_3]^+[Al(OR^F)_4]$ (S-Figure 16), two degenerate asymmetric stretching vibrations of the In–Al bonds are observed at 460 cm^{-1}. Moreover, the band at 496 cm^{-1} can be assigned to a symmetric stretching vibration. The molecular vibrations were calculated on bp86-d3bj/def2-svp-level of DFT and are visualized in S-Figure 17. 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.[9,10]

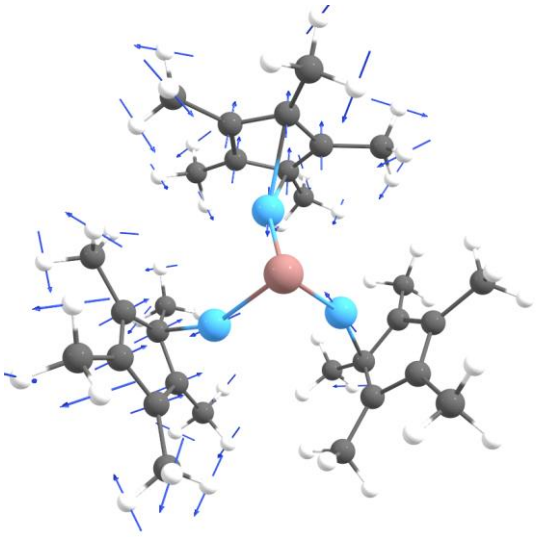


S-Figure 16: Experimental Raman spectrum of **2**.



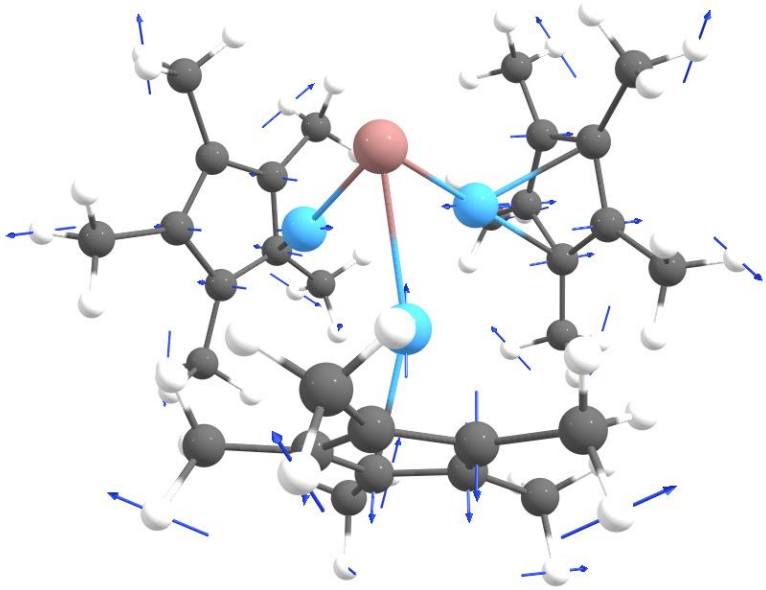
(Threshold for visualization: 0.12)

$\tilde{\nu}_1$($InAl_3$, calc.) = 455.3 cm^{-1}



(Threshold for visualization: 0.05)

$\tilde{\nu}_2$($InAl_3$,calc.) = 456.03 cm^{-1}



(Threshold for visualization: 0.18)

$\tilde{\nu}_3$($InAl_3$,calc.) = 503.3 cm^{-1}

S-Figure 17: Computed breathing vibrations of the $InAl_3^+$ unit (at bp86-d3bj/def2-svp level of DFT). The displacement vectors computed for the vibration are displayed as blue arrows.

Experimental data for $[Tl(AlCp^*)_3][Al(OR^F)_4]$ **3**

Procedure: Synthesis of $[Tl(AlCp^*)_3][Al(OR^F)_4]$ **3**

$Tl[Al(OR^F)_4]$ (50 mg, 43 μmol) and $[(AlCp^*)_4]$ (21 mg, 33 μmol, 0.75 equiv.) were weighed into a Schlenk tube and fluorobenzene (1.5 mL) was added. The yellow solution was stirred for 10 min at room temperature and canulated onto *n*-heptane (5 mL) forming a yellow precipitate. The title compound (50 mg, 30 μmol, 71 %) was isolated as yellow powder.

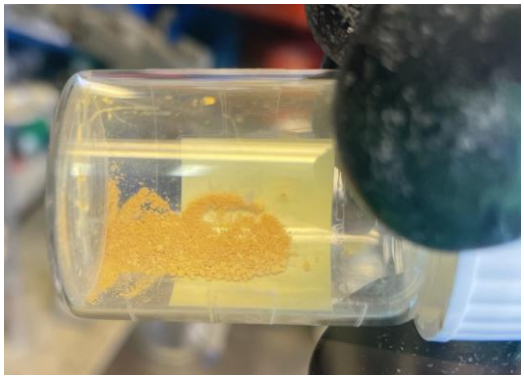
^{1}H NMR spectrum (400.16 MHz, PhF, 298 K): δ = 1.70 (s, 45 H, $[Tl(Al\mathbf{Cp^*})_3]^+$ ppm.

^{1}H, ^{13}C HMBC spectrum (400.16 MHz, 100.6 MHz, PhF, 298 K): $\delta(^{13}C)$ = 9.0 (-$\mathbf{C}H_3$), 115.7 ($\mathbf{C_5}Me_5$) ppm.

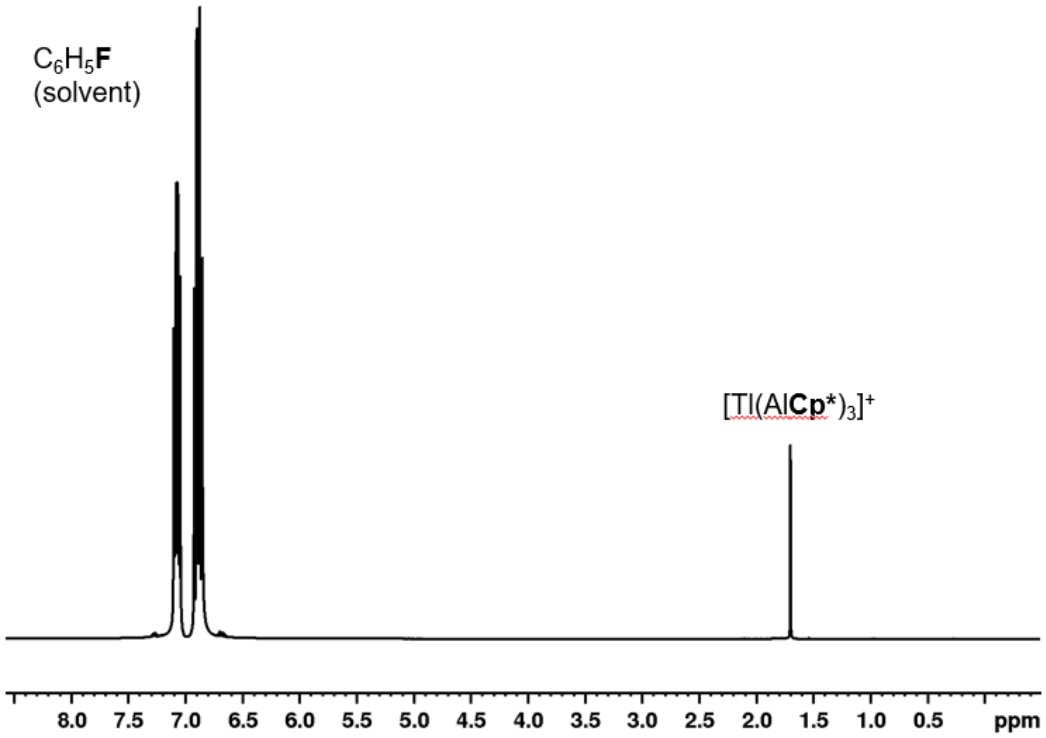
^{19}F NMR spectrum (376.54 MHz, PhF, 298 K): δ = −75.0 (s, 36 F, $[Al(OC_4F_9)_4]^-$) ppm.

^{27}Al NMR spectrum (78.22 MHz, PhF, 298 K): δ = 35.0 (s, $[Al(OC_4F_9)_4]^-$), −70.0 (d, $^1J(^{27}Al, ^{205}Tl)$ = 3577 Hz, $[Tl(\mathbf{Al}Cp^*)_3]^+$), −114.1 (s, $[AlCp^*_2]^+$) ppm.

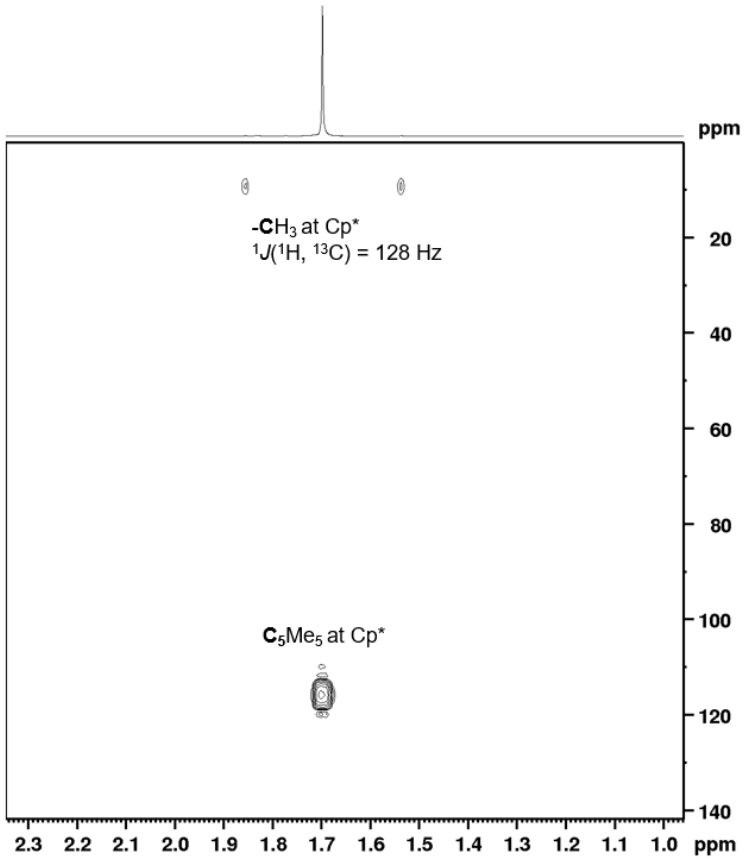
FTIR spectrum (ZnSe-ATR): $\tilde{\nu}$ = 1353 (vw), 1299 (w), 1276 (m), 1242 (s), 1218 (vs), 1164 (vw), 973 (vs), 833 (vw), 799 (vw), 756 (vw), 728 (s), 561 (vw) cm^{-1}.
Raman (25 mW, 10000 scans): $\tilde{\nu}$ = 2929 (m), 2757 (w), 1496 (w), 1488 (vw), 1421 (w), 1393 (w), 1077 (vw), 1030 (vw), 1002 (vw), 797 (vw), 744 (vw), 592 (vw), 495 (w), 452 (w), 399 (w), 80 (vs), 98 (vs), 320 (vw), 211 (vw), 285 (vw) cm^{-1}.



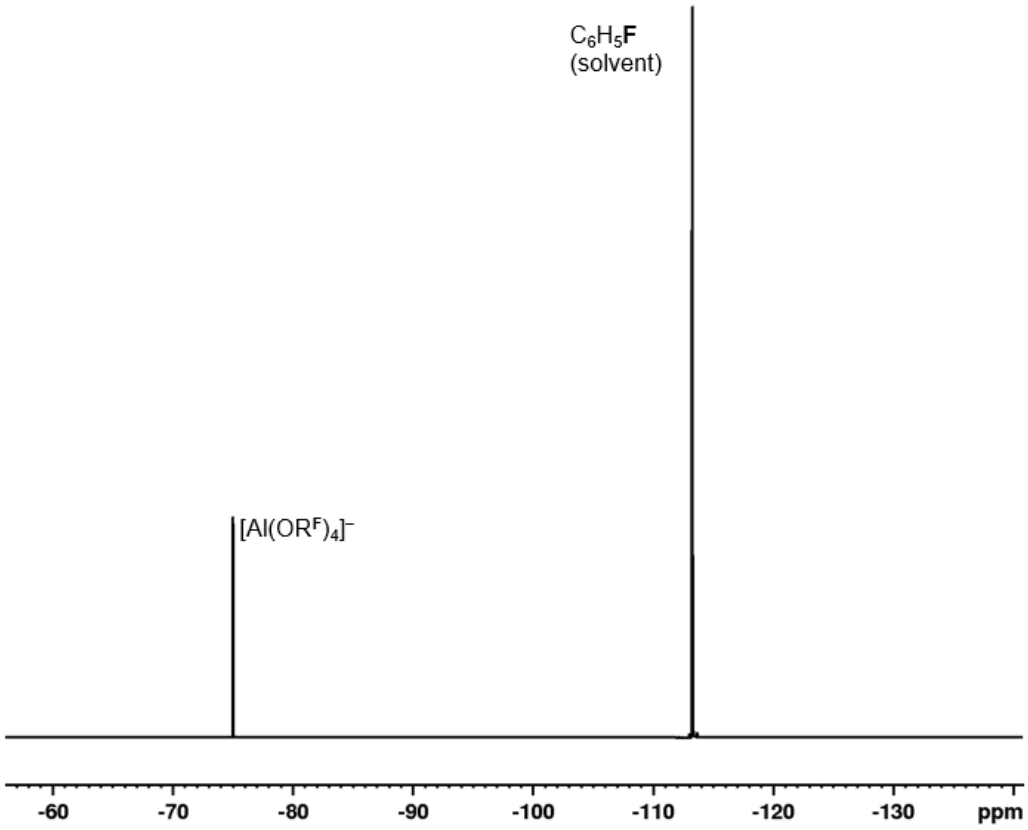
S-Figure 18: Picture of isolated yellow powder of **3**.



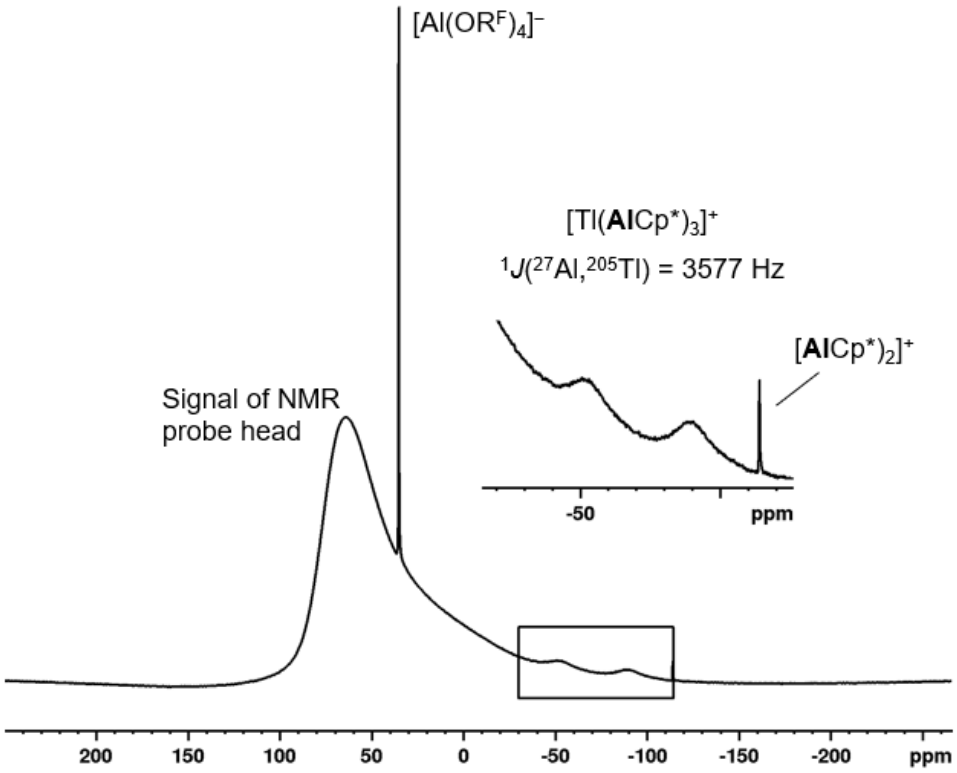
S-Figure 19: ^{1}H NMR spectrum (400.20 MHz, PhF, 300K) of [Tl(AlCp*)$_3$][Al(OR^F)$_4$] **3**.



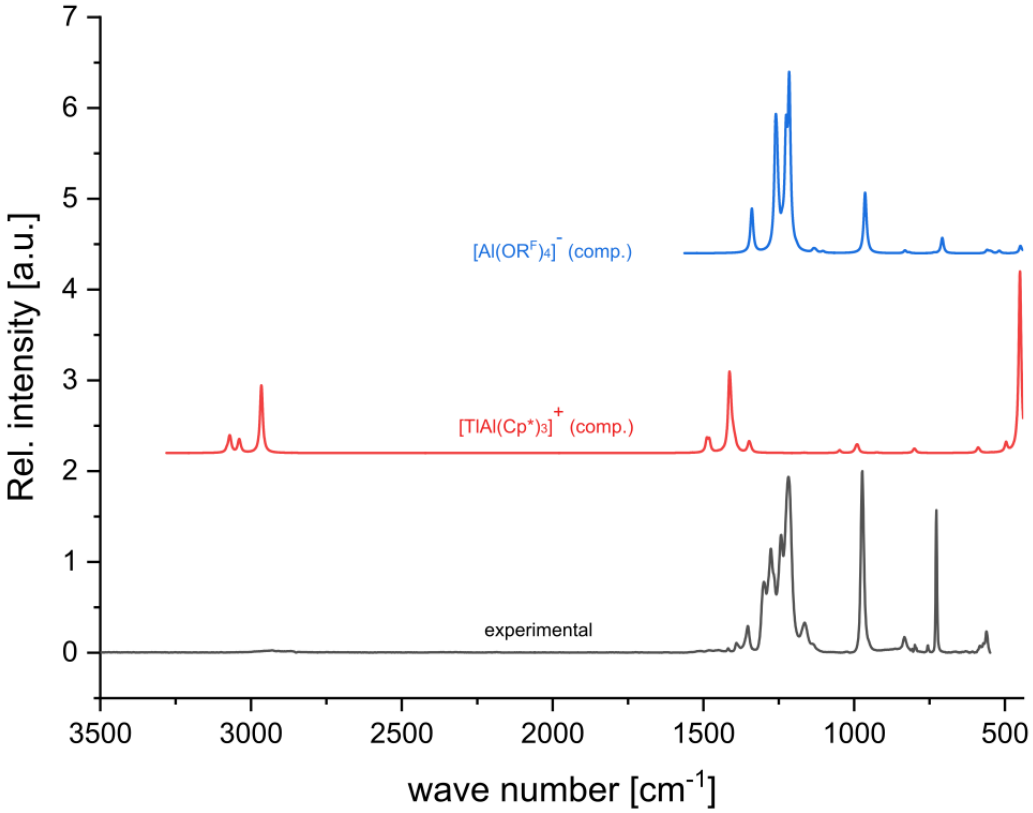
S-Figure 20: ^{1}H-^{13}C HMBC spectrum (400.20 MHz, 100.62 MHz, PhF, 300K) of [Tl(AlCp*)$_3$][Al(OR^F)$_4$] **3**.



S-Figure 21: ^{11}F NMR spectrum (376.5 MHz, PhF, 300K) of [Tl(AlCp*)$_3$][Al(OR^F)$_4$] **3**.



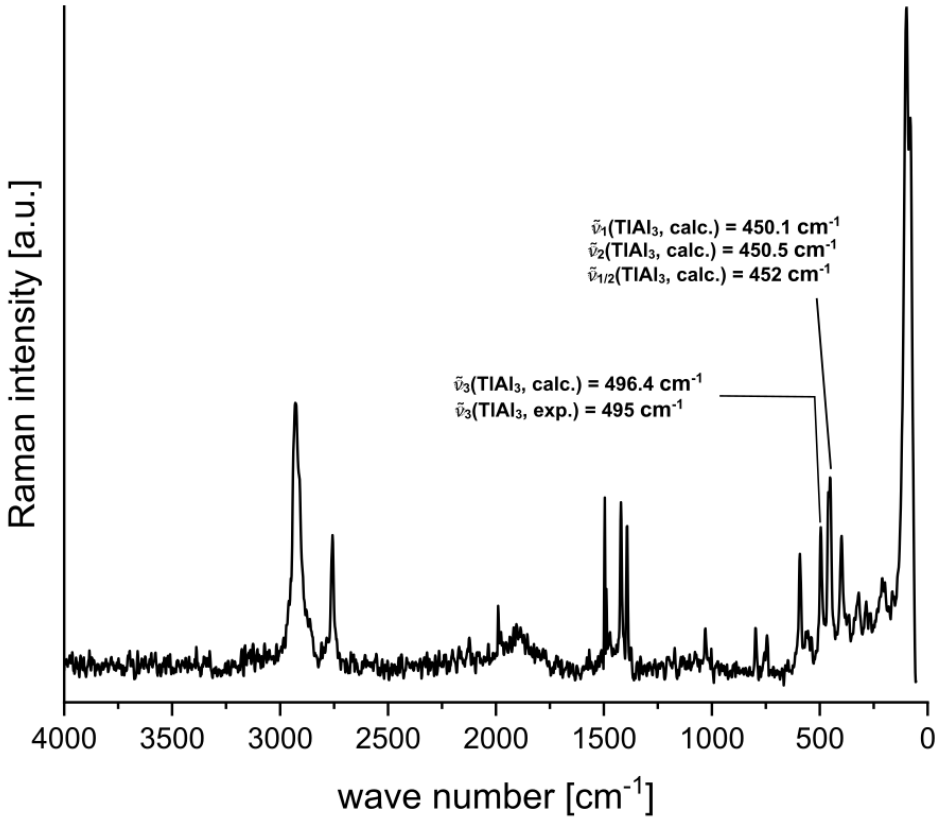
S-Figure 22: ^{27}Al NMR spectrum (104.3 MHz, PhF, 300K) of [Tl(AlCp*)$_3$][Al(OR^F)$_4$] **3**.



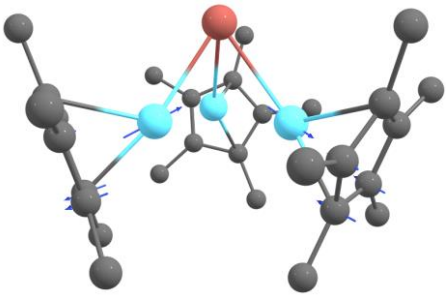
S-Figure 23: Experimental IR spectrum of **3** and computed IR spectra for the $[Tl(AlCp^*)_3]^+$ cation and the $[Al(OR^F)_4]^-$ anion (bp86-d3bj/def2-svp).

Raman spectrum of 3

In the Raman spectrum of $[Tl(AlCp^*)_3]^+[Al(OR^F)_4]$ (S-Figure 24), two degenerate asymmetric stretching vibrations of the In–Al bonds are observed at 452 cm^{-1}. Moreover, the band at 495 cm^{-1} can be assigned to a symmetric stretching vibration. The molecular vibrations were calculated on bp86-d3bj/def2-svp-level of DFT and are visualized in S-Figure 25. 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.[9,10]

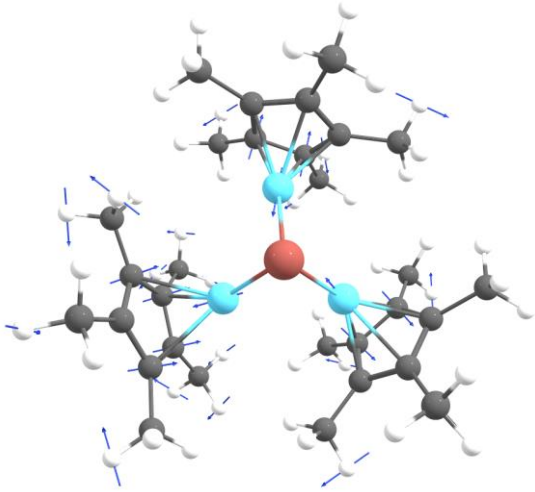


S-Figure 24: Experimental Raman spectrum of **3**.



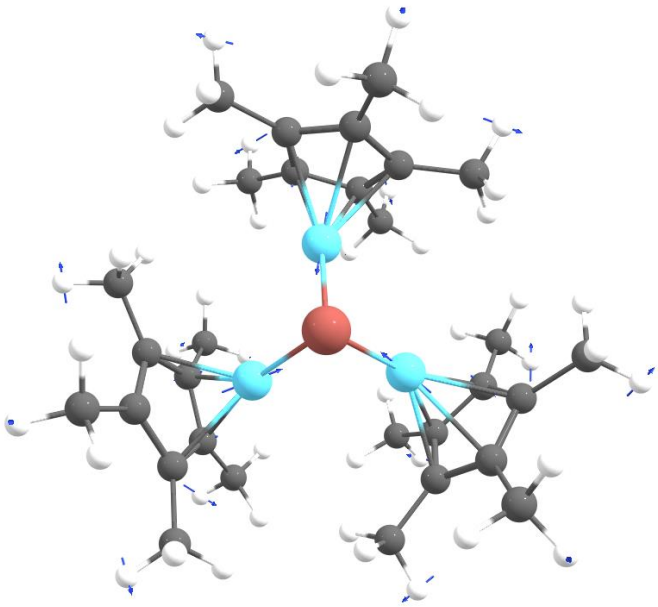
(Threshold for visualization: 0.12)

$\tilde{\nu}_1$($TlAl_3$, calc.) = 450.1 cm^{-1}



(Threshold for visualization: 0.09, Scale displacement 2)

$\tilde{\nu}_2$($GaAl_3$,calc.) = 450.5 cm^{-1}

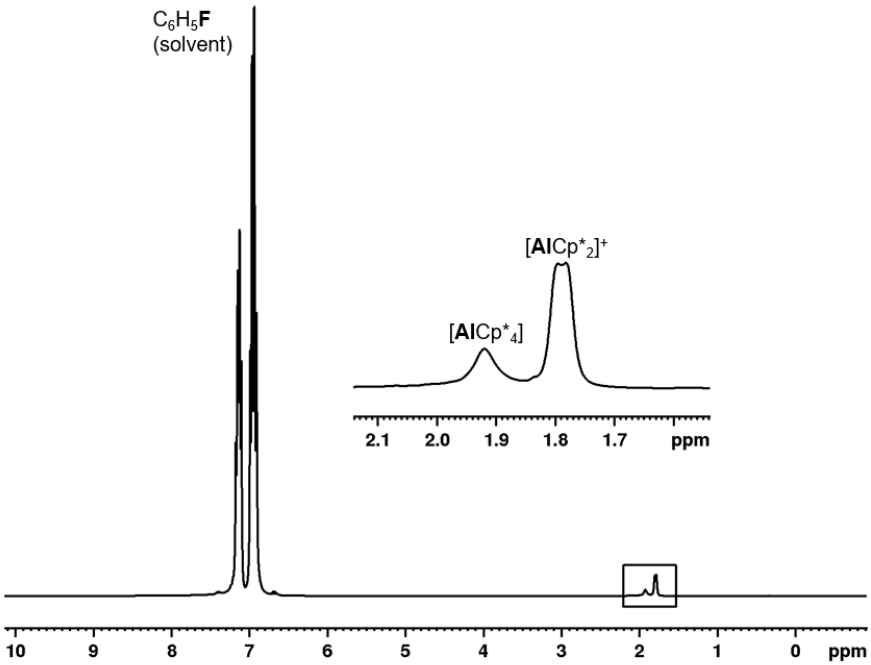


(Threshold for visualization: 0.09)

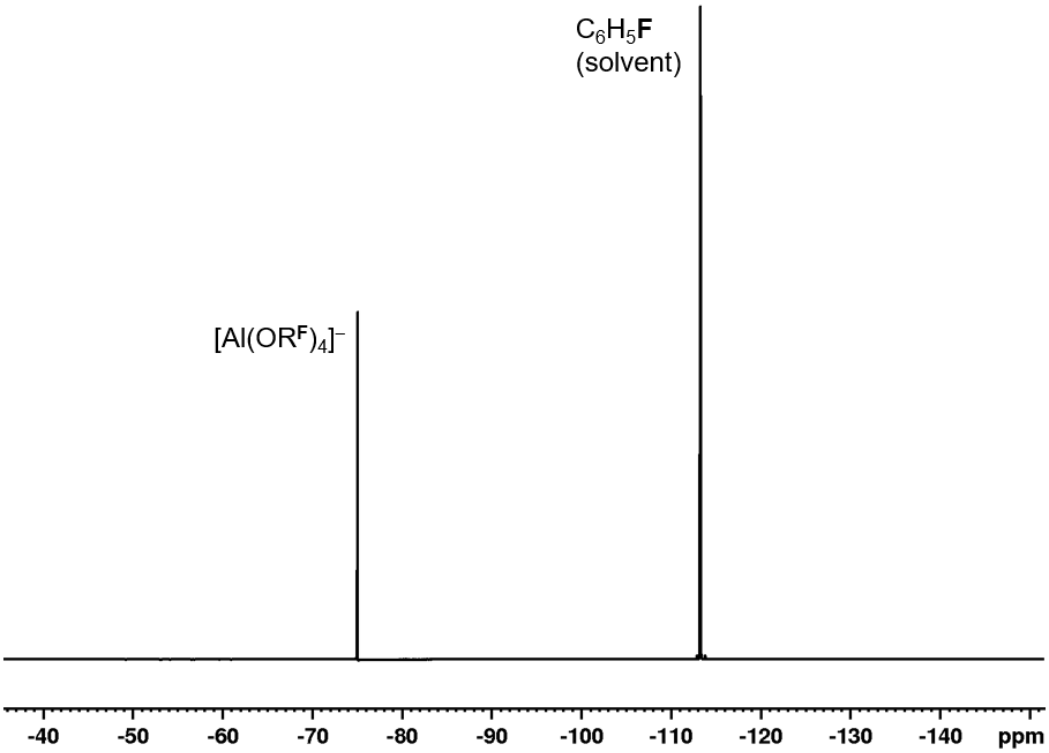
$\tilde{\nu}_3$($TlAl_3$,calc.) = 496.4 cm^{-1}

S-Figure 25: Computed breathing vibrations of the $TlAl_3^+$ unit (at bp86-d3bj/def2-svp level of DFT). The displacement vectors computed for the vibration are displayed as blue arrows.

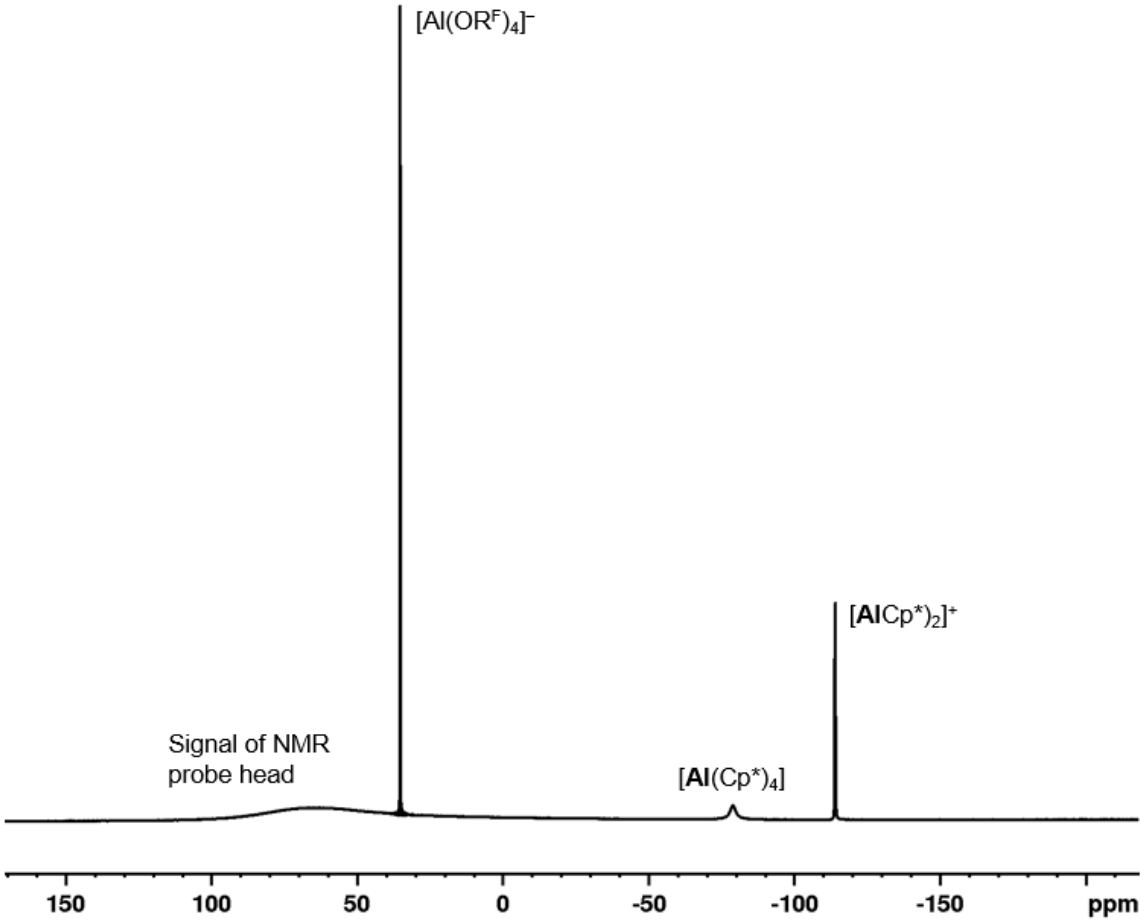
Decomposition of 3 after 4 days at room temperature



S-Figure 26: ^{1}H NMR spectrum (300.02 MHz, PhF, 300K) of the decomposition of $[Tl(AlCp^*)_3][Al(OR^F)_4]$ **3** after 4 days.



S-Figure 27: ^{11}F NMR spectrum (282.5 MHz, PhF, 300K) of the decomposition of $[Tl(AlCp^*)_3][Al(OR^F)_4]$ **3** after 4 days.



S-Figure 28: ^{27}Al NMR spectrum (78.2 MHz, PhF, 300K) of the decomposition of $[Tl(AlCp^*)_3][Al(OR^F)_4]$ **3** after 4 days.

Experimental data for $[Ga(Me_3TACN)][Al(OR^F)_4]$ **7**

Procedure: Synthesis of **7**

$[Ga(PhF)_{2\text{-}3}][Al(OR^F)_4]$ (100 mg, 81.4 μmol) was dissolved in PhF (2.5 mL). A solution of Me_3TACN in PhF (0.2 M, 0.45 mL, 90 μmol, 1.2 equiv.) were added to yield a slightly yellow solution which was layered with *n*-pentane. The title compound (89 mg, 74 μmol, 91 %) was isolated as colourless powder.

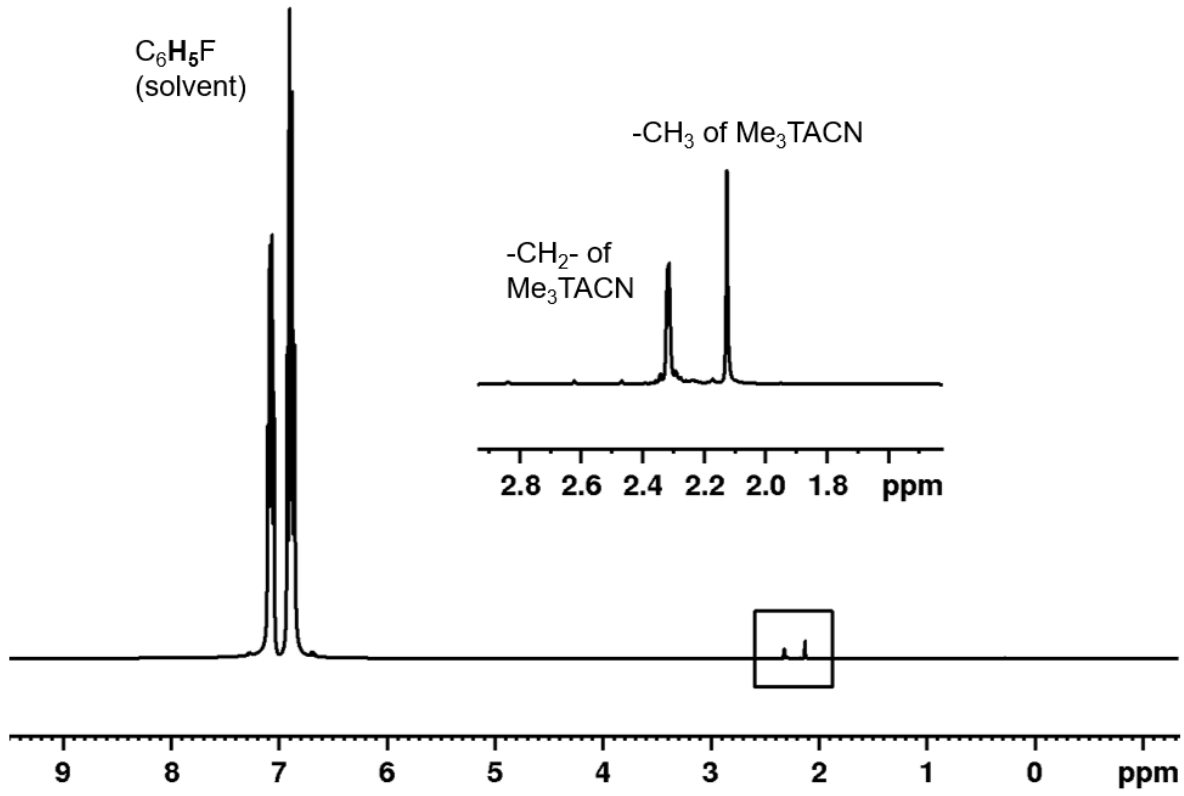
^{1}H NMR spectrum (400.16 MHz, PhF, 298 K): δ = 2.12 (s, 9 H, -CH_3), 2.32 (m_c, 8 H, -CH_2-) ppm.

^{1}H, ^{13}C HMBC spectrum (400.16 MHz, 100.6 MHz, PhF, 298 K): δ(^{13}C) = 43.7(-**C**H_3), 52.7 (-**C**H_2-) ppm.

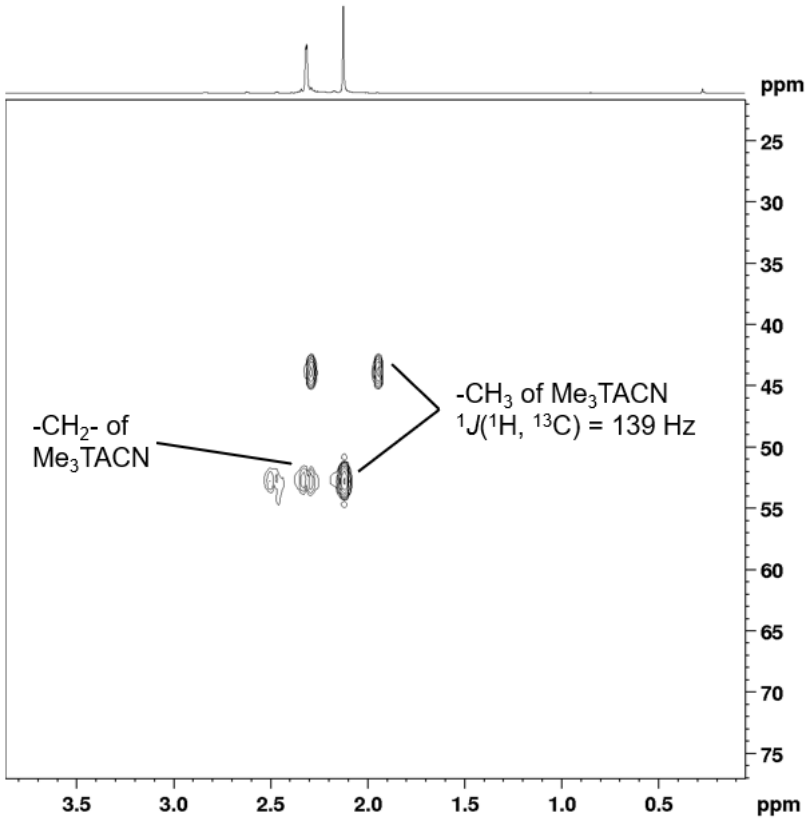
^{19}F NMR spectrum (376.54 MHz, PhF, 298 K): δ = –75.5 (s, 36 F, $[Al(OC_4F_9)_4]^-$) ppm.

^{27}Al NMR spectrum (78.22 MHz, PhF, 298 K): δ = 35.1 (s, $[Al(OC_4F_9)_4]^-$).

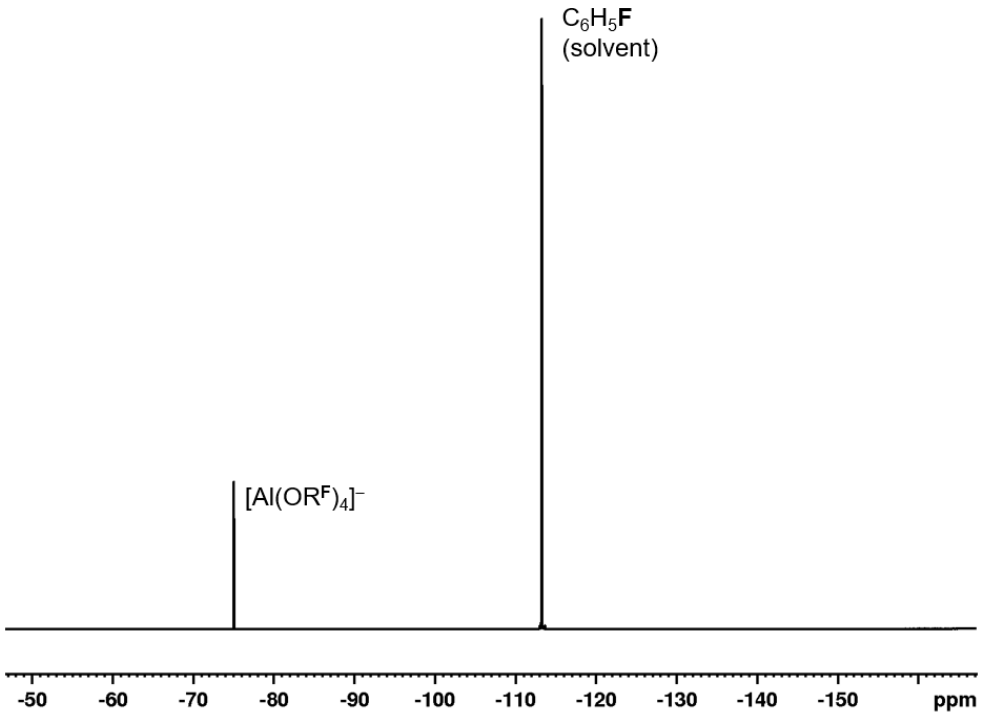
^{71}Ga NMR spectrum (122.04 MHz, PhF, 298 K): No signal.



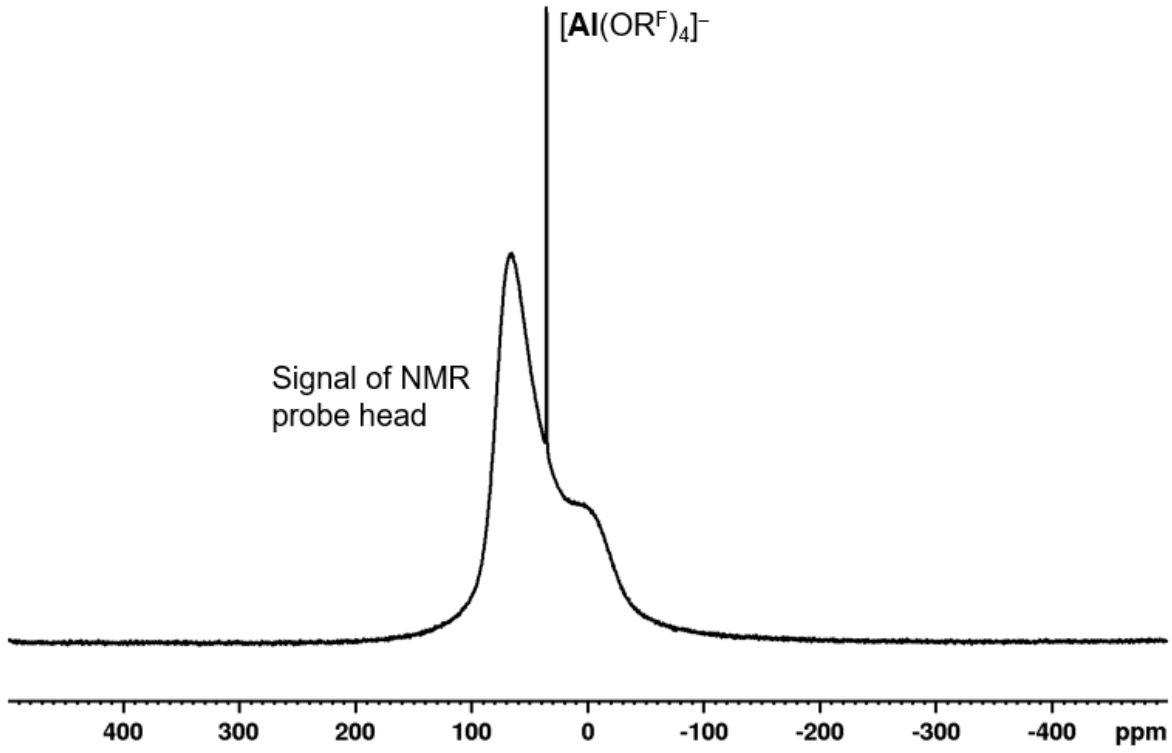
S-Figure 29: ^{1}H NMR spectrum (400.20 MHz, PhF, 300K) of $[Ga(Me_3TACN)]^+[Al(OR^F)_4]^-$ **7**.



S-Figure 30: ^{1}H-^{13}C HMBC spectrum (400.20 MHz, 100.62 MHz, PhF, 300K) of $[Ga(Me_3TACN)]^{+}[Al(OR^{F})_4]^{-}$ **7**.



S-Figure 31: ^{11}F NMR spectrum (376.5 MHz, PhF, 300K) of $[Ga(Me_3TACN)]^{+}[Al(OR^{F})_4]^{-}$ **7**.



S-Figure 32: ^{27}Al NMR spectrum (104.3 MHz, PhF, 300K) of $[Ga(Me_3TACN)]^+[Al(OR^F)_4]^-$ **7**.

Experimental data for $[Tl(Me_3TACN)][Al(OR^F)_4]$ **8**

Procedure: Synthesis of **8**

$Tl[Al(OR^F)_4]$ (170 mg, 145 μmol) was dissolved in PhF (1 mL). An excess of Me_3TACN (0.08 mL, 0.07 g, 0.4 mmol, 3 equiv.) were added. The colourless solution was layered with *n*-pentane. The title compound (160 mg, 137 μmol, 94 %) was isolated as colourless powder.

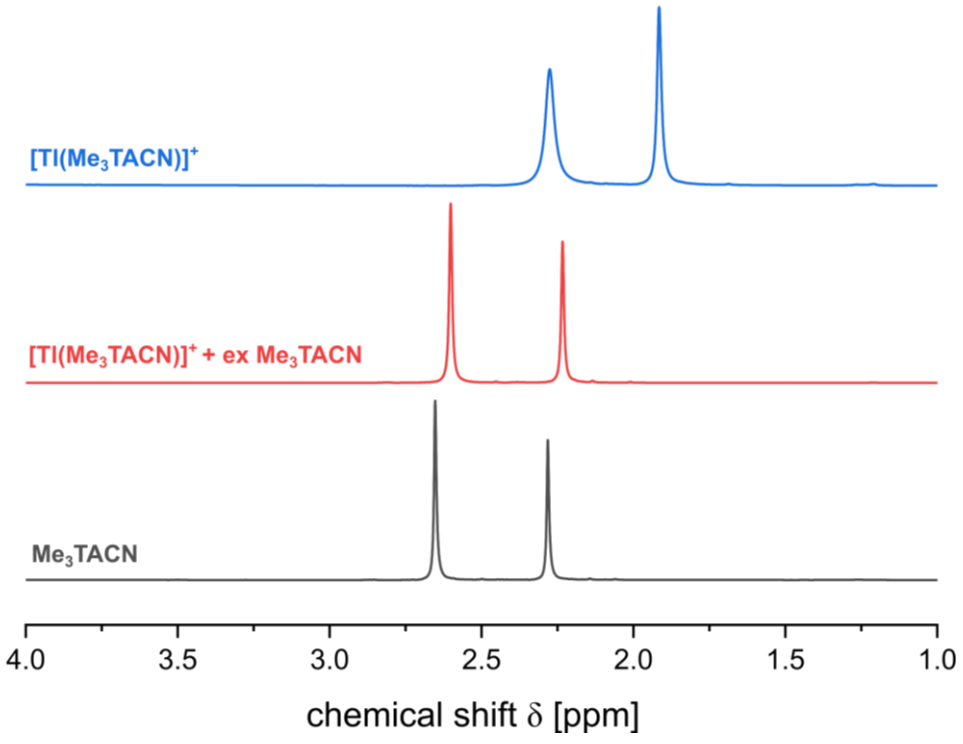
^{1}H NMR spectrum (300.17MHz, PhF, 298 K): δ = 1.92 (s, 9 H, -CH_3), 2.28 (s, 8 H, -CH_2-) ppm.

^{1}H, ^{13}C HMBC spectrum (300.17 MHz, 75.51 MHz, PhF, 298 K): δ(^{13}C) = 44.2 (-**C**H_3), 53.3 (-**C**H_2-) ppm.

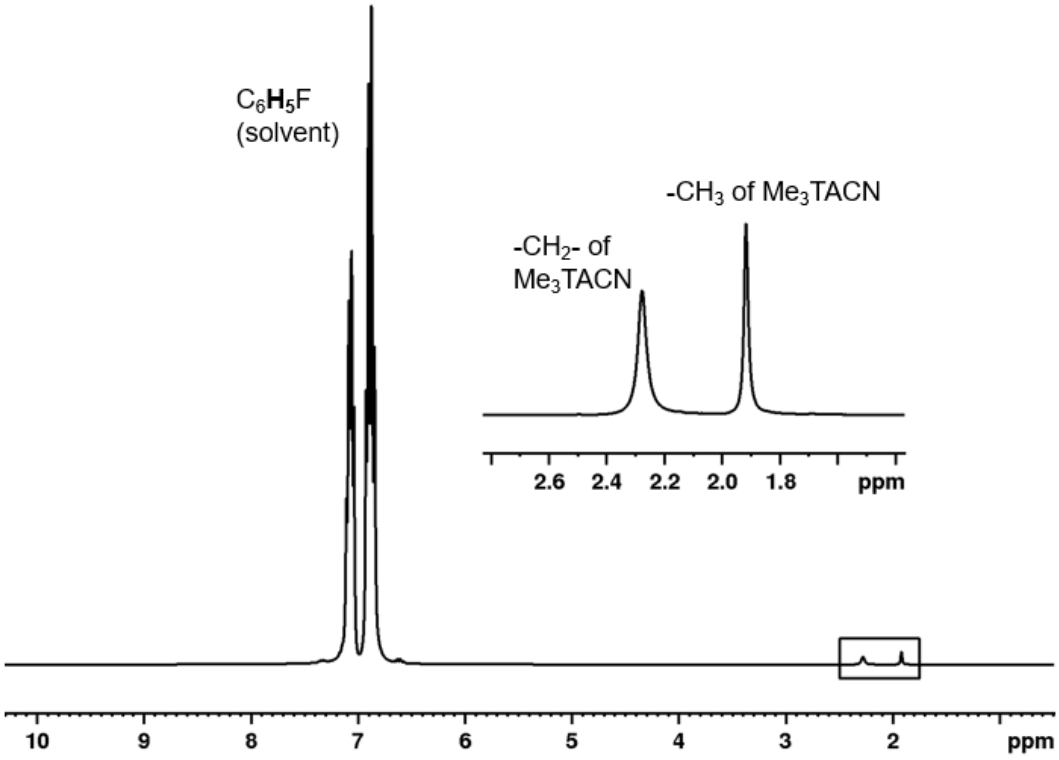
^{19}F NMR spectrum (282.45 MHz, PhF, 298 K): δ = –75.5 (s, 36 F, $[Al(OC_4F_9)_4]^-$) ppm.

^{27}Al NMR spectrum (78.22 MHz, PhF, 298 K): δ = 35.1 (s, $[Al(OC_4F_9)_4]^-$).

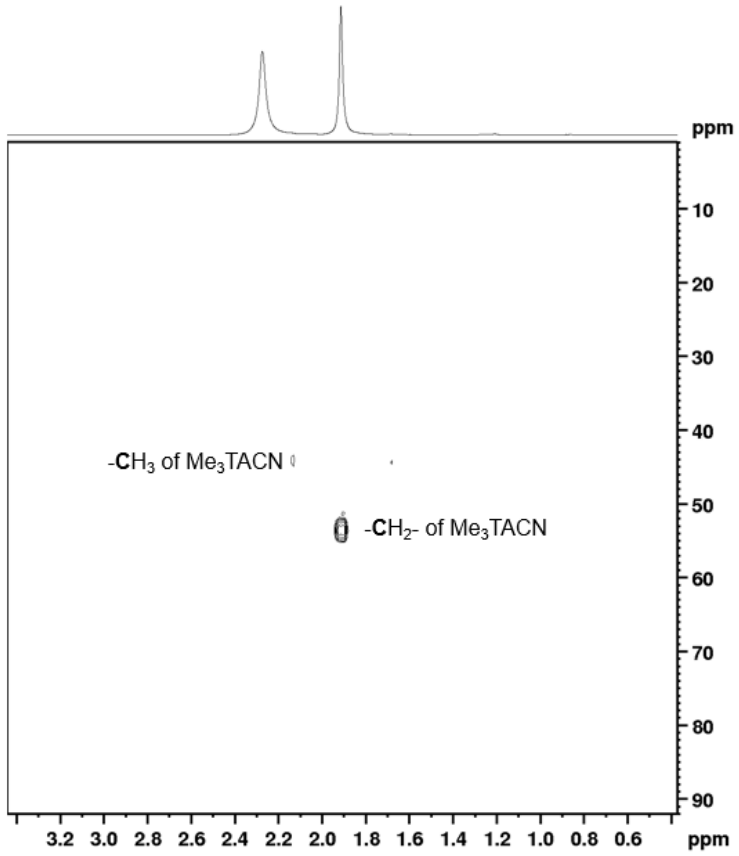
The $[Tl(Me_3TACN)]^+$ is already literature known as $[Tl(Me_3TACN)][PF_6]$.[11] Yet, no NMR signals have been reported. Interestingly, addition of an excess of Me_3TACN leads to significant shift of the Me_3TACN signal (S-Figure 33). This observation indicates a weak bonding of the Me_3TACN ligand to Tl^+ with dynamic ligand-exchange in solution.



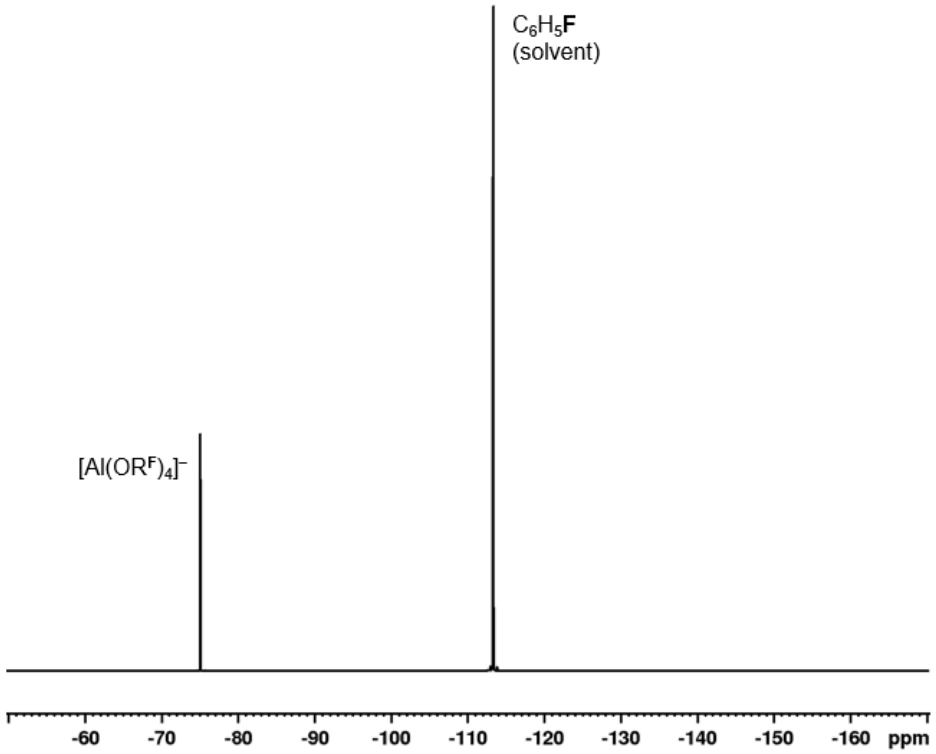
S-Figure 33: Comparison of ^{1}H NMR spectra (300.15 MHz, PhF, 300K) of $[Tl(Me_3TACN)]^+[Al(OR^F)_4]^-$ **8** before (top) and after (middle) addition of *ex* Me_3TACN (ca. 10 equiv, 0.03 mL) as well as the ^{1}H NMR spectrum of clean Me_3TACN.



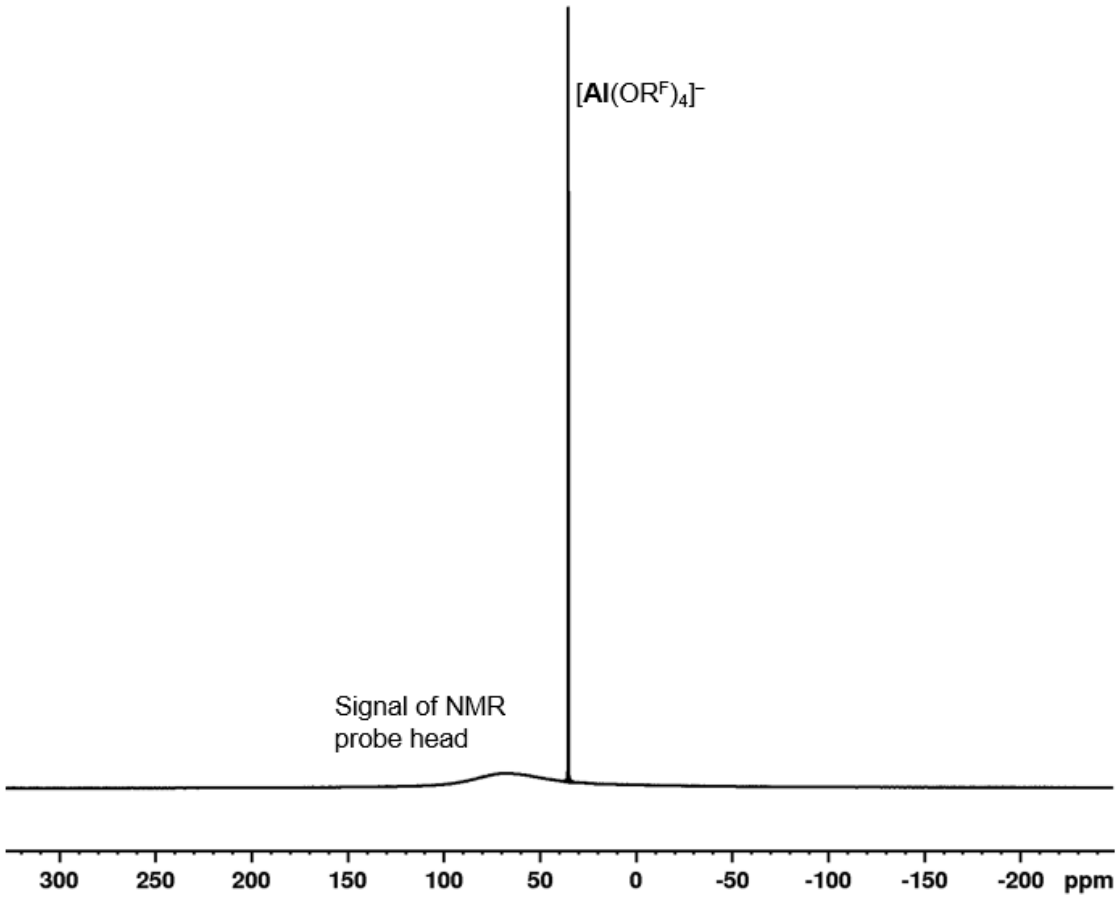
S-Figure 34: ^{1}H NMR spectrum (300.15 MHz, PhF, 300K) of $[Tl(Me_3TACN)]^{+}[Al(OR^{F})_4]^{-}$ **8**.



S-Figure 35: ^{1}H-^{13}C HMBC spectrum (300.17 MHz, 75.51 MHz, PhF, 300K) of $[Tl(Me_3TACN)]^{+}[Al(OR^{F})_4]^{-}$ **8**.



S-Figure 36: ^{11}F NMR spectrum (282.45 MHz, PhF, 300K) of $[Tl(Me_3TACN)]^+[Al(OR^F)_4]^-$ **8**.

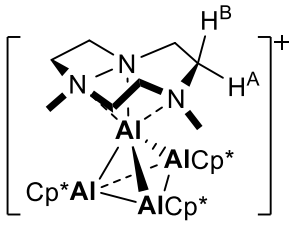


S-Figure 37: ^{27}Al NMR spectrum (78.22 MHz, PhF, 300K) of $[Tl(Me_3TACN)]^+[Al(OR^F)_4]^-$ **8**.

Experimental data for $[(Me_3TACN)Al(AlCp^*)_3][Al(OR^F)_4]$ **4**

Procedure 1: Synthesis of **4** from **8**

$[Tl(Me_3TACN)][Al(OR^F)_4]$ **8** (70 mg, 60 μmol) and $[(AlCp^*)_4]$ (39 mg, 0.24 mmol, 1 equiv.) were weighed into a Schlenk tube and fluorobenzene (3 mL) was added. The yellow suspension was heated to 60°C for 3h solution. The yellow solution was filtered off from minor metallic precipitate (S-Figure 38). Then, *n*-pentane (10 mL) was added to precipitate the product. The title compound (95 mg, 60 μmol, 95 %) was isolated as yellow powder.



^{1}H NMR spectrum (400.16 MHz, PhF, 298 K): δ = 1.85 (s, 45 H, $[(Me_3TACN)Al(Al\mathbf{Cp^*})_3]^+$), 2.34 ($m_c$, 6H, H^B), 2.39 (s, 9H, -CH_3), 2.63 (m_c, 6H, H^A) ppm.

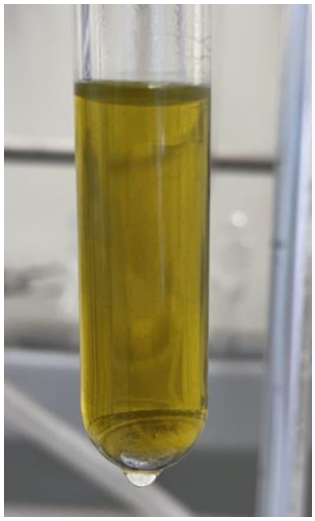
^{1}H, ^{13}C HMBC spectrum (400.16 MHz, 100.6 MHz, PhF, 298 K): δ(^{13}C) = 10.9 (-C**C**H_3), 48.9 (–N**C**H_3), 51.33 (–CH_2–) 114.4 (**C$_5$**Me_5) ppm.

^{19}F NMR spectrum (376.54 MHz, PhF, 298 K): δ = –75.0 (s, 36 F, $[Al(OC_4F_9)_4]^-$) ppm.

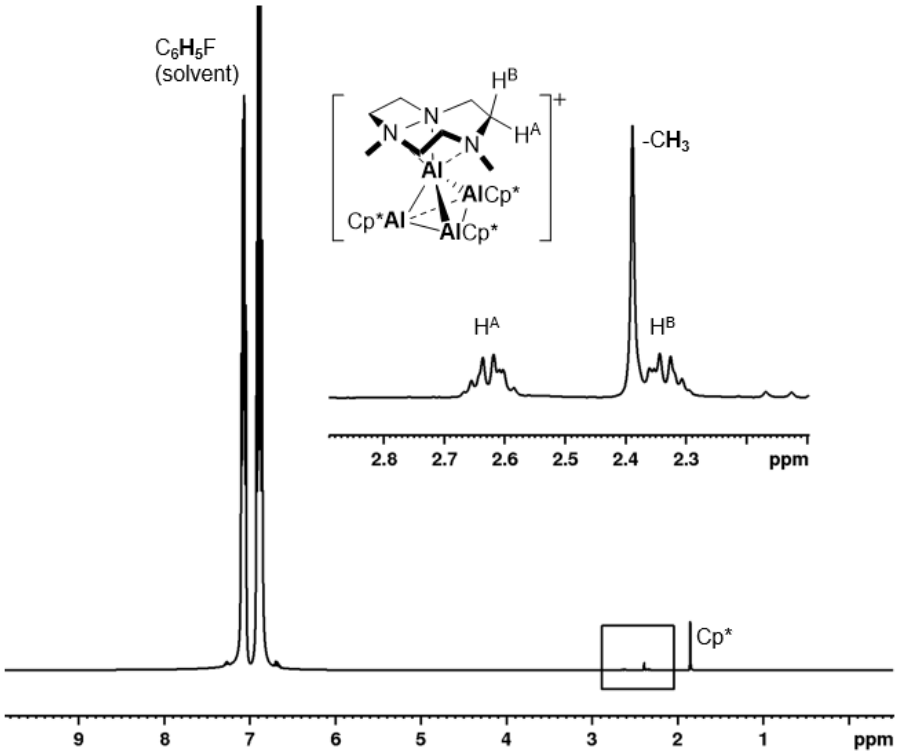
^{27}Al NMR spectrum (78.22 MHz, PhF, 298 K): δ = 35.0 (s, $[Al(OC_4F_9)_4]^-$), –77.0 (s, $[(TACN)Al(\mathbf{Al}Cp^*)_3]^+$) ppm.

FTIR spectrum (ZnSe-ATR): $\tilde{\nu}$ = 2919 (vw), 2865 (vw), 1499 (vw), 1458 (vw), 1426 (vw), 1385 (vw), 1376 (vw), 1351 (vw), 1299 (w), 1276 (m), 1240 (s), 1212 (vs), 1164 (w), 1069 (vw), 1056 (vw), 1003 (vw), 972 (vs), 899 (vw), 830 (vw), 809 (vw), 798 (vw), 778 (vw), 755 (vw), 740 (vw), 727 (vs), 671 (vw), 589 (vw), 571 (vw), 560 (vw) cm^{-1}.

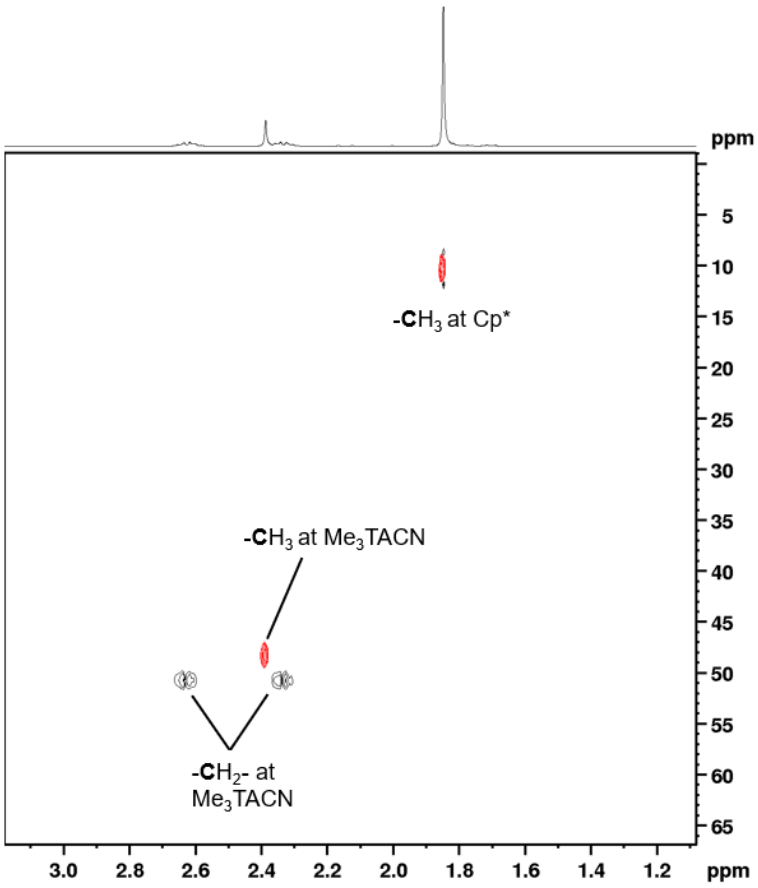
Raman (25 mW, 10000 scans): $\tilde{\nu}$ = 2927 (vs), 2826 (w), 2756 (w), 1503 (vw), 1489 (vw), 1458 (w), 1428 (m), 1386 (w), 797 (vw), 745 (vw), 595 (w), 553 (vw), 401 (w), 127 (vs), 114 (vs), 74 (s), 188 (w), 235 (vw), 321 (w), 370 (w), 538 (vw) cm^{-1}.



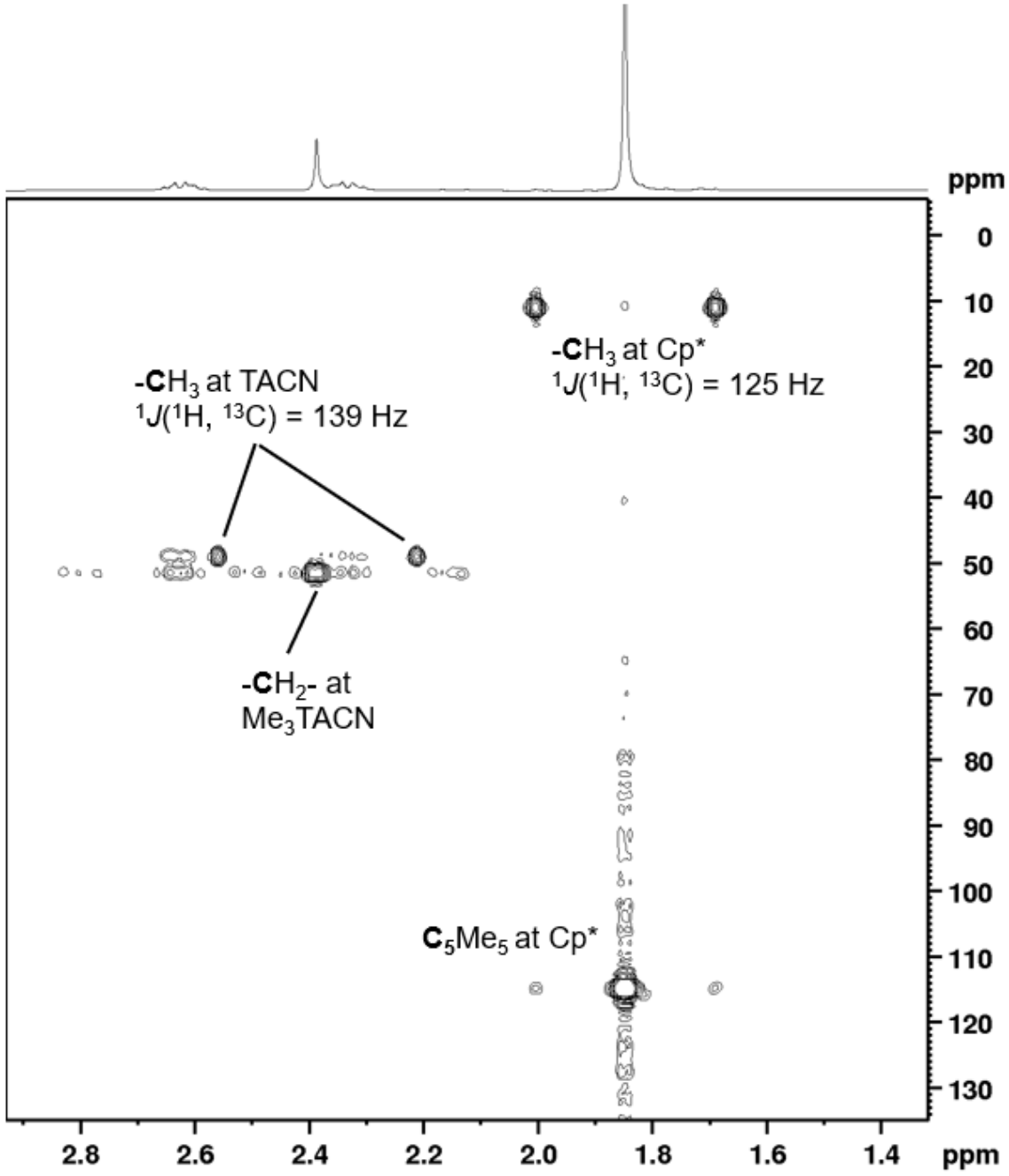
S-Figure 38: Reaction solution of **8** with $[(AlCp^*)_4]$ in PhF after heating showing the intense yellow colour of **4** along with metallic thallium formed at the stirring bar.



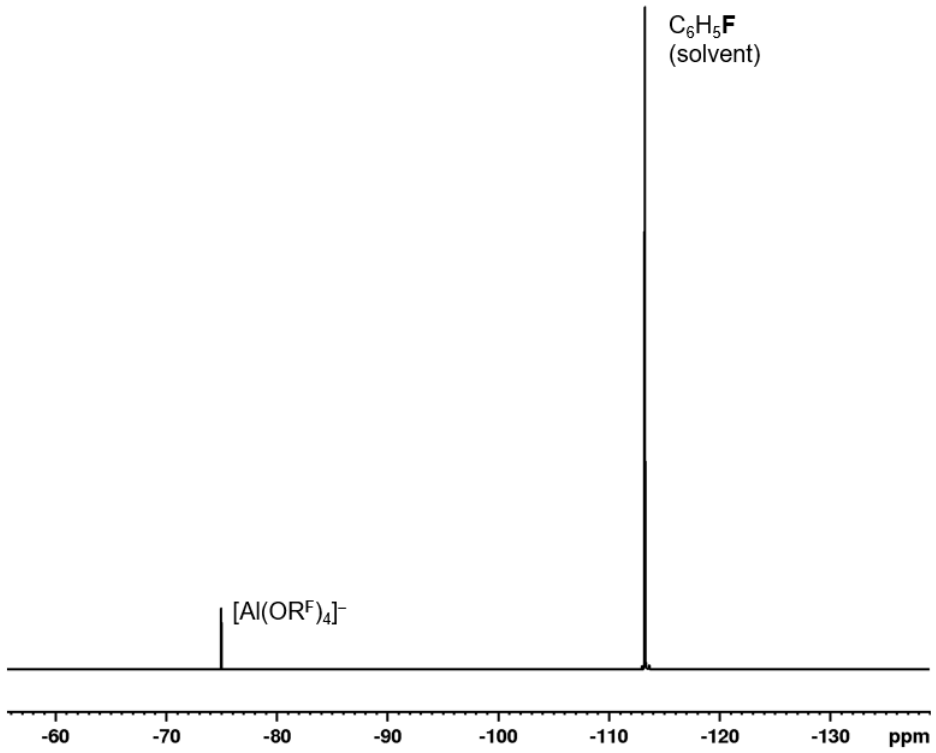
S-Figure 39: ^{1}H NMR spectrum (400.20 MHz, PhF, 300K) of $[(Me_3TACN)Al(AlCp^*)_3][Al(OR^F)_4]$ **4**.



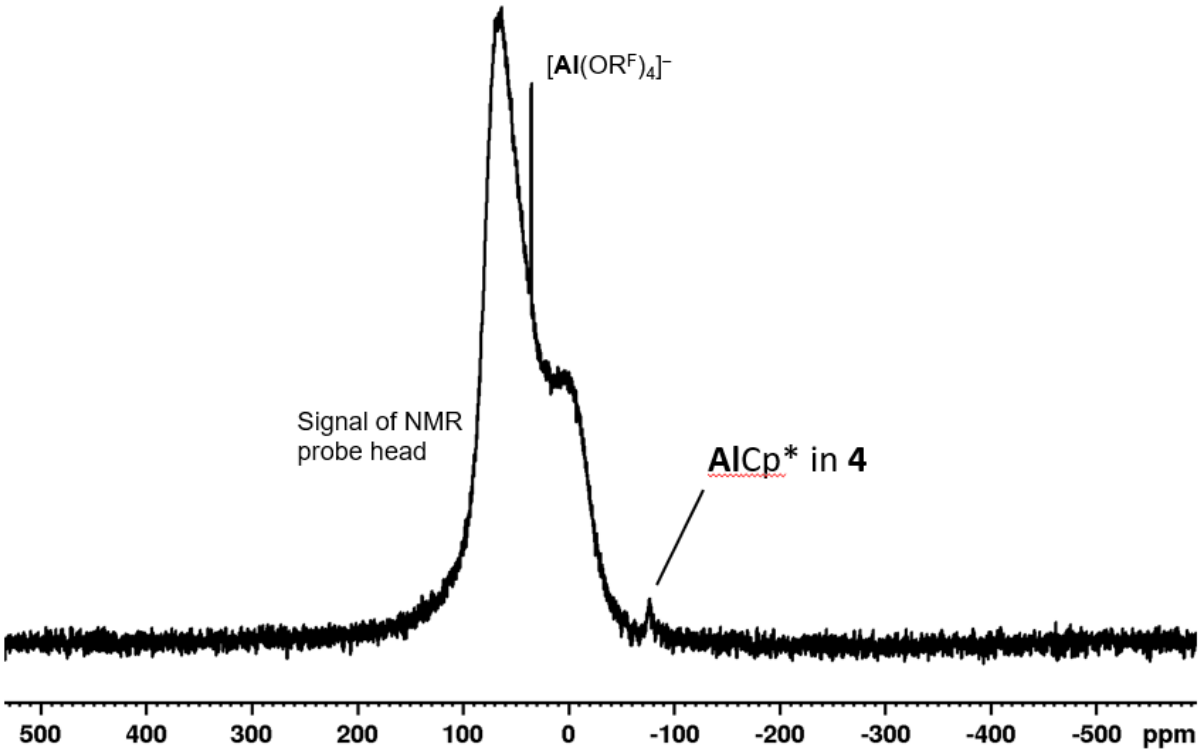
S-Figure 40: ^{1}H-^{13}C HSQC spectrum (400.20 MHz, 100.62 MHz, PhF, 300K) of $[(Me_3TACN)Al(AlCp^*)_3][Al(OR^F)_4]$ **4**.



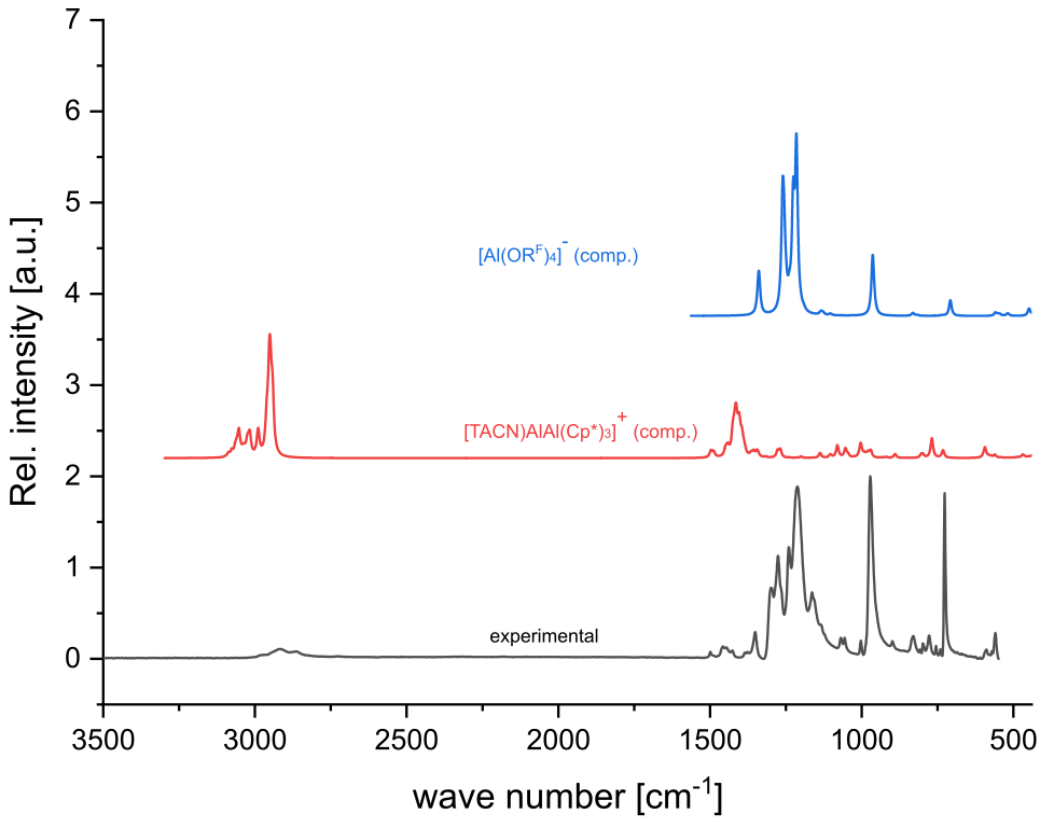
S-Figure 41: ^{1}H-^{13}C HMBC spectrum (400.20 MHz, 100.62 MHz, PhF, 300K) of $[(Me_3TACN)Al(AlCp^*)_3][Al(OR^F)_4]$ **4**.



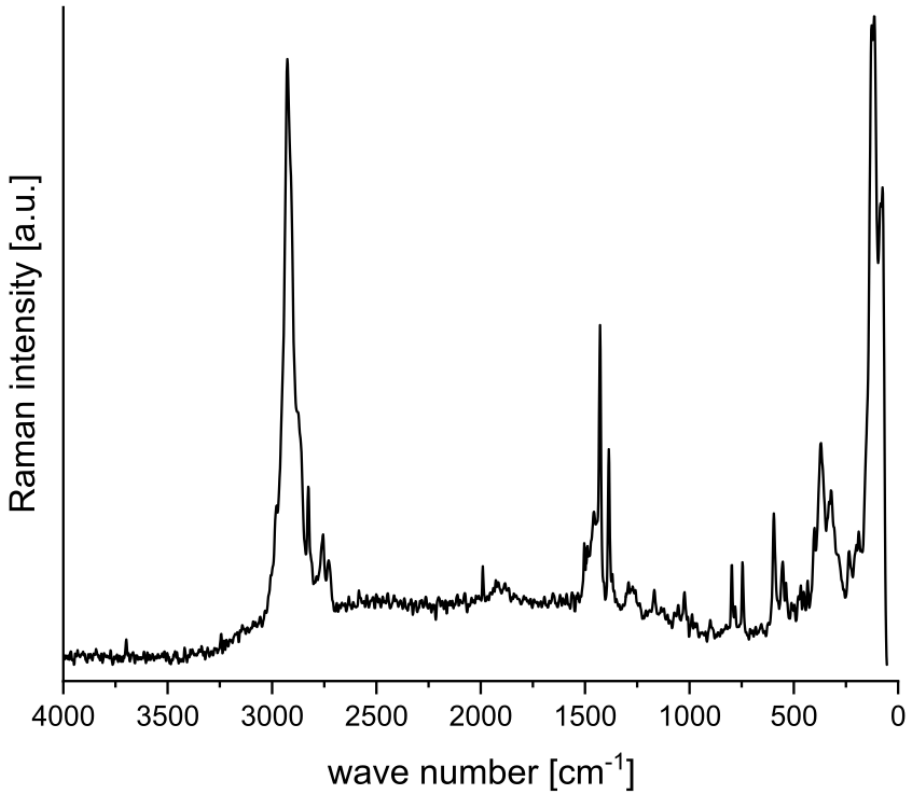
S-Figure 42: ^{11}F NMR spectrum (376.5 MHz, PhF, 300K) [(Me_3TACN)Al(AlCp*)$_3$][Al(OR^F)$_4$] **4**.



S-Figure 43: ^{27}Al NMR spectrum (104.3 MHz, PhF, 300K) of [(Me_3TACN)Al(AlCp*)$_3$][Al(OR^F)$_4$] **4**.



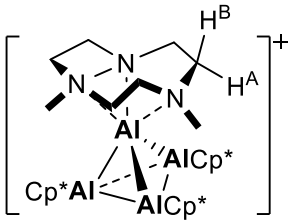
S-Figure 44: Experimental IR spectrum of **4** and computed IR spectra for the $[(Me_3TACN)Al(AlCp^*)_3]^+$ cation and the $[Al(OR^F)_4]^-$ anion (bp86-d3bj/def2-svp).



S-Figure 45: Experimental Raman spectrum of **4**.

Procedure 2: Synthesis of **4** from **7**

[Ga(TACN)][Al(OR^F)$_4$] **7** (60 mg, 50 μmol) and [(AlCp*)$_4$] (32 mg, 0.20 mmol, 1 equiv.) were weighed into a Schlenk tube and fluorobenzene (3 mL) was added. The yellow suspension was heated to 60°C for 5h solution. Then, the yellow solution was layered with *n*-pentane. The title compound (72 mg, 50 μmol, 88 %) was isolated as yellow crystals.

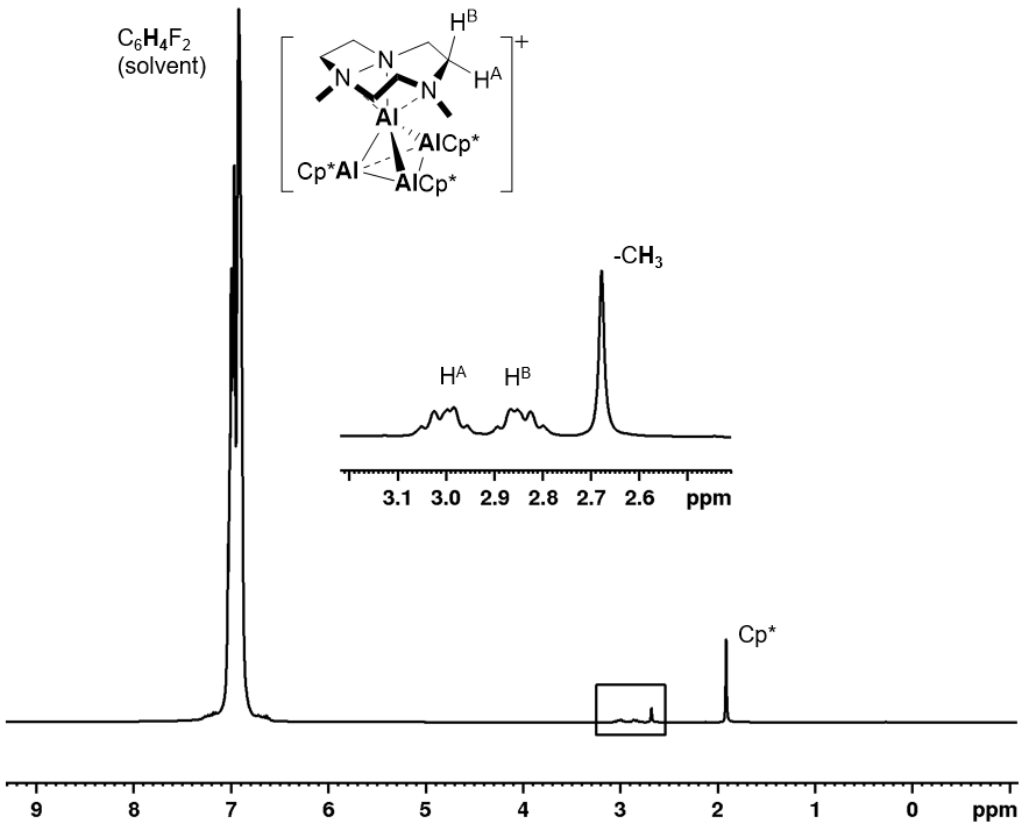


^{1}H NMR spectrum (400.16 MHz, 1,2-DFB, 298 K): δ = 1.91 (s, 45 H, [(Me_3TACN)Al(Al**Cp***)$_3$]$^+$), 2.68 (s, 9H, -CH_3), 2.85 (m_c, 6H, H^B), 3.00 (m_c, 6H, H^A) ppm.

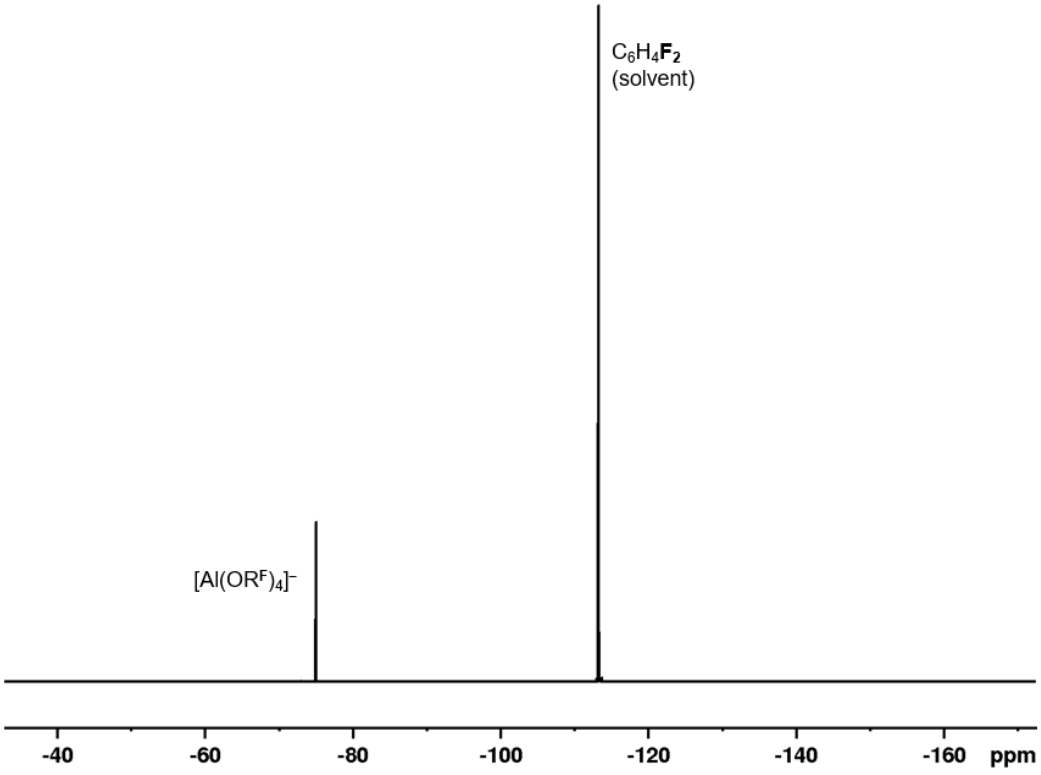
^{19}F NMR spectrum (376.54 MHz, 1,2-DFB, 298 K): δ = −75.0 (s, 36 F, [Al(OC_4F_9)$_4$]$^-$) ppm.

^{27}Al NMR spectrum (78.22 MHz, 1,2-DFB, 298 K): δ = 35.0 (s, [Al(OC_4F_9)$_4$]$^-$), −77.0 (s, [(TACN)Al(**Al**Cp*)$_3$]$^+$) ppm.

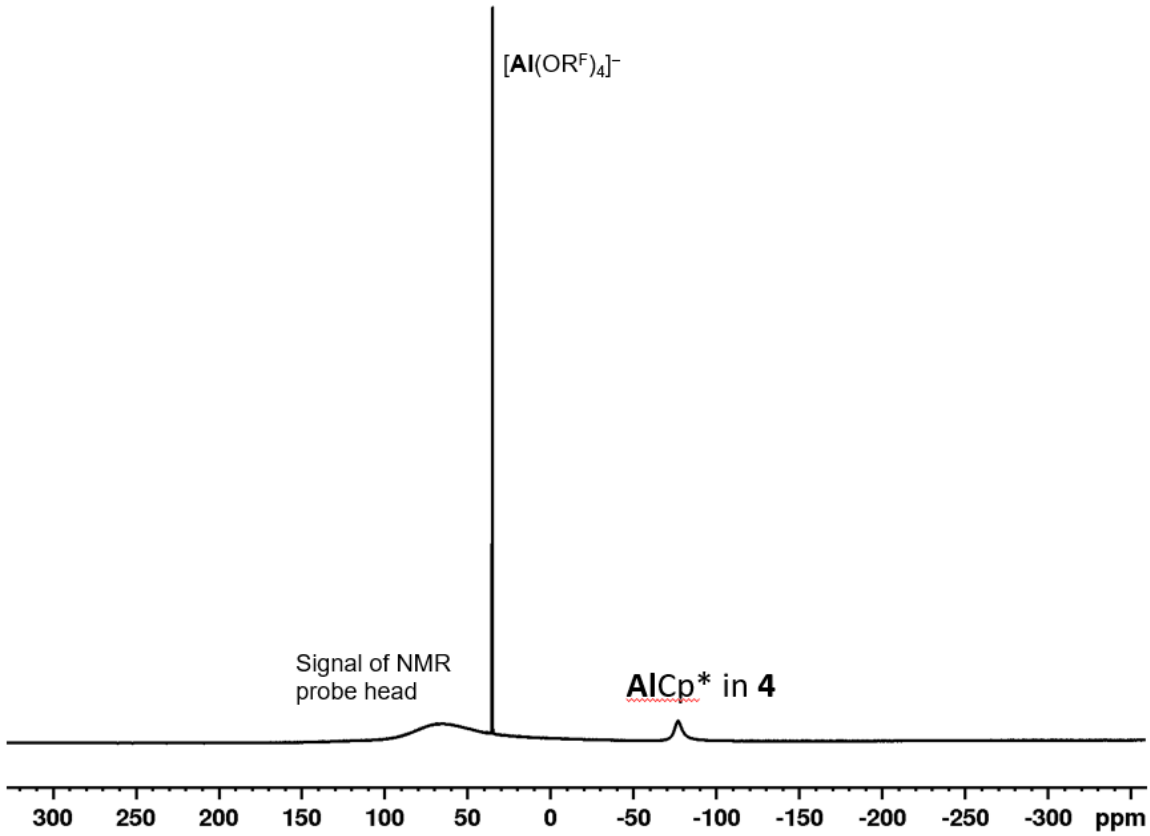
S-Figure 46: Yellow crystals of **4**.



S-Figure 47: ^{1}H NMR spectrum (300.17 MHz, 1,2-DFB, 300K) of [(Me-$_3$TACN)Al(AlCp*)$_3$][Al(OR^F)$_4$] **4**.



S-Figure 48: ^{11}F NMR spectrum (282.5 MHz, 1,2-DFB, 300K) [(Me$_3$TACN)Al(AlCp*)$_3$][Al(OR^F)$_4$] **4**.



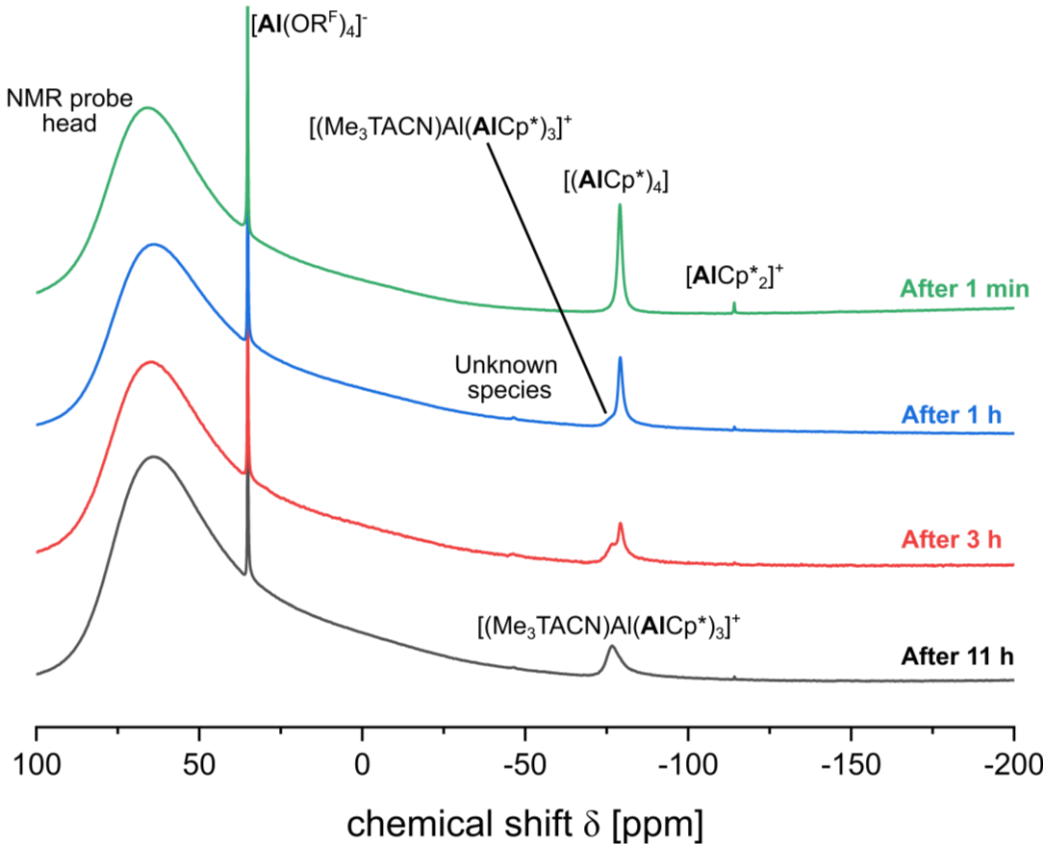
S-Figure 49: ^{27}Al NMR spectrum (78.2 MHz, 1,2-DFB, 300K) of [(Me_3TACN)Al(AlCp*)$_3$][Al(OR^F)$_4$] **4**.

S-2 Mechanistic studies on the reaction of $[Tl(AlCp^*)_3][Al(OR^F)_4]$ **3** with Me_3TACN

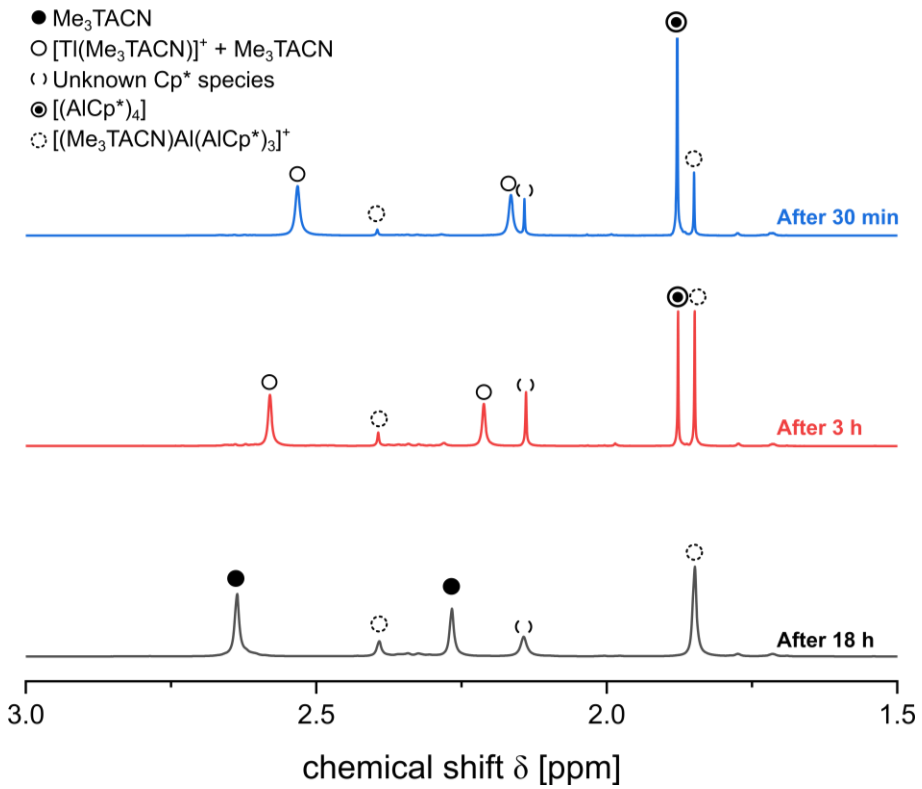
To study the reaction between **3** and TACN yielding **4** in PhF at room temperature, in situ NMR studies were performed. Hence, $[Tl(AlCp^*)_3][Al(OR^F)_4]$ **3** (25 mg, 15 μmol) was dissolved in PhF (0.5 mL) in a young NMR tube. Then, a solution of TACN in PhF was added (0.4 M, 0.08 mL, 0.03 mmol, 2 equiv.) at room temperature. After 1h already, the formation of a black precipitate was observed. Moreover, yellow crystals of Al_4^+ formed in the NMR tube.

The ^{27}Al NMR spectrum directly after addition of Me_3TACN shows the initial formation of $[(AlCp^*)_4]$ (S-Figure 49). Already after 1h, a shoulder of the Al_4^+ cluster can be observed at δ = −77.0 ppm. In the following hours, the product signal intensified whereas the intensity of the $[(AlCp^*)_4]$ decreased. After 11 h, the ^{27}Al NMR resonance of $[(AlCp^*)_4]$ has vanished. Besides a very weak singlet of an unknown species at δ = −46.2 ppm, no signals assignable to intermittent $TlAl_3^+$ clusters could be detected.

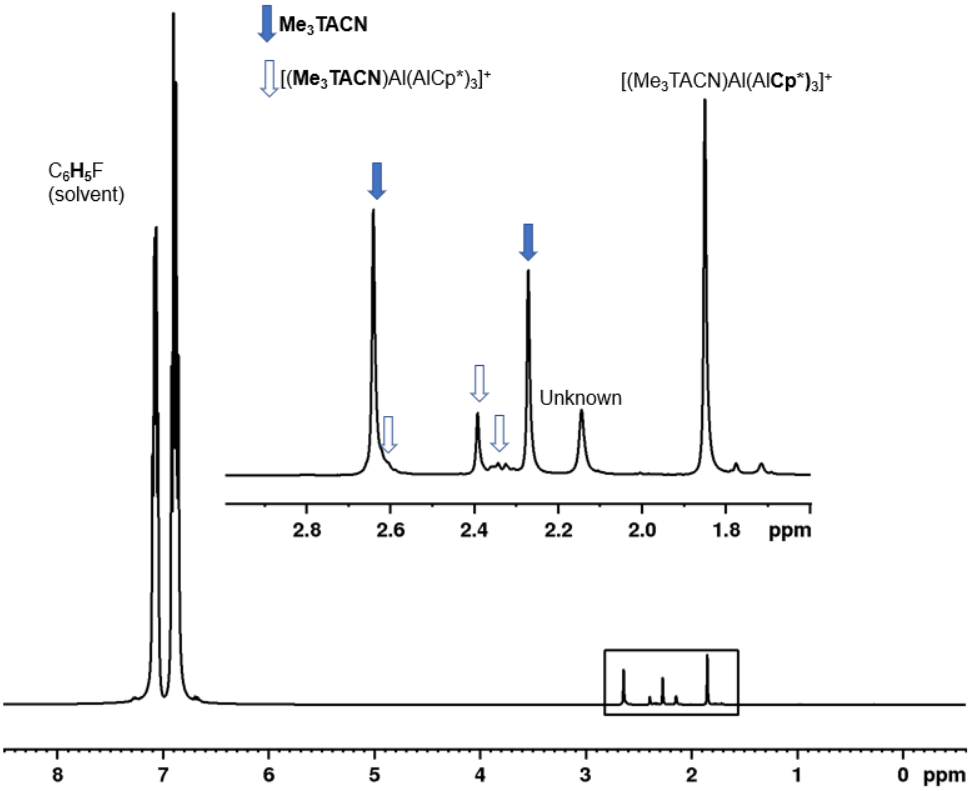
The first detected ^1H NMR spectrum verifies the initial formation of $[(AlCp^*)_4]$ via break-up of **3**. Moreover, ^1H NMR signals of $[Tl(Me_3TACN)]^+$ are detected as by-product. Yet, as previously shown for solutions of $[Tl(Me_3TACN)]^+$ **7** with excess Me_3TACN, a dynamic exchange of the Me_3TACN coordinated to the Tl^+ cation leads to the observation of an average peak for the two species (S-Figure 33). This dynamic behaviour can also be seen here. With removal of **7** by reaction with $[(AlCp^*)_4]$ to **4** and consecutively lowering of the concentration of $[Tl(Me_3TACN)]^+$, the average peaks shift to the chemical shifts detected for free Me_3TACN. Moreover, the ^1H NMR spectrum shows proton resonances assigned to **4** already after 30 min. After 18h, the $[(AlCp^*)_4]$ signal has depleted quantitatively. In addition to the proton resonances of **4**, a novel species is formed in the reaction which shows a singlet at δ = 2.15 ppm. The ^1H, ^{13}C HMBC spectrum shows that this species corresponds to a symmetrically coordinating Cp*-ligand. Most likely, the novel Cp* compound represents a TlCp* unit.



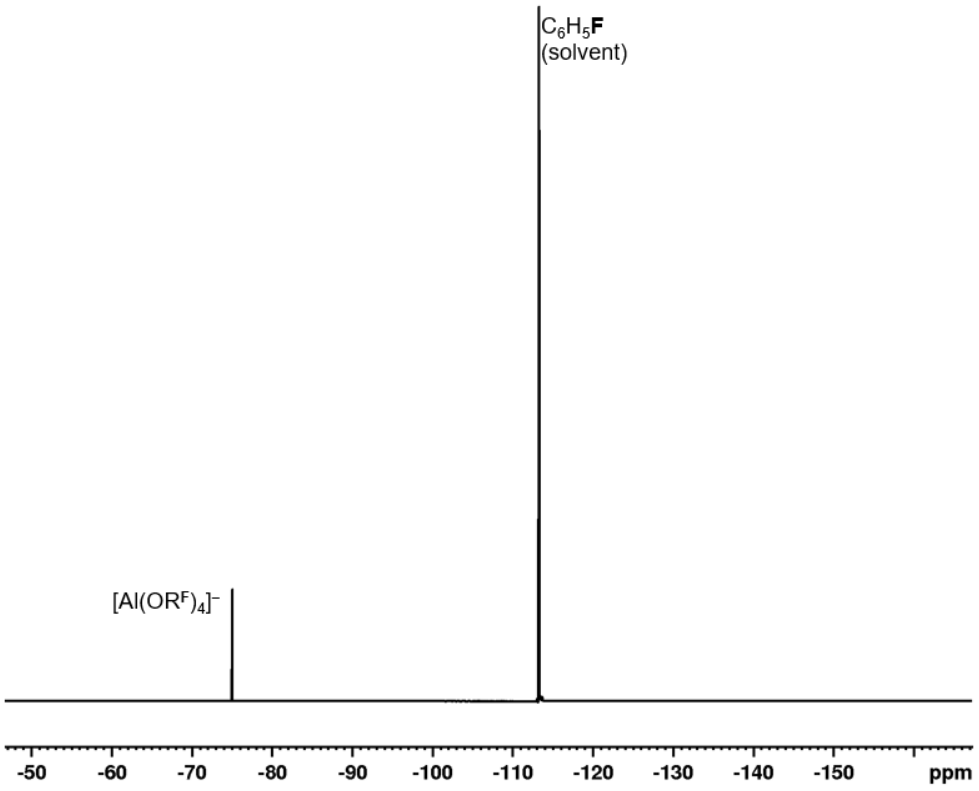
S-Figure 50: In situ ^{27}Al NMR spectra (104.27 MHz, PhF, 300K) for the reaction of **3** with Me_3TACN.



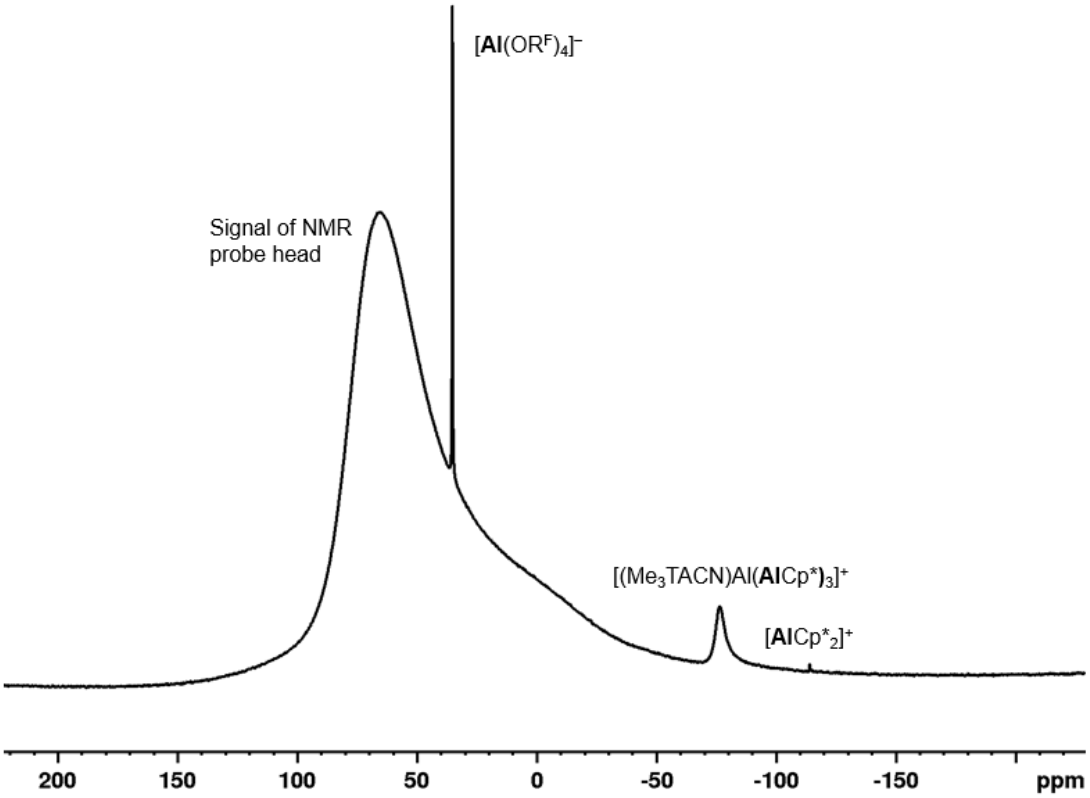
S-Figure 51: In situ ^{1}H NMR spectra (400.20 MHz, PhF, 300K) for the reaction of **3** with Me_3TACN.



S-Figure 52: ^{1}H NMR spectrum (400.20 MHz, PhF, 300K) of reaction of **3** with Me_3TACN after 18h.



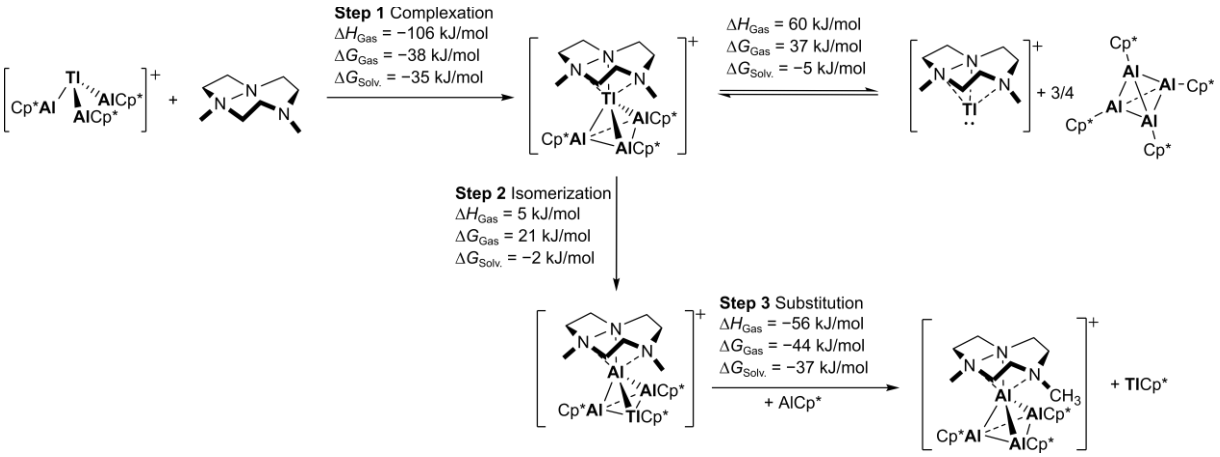
S-Figure 53: ^{11}F NMR spectrum (376.5 MHz, PhF, 300K) of reaction of **3** with Me_3TACN after 18h.



S-Figure 54: ^{27}Al NMR spectrum (104.3 MHz, PhF, 300K)) of reaction of **3** with Me_3TACN after 18h.

Computation of the thermodynamics in solution

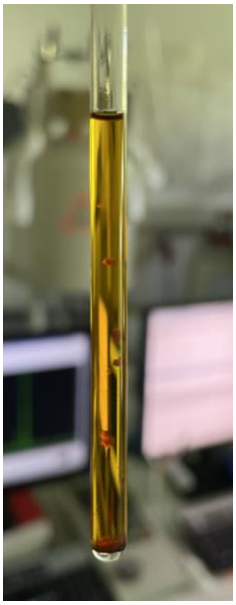
Although the NMR spectra for the mechanistic NMR study for the reaction of **3** with Me_3TACN did not allow for the observations of intermittent $TlAl_3^+$ clusters, we computed the thermodynamics of the reaction mechanism proposed for the reaction with the gallium complex **1** for thallium. Here, an in total exergonic reaction enthalpy to form TlCp* and the Al_4^+ cluster was calculated. Moreover, the formation of $[Tl(Me_3TACN)]^+$ and $[(AlCp^*)_4]$ is slightly exergonic, which coincides with the observations in the NMR spectrum.



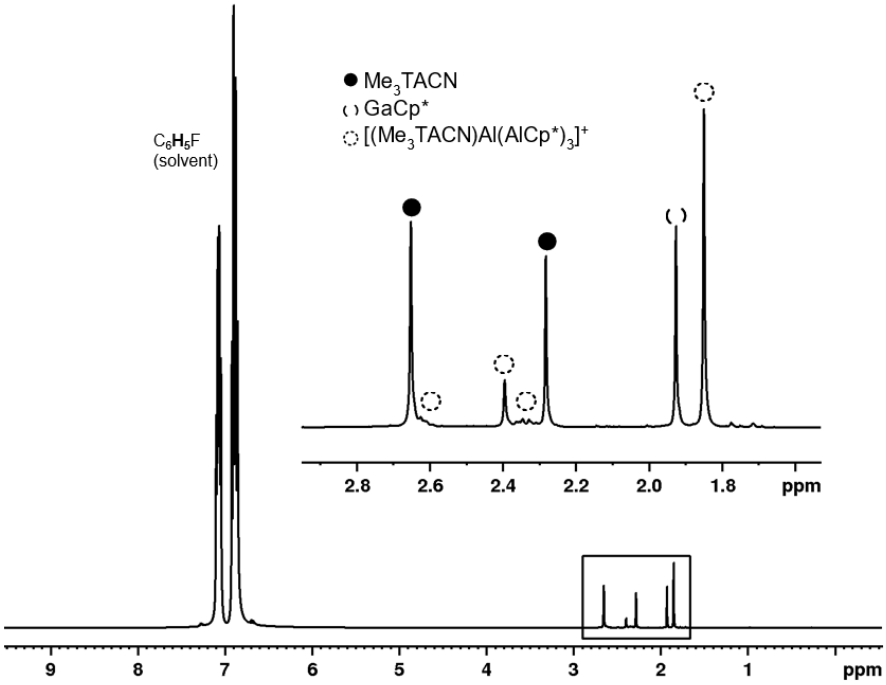
S-Figure 55: Postulated mechanism of the formation of $\mathbf{4}^+$ from $\mathbf{3}^+$ and Me_3TACN as well as computed thermodynamics (b3lyp-d3bj/def2-svp//bp86-d3bj/def2-svp with cosmo-rs in fluorobenzene).

S-3 Mechanistic studies on the reaction of $[Ga(AlCp^*)_3][Al(OR^F)_4]$ **1** with Me_3TACN

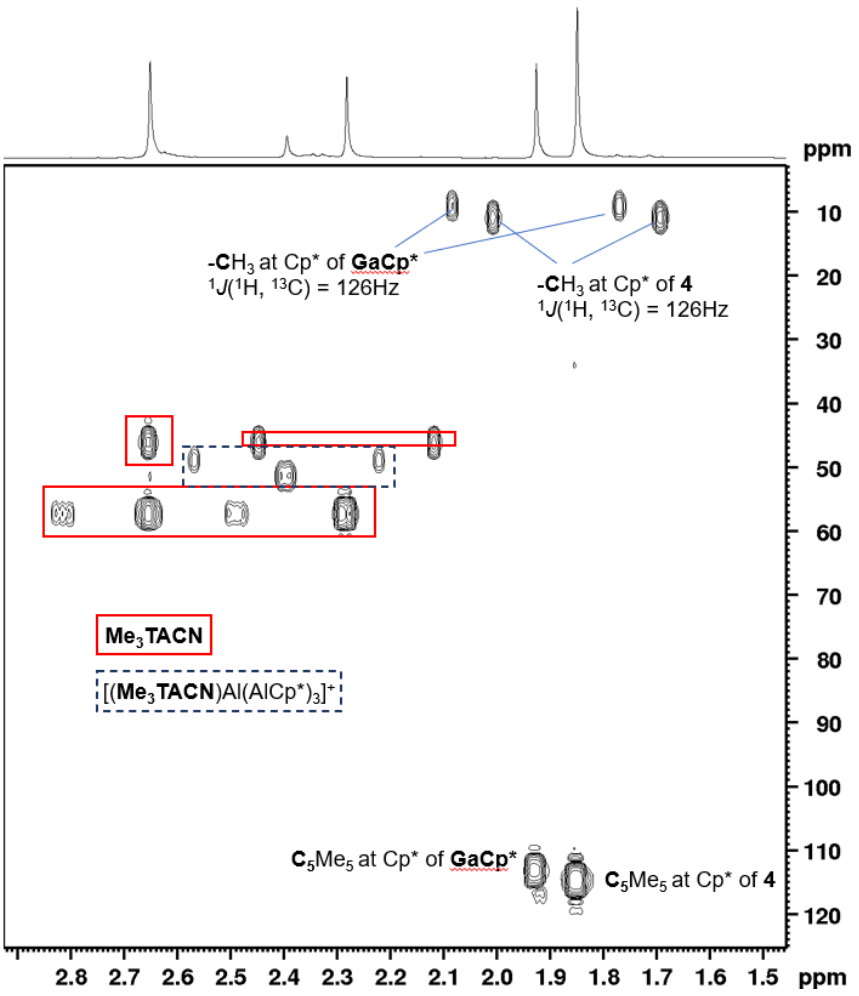
To study the reaction between **3** and Me_3TACN yielding **4** in PhF at room temperature, in situ NMR studies were performed. Hence, $[Ga(AlCp^*)_3][Al(OR^F)_4]$ **3** (32 mg, 21 μmol) was dissolved in PhF (0.5 mL) in a young NMR tube. Then, a solution of TACN in PhF was added (0.4 M, 0.11 mL, 0.04 mmol, 2 equiv.) at room temperature. After 24 h the formation of orange crystals could be observed, which were analysed by scXRD to be the product **4**.



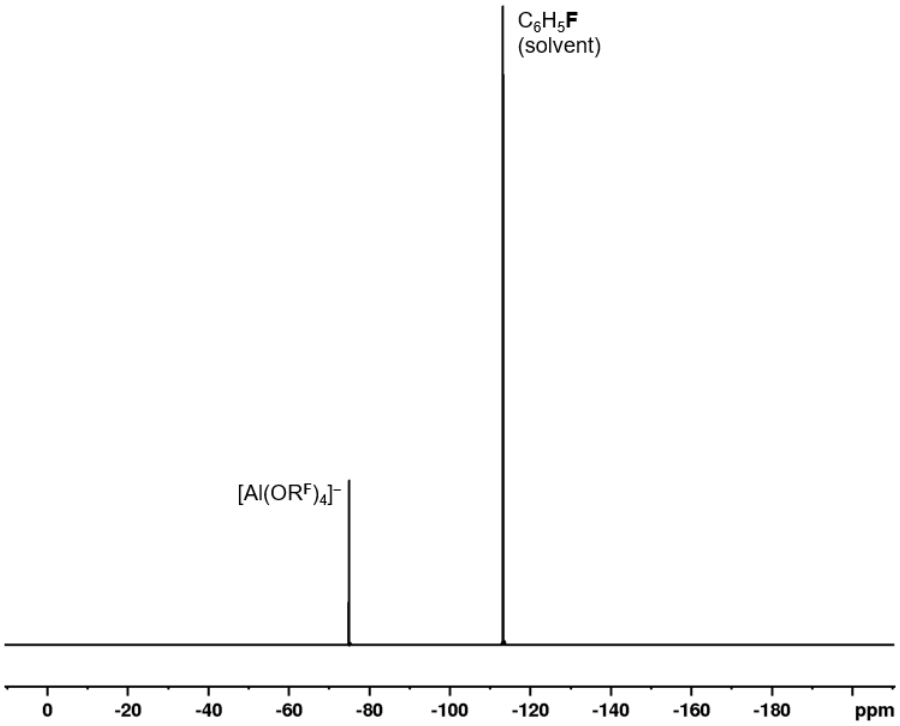
S-Figure 56: Young NMR with orange crystals of **4** after 24h.



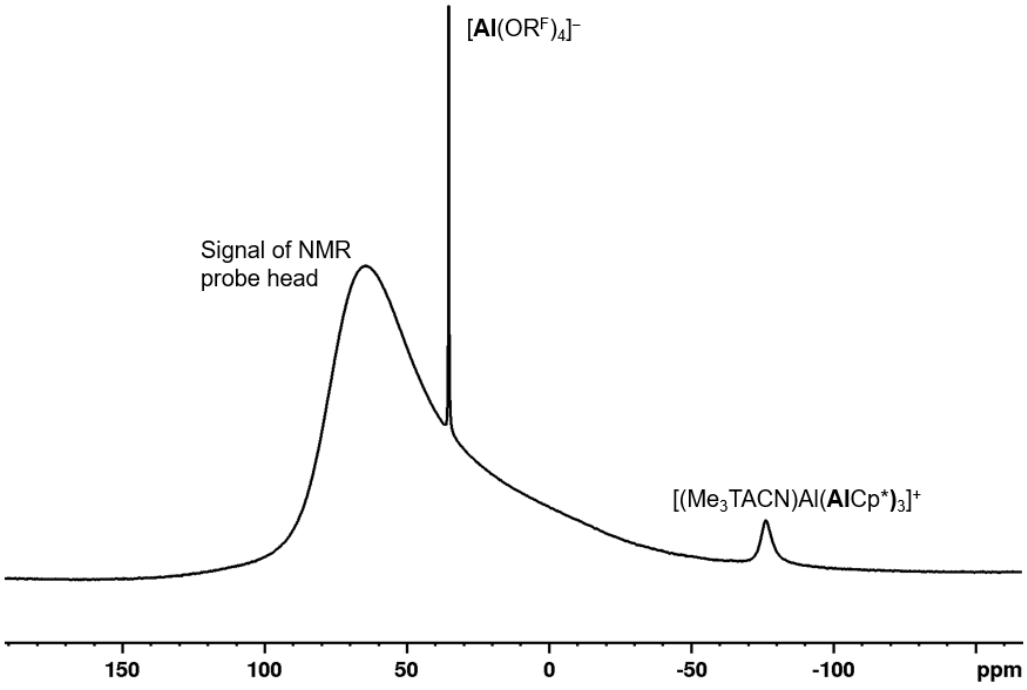
S-Figure 57: ^1H NMR spectrum (400.20 MHz, PhF, 300K) of reaction of **1** with Me_3TACN after 11 days.



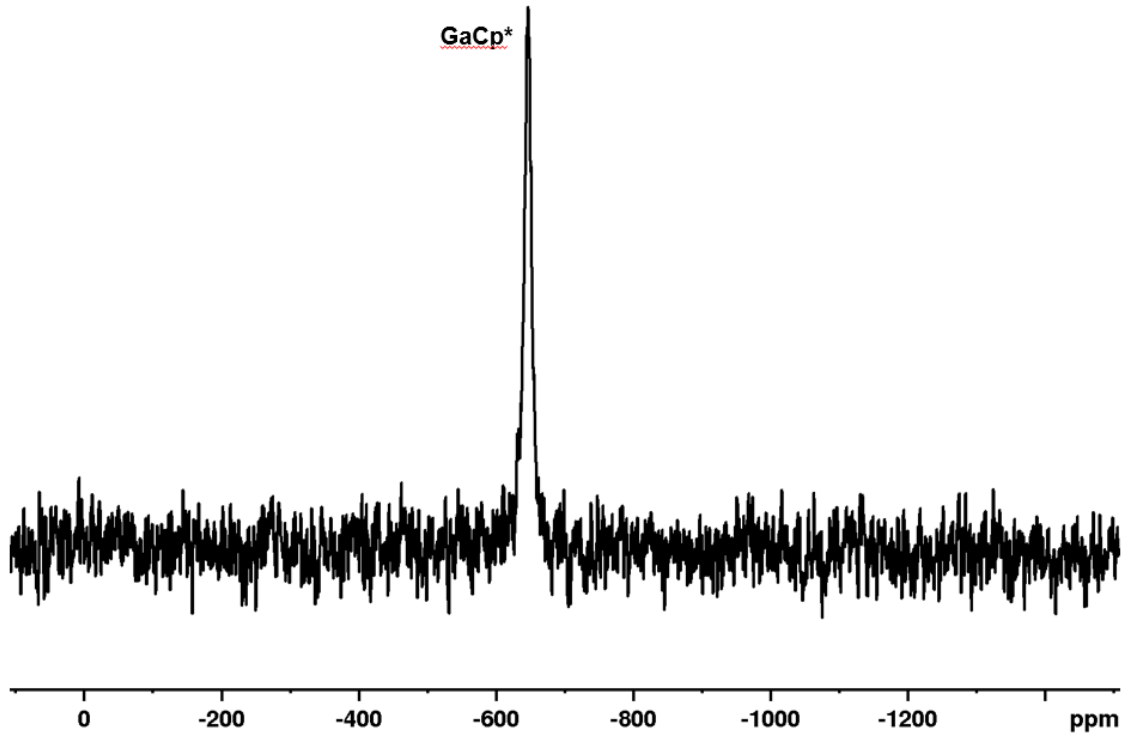
S-Figure 58: ^1H-^{13}C HMBC spectrum (400.20 MHz, 100.62 MHz, PhF, 300K) of reaction of **1** with Me_3TACN after 11 days.



S-Figure 59: ^{11}F NMR spectrum (376.5 MHz, PhF, 300K) of reaction of **1** with Me_3TACN after 11 days.



S-Figure 60: ^{27}Al NMR spectrum (104.3 MHz, PhF, 300K)) of reaction of **1** with Me_3TACN after 11 days.



S-Figure 61: ^{71}Ga NMR spectrum (122-04 MHz, PhF, 300K)) of reaction of **1** with Me_3TACN after 11 days.

S-4 Supporting quantum-chemical calculations

Computational details

Geometry optimizations were performed with the TURBOMOLE software[12] (v7.2 or v7.5) using DFT functionals bp86[13] with the def2-svp[14] basis set, the resolution-of-identity (RI) approximation[15], dispersion correction (d3bj)[16], 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[17]. 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[18] (20 excited states, singlet, with thermal smearing of occ. Numbers ($fermi)) starting from scXRD or bp96-d3bj/def2-svp structures. Computed NMR shifts were referenced against the experimental magnetic shielding of $[AlCp^*]_4$ ($\delta = -79.9$ ppm).

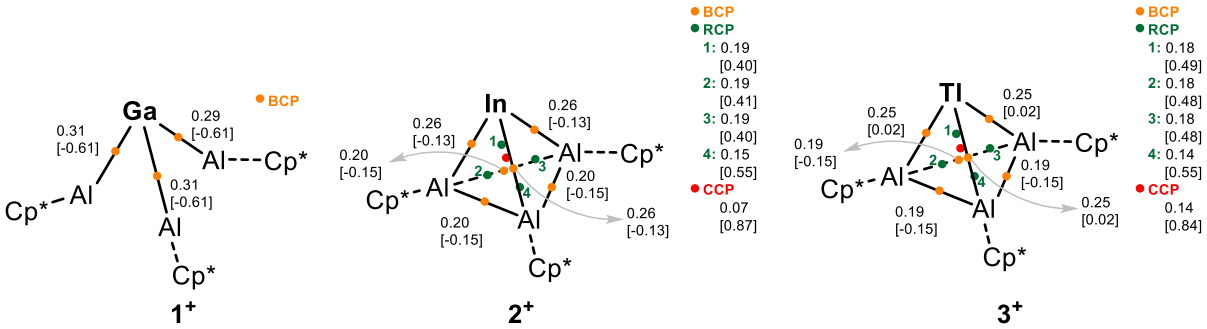
Gibbs free energies of solvation were calculated with the COSMO-RS model[19] at the bp86-d3/def2-tzvpd//bp86-d3/def2-tzvp[20] level of theory using the CosmoThermX[21] software (v C39_1501). Single-point calculations with the pbe0[22]-d3bj/def2-tzvpp or the b3lyp[23]-d3bj/def2tzvpp method were performed based on bp86-d3bj/def2-svp structures using TURBOMOLE.

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

QTAIM analysis of the cations

In the quantum theory of atoms in molecule analysis (QTAIM), the values computed at bond critical points (BCP) reflect the nature of interactions between the atoms. The most important values for description of the interaction are the electron density ρ(r) and the Laplacian of the electron density Δ_ρ(r). In general, large values of the electron density ρ(r) indicate a strong bonding interaction. Moreover, a negative Δ_ρ(r) value is indicative of a covalent, shared-shell interaction[27]. The ellipticity of electron density ε at the BCP reflects the anisotropy of the curvature of the electron density orthogonal to the bond. Hence, ε-values below 0.1 indicate no anisotropy (*e.g.* in σ-bonds) and values higher than 0.25 are typically calculated for double bonds[28].

The results of the QTAIM analyses of the $[M(AlCp^*)_3]^+$ cations are displayed in S-Figure 62. Here, the decrease of the electron densities on the BCPs of the M–Al bonds in the order Ga > In > Tl reveal the decreasing strength of these bonds. This observation coincides the decreasing wavenumber of the symmetric and asymmetric stretching vibrations in the same order as measured in the Raman spectra of the complexes. Surprisingly, for the In- and Tl-centred complexes, BCPs were computed between the Al_{Cp^*} atoms, indicating a weak bonding interaction. These interactions most likely result from the poor overlap of the AlCp* lone-pairs and the In/Tl accepting orbitals (see EDA-NOCV). Hence, remaining electron density at the Al-atoms allows for some delocalization as seen in the QTAIM analysis. Yet, the large, experimental, and computational Al_{Cp^*}–Al_{Cp^*} distances preclude a covalent Al–Al bonding interaction (average., comp. values for Al_{Cp^*}–Al_{Cp^*} distances: 2.986 Å in **1**$^+$, 3.008 Å **2**$^+$, 3.041 Å in **3**$^+$).



S-Figure 62: QTAIM analyses of the mixed group 13 cations.

EDA-NOCV of the clusters

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

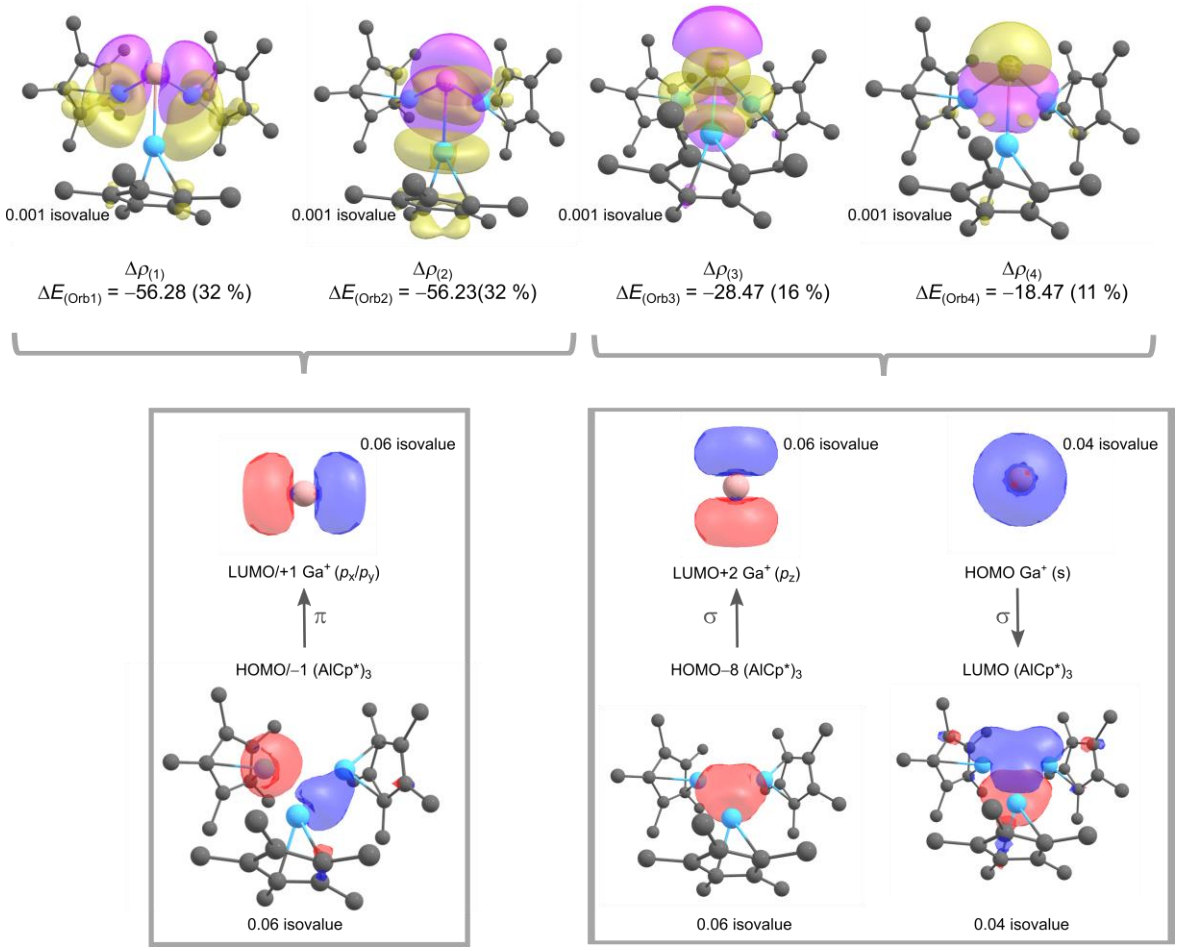
$$\boldsymbol{\Delta E_{int} = \Delta E_{elstat.} + \Delta E_{Pauli} + \Delta E_{disp} + \Delta E_{orb}.} \quad (2)$$

Moreover, the orbital interaction term ΔE_{orb} is further divided in the NOCV procedure into pairwise contributions $\Delta E^{k}{}_{orb}$. These $\Delta E^{k}{}_{orb}$ terms can be assigned to plots of deformation density $\Delta\varrho_k(r)$, which illustrate the orbital contributions to the bonding and the change in electron distribution in the molecule compared to the two fragments. More detailed information on the EDA-NOCV method can be found in recent reviews[29,30]. The EDA-NOCV method depends significantly on the charge and multiplicity of the fragments chosen. Here, the fragment combination leading to the lowest ΔE_{orb} is considered as the best bonding representation[30]. Similar to the previously reported $[Al(AlCp^*)_3]^+$ cation, the $[M(AlCp^*)_3]^+$ clusters are best described via the interaction of a M^+ cation with a $(s)^2(p)^0$-electron configuration with an $(AlCp^*)_3$ in its singlet state.

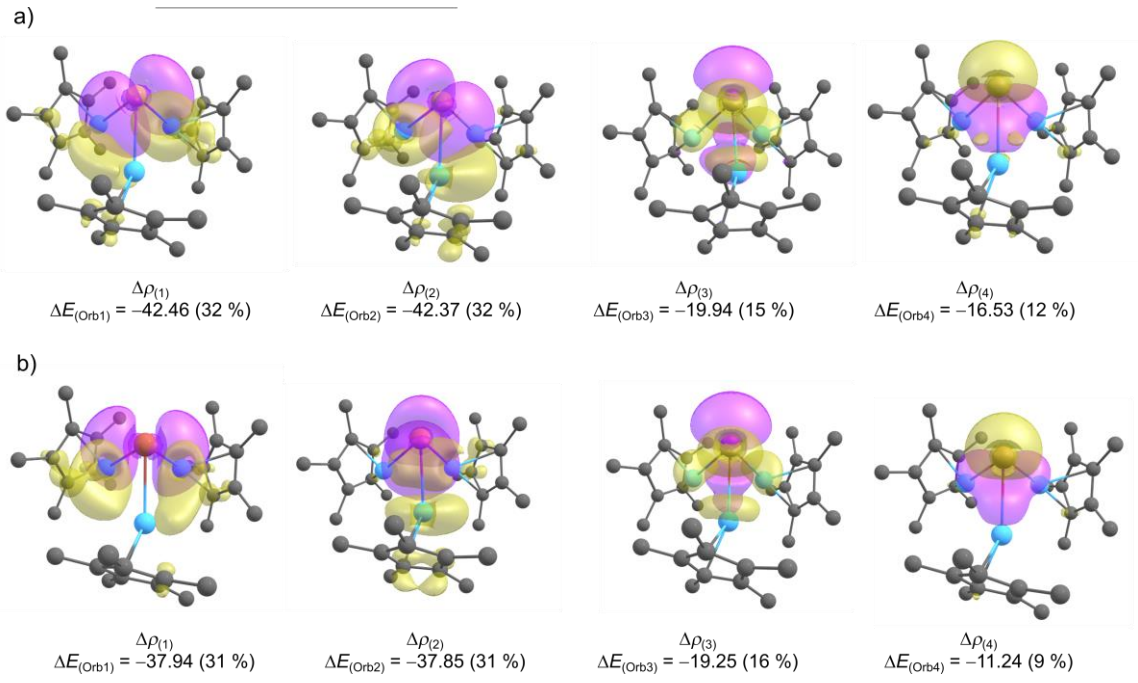
The plots of the deformation densities for the cations of type $[M(AlCp^*)_3]^+$ are displayed in S-Figure 63 and S-Figure 64. As further proven by the detailed analysis of the underlying symmetry-adapted fragment orbitals (SFOs) for $[Ga(AlCp^*)_3]^+$ (S-Figure 63), the major orbital interactions represent the electron donation from the degenerate HOMO/–1 orbitals of the $(AlCp^*)_3$ fragment into the empty p_x/p_y-orbitals at the metal cation. Furthermore, the back-donation from the metal cations lone-pair into the LUMO of the $(AlCp^*)_3$ fragment together with s-bonding interaction of the HOMO–8 at the $(AlCp^*)_3$ fragment with the metals p_z orbital are minor interactions. The latter two combine to the plots of deformation density $\Delta\rho_3$ and $\Delta\rho_4$. Interestingly, with lowering of the total magnitude of the orbital interaction in the order of $Ga^+ > In^+ > Tl^+$, the relative contributions of the bonding interactions to the total orbital interaction energies remain the same.

S-Table 1: Results of the EDA-NOCV analysis for the interaction of the M^+ atoms (S, electron configuration $(s^2)(p^0)$) with the $(AlCp^*)_3$ fragment (S) in **1**$^+$. Values are given in kcal/mol

		$[Ga(AlCp^*)_3]^+$	**$[In(AlCp^*)_3]^+$**	**$[Tl(AlCp^*)_3]^+$**
Energy terms	Orbital interaction			
ΔE_{int}		**-131.83**	**-112.14**	**-101.95**
ΔE_{Pauli}		152.96	129.70	127.55
ΔE_{elstat}		-99.47	-93.56	-94.65
ΔE_{Orb}		-174.59	-135.28	-120.80
$\Delta E_{Orb(1)}$	$(AlCp^*)_3 \rightarrow M^+ (p_y)$ π-donation	-56.28 (32%)	-42.46 (32%)	-37.94 (31%)
$\Delta E_{Orb(2)}$	$(AlCp^*)_3 \rightarrow M^+ (p_x)$ π-donation	-56.23 (32%)	-42.37 (32%)	-37.85 (31%)
$\Delta E_{Orb(3)}$	$(AlCp^*)_3 \rightleftarrows M^+ (s/p_z)$ σ-bonding	-28.47(16%)	-19.94 (15%)	-19.25 (16%)
$\Delta E_{Orb(4)}$	$(AlCp^*)_3 \rightleftarrows M^+ (s/p_z)$ σ-bonding	-18.47 (11%)	-16.53 (12%)	-11.24 (9%)
ΔE_{Rest}		-15.06	-13.98	-14.49
ΔE_{Disp}		-10.73	-12.99	-14.06



S-Figure 63: Plots of deformation densities $\Delta\rho_{(1)-(4)}$ of the pairwise orbital interaction in **1**$^+$ associated with energy terms $\Delta E_{Orb(1)-Orb(4)}$ (values in kcal/mol) as well as visualization of the underlying fragment orbitals of $(AlCp^*)_3$ and Ga^+. Charge flows from yellow to purple.



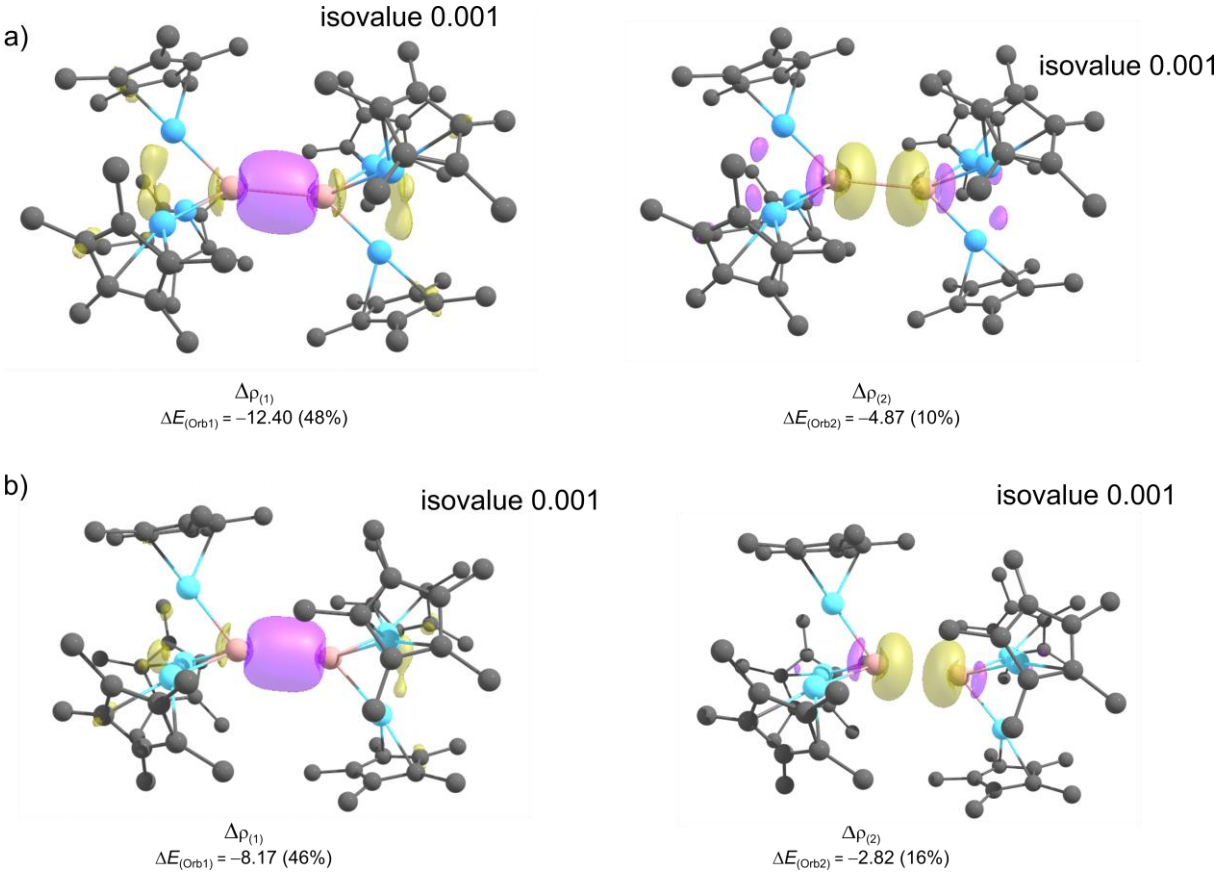
S-Figure 64: Plots of deformation densities $\Delta\rho_{(1)-(4)}$ of the pairwise orbital interaction in **2**$^+$ (a) and **3**$^+$ (b) associated with energy terms $\Delta E_{Orb(1)-Orb(4)}$ (values in kcal/mol) (isovalue 0.001). Charge flows from yellow to purple.

QC analysis of $[Ga_2(AlCp^*)_6]$

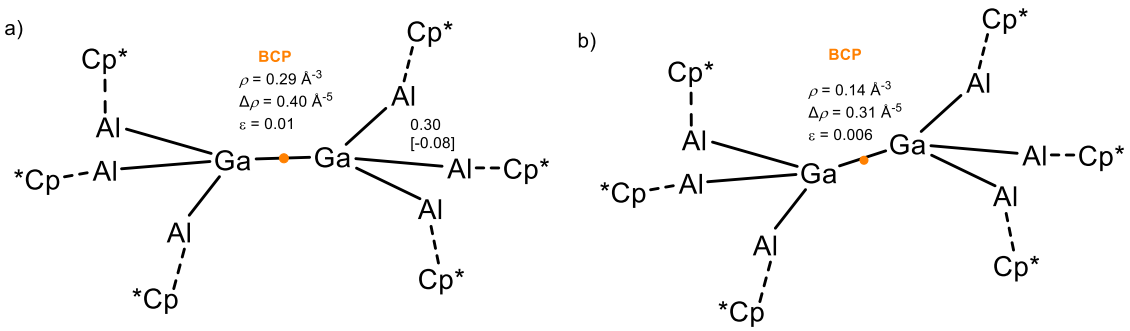
To study the interaction of the $[Ga(AlCp^*)_3]^+$ cations in the dimer $[Ga_2(AlCp^*)_6]^{2+}$, QTAIM and EDA-NOCV calculations were performed. In the latter, the dimer-interactions were found to be represented by a week σ-bonding interaction by double dative interaction of the lone-pair at one Ga atom with the p_z orbital of the other Ga atom. The σ-bonding nature is further validated by the low computed ellipticities at the BCPs of the Ga–Ga bonds (S-Figure 66). Yet, these interactions are very weak to that extent, that the covalent interaction energies are only slightly larger (short Ga–Ga distance) or even smaller (long Ga–Ga distance) than the dispersion forces.

S-Table 2: Results of the EDA-NOCV analysis for the interaction of two $[M(AlCp^*)_3]^+$ fragments; Values are given in kcal/mol

	Dimer with long Ga^+–Ga^+ bond (scXRD)		**Dimer with short Ga^+–Ga^+ bond (scXRD)**	
	$[Ga(AlCp^*)_3]^+$ (S) + $[Ga(AlCp^*)_3]^+$ (S)	**$[Ga(AlCp^*)_3]^+$ (T) + $[Ga(AlCp^*)_3]^+$ (T)**	**$[Ga(AlCp^*)_3]^+$ (S) + $[Ga(AlCp^*)_3]^+$ (S)**	**$[Ga(AlCp^*)_3]^+$ (T) + $[Ga(AlCp^*)_3]^+$ (T)**
Energy terms				
ΔE_{int}	**13.88**	**-116.98**	**12.73**	**-120.26**
ΔE_{Pauli}	26.05	49.71	40.96	73.52
ΔE_{elstat}	24.36	1.32	16.35	-20.88
ΔE_{Orb}	-17.77	-149.24	-25.61	-153.66
$\Delta E_{Orb(1)}$	-8.17 (46%)		-12.40 (48%)	
$\Delta E_{Orb(2)}$	-2.82 (16%)		-4.87 (10%)	
ΔE_{Rest}	-6.76		-8.34 (33%)	
ΔE_{Disp}	-18.77	-18.77	-18.96	-18.96



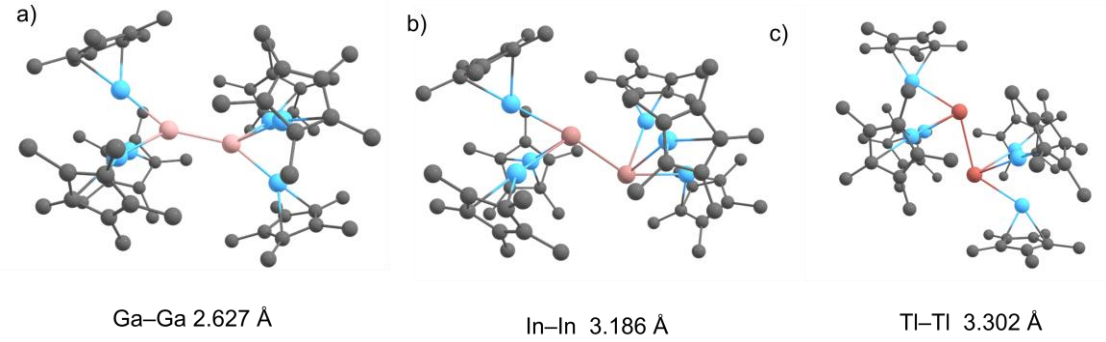
S-Figure 65: Plots of deformation densities $\Delta\rho_{(1)-(2)}$ of the pairwise orbital interaction in the $[Ga_2(AlCp^*)_6]^{2+}$ dimers with a short (a) and long (b) Ga^+–Ga^+ distance. Charge flows from yellow to purple.



S-Figure 66: Computed electron densities $\rho(r)$, Laplacian of the electron density $\Delta_\rho(r)$ and ellipticity ε of electron density at the critical points (BCP: bond critical point) of the scXRD structures of $[Ga_2(AlCp^*)_6]^{2+}$ with short (a) and long (b) Ga^+–Ga^+ distances.

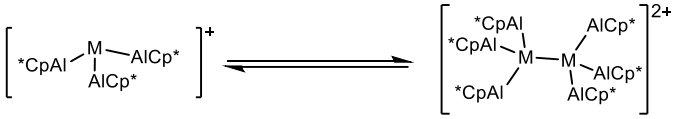
Comparison of dimerization for **1**$^{+}$, **2**$^{+}$, and **3**$^{+}$

The comparison of the computed structures of the dimeric $[M_2(AlCp^*)_6]^{2+}$ clusters shows a significant change to “slipped”-dimeric structures for the heavier indium- and thallium-centred clusters. These structural changes can be attributed to the significant decrease in orbital overlap between the s-type lone-pair and p_z-type LUMO of the complexes.



S-Figure 67: Computed gas-phase structures of $[Ga_2(AlCp^*)_6]^{2+}$ (a), $[In_2(AlCp^*)_6]^{2+}$ (b) and $[Tl_2(AlCp^*)_6]^{2+}$ (c).

The thermodynamics of the dimerization of $[M(AlCp^*)_3]^{+}$ cations (M = Ga^{+}, In^{+}, Tl^{+}) was computed on b3-lyp-d3bj/def2-tzvpp//bp86-d3bj/def2-svp level of DFT. The gas-phase structure of the $[Ga_2(AlCp^*)_6]^{2+}$ dimer was computed with a significant shorter Ga–Ga distance of 2.627 Å which deviates significantly from the values measured in the scXRD structures of 2.860(1) Å and 3.108(1) Å. Hence, the computed thermodynamics most likely do not accurately describe the dimerization observed in the experiment in solution and solid state. Hence, only the $\Delta(\Delta H^0_{gas})$ and $\Delta(\Delta G^0_{gas})$ for the dimers will be discussed. As expected, the enthalpies and free enthalpies of dimerization become less favourable in the order Ga > In > Tl.

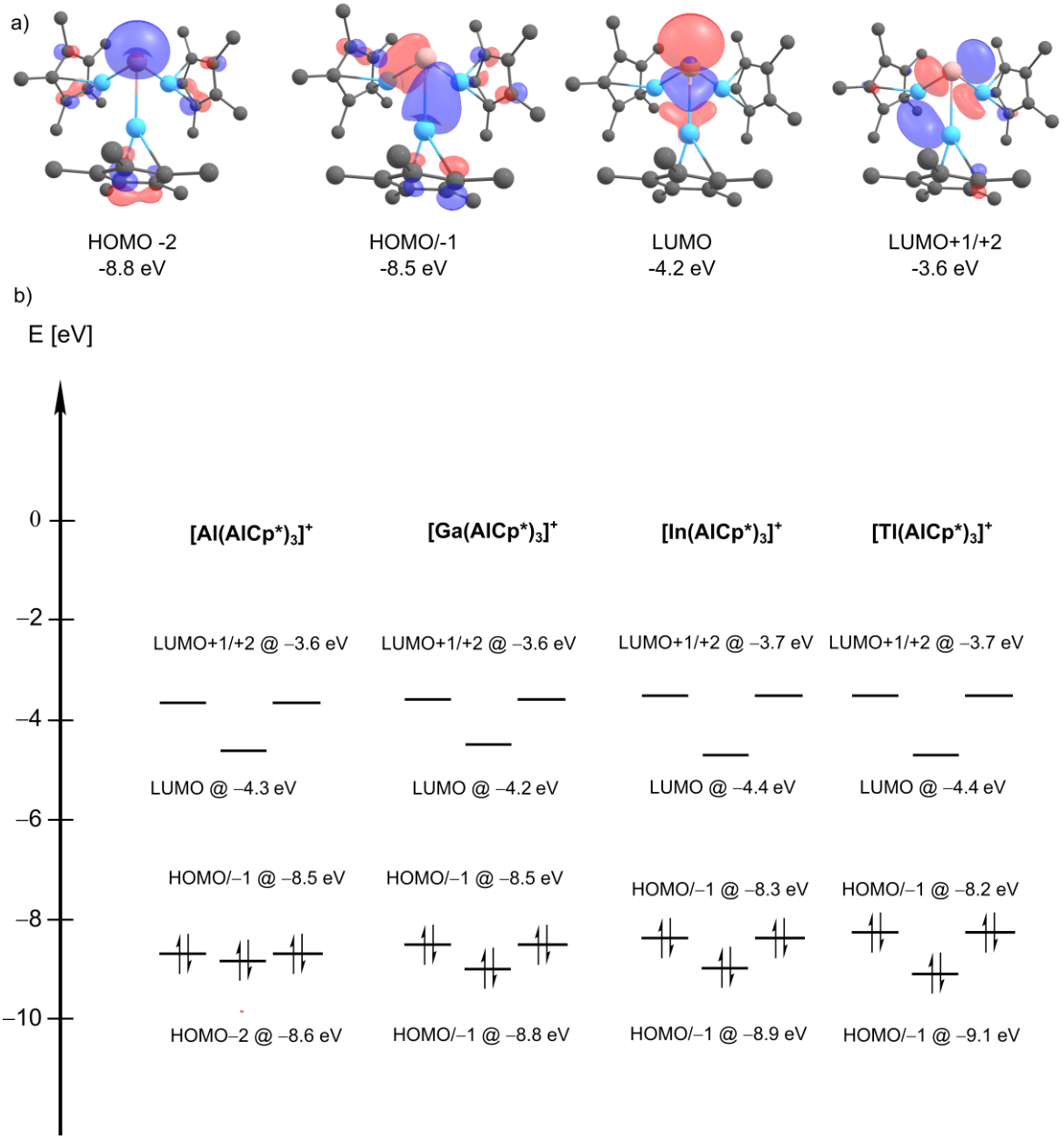


Calc. Gas-Phase Thermodynamics:
Ga-Dimer: ΔH^0_{gas}= 91 kJ/mol, ΔG^0_{gas}= 160 kJ/mol
In-Dimer: ΔH^0_{gas}= 102 kJ/mol, ΔG^0_{gas}= 179 kJ/mol
Tl-Dimer: ΔH^0_{gas}= 110 kJ/mol, ΔG^0_{gas}= 185 kJ/mol

S-Scheme 1: Computed gas-phase thermodynamics for the dimerization of $[M(AlCp^*)_3]^{+}$. Values computed at b3-lyp-d3bj/def2-tzvpp//bp86-d3bj/def2-svp level of DFT.[1]

[1] The optimized structure of $[In_2(AlCp^*)_6]^{2+}$ contained a small imaginary frequency of -5.33 cm^{-1}, which could not be removed despite various changes in the convergence criteria und start structures. Yet, the effect on the computed thermodynamics is negligible.

Frontier orbitals



S-Figure 68: a) Kohn-Sham orbitals of $[Ga(AlCp^*)_3]^+$ computed at pbe0-d3bj/def2-tzvpp//bp86-d3bj/def2-svp level of DFT (isovalue 0.05). b) Computed energy levels of frontier orbitals for the cations $[M(AlCp^*)_3]^+$ (pbe0-d3bj/def2-tzvpp//bp86-d3bj/def2-svp).

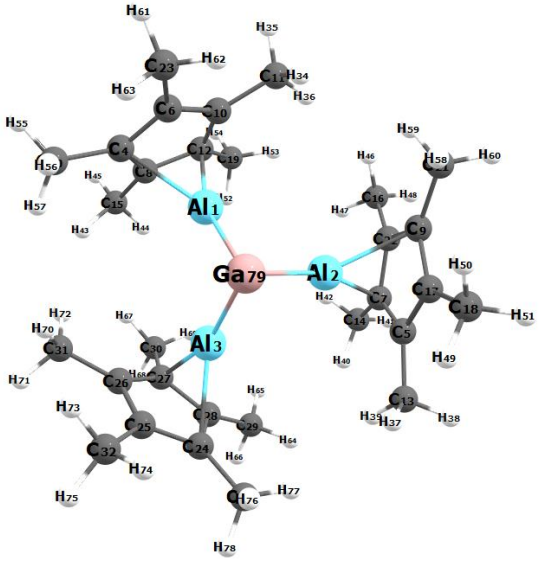
Energies

S-Table 3: Thermodynamic data for computed molecules (b3lyp-d3bj/def2-tzvpp//bp86-d3bj/def2-svp).

Compound	E(SCF) [Eh]	FreeH Energy [Eh]	FreeH entropy at 298 K [Eh]	COSMO-RS (in PhF) [kcalmol^{-1}]
[(AlCp*)$_4$]	-2529.835157	2426.51	1.37152	-76.5106156
AlCp*	-632.4399962	600.57	0.481	-15
[(Me$_3$TACN)Al(AlCp*)$_3$]$^+$	-2659.409	2654.2	1.32835	-202.844531
Me$_3$TACN	-519.703011	807.98	0.4746	-25
GaCp*	-2314.827134	599.08	0.49268	-12.1002582
[Ga(AlCp*)$_3$]$^+$	-3822.032286	1830.15	1.18065	-161.315915
[Ga(Me$_3$TACN)]$^+$	-2444.372119	826.54	0.4766	-166.865461
[(Me$_3$TACN)Ga(AlCp*)$_3$]$^+$	-4341.782125	2653.1	1.36149	-192.75364
[(Me$_3$TACN)Al(GaCp*)(AlCp*)$_2$]$^+$	-4341.791223	2652.12	1.35856	-205.911341
TlCp*	-562.5571331	597.52	0.50735	-13.7432522
[Tl(AlCp*)$_3$]$^+$	-2069.759043	1828.89	1.20231	-163
[Tl(Me$_3$TACN)]$^+$	-692.1058238	824.77	0.49836	-168.893325
[(Me$_3$TACN)Tl(AlCp*)$_3$]$^+$	-2589.506147	2649.11	1.44928	-184.894589
[(Me$_3$TACN)Tl(GaCp*)(AlCp*)$_2$]$^+$	-2589.504314	2649.62	1.39584	-208.01827

Optimized structures

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



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

Symmetry: c1

Cartesian coordinates in Ångström:

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Al	1.0852732	-0.1409108	1.3373517
Al	0.6160494	-0.1431440	-1.6113235
C	-3.8695401	-0.2282552	-0.3205289
C	3.2338526	0.2327248	1.8492381
C	-3.7286099	-0.8055956	0.9916860
C	2.4694712	1.4364635	2.0671232
C	-3.4368086	1.1448053	-0.2508155
C	1.6551312	-0.2128090	3.5092481
C	-3.2175523	0.2089726	1.8773542
C	-2.9465920	0.0247344	3.3415761
C	-3.0286603	1.4166294	1.1115476
C	4.3698019	0.0550894	0.8852399
C	2.7054714	2.7776930	1.4363745
C	-3.5261504	2.1635006	-1.3477758
C	0.5810925	2.1735416	3.7236710
C	2.7255954	-0.7845986	2.7332737
C	3.2304954	-2.1941234	2.8296956
C	-2.6000571	2.7557694	1.6361181
C	-4.3910855	-0.9324460	-1.5385578
C	0.8625321	-0.9220903	4.5677342
C	1.4927456	1.1594478	3.0995783
C	-4.0594878	-2.2176533	1.3760092
C	2.2110725	-0.1965617	-3.1918781
C	1.0077204	-0.7747864	-3.7329513
C	-0.0195393	0.2349998	-3.7255344
C	0.5428893	1.4403230	-3.1673011
C	1.9274677	1.1719826	-2.8400225
C	2.9161579	2.1904467	-2.3563399
C	-0.1322735	2.7751989	-3.0474022
C	-1.4213973	0.0498617	-4.2276009
C	0.8486712	-2.1829663	-4.2257027
C	3.5297064	-0.8962343	-3.0391719
H	-2.4560632	-0.9468535	3.5518747
H	-3.8905098	0.0482803	3.9250273
H	-2.2958096	0.8261739	3.7390967
H	4.3159070	-0.9186457	0.3582307
H	5.3458267	0.0885276	1.4126475
H	4.3834449	0.8542601	0.1203401
H	3.2515214	2.6895880	0.4795350
H	3.3142880	3.4223820	2.1047839
H	1.7585911	3.3177554	1.2370143
H	-3.4440265	1.7001423	-2.3496328
H	-2.7402724	2.9378472	-1.2602321
H	-4.5052372	2.6864966	-1.3123214
H	-0.3260919	1.7055043	4.1513643
H	0.2614401	2.9464139	2.9987805
H	1.0971152	2.6991066	4.5548890
H	3.6230032	-2.5571379	1.8599541
H	2.4361585	-2.8936973	3.1544284
H	4.0566773	-2.2679512	3.5680074
H	-1.9613675	3.3016218	0.9137049
H	-2.0361503	2.6632346	2.5821374
H	-3.4833752	3.3968408	1.8404558
H	-5.5006475	-0.9050328	-1.5664885
H	-4.0897895	-1.9982949	-1.5577978

H	-4.0267636	-0.4626154	-2.4718464
H	0.6920793	-1.9860625	4.3102098
H	-0.1263715	-0.4510747	4.7246599
H	1.3959577	-0.9020037	5.5412234
H	-5.1080702	-2.2942459	1.7333714
H	-3.4068351	-2.5850266	2.1918188
H	-3.9523414	-2.9121886	0.5205031
H	3.7433241	1.7247192	-1.7872399
H	2.4423285	2.9558118	-1.7124238
H	3.3744233	2.7244594	-3.2154665
H	-1.2329090	2.6768403	-3.0341155
H	0.1301339	3.4251848	-3.9085953
H	0.1706144	3.3147171	-2.1281140
H	-1.8431451	-0.9293669	-3.9242661
H	-1.4536237	0.0910296	-5.3363011
H	-2.0965731	0.8410619	-3.8507769
H	-0.1843864	-2.5547066	-4.0811721
H	1.5331572	-2.8800901	-3.7049510
H	1.0738005	-2.2491994	-5.3110885
H	3.4001790	-1.9647595	-2.7770925
H	4.1533164	-0.4298776	-2.2529357
H	4.1091686	-0.8588549	-3.9855129
Ga	0.0077276	-1.9950930	-0.0018957

SCF energy GEOOPT = -3821.663251952 H

ZPE = 1704. kJ/mol

FREEH energy = 1830.15 kJ/mol

FREEH entropy = 1.18065 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
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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	- -
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8	a	19.03	0.00610	YES YES
9	a	20.90	0.01453	YES YES
10	a	31.88	0.00568	YES YES
11	a	34.55	0.02087	YES YES
12	a	37.20	0.02549	YES YES
13	a	49.00	0.04367	YES YES
14	a	50.82	0.06740	YES YES
15	a	51.64	0.03164	YES YES
16	a	61.55	0.21493	YES YES
17	a	66.88	0.11379	YES YES
18	a	68.75	0.09243	YES YES
19	a	72.05	0.02188	YES YES
20	a	78.90	0.20373	YES YES
21	a	81.27	0.05455	YES YES
22	a	84.44	0.31918	YES YES
23	a	88.51	0.34979	YES YES
24	a	93.24	0.10044	YES YES
25	a	94.50	0.03078	YES YES
26	a	98.08	0.13642	YES YES
27	a	100.76	0.01274	YES YES
28	a	109.33	0.69000	YES YES
29	a	110.75	0.65261	YES YES
30	a	113.21	0.13041	YES YES
31	a	123.93	0.33518	YES YES
32	a	124.16	0.37147	YES YES
33	a	135.80	0.05448	YES YES
34	a	138.23	0.01217	YES YES
35	a	144.13	0.04898	YES YES
36	a	148.86	0.06057	YES YES
37	a	152.28	0.00075	YES YES
38	a	155.31	0.02628	YES YES
39	a	157.12	0.01683	YES YES
40	a	163.83	0.08110	YES YES
41	a	171.18	0.23595	YES YES
42	a	175.27	0.15766	YES YES
43	a	187.75	1.37746	YES YES
44	a	189.03	1.36762	YES YES
45	a	192.59	0.07754	YES YES
46	a	213.49	0.27760	YES YES

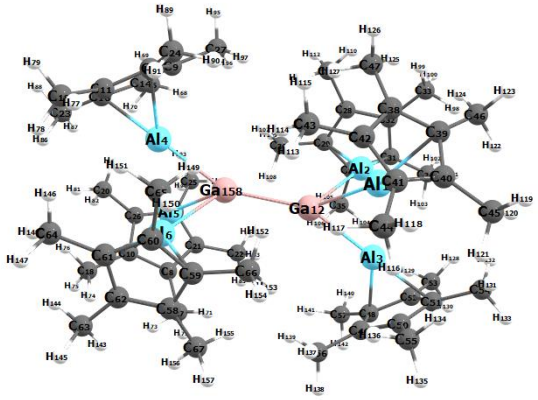
47	a	228.07	0.94008	YES	YES
48	a	229.70	1.06767	YES	YES
49	a	246.20	4.29183	YES	YES
50	a	252.30	7.25160	YES	YES
51	a	253.14	7.26408	YES	YES
52	a	272.81	0.03308	YES	YES
53	a	273.40	0.20723	YES	YES
54	a	274.10	0.27364	YES	YES
55	a	274.33	0.07583	YES	YES
56	a	276.09	0.26735	YES	YES
57	a	277.27	0.20900	YES	YES
58	a	282.51	0.12423	YES	YES
59	a	284.56	1.81087	YES	YES
60	a	284.81	1.72826	YES	YES
61	a	287.81	0.18222	YES	YES
62	a	289.92	1.32348	YES	YES
63	a	290.84	1.10541	YES	YES
64	a	379.52	0.37233	YES	YES
65	a	380.00	10.88434	YES	YES
66	a	380.66	11.29656	YES	YES
67	a	390.57	0.75556	YES	YES
68	a	394.10	1.34990	YES	YES
69	a	394.38	1.76726	YES	YES
70	a	471.70	360.42613	YES	YES
71	a	472.66	360.65502	YES	YES
72	a	523.23	26.29642	YES	YES
73	a	543.32	0.03343	YES	YES
74	a	544.17	0.03609	YES	YES
75	a	544.53	0.02109	YES	YES
76	a	544.73	0.10226	YES	YES
77	a	544.81	0.06416	YES	YES
78	a	545.26	0.14326	YES	YES
79	a	546.37	0.06519	YES	YES
80	a	546.73	0.04543	YES	YES
81	a	547.27	0.02525	YES	YES
82	a	588.36	6.31620	YES	YES
83	a	588.63	7.29255	YES	YES
84	a	589.67	0.79537	YES	YES
85	a	591.13	1.34444	YES	YES
86	a	591.76	1.06115	YES	YES
87	a	592.17	0.90808	YES	YES
88	a	604.23	0.19692	YES	YES
89	a	604.43	0.10604	YES	YES
90	a	605.09	0.12654	YES	YES
91	a	796.51	2.52528	YES	YES
92	a	797.84	2.90877	YES	YES
93	a	798.25	2.85180	YES	YES
94	a	801.81	6.71017	YES	YES
95	a	802.07	0.99379	YES	YES
96	a	802.49	1.64390	YES	YES
97	a	922.98	0.18527	YES	YES
98	a	923.72	0.28632	YES	YES
99	a	924.36	0.35055	YES	YES
100	a	925.75	0.28642	YES	YES
101	a	926.19	0.25103	YES	YES
102	a	927.57	0.15395	YES	YES
103	a	988.19	5.93467	YES	YES
104	a	988.62	8.31098	YES	YES
105	a	989.09	4.96394	YES	YES
106	a	992.73	6.67750	YES	YES
107	a	993.46	6.10285	YES	YES
108	a	993.93	5.45727	YES	YES
109	a	995.72	0.39885	YES	YES
110	a	996.59	0.24580	YES	YES
111	a	997.50	0.07776	YES	YES
112	a	998.83	0.21021	YES	YES
113	a	999.38	0.22821	YES	YES
114	a	1000.60	0.17120	YES	YES
115	a	1000.77	0.02083	YES	YES
116	a	1001.45	0.49174	YES	YES
117	a	1001.60	0.93557	YES	YES
118	a	1048.28	5.33512	YES	YES
119	a	1048.73	2.90306	YES	YES
120	a	1049.33	3.24328	YES	YES
121	a	1050.43	0.01353	YES	YES
122	a	1050.61	0.48561	YES	YES
123	a	1051.03	0.09963	YES	YES
124	a	1074.51	0.12086	YES	YES

125	a	1074.94	0.12371	YES	YES
126	a	1077.26	0.04565	YES	YES
127	a	1163.76	0.01124	YES	YES
128	a	1164.22	0.01713	YES	YES
129	a	1164.32	0.00328	YES	YES
130	a	1165.34	0.02319	YES	YES
131	a	1165.59	0.17181	YES	YES
132	a	1165.94	0.15725	YES	YES
133	a	1338.89	0.28156	YES	YES
134	a	1340.06	0.12985	YES	YES
135	a	1340.55	0.64543	YES	YES
136	a	1341.22	0.26633	YES	YES
137	a	1341.52	0.79799	YES	YES
138	a	1342.66	1.39255	YES	YES
139	a	1345.39	2.32263	YES	YES
140	a	1346.12	2.10208	YES	YES
141	a	1347.49	4.79623	YES	YES
142	a	1348.73	11.09100	YES	YES
143	a	1349.40	1.57250	YES	YES
144	a	1351.35	13.30355	YES	YES
145	a	1352.74	2.40651	YES	YES
146	a	1353.33	1.01765	YES	YES
147	a	1355.45	0.07755	YES	YES
148	a	1384.02	1.66294	YES	YES
149	a	1384.27	1.08256	YES	YES
150	a	1384.46	0.93540	YES	YES
151	a	1388.41	0.38246	YES	YES
152	a	1388.73	0.15804	YES	YES
153	a	1389.21	0.52809	YES	YES
154	a	1394.36	18.51464	YES	YES
155	a	1395.64	4.08743	YES	YES
156	a	1396.10	3.69335	YES	YES
157	a	1397.32	0.28654	YES	YES
158	a	1397.88	1.30752	YES	YES
159	a	1398.10	1.79474	YES	YES
160	a	1398.88	3.28683	YES	YES
161	a	1400.84	13.37064	YES	YES
162	a	1401.09	10.68011	YES	YES
163	a	1402.16	4.41823	YES	YES
164	a	1402.91	1.83180	YES	YES
165	a	1403.37	1.85933	YES	YES
166	a	1405.56	4.97556	YES	YES
167	a	1406.09	3.08118	YES	YES
168	a	1406.83	2.28346	YES	YES
169	a	1407.49	2.53716	YES	YES
170	a	1409.65	17.80986	YES	YES
171	a	1410.02	31.17688	YES	YES
172	a	1411.31	42.69557	YES	YES
173	a	1411.79	66.63948	YES	YES
174	a	1412.74	2.38510	YES	YES
175	a	1414.42	73.70869	YES	YES
176	a	1414.62	56.15901	YES	YES
177	a	1416.81	23.14322	YES	YES
178	a	1435.14	0.59929	YES	YES
179	a	1435.67	0.63637	YES	YES
180	a	1436.46	0.28754	YES	YES
181	a	1444.37	0.02297	YES	YES
182	a	1446.14	0.14440	YES	YES
183	a	1446.61	0.13163	YES	YES
184	a	1449.82	0.03206	YES	YES
185	a	1450.02	0.03916	YES	YES
186	a	1450.79	0.17101	YES	YES
187	a	1479.69	18.06371	YES	YES
188	a	1479.91	13.42923	YES	YES
189	a	1480.09	4.04798	YES	YES
190	a	1486.99	3.02725	YES	YES
191	a	1487.31	19.85745	YES	YES
192	a	1487.43	19.76636	YES	YES
193	a	2965.64	32.73820	YES	YES
194	a	2965.87	29.49706	YES	YES
195	a	2966.17	7.41347	YES	YES
196	a	2966.26	38.98387	YES	YES
197	a	2966.41	5.29680	YES	YES
198	a	2966.65	16.16597	YES	YES
199	a	2966.76	12.53130	YES	YES
200	a	2966.82	9.56284	YES	YES
201	a	2966.95	7.99047	YES	YES
202	a	2967.54	25.48082	YES	YES

203	a	2967.56	18.08403	YES	YES
204	a	2967.83	26.51411	YES	YES
205	a	2967.86	5.59371	YES	YES
206	a	2968.00	8.28532	YES	YES
207	a	2968.16	11.34067	YES	YES
208	a	3038.92	3.20149	YES	YES
209	a	3039.30	3.11758	YES	YES
210	a	3039.36	2.43674	YES	YES
211	a	3039.48	2.46972	YES	YES
212	a	3039.65	8.64664	YES	YES
213	a	3039.83	10.30085	YES	YES
214	a	3041.05	1.79176	YES	YES
215	a	3041.15	5.52179	YES	YES
216	a	3041.77	5.97306	YES	YES
217	a	3042.12	2.92045	YES	YES
218	a	3042.24	1.90250	YES	YES
219	a	3042.37	2.99738	YES	YES
220	a	3043.67	0.17209	YES	YES
221	a	3043.75	0.19972	YES	YES
222	a	3043.83	0.18223	YES	YES
223	a	3068.57	6.39954	YES	YES
224	a	3068.76	2.79659	YES	YES
225	a	3068.99	7.14348	YES	YES
226	a	3069.03	1.66714	YES	YES
227	a	3069.35	5.44832	YES	YES
228	a	3069.46	2.39735	YES	YES
229	a	3070.87	5.74635	YES	YES
230	a	3071.16	5.69489	YES	YES
231	a	3071.45	5.08322	YES	YES
232	a	3072.18	8.29691	YES	YES
233	a	3072.31	10.99669	YES	YES
234	a	3072.97	9.86484	YES	YES
235	a	3082.59	3.76844	YES	YES
236	a	3083.38	3.79974	YES	YES
237	a	3083.72	4.40870	YES	YES

$end

$[Ga_2(AlCp^*)_6]^{2+}$



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

Symmetry: c1

Cartesian coordinates in Ångström:

Al	3.1053937	0.1926431	-1.7077904
Al	2.8952540	-1.7242699	0.5157352
Al	3.3701596	1.1252726	1.0508621
Al	-3.3700947	-1.1271012	-1.0659406
Al	-3.1128171	-0.2047672	1.6980144
Al	-2.8985855	1.7208224	-0.5188383
C	-3.5667398	-2.1403447	-3.0586996
C	-3.1493136	1.0134367	3.5690910
C	-3.1665206	-3.1191432	-2.0809619
C	-4.4908295	0.6154502	3.2256134
C	-4.8467219	-1.6114469	-2.6595418
Ga	1.3004448	0.1665591	0.0297373
C	-3.2399570	-1.3164474	3.6490147
C	-4.1940328	-3.2009792	-1.0754278
C	-4.1809673	-4.1090986	0.1187764
C	-5.2354154	-2.2651280	-1.4269894
C	-2.6156297	2.4124374	3.6509693
C	-5.6527735	1.5223622	2.9485424
C	-5.6976325	-0.6559378	-3.4406443
C	-5.7822333	-1.6657359	3.1149742
C	-2.3804934	-0.1761847	3.8313743
C	-0.9245836	-0.1831260	4.2009819
C	-6.5370861	-2.0645770	-0.7088778
C	-2.7912438	-1.7678355	-4.2879463
C	-2.8885887	-2.7590041	3.8677989
C	-4.5459588	-0.8308166	3.2690661
C	-1.8985930	-3.9179866	-2.1159187
C	2.3527099	-3.9078342	0.3735169
C	1.7494504	-3.3523222	1.5554452
C	2.7994631	-2.8891607	2.4252571
C	4.0598653	-3.1375968	1.7719064
C	3.7817238	-3.7667181	0.4943904
C	4.8208992	-4.3203255	-0.4350804
C	5.4321034	-2.9251351	2.3395420
C	2.5883237	-2.2398129	3.7614855
C	0.2778708	-3.2674180	1.8339832
C	1.6055021	-4.5410082	-0.7616082
C	3.1394267	-1.0223612	-3.5807958
C	4.4815630	-0.6258240	-3.2379342
C	4.5375802	0.8204614	-3.2790138
C	3.2316636	1.3075856	-3.6571366
C	2.3712016	0.1682377	-3.8404884
C	0.9149322	0.1767985	-4.2086124
C	2.8811013	2.7509378	-3.8722768
C	5.7743013	1.6544831	-3.1233839
C	5.6432855	-1.5339029	-2.9637911
C	2.6049715	-2.4209011	-3.6652902
C	3.5650607	2.1364373	3.0449358
C	3.1649686	3.1161459	2.0680950
C	4.1930216	3.1996562	1.0632671
C	5.2346470	2.2638277	1.4144190
C	4.8454737	1.6086063	2.6460144
C	5.6959875	0.6518508	3.4260052
C	6.5373001	2.0653871	0.6974650
C	4.1809963	4.1099106	-0.1293333
C	1.8964092	3.9139430	2.1034198
C	2.7882193	1.7616120	4.2725873
C	-2.3569114	3.9045506	-0.3785474
C	-1.7538614	3.3483735	-1.5602922
C	-2.8040454	2.8842529	-2.4294087
C	-4.0642902	3.1326785	-1.7758178

C	-3.7859596	3.7628193	-0.4988591
C	-4.8249939	4.3175388	0.4300964
C	-5.4366476	2.9188979	-2.3426694
C	-2.5930300	2.2335364	-3.7650174
C	-0.2823478	3.2634393	-1.8393787
C	-1.6097286	4.5396053	0.7555675
H	-3.1621594	-4.2206901	0.5409424
H	-4.5396137	-5.1246405	-0.1491851
H	-4.8405302	-3.7317577	0.9231223
H	-1.6254807	2.5038862	3.1601153
H	-2.4926739	2.7300236	4.7075193
H	-3.2985131	3.1364729	3.1687663
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H	-6.2462414	1.6917459	3.8712875
H	-6.3400033	1.0962078	2.1915690
H	-5.0892185	0.0032695	-4.0887833
H	-6.3170379	-0.0172157	-2.7829460
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H	-5.5508863	-2.6849877	2.7501854
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H	-6.2935738	-1.7823089	4.0938828
H	-0.2851618	0.2070944	3.3787644
H	-0.5727599	-1.2028644	4.4433973
H	-0.7392234	0.4498819	5.0923666
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H	-3.3330393	-3.1312805	4.8142051
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H	-1.0557781	-3.3284465	-2.5289921
H	5.7272628	-3.6862233	-0.4727382
H	4.4378351	-4.4333241	-1.4672006
H	5.1433362	-5.3277253	-0.0969309
H	6.1415643	-2.5315666	1.5849574
H	5.8498627	-3.8852247	2.7085650
H	5.4204755	-2.2228551	3.1919841
H	3.5327049	-1.8340454	4.1694879
H	2.1964105	-2.9680612	4.5010313
H	1.8610981	-1.4040913	3.7012578
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H	0.0234271	-2.3526575	2.4031532
H	-0.0671968	-4.1398380	2.4283873
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H	3.2528612	3.3967135	-3.0520694
H	1.7885545	2.9007285	-3.9457342
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H	1.6147709	-2.5127578	-3.1746768
H	6.3145016	0.0130315	2.7675624
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H	6.3917638	1.2068637	4.0898502
H	6.4663797	2.3527975	-0.3677576
H	6.8803554	1.0132027	0.7433995
H	7.3339835	2.6894168	1.1540789
H	4.8392259	3.7327695	-0.9348870
H	4.5419535	5.1242138	0.1402581
H	3.1621320	4.2245007	-0.5505149
H	1.6088800	4.2674178	1.0949320
H	2.0085300	4.8124774	2.7459155
H	1.0532120	3.3221219	2.5124811

H	3.0742533	0.7626275	4.6518598
H	1.6970251	1.7493182	4.0794388
H	2.9678156	2.4889274	5.0919124
H	-4.4426083	4.4297966	1.4625636
H	-5.7322789	3.6847063	0.4668044
H	-5.1457755	5.3254800	0.0919664
H	-5.4247623	2.2164216	-3.1949544
H	-5.8555093	3.8785094	-2.7116810
H	-6.1453455	2.5247848	-1.5876291
H	-1.8676243	1.3962730	-3.7034989
H	-2.1988637	2.9604370	-4.5046949
H	-3.5379050	1.8294519	-4.1735693
H	-0.0278245	2.3475304	-2.4067277
H	0.3122105	3.2439718	-0.9050458
H	0.0621165	4.1346935	-2.4358472
H	-0.7781581	3.8988661	1.1097312
H	-2.2681385	4.7454702	1.6188295
H	-1.1675857	5.5075732	0.4405690
Ga	-1.3039303	-0.1709901	-0.0354580

SCF energy GEOOPT = -7643.312863159 H

ZPE = 3413. kJ/mol

FREEH energy = 3668.03 kJ/mol

FREEH entropy = 2.13217 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		-0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	6.05	0.01304	YES YES
8	a	13.57	0.00013	YES YES
9	a	15.34	0.04671	YES YES
10	a	16.67	0.00021	YES YES
11	a	20.77	0.13966	YES YES
12	a	22.13	0.03976	YES YES
13	a	23.27	0.00836	YES YES
14	a	26.48	0.06838	YES YES
15	a	28.55	0.04779	YES YES
16	a	29.88	0.08825	YES YES
17	a	30.34	0.00970	YES YES
18	a	35.36	0.00557	YES YES
19	a	35.96	0.81001	YES YES
20	a	39.64	0.01913	YES YES
21	a	41.77	0.00004	YES YES
22	a	44.08	0.00004	YES YES
23	a	45.48	0.05819	YES YES
24	a	45.73	0.00359	YES YES
25	a	55.06	0.07657	YES YES
26	a	55.17	0.00217	YES YES
27	a	56.47	0.28492	YES YES
28	a	57.93	3.26021	YES YES
29	a	62.20	0.00094	YES YES
30	a	68.12	1.90464	YES YES
31	a	68.88	0.00215	YES YES
32	a	69.37	0.03903	YES YES
33	a	71.06	11.64932	YES YES
34	a	73.71	0.01275	YES YES
35	a	78.15	0.01936	YES YES
36	a	79.50	2.92883	YES YES
37	a	88.45	1.49394	YES YES
38	a	88.97	1.34552	YES YES
39	a	91.33	2.25674	YES YES
40	a	92.52	0.00134	YES YES
41	a	94.48	0.01109	YES YES
42	a	95.42	0.38208	YES YES
43	a	98.89	0.34153	YES YES
44	a	99.76	0.03647	YES YES
45	a	102.38	0.12135	YES YES
46	a	102.64	1.35348	YES YES
47	a	103.93	0.46879	YES YES
48	a	104.17	0.74343	YES YES
49	a	108.09	1.27694	YES YES
50	a	108.51	0.48857	YES YES

51	a	109.92	1.22735	YES	YES
52	a	111.54	0.05456	YES	YES
53	a	111.79	0.37384	YES	YES
54	a	114.16	0.00910	YES	YES
55	a	120.73	0.07861	YES	YES
56	a	121.45	5.77454	YES	YES
57	a	122.53	0.02613	YES	YES
58	a	124.26	0.85373	YES	YES
59	a	127.89	0.00332	YES	YES
60	a	128.87	1.62316	YES	YES
61	a	131.28	0.00089	YES	YES
62	a	135.03	0.90831	YES	YES
63	a	135.77	0.33481	YES	YES
64	a	136.48	0.00133	YES	YES
65	a	137.39	1.18148	YES	YES
66	a	141.83	0.02396	YES	YES
67	a	142.98	0.43077	YES	YES
68	a	144.95	0.02847	YES	YES
69	a	148.73	2.20462	YES	YES
70	a	150.12	0.07164	YES	YES
71	a	152.46	0.00249	YES	YES
72	a	152.98	5.59160	YES	YES
73	a	153.93	0.04667	YES	YES
74	a	155.15	0.42656	YES	YES
75	a	156.25	0.01653	YES	YES
76	a	158.45	0.00135	YES	YES
77	a	160.11	0.07250	YES	YES
78	a	167.83	1.85418	YES	YES
79	a	168.03	0.35942	YES	YES
80	a	171.57	0.04860	YES	YES
81	a	171.69	0.07928	YES	YES
82	a	173.91	0.00048	YES	YES
83	a	175.36	0.64794	YES	YES
84	a	181.52	0.00012	YES	YES
85	a	189.11	1.99294	YES	YES
86	a	189.88	0.01363	YES	YES
87	a	190.67	2.44507	YES	YES
88	a	190.88	0.10057	YES	YES
89	a	193.40	5.38766	YES	YES
90	a	194.18	0.01749	YES	YES
91	a	209.07	65.30863	YES	YES
92	a	216.22	0.00037	YES	YES
93	a	224.74	0.00048	YES	YES
94	a	227.40	3.86910	YES	YES
95	a	228.42	2.28995	YES	YES
96	a	230.57	0.00026	YES	YES
97	a	246.35	0.02699	YES	YES
98	a	247.30	94.83544	YES	YES
99	a	251.14	0.00052	YES	YES
100	a	252.69	15.55453	YES	YES
101	a	254.27	7.71421	YES	YES
102	a	262.65	0.00039	YES	YES
103	a	265.19	2.00149	YES	YES
104	a	266.90	0.05345	YES	YES
105	a	267.29	1.71283	YES	YES
106	a	268.31	0.00601	YES	YES
107	a	268.90	0.24871	YES	YES
108	a	269.16	0.04336	YES	YES
109	a	274.87	0.37348	YES	YES
110	a	275.38	0.00357	YES	YES
111	a	276.73	0.06621	YES	YES
112	a	276.93	1.50815	YES	YES
113	a	277.29	2.88855	YES	YES
114	a	277.86	0.02372	YES	YES
115	a	282.01	3.32949	YES	YES
116	a	282.45	0.06472	YES	YES
117	a	283.81	0.00061	YES	YES
118	a	284.39	2.41387	YES	YES
119	a	286.04	8.48496	YES	YES
120	a	286.58	0.06420	YES	YES
121	a	288.65	0.00124	YES	YES
122	a	289.24	1.57789	YES	YES
123	a	290.28	1.78430	YES	YES
124	a	290.84	0.00007	YES	YES
125	a	292.20	0.01565	YES	YES
126	a	292.41	1.99741	YES	YES
127	a	375.04	0.09996	YES	YES
128	a	375.84	13.03411	YES	YES

129	a	378.51	14.32914	YES	YES
130	a	378.74	0.46333	YES	YES
131	a	381.56	15.31683	YES	YES
132	a	381.67	0.59232	YES	YES
133	a	389.87	9.63115	YES	YES
134	a	390.22	0.06225	YES	YES
135	a	392.87	0.10798	YES	YES
136	a	393.09	7.03859	YES	YES
137	a	397.76	0.00110	YES	YES
138	a	398.24	2.33422	YES	YES
139	a	467.23	0.00309	YES	YES
140	a	471.12	515.77303	YES	YES
141	a	473.25	0.00658	YES	YES
142	a	477.11	571.61814	YES	YES
143	a	505.75	570.85434	YES	YES
144	a	530.37	0.00292	YES	YES
145	a	543.00	0.00015	YES	YES
146	a	543.22	0.26865	YES	YES
147	a	543.85	0.00188	YES	YES
148	a	543.95	0.05081	YES	YES
149	a	544.48	0.51912	YES	YES
150	a	544.66	0.00033	YES	YES
151	a	545.11	0.00002	YES	YES
152	a	545.26	0.08502	YES	YES
153	a	545.46	0.10257	YES	YES
154	a	545.87	0.00010	YES	YES
155	a	546.97	0.11922	YES	YES
156	a	547.03	0.01909	YES	YES
157	a	547.44	0.08148	YES	YES
158	a	547.53	0.00368	YES	YES
159	a	547.78	0.22829	YES	YES
160	a	547.80	0.00308	YES	YES
161	a	549.13	0.00072	YES	YES
162	a	549.31	0.13434	YES	YES
163	a	587.48	8.45080	YES	YES
164	a	587.50	0.07342	YES	YES
165	a	587.73	0.03524	YES	YES
166	a	587.94	3.77974	YES	YES
167	a	589.21	0.00187	YES	YES
168	a	589.75	16.65485	YES	YES
169	a	590.61	9.86983	YES	YES
170	a	590.82	0.00172	YES	YES
171	a	591.92	0.13326	YES	YES
172	a	592.06	1.97261	YES	YES
173	a	592.13	8.07731	YES	YES
174	a	593.45	0.00063	YES	YES
175	a	602.78	0.97487	YES	YES
176	a	603.17	0.00007	YES	YES
177	a	603.30	0.03102	YES	YES
178	a	603.38	0.00812	YES	YES
179	a	604.75	0.43190	YES	YES
180	a	604.85	0.01030	YES	YES
181	a	795.73	3.28588	YES	YES
182	a	795.79	2.02308	YES	YES
183	a	796.83	0.90849	YES	YES
184	a	796.85	2.43869	YES	YES
185	a	798.78	4.21375	YES	YES
186	a	798.89	0.12347	YES	YES
187	a	802.80	7.22522	YES	YES
188	a	802.91	0.13419	YES	YES
189	a	803.35	4.48765	YES	YES
190	a	803.61	0.00603	YES	YES
191	a	803.74	0.00717	YES	YES
192	a	804.08	25.06184	YES	YES
193	a	921.74	0.03129	YES	YES
194	a	921.77	2.29412	YES	YES
195	a	923.54	1.56547	YES	YES
196	a	923.59	0.66860	YES	YES
197	a	924.70	0.67537	YES	YES
198	a	924.85	0.05358	YES	YES
199	a	927.21	0.46840	YES	YES
200	a	927.28	0.21729	YES	YES
201	a	927.56	1.00276	YES	YES
202	a	927.76	0.02579	YES	YES
203	a	929.17	0.00034	YES	YES
204	a	929.45	5.91556	YES	YES
205	a	987.83	0.12076	YES	YES
206	a	987.98	5.55746	YES	YES

207	a	989.15	7.28454	YES	YES
208	a	989.22	2.53329	YES	YES
209	a	989.34	7.15180	YES	YES
210	a	989.55	0.07467	YES	YES
211	a	991.47	6.41299	YES	YES
212	a	991.51	1.10067	YES	YES
213	a	992.95	0.00146	YES	YES
214	a	993.16	7.22793	YES	YES
215	a	994.51	2.60443	YES	YES
216	a	994.57	0.02395	YES	YES
217	a	994.84	0.48439	YES	YES
218	a	994.99	0.00623	YES	YES
219	a	995.74	0.00486	YES	YES
220	a	995.92	1.74767	YES	YES
221	a	996.60	2.15684	YES	YES
222	a	996.89	0.00499	YES	YES
223	a	997.42	0.00188	YES	YES
224	a	997.89	2.05254	YES	YES
225	a	998.37	0.79634	YES	YES
226	a	999.07	0.01874	YES	YES
227	a	999.15	0.19241	YES	YES
228	a	999.30	0.00458	YES	YES
229	a	999.90	0.00011	YES	YES
230	a	1000.52	0.38143	YES	YES
231	a	1007.20	0.07210	YES	YES
232	a	1007.32	0.00427	YES	YES
233	a	1010.70	0.00852	YES	YES
234	a	1010.73	0.06538	YES	YES
235	a	1047.94	3.10106	YES	YES
236	a	1048.07	0.02617	YES	YES
237	a	1048.84	0.00378	YES	YES
238	a	1049.09	1.84253	YES	YES
239	a	1049.21	3.95031	YES	YES
240	a	1049.36	0.07646	YES	YES
241	a	1049.88	2.23062	YES	YES
242	a	1050.00	0.01816	YES	YES
243	a	1051.08	0.37626	YES	YES
244	a	1051.11	0.98241	YES	YES
245	a	1051.87	0.16518	YES	YES
246	a	1051.94	1.51561	YES	YES
247	a	1073.57	0.25266	YES	YES
248	a	1073.62	0.09683	YES	YES
249	a	1074.04	0.00396	YES	YES
250	a	1074.28	0.53618	YES	YES
251	a	1076.85	0.11804	YES	YES
252	a	1077.00	0.00227	YES	YES
253	a	1162.47	6.25216	YES	YES
254	a	1162.63	0.20935	YES	YES
255	a	1163.43	1.89709	YES	YES
256	a	1163.88	0.00091	YES	YES
257	a	1164.46	1.77284	YES	YES
258	a	1164.58	0.02760	YES	YES
259	a	1164.59	3.89781	YES	YES
260	a	1164.73	0.00584	YES	YES
261	a	1165.06	0.00023	YES	YES
262	a	1165.53	0.13519	YES	YES
263	a	1165.81	0.00024	YES	YES
264	a	1165.99	0.41948	YES	YES
265	a	1337.92	4.84635	YES	YES
266	a	1338.26	0.00100	YES	YES
267	a	1339.08	3.01367	YES	YES
268	a	1339.28	0.00590	YES	YES
269	a	1339.85	0.02010	YES	YES
270	a	1340.01	0.28562	YES	YES
271	a	1340.44	0.00056	YES	YES
272	a	1340.70	11.06091	YES	YES
273	a	1341.70	0.00614	YES	YES
274	a	1342.11	1.31328	YES	YES
275	a	1342.43	0.54414	YES	YES
276	a	1342.65	0.00062	YES	YES
277	a	1344.04	3.86586	YES	YES
278	a	1344.13	2.14606	YES	YES
279	a	1344.70	5.18624	YES	YES
280	a	1345.04	0.00893	YES	YES
281	a	1345.59	0.00198	YES	YES
282	a	1346.39	10.12013	YES	YES
283	a	1347.30	12.93170	YES	YES
284	a	1347.56	0.01540	YES	YES

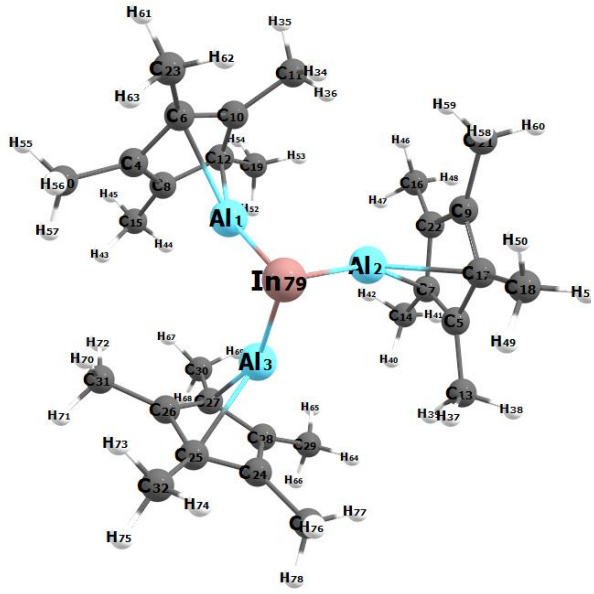
285	a	1348.84	10.38205	YES	YES
286	a	1349.11	0.27371	YES	YES
287	a	1349.79	11.47517	YES	YES
288	a	1350.05	0.00471	YES	YES
289	a	1352.72	0.00244	YES	YES
290	a	1352.85	3.15522	YES	YES
291	a	1352.90	0.04611	YES	YES
292	a	1353.34	0.51794	YES	YES
293	a	1355.13	0.10384	YES	YES
294	a	1355.22	0.00010	YES	YES
295	a	1381.67	0.00025	YES	YES
296	a	1382.46	14.22651	YES	YES
297	a	1383.26	5.60771	YES	YES
298	a	1383.85	0.04307	YES	YES
299	a	1383.99	0.08730	YES	YES
300	a	1384.05	0.91824	YES	YES
301	a	1386.87	0.00054	YES	YES
302	a	1387.43	0.58079	YES	YES
303	a	1388.23	11.25626	YES	YES
304	a	1388.75	0.00107	YES	YES
305	a	1389.72	0.00168	YES	YES
306	a	1390.34	2.21170	YES	YES
307	a	1392.62	6.57741	YES	YES
308	a	1393.33	0.01746	YES	YES
309	a	1394.80	11.06824	YES	YES
310	a	1395.05	0.00231	YES	YES
311	a	1396.24	2.28155	YES	YES
312	a	1396.31	0.03270	YES	YES
313	a	1396.43	2.76169	YES	YES
314	a	1396.62	0.00757	YES	YES
315	a	1397.01	4.09201	YES	YES
316	a	1397.52	0.00252	YES	YES
317	a	1398.05	23.53249	YES	YES
318	a	1398.72	7.41197	YES	YES
319	a	1398.81	0.34205	YES	YES
320	a	1399.62	0.01957	YES	YES
321	a	1399.88	0.00543	YES	YES
322	a	1400.62	45.13941	YES	YES
323	a	1401.07	0.16186	YES	YES
324	a	1401.23	2.56283	YES	YES
325	a	1402.47	0.40484	YES	YES
326	a	1402.59	2.27103	YES	YES
327	a	1403.15	0.02660	YES	YES
328	a	1403.39	3.02163	YES	YES
329	a	1404.32	1.93374	YES	YES
330	a	1404.38	24.47539	YES	YES
331	a	1404.68	6.23932	YES	YES
332	a	1405.42	0.01596	YES	YES
333	a	1405.96	0.00345	YES	YES
334	a	1406.26	3.73859	YES	YES
335	a	1406.30	5.86124	YES	YES
336	a	1406.65	0.04358	YES	YES
337	a	1407.10	36.62293	YES	YES
338	a	1408.03	21.38746	YES	YES
339	a	1409.02	9.00622	YES	YES
340	a	1409.12	0.05159	YES	YES
341	a	1410.54	12.76048	YES	YES
342	a	1410.77	0.00249	YES	YES
343	a	1411.35	156.59894	YES	YES
344	a	1411.48	2.13029	YES	YES
345	a	1412.56	0.08848	YES	YES
346	a	1413.14	43.42048	YES	YES
347	a	1413.96	123.54805	YES	YES
348	a	1414.09	0.04848	YES	YES
349	a	1414.71	48.93296	YES	YES
350	a	1415.61	0.00279	YES	YES
351	a	1416.21	149.67020	YES	YES
352	a	1416.50	0.01441	YES	YES
353	a	1417.13	40.83876	YES	YES
354	a	1417.34	0.00205	YES	YES
355	a	1430.33	0.06022	YES	YES
356	a	1430.40	3.15535	YES	YES
357	a	1431.11	11.70664	YES	YES
358	a	1431.23	0.00044	YES	YES
359	a	1435.96	12.41903	YES	YES
360	a	1436.15	0.18533	YES	YES
361	a	1442.36	6.86151	YES	YES
362	a	1442.73	0.07607	YES	YES

363	a	1444.93	0.09267	YES	YES
364	a	1445.00	1.83640	YES	YES
365	a	1446.94	0.02612	YES	YES
366	a	1447.10	1.21406	YES	YES
367	a	1447.91	0.18062	YES	YES
368	a	1448.07	0.00891	YES	YES
369	a	1449.71	0.02047	YES	YES
370	a	1449.83	4.60348	YES	YES
371	a	1450.57	0.00228	YES	YES
372	a	1450.87	0.70929	YES	YES
373	a	1475.48	0.12111	YES	YES
374	a	1475.66	33.91641	YES	YES
375	a	1478.83	0.25983	YES	YES
376	a	1479.05	34.97751	YES	YES
377	a	1479.60	7.11952	YES	YES
378	a	1479.67	26.32872	YES	YES
379	a	1486.23	11.57036	YES	YES
380	a	1486.32	8.30144	YES	YES
381	a	1489.52	24.76369	YES	YES
382	a	1489.83	0.01462	YES	YES
383	a	1490.19	0.03415	YES	YES
384	a	1490.69	30.05075	YES	YES
385	a	2944.56	0.15090	YES	YES
386	a	2944.64	26.24521	YES	YES
387	a	2959.82	0.92373	YES	YES
388	a	2959.94	17.97982	YES	YES
389	a	2962.64	12.50789	YES	YES
390	a	2962.69	15.20937	YES	YES
391	a	2962.75	7.95272	YES	YES
392	a	2962.88	10.59210	YES	YES
393	a	2963.82	10.53976	YES	YES
394	a	2964.02	11.87738	YES	YES
395	a	2966.13	9.70297	YES	YES
396	a	2966.14	32.94705	YES	YES
397	a	2966.82	9.01082	YES	YES
398	a	2966.84	7.14448	YES	YES
399	a	2967.70	18.39538	YES	YES
400	a	2967.79	14.39845	YES	YES
401	a	2968.36	21.17131	YES	YES
402	a	2968.41	11.54233	YES	YES
403	a	2969.72	20.25782	YES	YES
404	a	2969.78	11.57564	YES	YES
405	a	2970.31	26.50241	YES	YES
406	a	2970.33	3.50257	YES	YES
407	a	2970.68	6.45029	YES	YES
408	a	2970.68	18.10245	YES	YES
409	a	2971.28	2.37401	YES	YES
410	a	2971.31	5.73642	YES	YES
411	a	2971.36	43.65648	YES	YES
412	a	2971.41	9.58764	YES	YES
413	a	2971.67	12.63826	YES	YES
414	a	2971.79	10.56394	YES	YES
415	a	3024.46	7.84231	YES	YES
416	a	3024.51	3.68626	YES	YES
417	a	3034.95	2.54267	YES	YES
418	a	3035.09	2.58509	YES	YES
419	a	3036.28	9.19311	YES	YES
420	a	3036.38	8.00040	YES	YES
421	a	3036.55	6.75741	YES	YES
422	a	3036.72	8.75772	YES	YES
423	a	3038.52	1.22407	YES	YES
424	a	3038.55	4.48789	YES	YES
425	a	3040.10	0.25458	YES	YES
426	a	3040.16	0.38400	YES	YES
427	a	3040.86	3.43488	YES	YES
428	a	3040.87	0.86267	YES	YES
429	a	3041.99	6.97939	YES	YES
430	a	3042.05	7.76470	YES	YES
431	a	3042.37	5.16575	YES	YES
432	a	3042.45	6.05321	YES	YES
433	a	3043.95	2.08151	YES	YES
434	a	3044.00	2.01475	YES	YES
435	a	3044.04	0.15053	YES	YES
436	a	3044.06	2.29191	YES	YES
437	a	3044.07	1.71322	YES	YES
438	a	3044.17	2.40739	YES	YES
439	a	3044.17	4.11836	YES	YES
440	a	3044.29	0.70645	YES	YES

441	a	3045.67	1.74482	YES	YES
442	a	3045.75	1.85190	YES	YES
443	a	3045.89	1.28995	YES	YES
444	a	3045.90	1.03067	YES	YES
445	a	3064.04	2.21220	YES	YES
446	a	3064.22	2.11144	YES	YES
447	a	3065.27	1.66818	YES	YES
448	a	3065.28	7.62631	YES	YES
449	a	3066.39	3.76457	YES	YES
450	a	3066.49	3.79248	YES	YES
451	a	3070.19	5.08565	YES	YES
452	a	3070.27	5.45173	YES	YES
453	a	3070.88	3.21710	YES	YES
454	a	3070.99	4.71286	YES	YES
455	a	3071.97	3.90577	YES	YES
456	a	3072.18	3.79471	YES	YES
457	a	3072.99	4.64579	YES	YES
458	a	3073.03	4.05346	YES	YES
459	a	3073.18	1.96835	YES	YES
460	a	3073.20	9.79117	YES	YES
461	a	3073.90	7.02594	YES	YES
462	a	3074.01	7.75334	YES	YES
463	a	3075.78	5.30851	YES	YES
464	a	3075.79	6.69567	YES	YES
465	a	3080.51	3.06555	YES	YES
466	a	3080.54	3.40420	YES	YES
467	a	3081.67	2.74238	YES	YES
468	a	3081.74	2.74610	YES	YES
469	a	3082.15	4.14199	YES	YES
470	a	3082.26	4.27156	YES	YES
471	a	3083.55	4.40139	YES	YES
472	a	3083.60	5.18346	YES	YES
473	a	3089.23	3.44183	YES	YES
474	a	3089.26	3.74605	YES	YES

$end

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



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

Symmetry: c1

Cartesian coordinates in Ångström:

Al	-1.7311013	-0.1818795	0.1561599
Al	1.0038363	-0.1625950	1.4172197
Al	0.7256723	-0.1705174	-1.5800995
C	-3.9313651	-0.2142805	-0.3565855
C	3.1718862	0.2349994	1.8587414
C	-3.7551135	-0.7975212	0.9484950
C	2.4045074	1.4343772	2.0811632
C	-3.4698552	1.1490523	-0.2996521
C	1.6567228	-0.1951006	3.5803145
C	-3.1946017	0.2041869	1.8175050
C	-2.8601681	0.0046775	3.2662220
C	-3.0067779	1.4083749	1.0484630
C	4.2630094	0.0433007	0.8472711
C	2.6024617	2.7635797	1.4128831
C	-3.5959550	2.1753547	-1.3858335
C	0.5831076	2.1881229	3.8060435
C	2.7034006	-0.7709859	2.7758141
C	3.2269401	-2.1731351	2.8774346
C	-2.5251195	2.7342475	1.5605981
C	-4.5146858	-0.9019360	-1.5557860
C	0.9118547	-0.8901420	4.6818719
C	1.4678236	1.1677561	3.1541142
C	-4.1022447	-2.2023461	1.3441178
C	2.2705294	-0.1844257	-3.2281993
C	1.0537605	-0.7657945	-3.7343083
C	0.0187607	0.2331537	-3.6751511
C	0.5878280	1.4334404	-3.1162587
C	1.9872144	1.1747140	-2.8447742
C	2.9875589	2.1992694	-2.3993660
C	-0.0990159	2.7566075	-2.9435495
C	-1.4019866	0.0348584	-4.1144310
C	0.8885748	-2.1662461	-4.2461593
C	3.6016062	-0.8709544	-3.1382456
H	-2.3509014	-0.9646130	3.4420426
H	-3.7771834	0.0127171	3.8913842
H	-2.1979053	0.8064932	3.6429873
H	4.1656861	-0.9243684	0.3143654
H	5.2613055	0.0528330	1.3320492
H	4.2577889	0.8478781	0.0883438
H	3.0875160	2.6553467	0.4255682
H	3.2522695	3.4202438	2.0290066
H	1.6451880	3.3006539	1.2617378
H	-3.5322323	1.7236777	-2.3944537
H	-2.8191501	2.9596711	-1.3082943
H	-4.5806086	2.6853165	-1.3223413
H	-0.3198767	1.7303935	4.2535503
H	0.2575330	2.9708288	3.0946636
H	1.1263208	2.7010404	4.6279006
H	3.5758176	-2.5531769	1.8973446
H	2.4574199	-2.8730448	3.2567076
H	4.0894906	-2.2230591	3.5751454
H	-1.9245485	3.2786346	0.8053846
H	-1.9029185	2.6193681	2.4668571
H	-3.3822845	3.3868856	1.8297653
H	-5.6233889	-0.8421177	-1.5457350
H	-4.2460675	-1.9762877	-1.5851071
H	-4.1694286	-0.4424452	-2.5015598
H	0.7488892	-1.9623988	4.4556170

H	-0.0781480	-0.4299147	4.8626728
H	1.4781947	-0.8394639	5.6355674
H	-5.1347613	-2.2546234	1.7495643
H	-3.4223021	-2.5879399	2.1289017
H	-4.0525066	-2.8965185	0.4830206
H	3.8320271	1.7433551	-1.8478786
H	2.5302216	2.9731473	-1.7538367
H	3.4207623	2.7228421	-3.2778600
H	-1.1952069	2.6393850	-2.8646985
H	0.0999492	3.4194448	-3.8119944
H	0.2497458	3.2915121	-2.0380330
H	-1.8082100	-0.9379434	-3.7702491
H	-1.4823348	0.0517880	-5.2212377
H	-2.0617351	0.8322971	-3.7243001
H	-0.1318819	-2.5543035	-4.0592284
H	1.6071093	-2.8639751	-3.7743601
H	1.0603057	-2.2086641	-5.3425060
H	3.4939257	-1.9467440	-2.8965091
H	4.2479336	-0.4149027	-2.3642370
H	4.1466230	-0.8055255	-4.1034261
In	0.0128025	-2.2939869	0.0028360

SCF energy GEOOPT = -2087.046213110 H

ZPE = 1703. kJ/mol

FREEH energy = 1829.32 kJ/mol

FREEH entropy = 1.18798 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	14.27	0.01254	YES	YES
8	a	17.10	0.03555	YES	YES
9	a	20.24	0.02470	YES	YES
10	a	23.66	0.00693	YES	YES
11	a	28.07	0.00995	YES	YES
12	a	31.44	0.00320	YES	YES
13	a	48.79	0.16678	YES	YES
14	a	51.20	0.03026	YES	YES
15	a	52.88	0.04594	YES	YES
16	a	60.89	0.20586	YES	YES
17	a	65.43	0.04084	YES	YES
18	a	73.75	0.15778	YES	YES
19	a	76.16	0.29597	YES	YES
20	a	82.56	0.42426	YES	YES
21	a	85.13	0.20887	YES	YES
22	a	87.64	0.21078	YES	YES
23	a	91.79	0.30924	YES	YES
24	a	92.73	0.18563	YES	YES
25	a	93.74	0.04671	YES	YES
26	a	95.78	0.03885	YES	YES
27	a	100.02	0.19035	YES	YES
28	a	102.19	0.16800	YES	YES
29	a	105.08	0.01373	YES	YES
30	a	107.20	0.12821	YES	YES
31	a	109.11	0.01575	YES	YES
32	a	109.97	0.13345	YES	YES
33	a	121.04	0.14431	YES	YES
34	a	142.16	0.07191	YES	YES
35	a	147.07	0.01050	YES	YES
36	a	150.60	0.13385	YES	YES
37	a	153.93	0.04207	YES	YES
38	a	158.86	0.06771	YES	YES
39	a	160.19	0.09515	YES	YES
40	a	163.04	0.10640	YES	YES
41	a	168.40	0.25421	YES	YES
42	a	172.32	0.26623	YES	YES
43	a	187.08	1.30028	YES	YES
44	a	188.05	1.23019	YES	YES
45	a	189.92	0.23975	YES	YES
46	a	208.63	1.09467	YES	YES
47	a	222.47	3.14514	YES	YES
48	a	222.70	2.82537	YES	YES

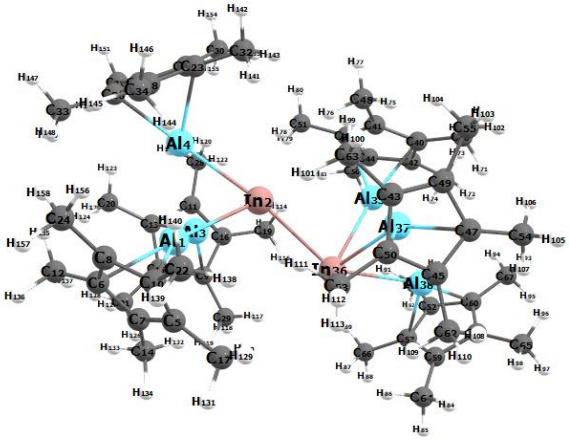
49	a	231.07	4.79689	YES	YES
50	a	237.21	4.33573	YES	YES
51	a	237.81	4.90433	YES	YES
52	a	271.63	0.05018	YES	YES
53	a	272.17	0.11358	YES	YES
54	a	272.93	0.14423	YES	YES
55	a	274.68	0.20613	YES	YES
56	a	276.00	0.06516	YES	YES
57	a	277.17	0.12897	YES	YES
58	a	280.47	0.14387	YES	YES
59	a	282.44	0.65344	YES	YES
60	a	282.92	0.70452	YES	YES
61	a	285.51	0.10613	YES	YES
62	a	287.10	0.82985	YES	YES
63	a	288.43	0.81637	YES	YES
64	a	378.21	0.15509	YES	YES
65	a	379.45	19.87863	YES	YES
66	a	379.95	19.79086	YES	YES
67	a	390.96	0.65387	YES	YES
68	a	392.65	2.78940	YES	YES
69	a	393.08	2.40814	YES	YES
70	a	455.33	337.18304	YES	YES
71	a	456.03	337.45631	YES	YES
72	a	503.34	35.52606	YES	YES
73	a	543.24	0.09353	YES	YES
74	a	543.83	0.02124	YES	YES
75	a	544.07	0.02243	YES	YES
76	a	544.35	0.10696	YES	YES
77	a	544.39	0.08723	YES	YES
78	a	544.95	0.08566	YES	YES
79	a	546.42	0.08244	YES	YES
80	a	546.73	0.07368	YES	YES
81	a	547.07	0.10162	YES	YES
82	a	586.85	3.85817	YES	YES
83	a	586.88	4.43669	YES	YES
84	a	587.00	0.95537	YES	YES
85	a	589.84	5.52924	YES	YES
86	a	590.05	5.01925	YES	YES
87	a	591.66	1.03984	YES	YES
88	a	600.81	0.16274	YES	YES
89	a	601.23	0.05772	YES	YES
90	a	601.34	0.06809	YES	YES
91	a	796.95	2.68190	YES	YES
92	a	798.04	2.73807	YES	YES
93	a	798.25	3.01071	YES	YES
94	a	801.81	3.42167	YES	YES
95	a	802.19	3.63257	YES	YES
96	a	803.08	2.56075	YES	YES
97	a	921.69	0.07406	YES	YES
98	a	923.12	0.68627	YES	YES
99	a	924.15	0.53952	YES	YES
100	a	925.50	0.17562	YES	YES
101	a	926.40	0.13998	YES	YES
102	a	927.21	0.28931	YES	YES
103	a	988.11	9.19845	YES	YES
104	a	988.25	5.88393	YES	YES
105	a	988.43	4.32896	YES	YES
106	a	992.52	6.17482	YES	YES
107	a	992.93	5.38575	YES	YES
108	a	993.06	5.95457	YES	YES
109	a	995.63	0.31132	YES	YES
110	a	995.79	0.40569	YES	YES
111	a	996.05	0.57251	YES	YES
112	a	998.28	0.20726	YES	YES
113	a	998.72	0.14834	YES	YES
114	a	999.21	0.30294	YES	YES
115	a	1000.64	0.38242	YES	YES
116	a	1001.10	0.20670	YES	YES
117	a	1001.43	0.79739	YES	YES
118	a	1048.18	3.98440	YES	YES
119	a	1048.43	2.98865	YES	YES
120	a	1048.75	3.15140	YES	YES
121	a	1050.24	0.26068	YES	YES
122	a	1050.61	0.10397	YES	YES
123	a	1050.97	0.03381	YES	YES
124	a	1074.34	0.13077	YES	YES
125	a	1074.63	0.10384	YES	YES
126	a	1077.18	0.02607	YES	YES

127	a	1163.83	0.01599	YES	YES
128	a	1163.93	0.02154	YES	YES
129	a	1164.20	0.00510	YES	YES
130	a	1165.36	0.13767	YES	YES
131	a	1165.81	0.36987	YES	YES
132	a	1165.87	0.38108	YES	YES
133	a	1338.79	0.08310	YES	YES
134	a	1340.12	0.14682	YES	YES
135	a	1340.71	1.08982	YES	YES
136	a	1341.09	0.22238	YES	YES
137	a	1341.49	0.24247	YES	YES
138	a	1342.05	2.53847	YES	YES
139	a	1345.34	2.52976	YES	YES
140	a	1345.67	3.80012	YES	YES
141	a	1346.55	6.79447	YES	YES
142	a	1348.48	5.08457	YES	YES
143	a	1349.16	5.52026	YES	YES
144	a	1349.79	15.49377	YES	YES
145	a	1351.77	2.24217	YES	YES
146	a	1352.07	0.51600	YES	YES
147	a	1353.96	1.94139	YES	YES
148	a	1383.88	1.92631	YES	YES
149	a	1384.33	2.22462	YES	YES
150	a	1384.73	0.57453	YES	YES
151	a	1388.81	0.51493	YES	YES
152	a	1389.04	0.63844	YES	YES
153	a	1389.65	0.03715	YES	YES
154	a	1394.63	17.76307	YES	YES
155	a	1395.43	3.07932	YES	YES
156	a	1395.88	2.77753	YES	YES
157	a	1397.29	1.87003	YES	YES
158	a	1397.76	1.79396	YES	YES
159	a	1398.31	3.03702	YES	YES
160	a	1399.11	0.96118	YES	YES
161	a	1401.28	9.99204	YES	YES
162	a	1401.67	10.07459	YES	YES
163	a	1402.72	4.80641	YES	YES
164	a	1402.99	0.71552	YES	YES
165	a	1403.54	1.28041	YES	YES
166	a	1405.89	3.29828	YES	YES
167	a	1406.09	3.18050	YES	YES
168	a	1407.32	10.66110	YES	YES
169	a	1407.85	1.02434	YES	YES
170	a	1409.30	15.50047	YES	YES
171	a	1409.67	34.72388	YES	YES
172	a	1411.08	17.57185	YES	YES
173	a	1411.30	22.80791	YES	YES
174	a	1412.36	8.07620	YES	YES
175	a	1413.54	107.50750	YES	YES
176	a	1414.43	87.78840	YES	YES
177	a	1415.50	26.66863	YES	YES
178	a	1435.21	0.53136	YES	YES
179	a	1436.07	0.45700	YES	YES
180	a	1436.23	0.45826	YES	YES
181	a	1444.72	0.02629	YES	YES
182	a	1446.73	0.06318	YES	YES
183	a	1446.95	0.06988	YES	YES
184	a	1450.13	0.24940	YES	YES
185	a	1450.27	0.19815	YES	YES
186	a	1451.04	0.33000	YES	YES
187	a	1480.20	26.71699	YES	YES
188	a	1480.35	3.67697	YES	YES
189	a	1480.61	7.79323	YES	YES
190	a	1488.27	5.12249	YES	YES
191	a	1488.62	18.13773	YES	YES
192	a	1488.82	19.63717	YES	YES
193	a	2964.39	24.45203	YES	YES
194	a	2964.92	32.07607	YES	YES
195	a	2964.98	15.54981	YES	YES
196	a	2965.55	45.18339	YES	YES
197	a	2965.64	7.78756	YES	YES
198	a	2965.68	14.47990	YES	YES
199	a	2965.84	6.53782	YES	YES
200	a	2965.89	3.85216	YES	YES
201	a	2966.06	7.58310	YES	YES
202	a	2966.76	24.05429	YES	YES
203	a	2967.05	26.56194	YES	YES
204	a	2967.12	18.17402	YES	YES

205	a	2967.35	6.39695	YES	YES
206	a	2967.66	4.93947	YES	YES
207	a	2967.79	21.39381	YES	YES
208	a	3037.18	4.54167	YES	YES
209	a	3037.32	4.54106	YES	YES
210	a	3037.44	4.52159	YES	YES
211	a	3039.50	4.80347	YES	YES
212	a	3039.67	8.36046	YES	YES
213	a	3039.71	10.40187	YES	YES
214	a	3040.48	2.65836	YES	YES
215	a	3040.58	2.39333	YES	YES
216	a	3040.95	2.46536	YES	YES
217	a	3041.00	1.83275	YES	YES
218	a	3041.08	2.40234	YES	YES
219	a	3041.21	2.42770	YES	YES
220	a	3042.19	0.20792	YES	YES
221	a	3042.31	0.36711	YES	YES
222	a	3042.37	0.55239	YES	YES
223	a	3067.23	4.54212	YES	YES
224	a	3067.73	3.68760	YES	YES
225	a	3067.76	5.17092	YES	YES
226	a	3068.97	3.56452	YES	YES
227	a	3069.72	6.00183	YES	YES
228	a	3070.16	4.22410	YES	YES
229	a	3070.30	4.31002	YES	YES
230	a	3070.38	8.82050	YES	YES
231	a	3070.50	1.47992	YES	YES
232	a	3072.69	7.75680	YES	YES
233	a	3072.88	6.83322	YES	YES
234	a	3073.12	13.24153	YES	YES
235	a	3081.64	3.42563	YES	YES
236	a	3081.75	3.25677	YES	YES
237	a	3082.15	3.40441	YES	YES

$end

$[In_2(AlCp^*)_6]^{2+}$



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

Symmetry: c1

Cartesian coordinates in Ångström:

Al	3.2826093	-1.7027056	0.5138570
In	1.1996287	-0.2102717	-0.5101412
Al	2.4379281	0.9496327	1.6547485
Al	3.6841980	0.8136567	-1.0839604
C	2.9039611	-3.6764672	1.5714409
C	4.9059020	-2.5027997	1.8052891
C	3.6493505	-2.8082731	2.4413718
C	4.9408299	-3.2106344	0.5436847
C	1.6239899	1.6995456	3.6317485
C	3.6970331	-3.9254515	0.3957737
C	2.5247922	3.1690209	2.0583183
C	6.0274135	-1.6834151	2.3744150
C	3.6179374	2.5059636	2.7187885
C	3.1752343	-2.3628006	3.7913394
C	3.0606345	1.6128642	3.7124019
C	1.2968469	2.6610895	2.6104849
C	1.5617641	-4.2537996	1.9117376
C	4.9675422	0.1407430	-2.8029191
C	-0.0831037	3.1057916	2.2253057
C	5.0805680	2.7699679	2.5113526
C	3.8561757	0.9229353	4.7787741
C	3.3394460	-4.8251363	-0.7510241
C	3.9059894	0.9571786	-3.3295659
C	6.1381753	-3.3438968	-0.3473922
C	4.0392481	2.2795019	-2.7795598
C	5.7501034	0.9506835	-1.9024363
C	5.1742092	2.2802561	-1.8918057
C	2.6417341	4.2018400	0.9750773
C	0.6386762	0.9647145	4.4936553
C	3.2011015	3.4716455	-3.1302463
C	5.7693470	3.4879420	-1.2309062
C	2.8683107	0.4925399	-4.3078213
C	7.0050860	0.5472759	-1.1853690
C	5.1940595	-1.2971841	-3.1658853
Al	-2.5092998	1.6359330	-0.6705378
In	-1.5853831	-0.2900734	1.0373222
Al	-2.4326330	-1.2631822	-1.4158203
Al	-4.3784814	-0.2459582	0.7411312
C	-1.4836299	3.3769027	-1.6955035
C	-3.3552756	2.3265191	-2.6033447
C	-1.9199713	2.4239183	-2.6818526
C	-3.8027273	3.2231877	-1.5631430
C	-1.3617753	-2.6136623	-2.8928697
C	-2.6460450	3.8746840	-1.0032873
C	-3.0417327	-3.4158838	-1.4876900
C	-4.2570443	1.4928889	-3.4630861
C	-3.6758662	-2.7087081	-2.5700536
C	-1.0080922	1.6744636	-3.6063544
C	-2.6329123	-2.2220091	-3.4503328
C	-1.6170992	-3.3500405	-1.6850724
C	-0.0618630	3.8096947	-1.5001379
C	-5.6242963	0.9494784	2.1945271
C	-0.5862318	-3.9422607	-0.7757858
C	-5.1532617	-2.5728795	-2.7944168
C	-2.8367894	-1.6467602	-4.8199951
C	-2.6734005	4.9323694	0.0604592
C	-4.9112805	-0.0607468	2.9301223
C	-5.2347932	3.5107803	-1.2300177
C	-5.3445992	-1.3531913	2.4639793
C	-6.4877508	0.2855063	1.2498949
C	-6.3117321	-1.1457412	1.4182965

C	-3.7328166	-4.0947544	-0.3439518
C	-0.0198197	-2.3651452	-3.5169815
C	-4.8721498	-2.6686484	3.0074285
C	-7.1371465	-2.1943652	0.7325953
C	-3.9226122	0.1949809	4.0285055
C	-7.5204738	0.9183543	0.3634149
C	-5.4821204	2.4270635	2.4150886
H	-3.6957938	0.6991381	-3.9860238
H	-4.7524542	2.1139965	-4.2382521
H	-5.0585856	1.0073642	-2.8702009
H	-5.8661360	2.6056985	-1.3134554
H	-5.6515174	4.2652280	-1.9302125
H	-5.3464022	3.9168994	-0.2078426
H	-1.5196782	0.8111304	-4.0702797
H	-0.1165234	1.2854471	-3.0707951
H	-0.6458685	2.3259096	-4.4294093
H	0.6285822	2.9474369	-1.3907225
H	0.0522170	4.4482306	-0.6063795
H	0.2866295	4.4029618	-2.3708161
H	-3.4350163	4.7200366	0.8364500
H	-2.9214027	5.9223294	-0.3765125
H	-1.6961793	5.0325491	0.5682629
H	-5.1835033	-3.5148823	2.3680337
H	-5.2911783	-2.8474500	4.0193750
H	-3.7667809	-2.7022101	3.1017686
H	-3.1874836	-0.6285857	4.1197104
H	-4.4371928	0.2844053	5.0087256
H	-3.3631960	1.1374311	3.8657607
H	-6.1000496	3.0070155	1.7058037
H	-4.4293014	2.7636505	2.3036814
H	-5.8065983	2.7041035	3.4387890
H	-7.5281253	0.4828623	-0.6554984
H	-7.3691614	2.0086261	0.2666162
H	-8.5349839	0.7649488	0.7876366
H	-7.3860842	-1.9145495	-0.3093772
H	-8.1005766	-2.3354769	1.2668281
H	-6.6328461	-3.1791424	0.7142454
H	0.0256884	-1.3814220	-4.0233902
H	0.2094241	-3.1390281	-4.2800327
H	0.7927230	-2.3934032	-2.7641369
H	-3.8304314	-1.1764907	-4.9371542
H	-2.7752150	-2.4578383	-5.5766758
H	-2.0634023	-0.9020981	-5.0905939
H	-5.5506257	-3.4438889	-3.3564410
H	-5.4001972	-1.6642386	-3.3761185
H	-5.7069808	-2.5209832	-1.8370717
H	-4.7676619	-3.7245537	-0.2230807
H	-3.2026244	-3.9300867	0.6151450
H	-3.7911170	-5.1908326	-0.5082999
H	0.3460523	-3.3428691	-0.7676070
H	-0.3228522	-4.9743643	-1.0907468
H	-0.9536162	-3.9987429	0.2661784
H	-0.2614338	3.0250937	1.1354862
H	-0.2493084	4.1640326	2.5179118
H	-0.8604075	2.5006438	2.7282257
H	-0.2654836	0.6687168	3.9231762
H	0.3016471	1.5954289	5.3428527
H	1.0759680	0.0433629	4.9233826
H	2.6622293	3.7477817	-0.0398372
H	3.5640116	4.8018563	1.0917742
H	1.7859075	4.9030146	1.0028020
H	5.2840254	3.1539685	1.4951797
H	5.6892861	1.8558445	2.6550717
H	5.4523387	3.5266332	3.2341525
H	3.2748938	0.1379282	5.2942640
H	4.1633705	1.6613970	5.5491825
H	4.7865437	0.4676484	4.3869657
H	1.2052972	-4.9476437	1.1301484
H	0.7896375	-3.4689786	2.0551753
H	1.6202507	-4.8279818	2.8594677
H	2.2759331	-1.7130249	3.7277162
H	3.9595570	-1.8083477	4.3338464
H	2.8983058	-3.2389445	4.4125164
H	6.5808714	-1.1389384	1.5847687
H	6.7600314	-2.3264440	2.9055465
H	5.6580804	-0.9351418	3.1013425
H	2.2443380	-4.9215967	-0.8720337
H	3.7464878	-5.8460380	-0.5933962

H	3.7523171	-4.4553096	-1.7100287
H	2.5592101	-0.5524647	-4.1088787
H	3.2587899	0.5284698	-5.3467316
H	1.9621646	1.1267700	-4.2755248
H	4.3456353	-1.9456005	-2.8567801
H	6.1100954	-1.6945530	-2.6955242
H	5.3083558	-1.4095818	-4.2629694
H	7.9028420	0.8508184	-1.7634246
H	7.0615356	-0.5480675	-1.0446446
H	7.0836853	1.0204103	-0.1869783
H	4.9975049	4.1998345	-0.8823884
H	6.4162752	4.0359336	-1.9483297
H	6.4060544	3.2168627	-0.3679256
H	2.1897793	3.1766110	-3.4680025
H	3.6690442	4.0462355	-3.9573732
H	3.0869098	4.1677004	-2.2765727
H	5.8602210	-3.6030966	-1.3853008
H	6.7977054	-4.1555908	0.0261897
H	6.7491355	-2.4214599	-0.3697850

SCF energy GEOOPT = -4174.075387183 H

ZPE = 3410. kJ/mol

FREEH energy = 3663.86 kJ/mol

FREEH entropy = 2.11740 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a	-5.33	0.00000	YES	YES
2		-0.00	0.00000	-	-
3		-0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	a	11.24	0.04317	YES	YES
9	a	12.79	0.01899	YES	YES
10	a	16.13	0.01404	YES	YES
11	a	18.44	0.05050	YES	YES
12	a	20.48	0.02598	YES	YES
13	a	21.24	0.05269	YES	YES
14	a	23.76	0.02347	YES	YES
15	a	30.47	0.10846	YES	YES
16	a	33.48	0.01610	YES	YES
17	a	35.73	0.09171	YES	YES
18	a	37.56	0.36316	YES	YES
19	a	38.02	0.12522	YES	YES
20	a	43.02	0.15269	YES	YES
21	a	44.98	0.07175	YES	YES
22	a	47.67	0.04169	YES	YES
23	a	48.86	0.25887	YES	YES
24	a	51.96	0.40162	YES	YES
25	a	53.71	0.24268	YES	YES
26	a	56.09	0.32593	YES	YES
27	a	58.10	0.33272	YES	YES
28	a	58.80	1.13474	YES	YES
29	a	61.50	0.22604	YES	YES
30	a	65.81	0.42477	YES	YES
31	a	68.14	0.59010	YES	YES
32	a	71.01	0.94114	YES	YES
33	a	71.72	0.02635	YES	YES
34	a	73.63	0.64564	YES	YES
35	a	74.66	1.29160	YES	YES
36	a	76.31	0.49217	YES	YES
37	a	78.27	0.28975	YES	YES
38	a	80.97	1.20114	YES	YES
39	a	84.52	2.23354	YES	YES
40	a	86.59	0.28346	YES	YES
41	a	87.31	0.33718	YES	YES
42	a	88.64	0.66549	YES	YES
43	a	89.56	0.11490	YES	YES
44	a	90.75	0.00795	YES	YES
45	a	93.31	0.25467	YES	YES
46	a	94.11	0.10352	YES	YES
47	a	95.23	0.10456	YES	YES
48	a	96.11	0.25507	YES	YES
49	a	97.03	0.54053	YES	YES
50	a	99.49	1.27559	YES	YES

51	a	102.87	1.03323	YES	YES
52	a	103.90	0.88250	YES	YES
53	a	106.28	0.10947	YES	YES
54	a	107.63	0.50896	YES	YES
55	a	109.50	0.07574	YES	YES
56	a	110.11	0.18145	YES	YES
57	a	110.99	0.10824	YES	YES
58	a	115.01	0.29495	YES	YES
59	a	115.70	0.59666	YES	YES
60	a	120.11	0.26339	YES	YES
61	a	124.92	3.06380	YES	YES
62	a	127.63	1.00212	YES	YES
63	a	129.58	0.10492	YES	YES
64	a	132.44	0.17896	YES	YES
65	a	140.17	0.47726	YES	YES
66	a	142.72	0.28034	YES	YES
67	a	147.09	0.68631	YES	YES
68	a	150.08	0.25448	YES	YES
69	a	151.37	0.49968	YES	YES
70	a	157.96	0.12114	YES	YES
71	a	159.12	0.86334	YES	YES
72	a	161.43	0.83184	YES	YES
73	a	162.79	1.00887	YES	YES
74	a	163.54	0.10493	YES	YES
75	a	165.29	0.40788	YES	YES
76	a	167.20	0.06855	YES	YES
77	a	171.16	0.42566	YES	YES
78	a	172.69	0.16212	YES	YES
79	a	175.39	1.75837	YES	YES
80	a	176.56	0.02682	YES	YES
81	a	179.15	0.90437	YES	YES
82	a	180.47	0.35743	YES	YES
83	a	186.00	0.44404	YES	YES
84	a	188.11	2.37285	YES	YES
85	a	190.42	0.92147	YES	YES
86	a	190.68	1.21461	YES	YES
87	a	191.21	0.20418	YES	YES
88	a	192.28	1.72630	YES	YES
89	a	193.99	0.18222	YES	YES
90	a	200.62	0.41633	YES	YES
91	a	205.22	5.60049	YES	YES
92	a	208.58	20.82909	YES	YES
93	a	213.39	1.45389	YES	YES
94	a	216.44	8.21960	YES	YES
95	a	218.17	6.49279	YES	YES
96	a	220.52	2.17451	YES	YES
97	a	226.32	23.60300	YES	YES
98	a	227.71	8.30454	YES	YES
99	a	228.89	2.86115	YES	YES
100	a	233.23	3.29713	YES	YES
101	a	233.37	7.79662	YES	YES
102	a	236.62	1.69791	YES	YES
103	a	263.88	0.31875	YES	YES
104	a	266.11	0.09739	YES	YES
105	a	266.28	0.03164	YES	YES
106	a	266.74	0.04964	YES	YES
107	a	267.35	0.71230	YES	YES
108	a	268.24	0.18691	YES	YES
109	a	269.65	0.16879	YES	YES
110	a	269.88	0.14289	YES	YES
111	a	272.09	0.24425	YES	YES
112	a	272.41	0.28030	YES	YES
113	a	274.15	0.08357	YES	YES
114	a	278.30	0.52870	YES	YES
115	a	278.53	0.77438	YES	YES
116	a	279.37	0.15544	YES	YES
117	a	280.52	0.64047	YES	YES
118	a	281.43	0.06434	YES	YES
119	a	281.98	0.98199	YES	YES
120	a	284.14	1.85616	YES	YES
121	a	285.22	0.17719	YES	YES
122	a	286.24	0.97292	YES	YES
123	a	286.91	0.27587	YES	YES
124	a	287.29	0.37534	YES	YES
125	a	288.53	0.15248	YES	YES
126	a	289.95	0.79196	YES	YES
127	a	366.20	3.16027	YES	YES
128	a	371.33	5.05545	YES	YES

129	a	372.83	12.60395	YES	YES
130	a	375.35	3.40027	YES	YES
131	a	375.82	6.00482	YES	YES
132	a	380.47	3.08779	YES	YES
133	a	386.70	6.10556	YES	YES
134	a	388.70	9.50985	YES	YES
135	a	389.52	3.69448	YES	YES
136	a	392.97	1.88540	YES	YES
137	a	393.65	4.85773	YES	YES
138	a	395.08	0.74003	YES	YES
139	a	444.88	160.78106	YES	YES
140	a	449.73	348.90643	YES	YES
141	a	450.87	89.24642	YES	YES
142	a	455.27	437.30565	YES	YES
143	a	482.66	387.08875	YES	YES
144	a	498.56	18.65710	YES	YES
145	a	541.74	0.14492	YES	YES
146	a	543.45	0.20872	YES	YES
147	a	543.79	1.14505	YES	YES
148	a	544.16	0.50400	YES	YES
149	a	544.24	0.67548	YES	YES
150	a	544.43	0.27791	YES	YES
151	a	544.72	0.26166	YES	YES
152	a	544.80	0.15215	YES	YES
153	a	545.10	0.09720	YES	YES
154	a	545.41	0.03234	YES	YES
155	a	545.95	0.05555	YES	YES
156	a	546.60	0.01988	YES	YES
157	a	546.91	0.45948	YES	YES
158	a	547.32	0.08645	YES	YES
159	a	547.80	0.35296	YES	YES
160	a	548.90	0.28496	YES	YES
161	a	550.15	0.29981	YES	YES
162	a	550.60	0.09069	YES	YES
163	a	580.85	0.72130	YES	YES
164	a	583.17	2.57147	YES	YES
165	a	583.28	3.32749	YES	YES
166	a	583.51	2.75082	YES	YES
167	a	584.00	4.45230	YES	YES
168	a	587.77	16.00959	YES	YES
169	a	588.04	2.90142	YES	YES
170	a	589.48	3.42709	YES	YES
171	a	591.14	10.48656	YES	YES
172	a	592.67	5.60194	YES	YES
173	a	594.91	5.95752	YES	YES
174	a	595.22	0.53003	YES	YES
175	a	595.34	8.84273	YES	YES
176	a	595.59	1.23781	YES	YES
177	a	596.90	2.08171	YES	YES
178	a	597.39	2.97485	YES	YES
179	a	597.72	1.53753	YES	YES
180	a	599.64	0.33562	YES	YES
181	a	795.02	2.29790	YES	YES
182	a	796.59	4.76094	YES	YES
183	a	797.07	3.26414	YES	YES
184	a	797.79	1.19079	YES	YES
185	a	798.32	1.83179	YES	YES
186	a	800.81	2.99882	YES	YES
187	a	802.50	8.23950	YES	YES
188	a	803.36	3.70569	YES	YES
189	a	803.66	3.50541	YES	YES
190	a	804.65	2.71064	YES	YES
191	a	805.90	2.41796	YES	YES
192	a	805.96	3.51086	YES	YES
193	a	919.86	2.06818	YES	YES
194	a	920.86	2.44297	YES	YES
195	a	922.50	0.72237	YES	YES
196	a	922.76	0.80357	YES	YES
197	a	924.74	1.05300	YES	YES
198	a	925.54	0.64672	YES	YES
199	a	929.05	1.51341	YES	YES
200	a	929.91	1.29289	YES	YES
201	a	930.09	0.17272	YES	YES
202	a	930.50	1.44020	YES	YES
203	a	932.02	0.13650	YES	YES
204	a	932.47	0.36387	YES	YES
205	a	985.12	7.06680	YES	YES
206	a	985.68	3.40854	YES	YES

207	a	987.91	3.04178	YES	YES
208	a	988.60	2.48693	YES	YES
209	a	989.28	3.70539	YES	YES
210	a	990.22	2.10155	YES	YES
211	a	990.63	4.21880	YES	YES
212	a	991.92	1.87438	YES	YES
213	a	992.30	4.94848	YES	YES
214	a	992.40	0.83258	YES	YES
215	a	992.98	6.55500	YES	YES
216	a	993.20	2.35978	YES	YES
217	a	993.55	0.16245	YES	YES
218	a	993.75	0.55312	YES	YES
219	a	994.27	0.91233	YES	YES
220	a	994.75	1.68229	YES	YES
221	a	995.37	0.25013	YES	YES
222	a	995.63	0.37833	YES	YES
223	a	996.66	0.12813	YES	YES
224	a	996.81	1.26342	YES	YES
225	a	997.10	0.67093	YES	YES
226	a	997.69	0.30016	YES	YES
227	a	997.81	1.11451	YES	YES
228	a	999.81	0.43872	YES	YES
229	a	1002.72	0.06673	YES	YES
230	a	1005.31	1.11227	YES	YES
231	a	1005.44	0.20152	YES	YES
232	a	1007.08	0.13950	YES	YES
233	a	1010.36	0.03563	YES	YES
234	a	1013.39	0.45413	YES	YES
235	a	1046.77	1.02895	YES	YES
236	a	1047.20	2.24046	YES	YES
237	a	1048.66	1.37897	YES	YES
238	a	1048.81	2.77270	YES	YES
239	a	1049.21	2.18071	YES	YES
240	a	1049.59	2.69151	YES	YES
241	a	1049.88	0.15660	YES	YES
242	a	1050.96	0.68197	YES	YES
243	a	1051.59	1.85732	YES	YES
244	a	1051.93	0.36203	YES	YES
245	a	1052.40	0.46332	YES	YES
246	a	1052.79	0.34768	YES	YES
247	a	1072.23	0.19989	YES	YES
248	a	1073.56	0.25123	YES	YES
249	a	1074.01	0.32124	YES	YES
250	a	1075.22	0.25855	YES	YES
251	a	1076.46	0.11107	YES	YES
252	a	1077.68	0.06206	YES	YES
253	a	1161.82	0.86968	YES	YES
254	a	1162.50	0.25073	YES	YES
255	a	1163.40	0.08632	YES	YES
256	a	1163.92	0.42702	YES	YES
257	a	1164.35	0.15693	YES	YES
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259	a	1165.38	0.53380	YES	YES
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261	a	1166.10	0.21218	YES	YES
262	a	1166.23	0.33324	YES	YES
263	a	1166.78	0.18694	YES	YES
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265	a	1338.20	1.34109	YES	YES
266	a	1338.40	0.95652	YES	YES
267	a	1339.40	1.74396	YES	YES
268	a	1339.71	2.92347	YES	YES
269	a	1339.89	0.20135	YES	YES
270	a	1340.26	1.87945	YES	YES
271	a	1340.41	0.53251	YES	YES
272	a	1340.93	2.96704	YES	YES
273	a	1341.16	0.39080	YES	YES
274	a	1341.27	0.41667	YES	YES
275	a	1342.12	0.76568	YES	YES
276	a	1342.60	0.64365	YES	YES
277	a	1344.38	2.46406	YES	YES
278	a	1345.57	3.77966	YES	YES
279	a	1345.78	0.78672	YES	YES
280	a	1345.96	2.79402	YES	YES
281	a	1346.36	5.64642	YES	YES
282	a	1346.47	2.22237	YES	YES
283	a	1347.43	5.24215	YES	YES
284	a	1347.51	2.95622	YES	YES

285	a	1347.97	2.50374	YES	YES
286	a	1348.31	14.41930	YES	YES
287	a	1348.53	6.63290	YES	YES
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290	a	1350.82	0.06499	YES	YES
291	a	1351.28	3.12292	YES	YES
292	a	1351.63	0.69614	YES	YES
293	a	1351.82	0.13110	YES	YES
294	a	1352.82	1.53046	YES	YES
295	a	1380.04	1.65836	YES	YES
296	a	1381.16	2.74248	YES	YES
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298	a	1382.96	8.33724	YES	YES
299	a	1383.78	1.28158	YES	YES
300	a	1384.26	3.69216	YES	YES
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304	a	1388.77	6.87161	YES	YES
305	a	1390.19	2.90309	YES	YES
306	a	1390.51	0.41525	YES	YES
307	a	1392.52	1.22359	YES	YES
308	a	1393.28	3.25892	YES	YES
309	a	1393.99	5.05509	YES	YES
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311	a	1394.76	1.94745	YES	YES
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313	a	1396.14	1.38136	YES	YES
314	a	1396.48	7.57897	YES	YES
315	a	1396.70	0.30563	YES	YES
316	a	1397.28	1.11188	YES	YES
317	a	1398.35	2.10005	YES	YES
318	a	1398.64	0.86661	YES	YES
319	a	1399.02	10.24760	YES	YES
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321	a	1400.02	0.63091	YES	YES
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324	a	1401.59	10.95896	YES	YES
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327	a	1403.02	0.23185	YES	YES
328	a	1403.08	9.96578	YES	YES
329	a	1403.70	12.27724	YES	YES
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332	a	1405.18	17.56376	YES	YES
333	a	1405.50	13.93135	YES	YES
334	a	1405.90	1.57435	YES	YES
335	a	1406.44	10.34606	YES	YES
336	a	1407.48	2.25441	YES	YES
337	a	1407.83	3.07104	YES	YES
338	a	1408.70	5.25993	YES	YES
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349	a	1415.63	75.03880	YES	YES
350	a	1416.77	58.22957	YES	YES
351	a	1417.64	14.13728	YES	YES
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353	a	1419.95	8.52082	YES	YES
354	a	1420.45	16.52209	YES	YES
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356	a	1432.99	16.10448	YES	YES
357	a	1434.31	3.64133	YES	YES
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359	a	1436.10	0.78493	YES	YES
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363	a	1444.51	1.75146	YES	YES
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366	a	1446.40	0.72415	YES	YES
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371	a	1450.77	1.40435	YES	YES
372	a	1451.90	1.05458	YES	YES
373	a	1477.31	19.00749	YES	YES
374	a	1479.63	12.31034	YES	YES
375	a	1479.85	11.17296	YES	YES
376	a	1480.14	10.37715	YES	YES
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378	a	1481.58	14.65101	YES	YES
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381	a	1489.12	20.32225	YES	YES
382	a	1489.65	14.57517	YES	YES
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384	a	1490.54	12.28508	YES	YES
385	a	2948.16	11.51027	YES	YES
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394	a	2960.16	12.41375	YES	YES
395	a	2961.28	7.63134	YES	YES
396	a	2963.03	9.32270	YES	YES
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399	a	2966.61	15.88381	YES	YES
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403	a	2967.98	9.14704	YES	YES
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405	a	2969.20	24.36942	YES	YES
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407	a	2969.72	24.11888	YES	YES
408	a	2969.74	19.31396	YES	YES
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417	a	3025.50	1.78016	YES	YES
418	a	3029.49	0.32278	YES	YES
419	a	3030.02	6.39663	YES	YES
420	a	3030.75	6.36176	YES	YES
421	a	3031.11	5.37430	YES	YES
422	a	3032.14	3.87168	YES	YES
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424	a	3033.75	6.27055	YES	YES
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426	a	3036.41	2.35066	YES	YES
427	a	3037.09	6.37186	YES	YES
428	a	3039.14	4.03047	YES	YES
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430	a	3040.59	4.03167	YES	YES
431	a	3041.11	3.18077	YES	YES
432	a	3041.74	0.30318	YES	YES
433	a	3041.83	3.88071	YES	YES
434	a	3042.17	4.90139	YES	YES
435	a	3042.45	5.46564	YES	YES
436	a	3043.88	2.26842	YES	YES
437	a	3044.14	2.94474	YES	YES
438	a	3044.28	1.37208	YES	YES
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440	a	3045.31	3.78164	YES	YES

441	a	3045.71	1.83082	YES	YES
442	a	3046.29	1.36894	YES	YES
443	a	3046.53	0.91220	YES	YES
444	a	3047.44	1.48320	YES	YES
445	a	3059.56	5.01342	YES	YES
446	a	3060.79	3.85611	YES	YES
447	a	3062.87	6.02680	YES	YES
448	a	3064.83	3.00652	YES	YES
449	a	3068.51	4.70473	YES	YES
450	a	3069.68	2.24576	YES	YES
451	a	3070.69	3.93447	YES	YES
452	a	3070.75	2.72040	YES	YES
453	a	3071.08	2.67456	YES	YES
454	a	3072.45	4.09416	YES	YES
455	a	3073.13	4.16661	YES	YES
456	a	3074.89	5.10896	YES	YES
457	a	3075.15	4.58752	YES	YES
458	a	3075.46	4.34165	YES	YES
459	a	3075.96	4.09184	YES	YES
460	a	3076.17	5.23120	YES	YES
461	a	3079.24	4.27090	YES	YES
462	a	3080.92	3.66634	YES	YES
463	a	3081.05	3.95184	YES	YES
464	a	3081.71	5.64506	YES	YES
465	a	3082.83	1.69465	YES	YES
466	a	3083.16	10.31738	YES	YES
467	a	3085.18	1.49866	YES	YES
468	a	3085.40	0.96438	YES	YES
469	a	3085.51	4.41574	YES	YES
470	a	3090.08	4.05885	YES	YES
471	a	3090.32	3.44866	YES	YES
472	a	3095.31	1.15502	YES	YES
473	a	3096.07	2.55273	YES	YES
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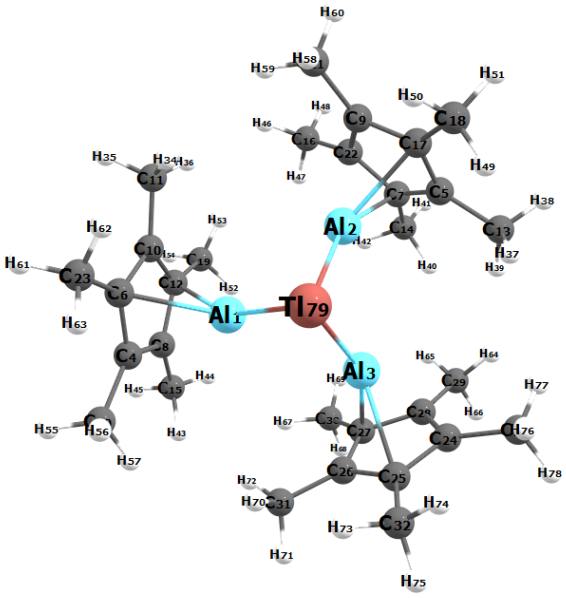
[Tl(AlCp*)$_3$]$^+$



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

Symmetry: c1

Cartesian coordinates in Ångström:

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Al	0.8048662	-0.1813994	-1.5606852
C	-3.9651612	-0.2045597	-0.3804434
C	3.1320611	0.2303424	1.8635867
C	-3.7629266	-0.7961948	0.9174755
C	2.3640431	1.4282125	2.0878913
C	-3.4965306	1.1559728	-0.3259156
C	1.6576920	-0.1851711	3.6236940
C	-3.1814038	0.1987438	1.7800323
C	-2.8118574	-0.0112930	3.2185444
C	-3.0025274	1.4051251	1.0135024
C	4.1958787	0.0298296	0.8253085
C	2.5359537	2.7459856	1.3901565
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C	0.5817485	2.1955038	3.8493087
C	2.6879176	-0.7670342	2.8016586
C	3.2227278	-2.1646284	2.9099665
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C	-4.5800135	-0.8824121	-1.5694399
C	0.9428475	-0.8677407	4.7526496
C	1.4541119	1.1716050	3.1861859
C	-4.1109127	-2.2007835	1.3138032
C	2.3076671	-0.1789524	-3.2518446
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C	0.0435394	0.2323289	-3.6371712
C	0.6218513	1.4308032	-3.0857725
C	2.0296705	1.1769824	-2.8545252
C	3.0409456	2.2026191	-2.4365453
C	-0.0708753	2.7462251	-2.8791824
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H	2.9653302	2.6182864	0.3794340
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H	1.5756042	3.2877474	1.2826655
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H	4.1005875	-2.1996393	3.5892656
H	-1.9288000	3.2771096	0.7500957
H	-1.8365875	2.5946599	2.3997694
H	-3.3404258	3.3737110	1.8384538
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H	-4.3151148	-1.9572244	-1.6129117
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H	-0.0509918	-0.4189128	4.9415784
H	1.5249020	-0.7879262	5.6948899
H	-5.1358423	-2.2484906	1.7386112
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H	-4.0818874	-2.8916105	0.4491091
H	3.8916817	1.7516535	-1.8903867
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SCF energy GEOOPT = -2069.456513958 H

ZPE = 1702. kJ/mol

FREEH energy = 1828.89 kJ/mol

FREEH entropy = 1.20231 kJ/mol/K

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity 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	14.90	0.05186	YES	YES
8	a	16.42	0.03324	YES	YES
9	a	19.46	0.02358	YES	YES
10	a	24.08	0.01391	YES	YES
11	a	25.01	0.01446	YES	YES
12	a	30.07	0.01132	YES	YES
13	a	43.50	0.20431	YES	YES
14	a	47.57	0.02244	YES	YES
15	a	49.84	0.11547	YES	YES
16	a	54.74	0.18745	YES	YES
17	a	61.39	0.04264	YES	YES
18	a	64.51	0.11405	YES	YES
19	a	72.10	0.01447	YES	YES
20	a	74.05	0.29654	YES	YES
21	a	77.28	0.24444	YES	YES
22	a	85.44	0.35523	YES	YES
23	a	87.77	0.06178	YES	YES
24	a	91.31	0.13189	YES	YES
25	a	92.84	0.08631	YES	YES
26	a	96.22	0.08109	YES	YES
27	a	96.57	0.17043	YES	YES
28	a	100.11	0.10504	YES	YES
29	a	103.22	0.14793	YES	YES
30	a	104.16	0.23909	YES	YES
31	a	107.74	0.07916	YES	YES
32	a	110.73	0.03051	YES	YES
33	a	112.93	0.25330	YES	YES
34	a	144.49	0.00860	YES	YES
35	a	146.74	0.00166	YES	YES
36	a	150.53	0.14790	YES	YES
37	a	155.67	0.04227	YES	YES
38	a	157.38	0.05260	YES	YES
39	a	159.88	0.00338	YES	YES
40	a	161.77	0.21812	YES	YES
41	a	169.96	0.24117	YES	YES
42	a	171.71	0.22889	YES	YES
43	a	186.40	1.04041	YES	YES
44	a	187.19	0.97880	YES	YES
45	a	188.35	0.43176	YES	YES
46	a	205.05	0.99404	YES	YES
47	a	217.94	4.88926	YES	YES
48	a	218.22	5.03397	YES	YES

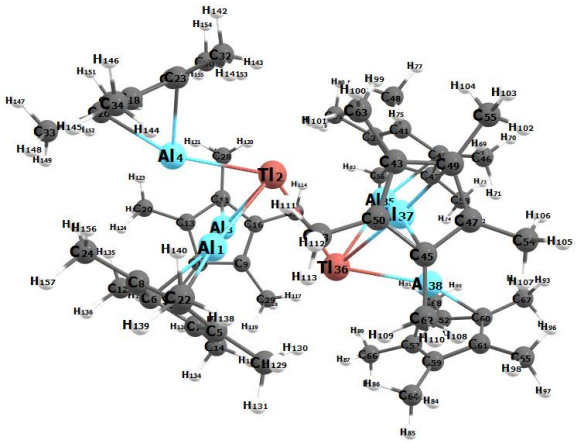
49	a	223.88	4.42410	YES	YES
50	a	230.33	2.16994	YES	YES
51	a	231.01	2.31891	YES	YES
52	a	271.06	0.07472	YES	YES
53	a	271.87	0.01420	YES	YES
54	a	272.94	0.11615	YES	YES
55	a	274.25	0.05478	YES	YES
56	a	274.93	0.31750	YES	YES
57	a	277.08	0.09643	YES	YES
58	a	279.72	0.07592	YES	YES
59	a	281.67	0.63231	YES	YES
60	a	282.49	0.40026	YES	YES
61	a	284.40	0.22389	YES	YES
62	a	285.87	0.78546	YES	YES
63	a	287.89	0.81503	YES	YES
64	a	378.38	0.21864	YES	YES
65	a	380.87	23.40824	YES	YES
66	a	381.05	23.70502	YES	YES
67	a	392.00	2.56755	YES	YES
68	a	392.53	1.57778	YES	YES
69	a	392.81	3.59138	YES	YES
70	a	450.07	327.49208	YES	YES
71	a	450.50	327.27913	YES	YES
72	a	496.39	32.81921	YES	YES
73	a	543.02	0.12933	YES	YES
74	a	543.57	0.07618	YES	YES
75	a	544.02	0.00781	YES	YES
76	a	544.24	0.11061	YES	YES
77	a	544.29	0.07320	YES	YES
78	a	544.54	0.07106	YES	YES
79	a	546.27	0.12753	YES	YES
80	a	546.84	0.08193	YES	YES
81	a	547.02	0.11237	YES	YES
82	a	585.43	2.50485	YES	YES
83	a	585.74	2.50091	YES	YES
84	a	586.31	2.65928	YES	YES
85	a	589.76	6.61409	YES	YES
86	a	589.85	6.21618	YES	YES
87	a	591.46	1.08637	YES	YES
88	a	598.52	0.20244	YES	YES
89	a	599.04	0.05311	YES	YES
90	a	599.28	0.03163	YES	YES
91	a	797.32	2.63377	YES	YES
92	a	797.67	2.90215	YES	YES
93	a	798.68	3.03780	YES	YES
94	a	801.28	3.26867	YES	YES
95	a	802.20	3.23794	YES	YES
96	a	802.94	2.74213	YES	YES
97	a	921.17	0.09428	YES	YES
98	a	922.45	0.75422	YES	YES
99	a	924.25	0.55678	YES	YES
100	a	925.20	0.11571	YES	YES
101	a	926.28	0.26941	YES	YES
102	a	927.48	0.30849	YES	YES
103	a	987.76	11.92751	YES	YES
104	a	987.92	3.55571	YES	YES
105	a	988.04	3.53110	YES	YES
106	a	992.10	5.94634	YES	YES
107	a	992.56	5.66712	YES	YES
108	a	993.21	5.16032	YES	YES
109	a	994.68	0.69713	YES	YES
110	a	995.09	0.92257	YES	YES
111	a	995.88	1.47957	YES	YES
112	a	998.03	0.12703	YES	YES
113	a	998.94	0.24709	YES	YES
114	a	999.50	0.05155	YES	YES
115	a	1000.17	0.18387	YES	YES
116	a	1000.69	0.39937	YES	YES
117	a	1001.18	1.05432	YES	YES
118	a	1048.12	3.06225	YES	YES
119	a	1048.36	3.28001	YES	YES
120	a	1048.48	3.12421	YES	YES
121	a	1050.27	0.14022	YES	YES
122	a	1050.50	0.23279	YES	YES
123	a	1050.77	0.13202	YES	YES
124	a	1074.06	0.11931	YES	YES
125	a	1074.73	0.09548	YES	YES
126	a	1077.12	0.02094	YES	YES

127	a	1163.60	0.04848	YES	YES
128	a	1163.74	0.02455	YES	YES
129	a	1163.97	0.02651	YES	YES
130	a	1165.33	0.09095	YES	YES
131	a	1165.66	0.41821	YES	YES
132	a	1165.86	0.33183	YES	YES
133	a	1338.56	0.01421	YES	YES
134	a	1339.91	0.66152	YES	YES
135	a	1340.45	0.63465	YES	YES
136	a	1340.65	0.73750	YES	YES
137	a	1341.40	1.42826	YES	YES
138	a	1341.99	0.87399	YES	YES
139	a	1344.84	5.27725	YES	YES
140	a	1345.62	4.64435	YES	YES
141	a	1346.32	5.57866	YES	YES
142	a	1348.34	2.72338	YES	YES
143	a	1349.14	13.66501	YES	YES
144	a	1349.35	8.60525	YES	YES
145	a	1351.20	1.14280	YES	YES
146	a	1351.82	0.38395	YES	YES
147	a	1353.41	2.78601	YES	YES
148	a	1383.88	1.47143	YES	YES
149	a	1384.33	1.23629	YES	YES
150	a	1384.85	0.61032	YES	YES
151	a	1388.87	0.23487	YES	YES
152	a	1389.06	0.54766	YES	YES
153	a	1389.90	0.22977	YES	YES
154	a	1394.71	18.66554	YES	YES
155	a	1395.32	0.94565	YES	YES
156	a	1395.53	1.83896	YES	YES
157	a	1397.27	2.52848	YES	YES
158	a	1397.62	0.72501	YES	YES
159	a	1398.14	1.83517	YES	YES
160	a	1399.94	1.05672	YES	YES
161	a	1400.60	12.33613	YES	YES
162	a	1401.11	12.37257	YES	YES
163	a	1402.75	1.82963	YES	YES
164	a	1403.33	3.25656	YES	YES
165	a	1403.46	2.96143	YES	YES
166	a	1405.70	4.76065	YES	YES
167	a	1406.20	3.20791	YES	YES
168	a	1407.25	10.78501	YES	YES
169	a	1408.70	2.43694	YES	YES
170	a	1409.46	27.13331	YES	YES
171	a	1409.57	30.10726	YES	YES
172	a	1410.49	8.66265	YES	YES
173	a	1410.62	17.17076	YES	YES
174	a	1411.84	3.64102	YES	YES
175	a	1413.81	106.01647	YES	YES
176	a	1414.18	93.79131	YES	YES
177	a	1414.85	23.28374	YES	YES
178	a	1435.55	0.83120	YES	YES
179	a	1436.16	0.31452	YES	YES
180	a	1436.63	0.54115	YES	YES
181	a	1444.94	0.00564	YES	YES
182	a	1446.86	0.16853	YES	YES
183	a	1447.13	0.15232	YES	YES
184	a	1450.24	0.47647	YES	YES
185	a	1450.41	0.31683	YES	YES
186	a	1451.05	0.39113	YES	YES
187	a	1480.24	26.16181	YES	YES
188	a	1480.35	5.76572	YES	YES
189	a	1480.71	9.29490	YES	YES
190	a	1488.42	2.81200	YES	YES
191	a	1488.74	19.89221	YES	YES
192	a	1488.87	20.72391	YES	YES
193	a	2963.87	20.35635	YES	YES
194	a	2963.90	25.65527	YES	YES
195	a	2963.94	17.01050	YES	YES
196	a	2965.33	28.99203	YES	YES
197	a	2965.41	20.10996	YES	YES
198	a	2965.58	14.87014	YES	YES
199	a	2965.64	15.23362	YES	YES
200	a	2965.69	8.86204	YES	YES
201	a	2965.85	4.52566	YES	YES
202	a	2966.56	24.37442	YES	YES
203	a	2966.86	27.65889	YES	YES
204	a	2966.95	17.97930	YES	YES

205	a	2967.18	7.46689	YES	YES
206	a	2967.69	1.52960	YES	YES
207	a	2967.74	23.40397	YES	YES
208	a	3036.17	4.99674	YES	YES
209	a	3036.33	4.79770	YES	YES
210	a	3036.55	4.99775	YES	YES
211	a	3039.00	5.57960	YES	YES
212	a	3039.24	8.53195	YES	YES
213	a	3039.65	8.90651	YES	YES
214	a	3040.64	0.72048	YES	YES
215	a	3040.83	2.32882	YES	YES
216	a	3040.88	3.86823	YES	YES
217	a	3040.97	1.31029	YES	YES
218	a	3041.23	4.02993	YES	YES
219	a	3041.71	1.64473	YES	YES
220	a	3042.00	0.66230	YES	YES
221	a	3042.14	0.78307	YES	YES
222	a	3042.30	0.27781	YES	YES
223	a	3067.23	4.44447	YES	YES
224	a	3067.56	4.22567	YES	YES
225	a	3068.06	4.51668	YES	YES
226	a	3069.04	5.78815	YES	YES
227	a	3069.41	2.85787	YES	YES
228	a	3069.78	7.52031	YES	YES
229	a	3069.88	0.71899	YES	YES
230	a	3070.02	5.22561	YES	YES
231	a	3070.24	4.72727	YES	YES
232	a	3072.34	6.14405	YES	YES
233	a	3072.49	7.42927	YES	YES
234	a	3072.69	14.71507	YES	YES
235	a	3078.83	3.11269	YES	YES
236	a	3080.29	3.18090	YES	YES
237	a	3080.55	3.31488	YES	YES

$end

$[Tl_2(AlCp^*)_6]^{2+}$



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

Symmetry: c1

Cartesian coordinates in Ångström:

Al	2.2629598	-1.4265453	1.2959558
Tl	1.3187600	-0.0278342	-0.9934359
Al	2.2381120	1.6415384	1.1531365
Al	4.1764699	-0.1134648	-0.6103345
C	1.4976589	-2.6127827	3.1123688
C	3.4463597	-1.3348452	3.1719710
C	2.0526976	-1.3558823	3.5385600
C	3.7486926	-2.5829350	2.5180856
C	1.2968553	3.3287817	2.3824139
C	2.5473885	-3.3740566	2.4792818
C	2.6431033	3.7489349	0.5246096
C	4.4416987	-0.2528042	3.4633455
C	3.5065758	3.4227990	1.6291599
C	1.3049216	-0.2695792	4.2509222
C	2.6726037	3.1724900	2.7855883
C	1.2818164	3.6882489	0.9933410
C	0.0904316	-3.0615320	3.3871581
C	5.4247085	-1.6023833	-1.7779008
C	0.0640459	4.0136456	0.1885648
C	5.0061940	3.4266999	1.6164838
C	3.1558597	3.0449006	4.2000241
C	2.4720415	-4.7846707	1.9714141
C	4.5688649	-0.9116082	-2.7036216
C	5.1108639	-3.0191585	2.0745995
C	4.9086822	0.4878868	-2.6798215
C	6.2869214	-0.6260664	-1.1574667
C	5.9664293	0.6708719	-1.7234812
C	3.0718667	4.1044344	-0.8677821
C	0.0918992	3.2286099	3.2705820
C	4.2739138	1.5418114	-3.5367137
C	6.7325033	1.9344633	-1.4658960
C	3.5490951	-1.5526157	-3.5964806
C	7.4326913	-0.8936889	-0.2248812
C	5.4247603	-3.0868957	-1.5576744
Al	-2.2628747	1.4266964	-1.2960576
Tl	-1.3186166	0.0280053	0.9933134
Al	-2.2380068	-1.6413894	-1.1532223
Al	-4.1763243	0.1136115	0.6102780
C	-1.4975893	2.6129529	-3.1124619
C	-3.4462864	1.3350087	-3.1720635
C	-2.0526251	1.3560534	-3.5386599
C	-3.7486197	2.5830919	-2.5181646
C	-1.2967498	-3.3286249	-2.3825169
C	-2.5473151	3.3742185	-2.4793599
C	-2.6429967	-3.7487891	-0.5247133
C	-4.4416217	0.2529667	-3.4634419
C	-3.5064691	-3.4226452	-1.6292627
C	-1.3048448	0.2697604	-4.2510330
C	-2.6724969	-3.1723304	-2.7856901
C	-1.2817081	-3.6880982	-0.9934468
C	-0.0903636	3.0617086	-3.3872480
C	-5.4245599	1.6025125	1.7778683
C	-0.0639379	-4.0135058	-0.1886780
C	-5.0060869	-3.4265514	-1.6165843
C	-3.1557535	-3.0447313	-4.2001246
C	-2.4719714	4.7848291	-1.9714843
C	-4.5687085	0.9117265	2.7035754
C	-5.1107883	3.0192996	-2.0746557
C	-4.9085220	-0.4877689	2.6797587
C	-6.2867762	0.6262021	1.1574304

C	-5.9662752	-0.6707437	1.7234228
C	-3.0717643	-4.1043047	0.8676716
C	-0.0917947	-3.2284454	-3.2706865
C	-4.2737453	-1.5417015	3.5366340
C	-6.7323500	-1.9343326	1.4658289
C	-3.5489329	1.5527226	3.5964358
C	-7.4325549	0.8938336	0.2248588
C	-5.4246159	3.0870274	1.5576588
H	-3.9402321	-0.6890912	-3.7428699
H	-5.1061204	0.5382531	-4.3057099
H	-5.0920627	0.0446847	-2.5882312
H	-5.6934461	2.1767076	-1.6539969
H	-5.6904439	3.4178933	-2.9341539
H	-5.0601266	3.8180444	-1.3125160
H	-1.4429014	-0.7104652	-3.7489803
H	-0.2179087	0.4738141	-4.2729060
H	-1.6479766	0.1594198	-5.3002831
H	0.6664209	2.3743737	-2.9521623
H	0.1026950	4.0725945	-2.9839222
H	0.0993730	3.1076973	-4.4791957
H	-2.8602528	4.8828900	-0.9376241
H	-3.0782811	5.4590874	-2.6111037
H	-1.4374066	5.1717158	-1.9783462
H	-4.5192608	-2.5614065	3.1875007
H	-4.6221175	-1.4577587	4.5870583
H	-3.1675956	-1.4470365	3.5511641
H	-2.6913429	0.8791635	3.7962840
H	-3.9951571	1.8108724	4.5802861
H	-3.1536479	2.4901260	3.1601180
H	-6.1333922	3.3838416	0.7640538
H	-4.4200331	3.4666558	1.2753151
H	-5.7258969	3.6178294	2.4839208
H	-7.4884476	0.1549087	-0.5987840
H	-7.3731186	1.9014190	-0.2264440
H	-8.3958123	0.8395515	0.7744519
H	-7.1163599	-1.9859376	0.4292535
H	-7.6127846	-1.9942104	2.1402191
H	-6.1222522	-2.8386869	1.6537461
H	-0.2946040	-2.6366373	-4.1827178
H	0.2391176	-4.2355671	-3.6012397
H	0.7641104	-2.7567537	-2.7475329
H	-4.2106870	-2.7194005	-4.2552207
H	-3.1001576	-4.0354744	-4.6993539
H	-2.5451781	-2.3472934	-4.8041808
H	-5.4015272	-4.4268710	-1.8915288
H	-5.4277644	-2.6966038	-2.3341829
H	-5.4039936	-3.1808257	-0.6148202
H	-4.0943738	-3.7398263	1.0795516
H	-2.3964907	-3.6700364	1.6308522
H	-3.0766632	-5.2046169	1.0139554
H	0.8459213	-3.5429626	-0.6080553
H	0.1064433	-5.1102736	-0.1645112
H	-0.1633982	-3.6684982	0.8558129
H	0.1635111	3.6686203	-0.8559199
H	-0.1063357	5.1104127	0.1643805
H	-0.8458140	3.5431057	0.6079442
H	-0.7640072	2.7569228	2.7474266
H	-0.2390076	4.2357347	3.6011314
H	0.2947022	2.6368019	4.1826147
H	2.3966054	3.6701342	-1.6309560
H	4.0944852	3.7399746	-1.0796521
H	3.0767407	5.2047434	-1.0140901
H	5.4041009	3.1809754	0.6147194
H	5.4278697	2.6967502	2.3340813
H	5.4016352	4.4270188	1.8914304
H	2.5452820	2.3474695	4.8040859
H	3.1002694	4.0356486	4.6992440
H	4.2107916	2.7195643	4.2551221
H	-0.1026262	-4.0724242	2.9838478
H	-0.6663530	-2.3742045	2.9520611
H	-0.0993049	-3.1074984	4.4791067
H	0.2179809	-0.4736124	4.2727678
H	1.4430093	0.7106455	3.7488770
H	1.6480321	-0.1592497	5.3001805
H	5.0921456	-0.0445326	2.5881367
H	5.1061896	-0.5380876	4.3056209
H	3.9403108	0.6892579	3.7427625
H	1.4374739	-5.1715488	1.9782686

H	3.0783415	-5.4589293	2.6110423
H	2.8603290	-4.8827403	0.9375572
H	3.1537922	-2.4900028	-3.1601436
H	3.9953285	-1.8107970	-4.5803183
H	2.6915166	-0.8790506	-3.7963578
H	4.4201725	-3.4665205	-1.2753440
H	6.1335228	-3.3837004	-0.7640537
H	5.7260574	-3.6177084	-2.4839249
H	8.3959526	-0.8394252	-0.7744696
H	7.3732444	-1.9012650	0.2264416
H	7.4885840	-0.1547475	0.5987468
H	6.1224117	2.8388156	-1.6538433
H	7.6129531	1.9943256	-2.1402675
H	7.1164893	1.9860875	-0.4293123
H	3.1677625	1.4471611	-3.5512386
H	4.6222806	1.4578439	-4.5871379
H	4.5194442	2.5615199	-3.1876006
H	5.0602070	-3.8179151	1.3124723
H	5.6905054	-3.4177417	2.9341120
H	5.6935321	-2.1765768	1.6539339

SCF energy GEOOPT = -4138.899540142 H

ZPE = 3409. kJ/mol

FREEH energy = 3665.86 kJ/mol

FREEH entropy = 2.15378 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	5.13	0.07948	YES	YES
8		a	11.25	0.00000	YES	YES
9		a	13.98	0.09617	YES	YES
10		a	15.49	0.00000	YES	YES
11		a	19.63	0.15261	YES	YES
12		a	21.00	0.00000	YES	YES
13		a	21.33	0.11034	YES	YES
14		a	28.84	0.00000	YES	YES
15		a	34.09	0.06911	YES	YES
16		a	34.10	0.00058	YES	YES
17		a	35.33	0.00000	YES	YES
18		a	36.19	0.20470	YES	YES
19		a	39.54	0.29688	YES	YES
20		a	39.66	0.00001	YES	YES
21		a	44.23	0.23785	YES	YES
22		a	45.40	0.00000	YES	YES
23		a	50.32	0.00000	YES	YES
24		a	50.77	0.09138	YES	YES
25		a	56.82	0.39279	YES	YES
26		a	57.40	0.00000	YES	YES
27		a	59.55	0.10370	YES	YES
28		a	61.10	0.00000	YES	YES
29		a	63.52	0.60435	YES	YES
30		a	64.89	0.79328	YES	YES
31		a	66.25	0.00000	YES	YES
32		a	71.66	0.88450	YES	YES
33		a	71.72	0.00001	YES	YES
34		a	73.64	1.09495	YES	YES
35		a	74.36	0.00000	YES	YES
36		a	75.76	0.00000	YES	YES
37		a	77.54	2.30379	YES	YES
38		a	78.05	0.00001	YES	YES
39		a	81.88	0.00000	YES	YES
40		a	82.86	0.58514	YES	YES
41		a	85.40	1.28614	YES	YES
42		a	88.01	0.00000	YES	YES
43		a	88.52	0.00000	YES	YES
44		a	89.24	0.42381	YES	YES
45		a	92.27	0.00000	YES	YES
46		a	93.56	0.51195	YES	YES
47		a	97.37	1.11713	YES	YES
48		a	98.93	0.00000	YES	YES
49		a	99.91	0.05346	YES	YES

50	a	101.31	0.00000	YES	YES
51	a	103.05	0.01708	YES	YES
52	a	105.24	0.00000	YES	YES
53	a	108.96	0.00000	YES	YES
54	a	109.83	0.65027	YES	YES
55	a	111.45	0.77268	YES	YES
56	a	112.13	0.00000	YES	YES
57	a	118.33	1.07319	YES	YES
58	a	118.66	0.00001	YES	YES
59	a	129.21	0.00869	YES	YES
60	a	129.23	0.15511	YES	YES
61	a	130.55	2.44145	YES	YES
62	a	131.14	0.00000	YES	YES
63	a	139.35	0.00000	YES	YES
64	a	140.08	2.53055	YES	YES
65	a	140.34	0.14014	YES	YES
66	a	140.87	0.00000	YES	YES
67	a	156.18	0.00002	YES	YES
68	a	156.40	1.38847	YES	YES
69	a	157.62	0.19521	YES	YES
70	a	158.25	0.00000	YES	YES
71	a	160.10	1.25410	YES	YES
72	a	161.24	0.00000	YES	YES
73	a	165.61	0.00000	YES	YES
74	a	167.09	0.29243	YES	YES
75	a	168.92	0.52466	YES	YES
76	a	168.98	0.00000	YES	YES
77	a	172.91	0.12433	YES	YES
78	a	172.97	0.00000	YES	YES
79	a	179.23	0.00001	YES	YES
80	a	179.41	0.58596	YES	YES
81	a	180.88	0.71129	YES	YES
82	a	183.07	0.00000	YES	YES
83	a	187.57	2.47358	YES	YES
84	a	187.77	0.00001	YES	YES
85	a	188.26	2.14767	YES	YES
86	a	188.63	0.00000	YES	YES
87	a	189.22	0.00000	YES	YES
88	a	191.01	1.31005	YES	YES
89	a	193.14	0.40890	YES	YES
90	a	193.25	0.00000	YES	YES
91	a	201.21	9.01975	YES	YES
92	a	202.31	0.00000	YES	YES
93	a	206.10	0.00000	YES	YES
94	a	209.33	7.56922	YES	YES
95	a	215.43	2.09693	YES	YES
96	a	215.50	0.00003	YES	YES
97	a	218.28	7.82417	YES	YES
98	a	221.58	22.00962	YES	YES
99	a	222.13	0.00000	YES	YES
100	a	224.33	0.00006	YES	YES
101	a	224.46	6.97050	YES	YES
102	a	229.67	0.00000	YES	YES
103	a	263.86	0.14966	YES	YES
104	a	264.09	0.00000	YES	YES
105	a	265.14	0.06236	YES	YES
106	a	265.16	0.00001	YES	YES
107	a	268.60	0.00000	YES	YES
108	a	269.47	0.22915	YES	YES
109	a	269.70	0.00000	YES	YES
110	a	269.88	0.86471	YES	YES
111	a	270.74	0.73690	YES	YES
112	a	271.94	0.00000	YES	YES
113	a	272.77	0.39545	YES	YES
114	a	273.14	0.00000	YES	YES
115	a	277.15	0.65949	YES	YES
116	a	277.88	0.00000	YES	YES
117	a	281.25	0.00000	YES	YES
118	a	281.76	1.29836	YES	YES
119	a	282.51	0.41037	YES	YES
120	a	282.71	0.00000	YES	YES
121	a	284.05	0.00000	YES	YES
122	a	284.75	1.48644	YES	YES
123	a	286.62	0.26303	YES	YES
124	a	286.78	0.00000	YES	YES
125	a	289.49	1.77433	YES	YES
126	a	290.06	0.00000	YES	YES
127	a	366.38	10.83773	YES	YES

128	a	367.76	0.00001	YES	YES
129	a	373.03	17.05143	YES	YES
130	a	374.89	0.00000	YES	YES
131	a	377.72	0.00000	YES	YES
132	a	378.83	18.03046	YES	YES
133	a	380.50	13.55802	YES	YES
134	a	381.47	0.00000	YES	YES
135	a	384.16	7.89991	YES	YES
136	a	384.82	0.00000	YES	YES
137	a	392.54	0.00000	YES	YES
138	a	393.00	4.22449	YES	YES
139	a	433.22	0.00001	YES	YES
140	a	435.35	557.32717	YES	YES
141	a	440.04	0.00001	YES	YES
142	a	443.50	403.84361	YES	YES
143	a	466.00	337.40917	YES	YES
144	a	480.97	0.00000	YES	YES
145	a	541.26	0.00001	YES	YES
146	a	541.31	0.62164	YES	YES
147	a	543.14	0.00000	YES	YES
148	a	543.18	0.44269	YES	YES
149	a	543.55	0.00000	YES	YES
150	a	543.60	0.88061	YES	YES
151	a	544.33	0.79204	YES	YES
152	a	544.37	0.00001	YES	YES
153	a	545.51	0.03848	YES	YES
154	a	545.55	0.00000	YES	YES
155	a	545.84	0.03894	YES	YES
156	a	546.14	0.00000	YES	YES
157	a	547.81	0.00476	YES	YES
158	a	547.81	0.73820	YES	YES
159	a	549.10	0.00000	YES	YES
160	a	549.24	0.15870	YES	YES
161	a	549.50	0.00009	YES	YES
162	a	549.51	0.13762	YES	YES
163	a	578.59	0.70137	YES	YES
164	a	578.60	0.03188	YES	YES
165	a	582.05	8.29036	YES	YES
166	a	582.06	0.18057	YES	YES
167	a	585.53	0.00031	YES	YES
168	a	585.59	1.30034	YES	YES
169	a	586.45	22.59256	YES	YES
170	a	586.55	0.00032	YES	YES
171	a	591.37	0.13662	YES	YES
172	a	591.37	4.31697	YES	YES
173	a	592.87	5.75808	YES	YES
174	a	593.04	0.00003	YES	YES
175	a	594.08	15.55548	YES	YES
176	a	594.18	0.00005	YES	YES
177	a	594.97	10.97109	YES	YES
178	a	595.38	0.00000	YES	YES
179	a	596.87	10.60876	YES	YES
180	a	597.18	0.00000	YES	YES
181	a	795.66	0.00000	YES	YES
182	a	795.82	4.07705	YES	YES
183	a	799.10	0.00000	YES	YES
184	a	799.22	4.14353	YES	YES
185	a	800.43	0.00002	YES	YES
186	a	800.53	4.82541	YES	YES
187	a	802.37	0.96012	YES	YES
188	a	802.72	0.00000	YES	YES
189	a	803.10	18.13349	YES	YES
190	a	803.14	0.00032	YES	YES
191	a	806.67	4.83740	YES	YES
192	a	806.79	0.00006	YES	YES
193	a	918.89	2.73260	YES	YES
194	a	919.20	0.00001	YES	YES
195	a	919.51	0.00000	YES	YES
196	a	919.90	1.86859	YES	YES
197	a	920.21	0.00025	YES	YES
198	a	920.25	1.66766	YES	YES
199	a	928.91	0.00001	YES	YES
200	a	929.11	3.25470	YES	YES
201	a	930.55	1.71549	YES	YES
202	a	931.01	0.00000	YES	YES
203	a	940.46	0.00019	YES	YES
204	a	940.55	1.19991	YES	YES
205	a	984.61	8.24329	YES	YES

206	a	984.75	0.00002	YES	YES
207	a	986.96	15.63814	YES	YES
208	a	986.99	0.00711	YES	YES
209	a	989.30	8.71965	YES	YES
210	a	989.40	0.00010	YES	YES
211	a	990.84	7.28615	YES	YES
212	a	990.88	0.00208	YES	YES
213	a	991.59	3.37691	YES	YES
214	a	991.61	0.00139	YES	YES
215	a	993.09	0.00160	YES	YES
216	a	993.12	4.94817	YES	YES
217	a	993.21	5.28694	YES	YES
218	a	993.32	0.00011	YES	YES
219	a	994.12	1.57048	YES	YES
220	a	994.12	0.00009	YES	YES
221	a	994.80	1.72117	YES	YES
222	a	994.81	0.00964	YES	YES
223	a	997.06	0.00000	YES	YES
224	a	997.51	0.52739	YES	YES
225	a	998.66	1.67755	YES	YES
226	a	998.88	0.00000	YES	YES
227	a	999.99	0.53902	YES	YES
228	a	999.99	0.00274	YES	YES
229	a	1002.00	0.00000	YES	YES
230	a	1002.02	0.01994	YES	YES
231	a	1003.06	0.65587	YES	YES
232	a	1003.50	0.00000	YES	YES
233	a	1005.29	0.00000	YES	YES
234	a	1005.52	0.21210	YES	YES
235	a	1046.92	0.00000	YES	YES
236	a	1047.22	3.65884	YES	YES
237	a	1048.72	0.00001	YES	YES
238	a	1048.89	4.02535	YES	YES
239	a	1049.06	0.40757	YES	YES
240	a	1049.08	0.00017	YES	YES
241	a	1050.42	1.12311	YES	YES
242	a	1050.64	0.00000	YES	YES
243	a	1051.09	1.88726	YES	YES
244	a	1051.17	0.00000	YES	YES
245	a	1052.00	2.74485	YES	YES
246	a	1052.45	0.00000	YES	YES
247	a	1073.32	0.00000	YES	YES
248	a	1073.67	0.69513	YES	YES
249	a	1075.09	2.12634	YES	YES
250	a	1075.31	0.00001	YES	YES
251	a	1076.35	1.00484	YES	YES
252	a	1076.42	0.00003	YES	YES
253	a	1162.24	0.03880	YES	YES
254	a	1162.24	1.13311	YES	YES
255	a	1163.24	0.00001	YES	YES
256	a	1163.37	0.48593	YES	YES
257	a	1164.09	0.00000	YES	YES
258	a	1164.17	0.44961	YES	YES
259	a	1165.01	0.58352	YES	YES
260	a	1165.31	0.00000	YES	YES
261	a	1167.60	1.09200	YES	YES
262	a	1167.63	0.00019	YES	YES
263	a	1170.83	0.00000	YES	YES
264	a	1171.05	0.33560	YES	YES
265	a	1337.42	0.00000	YES	YES
266	a	1337.68	3.29875	YES	YES
267	a	1339.18	3.64410	YES	YES
268	a	1339.21	0.00016	YES	YES
269	a	1339.51	0.20266	YES	YES
270	a	1339.98	0.00000	YES	YES
271	a	1340.63	1.52930	YES	YES
272	a	1340.89	0.00000	YES	YES
273	a	1341.14	3.57143	YES	YES
274	a	1341.42	0.00000	YES	YES
275	a	1342.52	3.44987	YES	YES
276	a	1342.61	0.00000	YES	YES
277	a	1343.39	0.00000	YES	YES
278	a	1344.31	0.81239	YES	YES
279	a	1344.85	13.40646	YES	YES
280	a	1345.01	0.00005	YES	YES
281	a	1346.02	17.32133	YES	YES
282	a	1346.09	0.00104	YES	YES
283	a	1346.79	14.59009	YES	YES

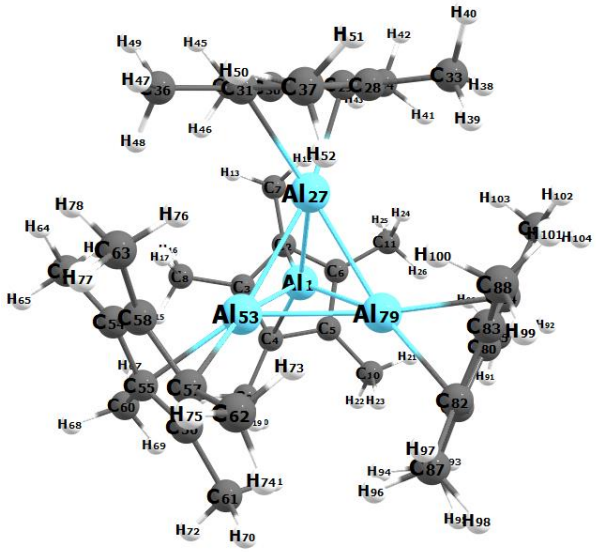
284	a	1347.09	0.00004	YES	YES
285	a	1347.65	14.43115	YES	YES
286	a	1348.00	0.00006	YES	YES
287	a	1349.02	0.00197	YES	YES
288	a	1349.07	14.63373	YES	YES
289	a	1350.78	0.00000	YES	YES
290	a	1351.47	0.90306	YES	YES
291	a	1352.28	0.00001	YES	YES
292	a	1352.56	1.87933	YES	YES
293	a	1353.91	3.11760	YES	YES
294	a	1353.92	0.00294	YES	YES
295	a	1380.42	0.00002	YES	YES
296	a	1380.62	6.17916	YES	YES
297	a	1381.70	4.06903	YES	YES
298	a	1382.06	0.00000	YES	YES
299	a	1383.00	0.00000	YES	YES
300	a	1383.64	12.01632	YES	YES
301	a	1387.61	0.53153	YES	YES
302	a	1387.75	0.00001	YES	YES
303	a	1390.26	0.00001	YES	YES
304	a	1390.36	9.47947	YES	YES
305	a	1390.99	0.00000	YES	YES
306	a	1391.55	8.99693	YES	YES
307	a	1391.84	3.91140	YES	YES
308	a	1393.24	0.00000	YES	YES
309	a	1393.47	3.14781	YES	YES
310	a	1393.92	0.00000	YES	YES
311	a	1394.50	0.00000	YES	YES
312	a	1395.37	7.33843	YES	YES
313	a	1395.74	0.00004	YES	YES
314	a	1395.85	1.15981	YES	YES
315	a	1395.96	0.00000	YES	YES
316	a	1396.31	15.08295	YES	YES
317	a	1397.37	0.00002	YES	YES
318	a	1398.12	26.30243	YES	YES
319	a	1398.40	17.13530	YES	YES
320	a	1398.82	0.00005	YES	YES
321	a	1399.25	49.05136	YES	YES
322	a	1399.28	0.00256	YES	YES
323	a	1401.07	0.00002	YES	YES
324	a	1401.22	3.64321	YES	YES
325	a	1401.80	1.54567	YES	YES
326	a	1402.08	0.00000	YES	YES
327	a	1402.68	2.66578	YES	YES
328	a	1403.87	11.96451	YES	YES
329	a	1403.94	0.00034	YES	YES
330	a	1404.48	0.00002	YES	YES
331	a	1405.80	6.15614	YES	YES
332	a	1405.80	0.06767	YES	YES
333	a	1406.30	7.68269	YES	YES
334	a	1406.41	0.00001	YES	YES
335	a	1407.93	17.89689	YES	YES
336	a	1408.03	0.00003	YES	YES
337	a	1408.67	18.81068	YES	YES
338	a	1408.71	0.00136	YES	YES
339	a	1409.71	0.00001	YES	YES
340	a	1409.92	37.24402	YES	YES
341	a	1411.03	49.80652	YES	YES
342	a	1411.09	0.00202	YES	YES
343	a	1411.60	81.19542	YES	YES
344	a	1412.02	0.00001	YES	YES
345	a	1412.64	0.00002	YES	YES
346	a	1413.03	165.57374	YES	YES
347	a	1414.86	0.00009	YES	YES
348	a	1415.36	23.77709	YES	YES
349	a	1415.42	0.00135	YES	YES
350	a	1416.10	96.53735	YES	YES
351	a	1418.25	23.19811	YES	YES
352	a	1418.88	0.00000	YES	YES
353	a	1420.31	55.25718	YES	YES
354	a	1420.90	0.00018	YES	YES
355	a	1431.04	26.07728	YES	YES
356	a	1431.45	0.00001	YES	YES
357	a	1437.25	0.00000	YES	YES
358	a	1437.86	6.72648	YES	YES
359	a	1439.55	10.53935	YES	YES
360	a	1439.80	0.00000	YES	YES
361	a	1442.49	0.00085	YES	YES

362	a	1442.56	1.62119	YES	YES
363	a	1446.03	0.39202	YES	YES
364	a	1446.05	0.00015	YES	YES
365	a	1448.04	3.06730	YES	YES
366	a	1448.33	0.00000	YES	YES
367	a	1448.92	3.91060	YES	YES
368	a	1449.17	0.00001	YES	YES
369	a	1450.01	2.84498	YES	YES
370	a	1450.22	0.00000	YES	YES
371	a	1451.93	0.00000	YES	YES
372	a	1452.27	3.79312	YES	YES
373	a	1478.07	34.35231	YES	YES
374	a	1478.49	0.00000	YES	YES
375	a	1481.65	0.00000	YES	YES
376	a	1481.92	30.83480	YES	YES
377	a	1485.57	24.99663	YES	YES
378	a	1485.69	0.00037	YES	YES
379	a	1487.46	0.00083	YES	YES
380	a	1487.62	24.56538	YES	YES
381	a	1490.85	0.00000	YES	YES
382	a	1491.04	30.68069	YES	YES
383	a	1491.94	20.28245	YES	YES
384	a	1492.04	0.00034	YES	YES
385	a	2947.71	0.03436	YES	YES
386	a	2947.72	27.54493	YES	YES
387	a	2955.03	0.00155	YES	YES
388	a	2955.06	13.71254	YES	YES
389	a	2958.18	14.91477	YES	YES
390	a	2958.19	0.76598	YES	YES
391	a	2958.39	21.51756	YES	YES
392	a	2958.40	0.30642	YES	YES
393	a	2959.70	0.12241	YES	YES
394	a	2959.70	19.13567	YES	YES
395	a	2961.49	23.03449	YES	YES
396	a	2961.49	0.02030	YES	YES
397	a	2962.26	0.00475	YES	YES
398	a	2962.27	20.60425	YES	YES
399	a	2966.87	0.00108	YES	YES
400	a	2966.97	17.43947	YES	YES
401	a	2967.01	48.99780	YES	YES
402	a	2967.04	0.00423	YES	YES
403	a	2967.54	39.26420	YES	YES
404	a	2967.56	0.00850	YES	YES
405	a	2967.62	0.13434	YES	YES
406	a	2967.63	9.51458	YES	YES
407	a	2969.46	22.45237	YES	YES
408	a	2969.47	0.05783	YES	YES
409	a	2970.88	32.42246	YES	YES
410	a	2970.89	0.06066	YES	YES
411	a	2971.03	16.35909	YES	YES
412	a	2971.04	0.15420	YES	YES
413	a	2971.72	21.43573	YES	YES
414	a	2971.73	0.07049	YES	YES
415	a	3023.00	9.16524	YES	YES
416	a	3023.02	0.00027	YES	YES
417	a	3024.30	8.77021	YES	YES
418	a	3024.31	1.60324	YES	YES
419	a	3028.20	4.58031	YES	YES
420	a	3028.20	8.49108	YES	YES
421	a	3028.52	4.53171	YES	YES
422	a	3028.53	0.00424	YES	YES
423	a	3031.51	0.01555	YES	YES
424	a	3031.51	17.38841	YES	YES
425	a	3032.99	0.29047	YES	YES
426	a	3033.00	0.00001	YES	YES
427	a	3034.24	0.00060	YES	YES
428	a	3034.25	8.37343	YES	YES
429	a	3039.10	0.08649	YES	YES
430	a	3039.10	6.56056	YES	YES
431	a	3040.37	8.53903	YES	YES
432	a	3040.38	0.00768	YES	YES
433	a	3041.71	0.13730	YES	YES
434	a	3041.72	1.69645	YES	YES
435	a	3042.25	2.91061	YES	YES
436	a	3042.26	0.03243	YES	YES
437	a	3043.85	4.40877	YES	YES
438	a	3043.85	4.54403	YES	YES
439	a	3044.84	5.70343	YES	YES

440	a	3044.84	0.68927	YES	YES
441	a	3045.96	0.00386	YES	YES
442	a	3046.03	12.28868	YES	YES
443	a	3048.87	2.03671	YES	YES
444	a	3048.88	0.02543	YES	YES
445	a	3063.24	0.26766	YES	YES
446	a	3063.25	7.72390	YES	YES
447	a	3066.93	0.00418	YES	YES
448	a	3066.99	12.00227	YES	YES
449	a	3070.74	0.94480	YES	YES
450	a	3070.75	3.21091	YES	YES
451	a	3072.04	0.00302	YES	YES
452	a	3072.06	8.16910	YES	YES
453	a	3073.16	1.40792	YES	YES
454	a	3073.16	12.80498	YES	YES
455	a	3073.57	0.14711	YES	YES
456	a	3073.58	8.48294	YES	YES
457	a	3077.18	1.05117	YES	YES
458	a	3077.18	7.33295	YES	YES
459	a	3078.72	0.78943	YES	YES
460	a	3078.72	11.08112	YES	YES
461	a	3082.10	4.10560	YES	YES
462	a	3082.10	0.41173	YES	YES
463	a	3084.01	0.42562	YES	YES
464	a	3084.02	6.99251	YES	YES
465	a	3085.68	0.05418	YES	YES
466	a	3085.69	5.63266	YES	YES
467	a	3085.77	6.85952	YES	YES
468	a	3085.77	0.16259	YES	YES
469	a	3086.53	3.36904	YES	YES
470	a	3086.53	5.62447	YES	YES
471	a	3088.28	4.03702	YES	YES
472	a	3088.29	0.02194	YES	YES
473	a	3102.99	1.29795	YES	YES
474	a	3103.00	0.00566	YES	YES

$end

[(AlCp*)$_4$]



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

Symmetry: c1

Cartesian coordinates in Ångström:

Al	4.7942950	5.0790550	7.2666824
C	3.4937503	5.5197319	9.1696205
C	3.2094391	6.5387150	8.1963420
C	4.4165175	7.2857355	7.9697539
C	5.4468136	6.7285630	8.8029617
C	4.8766314	5.6369876	9.5443613
C	2.5047481	4.5438781	9.7408564
C	1.8712026	6.8141755	7.5717900
C	4.5597504	8.4781094	7.0673427
C	6.8552496	7.2368473	8.9238032
C	5.5849219	4.8048530	10.5752064
H	2.9898462	3.5953492	10.0446605
H	1.7072420	4.2922856	9.0142937
H	2.0062888	4.9604880	10.6431677
H	1.9709762	7.2473640	6.5570060
H	1.2862263	7.5375043	8.1806587
H	1.2606496	5.8940985	7.4822615
H	3.8718095	8.4243951	6.2006001
H	5.5893944	8.5729624	6.6696594
H	4.3301681	9.4210080	7.6098794
H	7.5641102	6.4281417	9.1900203
H	6.9339875	8.0147413	9.7142500
H	7.2111463	7.6938923	7.9794716
H	5.1659618	3.7811542	10.6375342
H	5.4949269	5.2578544	11.5865419
H	6.6665670	4.7090897	10.3556545

SCF energy GEOOPT = -632.2715013140 H

ZPE = 563.5 kJ/mol

FREEH energy = 600.57 kJ/mol

FREEH entropy = 0.48100 kJ/mol/K

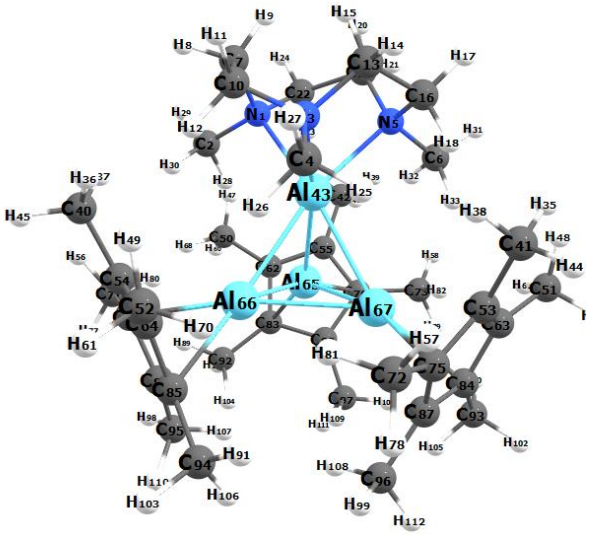
$vibrational spectrum

# mode	symmetry	wave number 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	93.85	0.00098	YES	YES
8	a	95.73	0.00075	YES	YES
9	a	110.60	0.08440	YES	YES
10	a	114.26	0.08981	YES	YES
11	a	117.50	0.00230	YES	YES
12	a	150.18	0.00005	YES	YES
13	a	150.35	0.00007	YES	YES
14	a	169.23	0.05382	YES	YES
15	a	169.99	0.05312	YES	YES
16	a	178.31	1.61169	YES	YES
17	a	271.86	0.10475	YES	YES
18	a	274.84	0.06538	YES	YES
19	a	277.00	0.43208	YES	YES
20	a	277.12	0.51002	YES	YES
21	a	379.95	3.40203	YES	YES
22	a	380.09	3.39259	YES	YES
23	a	399.72	114.44140	YES	YES
24	a	542.39	0.00004	YES	YES
25	a	542.54	0.00001	YES	YES

26	a	544.07	0.00012	YES	YES
27	a	577.25	0.00000	YES	YES
28	a	577.32	0.00004	YES	YES
29	a	590.72	2.79551	YES	YES
30	a	799.98	3.83572	YES	YES
31	a	801.13	3.81134	YES	YES
32	a	922.45	0.00060	YES	YES
33	a	924.03	0.00006	YES	YES
34	a	993.91	7.15065	YES	YES
35	a	994.11	7.15438	YES	YES
36	a	1000.54	0.01489	YES	YES
37	a	1000.60	0.00621	YES	YES
38	a	1001.10	0.05180	YES	YES
39	a	1046.07	1.79150	YES	YES
40	a	1046.96	1.80373	YES	YES
41	a	1073.46	0.00091	YES	YES
42	a	1164.10	0.00001	YES	YES
43	a	1164.36	0.00008	YES	YES
44	a	1340.17	0.16384	YES	YES
45	a	1341.45	0.00155	YES	YES
46	a	1346.21	1.46406	YES	YES
47	a	1347.46	1.44571	YES	YES
48	a	1350.80	5.69176	YES	YES
49	a	1391.01	0.00038	YES	YES
50	a	1391.12	0.00120	YES	YES
51	a	1401.42	9.81779	YES	YES
52	a	1401.79	9.74744	YES	YES
53	a	1403.42	0.23077	YES	YES
54	a	1403.94	0.04765	YES	YES
55	a	1405.83	0.00103	YES	YES
56	a	1407.80	0.19744	YES	YES
57	a	1408.85	0.07348	YES	YES
58	a	1414.41	38.92017	YES	YES
59	a	1442.19	0.03081	YES	YES
60	a	1452.91	0.00086	YES	YES
61	a	1452.99	0.00038	YES	YES
62	a	1492.00	13.61848	YES	YES
63	a	1492.26	13.58872	YES	YES
64	a	2952.64	33.37904	YES	YES
65	a	2952.84	33.32803	YES	YES
66	a	2952.87	70.15541	YES	YES
67	a	2952.97	47.07046	YES	YES
68	a	2954.27	26.44482	YES	YES
69	a	3026.79	28.06994	YES	YES
70	a	3027.10	5.14003	YES	YES
71	a	3027.25	4.32737	YES	YES
72	a	3028.46	0.15283	YES	YES
73	a	3028.70	0.03439	YES	YES
74	a	3058.52	2.22196	YES	YES
75	a	3058.85	2.69835	YES	YES
76	a	3059.08	4.32815	YES	YES
77	a	3059.51	22.71835	YES	YES
78	a	3059.85	22.98720	YES	YES

$end

$[(Me_3TACN)Al(AlCp^*)_3]^+$



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

Symmetry: c1

Cartesian coordinates in Ångström:

N	-2.0430972	2.3364798	15.5351394
C	-2.5926762	1.0555079	16.0230238
N	-0.6216260	3.0048000	13.1593342
C	-0.2850350	2.5835513	11.7844442
N	-2.6203038	4.7663921	14.1663356
C	-3.8960404	5.4510038	13.8752319
C	-0.5546339	2.3273240	15.5483141
H	-0.1726674	1.5424744	16.2336485
H	-0.1854892	3.2882714	15.9554769
C	-0.0023481	2.0889117	14.1453364
H	1.1081336	2.1749992	14.1447957
H	-0.2570057	1.0621115	13.8183606
C	-0.2852092	4.4372373	13.3851005
H	0.4538179	4.7900305	12.6360123
H	0.2083815	4.5472230	14.3697930
C	-1.5381680	5.3062254	13.3106145
H	-1.2954677	6.3613188	13.5722316
H	-1.9292202	5.3013333	12.2748585
C	-2.3038428	4.8054083	15.6203885
H	-1.2337906	5.0544626	15.7563307
H	-2.8690116	5.6170964	16.1237314
C	-2.6345625	3.4703259	16.2828355
H	-3.7305252	3.3135357	16.2695896
H	-2.3095271	3.4740929	17.3481478
H	-0.8114963	3.2307227	11.0608886
H	-0.6536010	1.5540681	11.6253104
H	0.8114115	2.6298118	11.6059796
H	-3.6895675	1.0629653	15.8901722
H	-2.3371672	0.8883593	17.0921474
H	-2.1984112	0.2269515	15.4083793
H	-3.8317885	6.5372116	14.1038658
H	-4.7060908	4.9895039	14.4672305
H	-4.1480675	5.3001097	12.8100188
H	-5.6973480	3.0853004	17.1642295
H	-2.4284745	6.1896681	10.3579033
H	0.1871970	-0.9825031	13.2385608
H	-0.9779495	-1.0438995	14.5973452
H	-1.3574744	4.7888602	10.0449476
H	-5.7886302	4.4154450	15.9683943
C	-0.7200262	-1.4928783	13.6167784
C	-2.2650021	5.3196527	9.6924236
C	-6.3234712	3.5289632	16.3656262
Al	-2.8128971	2.6516347	13.4562842
H	-2.0158105	5.7320660	8.6910333
H	-0.4262829	-2.5445635	13.8231330
H	-7.2398438	3.9145736	16.8620774
H	-5.5260543	0.9468015	17.3352388
H	-4.4240251	6.7177570	10.9682715
H	0.3572734	-0.5003181	11.1483028
C	-6.1290228	0.3284796	16.6420140
C	-5.2604979	6.1285722	10.5443274
C	-0.4589806	-0.8343442	10.4785915
C	-3.4758331	4.4350614	9.6232783
C	-1.8468560	-1.4340099	12.6267642
C	-6.6690164	2.5245776	15.3049251
H	-2.9774982	-2.4818286	14.9340461
H	-1.4867112	3.0287949	8.2945030
H	-7.5592329	4.9551046	14.3050624
H	-5.7212401	6.7532298	9.7488899

H	-6.9945861	-0.0542813	17.2247204
H	-0.0830174	-1.7291488	9.9370561
C	-6.5885368	1.1001419	15.4396065
C	-4.8087596	4.8063471	9.9962817
C	-1.7205536	-1.1492493	11.2280418
Al	-5.3239119	1.7139060	13.4684323
Al	-3.3605686	0.3854562	12.1343109
Al	-4.2581232	2.7792084	11.2036297
H	-5.5213932	-0.5565319	16.3623638
H	-6.0277111	6.0114656	11.3369713
H	-0.6138177	-0.0453933	9.7141466
C	-3.7773290	-2.1966172	14.2239431
C	-2.3496681	2.3623332	8.4853289
C	-7.5706048	4.1949950	13.5004203
C	-3.2118790	-1.8076337	12.8870969
C	-3.5250610	3.1270447	9.0254628
C	-7.2853223	2.8213371	14.0388626
H	-4.4622045	-3.0638861	14.1369869
H	-2.5966104	1.8638275	7.5265980
H	-8.5682361	4.2423795	13.0196282
H	-4.3576749	-1.3708246	14.6913919
H	-2.0077520	1.5681836	9.1852740
H	-6.8266052	4.5095597	12.7357825
C	-7.1612563	0.5103215	14.2613380
C	-5.6885023	3.7330101	9.6243329
C	-3.0045859	-1.3527897	10.6164101
C	-3.9251350	-1.7731604	11.6377369
C	-4.8989363	2.6993247	9.0115123
C	-7.6053066	1.5723015	13.3999697
H	-6.5862407	-1.5830326	14.4046596
H	-7.5575058	4.2368103	10.6175330
H	-2.7689572	-0.4850626	8.6355108
C	-7.4287669	-0.9518983	14.0629983
C	-7.1864325	3.7754840	9.6824346
C	-3.2798774	-1.3258234	9.1425401
C	-5.3650199	-2.1294835	11.4082928
C	-5.4429102	1.4210188	8.4430528
C	-8.3007581	1.3816742	12.0835204
H	-5.7880804	-2.6708830	12.2742724
H	-4.6937228	0.9118573	7.8095840
H	-8.7654246	2.3218534	11.7342728
H	-8.3243907	-1.2661332	14.6415325
H	-7.5921202	4.3776458	8.8407525
H	-2.9198028	-2.2610687	8.6616936
H	-7.6211406	-1.1938535	13.0021933
H	-7.6287633	2.7657475	9.6076082
H	-4.3604462	-1.2405202	8.9283479
H	-5.9977214	-1.2293627	11.2427618
H	-5.7425559	0.7034076	9.2387091
H	-7.6021571	1.0445327	11.2860763
H	-5.4783828	-2.7807200	10.5187633
H	-9.1030160	0.6210737	12.1624863
H	-6.3370360	1.6113212	7.8163866

SCF energy GEOOPT = -2658.723053696 H

ZPE = 2496. kJ/mol

FREEH energy = 2654.20 kJ/mol

FREEH entropy = 1.32835 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	24.76	0.12432	YES YES
8	a	32.85	0.09116	YES YES
9	a	33.85	0.08330	YES YES
10	a	42.02	0.18628	YES YES
11	a	42.43	0.00801	YES YES
12	a	49.01	0.05052	YES YES
13	a	56.87	0.07412	YES YES
14	a	61.77	0.15007	YES YES
15	a	64.67	0.08015	YES YES
16	a	68.53	0.32839	YES YES

17	a	74.72	0.05154	YES	YES
18	a	79.47	0.16462	YES	YES
19	a	83.47	0.22820	YES	YES
20	a	88.90	0.25696	YES	YES
21	a	97.31	0.17263	YES	YES
22	a	97.96	0.35905	YES	YES
23	a	103.41	0.05569	YES	YES
24	a	107.88	0.09489	YES	YES
25	a	111.61	0.37688	YES	YES
26	a	113.27	0.54841	YES	YES
27	a	118.77	0.44714	YES	YES
28	a	124.89	0.09047	YES	YES
29	a	126.16	0.16406	YES	YES
30	a	128.39	0.02887	YES	YES
31	a	136.07	0.22153	YES	YES
32	a	138.80	0.02866	YES	YES
33	a	141.00	0.08679	YES	YES
34	a	143.05	0.24258	YES	YES
35	a	145.68	0.18980	YES	YES
36	a	148.38	8.30259	YES	YES
37	a	149.15	2.45696	YES	YES
38	a	153.76	6.94866	YES	YES
39	a	157.67	0.15373	YES	YES
40	a	160.92	1.02831	YES	YES
41	a	163.01	0.50941	YES	YES
42	a	165.12	0.22380	YES	YES
43	a	169.09	0.16534	YES	YES
44	a	174.06	1.57132	YES	YES
45	a	174.39	0.86165	YES	YES
46	a	182.61	0.06430	YES	YES
47	a	184.82	0.26838	YES	YES
48	a	186.06	0.17230	YES	YES
49	a	189.52	0.98572	YES	YES
50	a	190.01	0.82754	YES	YES
51	a	195.22	5.53318	YES	YES
52	a	201.68	0.73173	YES	YES
53	a	202.94	0.15457	YES	YES
54	a	215.91	2.60578	YES	YES
55	a	218.83	1.30965	YES	YES
56	a	220.21	1.26691	YES	YES
57	a	238.73	9.11988	YES	YES
58	a	239.04	1.03848	YES	YES
59	a	241.47	6.24244	YES	YES
60	a	245.04	2.81205	YES	YES
61	a	247.13	0.13527	YES	YES
62	a	259.82	7.86919	YES	YES
63	a	264.44	3.17229	YES	YES
64	a	265.45	3.97497	YES	YES
65	a	267.63	2.57294	YES	YES
66	a	271.06	1.01749	YES	YES
67	a	272.86	1.13557	YES	YES
68	a	274.68	0.49945	YES	YES
69	a	278.35	0.76410	YES	YES
70	a	278.95	0.78896	YES	YES
71	a	280.53	1.26665	YES	YES
72	a	282.45	1.24505	YES	YES
73	a	285.03	9.27113	YES	YES
74	a	286.54	4.59235	YES	YES
75	a	289.13	6.74848	YES	YES
76	a	291.44	17.29626	YES	YES
77	a	292.36	10.14156	YES	YES
78	a	319.48	138.03823	YES	YES
79	a	321.41	8.10114	YES	YES
80	a	323.76	12.96405	YES	YES
81	a	336.61	48.38835	YES	YES
82	a	337.37	51.86975	YES	YES
83	a	338.85	11.05704	YES	YES
84	a	357.78	22.40892	YES	YES
85	a	361.06	31.98888	YES	YES
86	a	361.35	39.89567	YES	YES
87	a	383.27	101.37289	YES	YES
88	a	385.46	185.59980	YES	YES
89	a	385.71	159.62169	YES	YES
90	a	389.02	103.46693	YES	YES
91	a	389.51	86.60572	YES	YES
92	a	417.47	10.41830	YES	YES
93	a	437.12	0.49561	YES	YES
94	a	438.33	0.54994	YES	YES

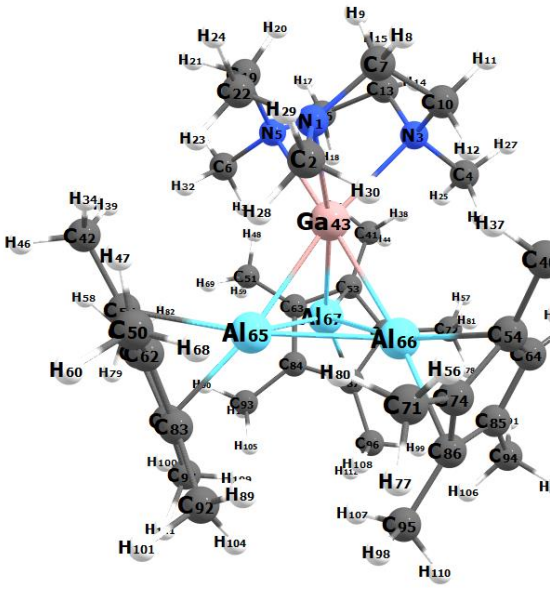
95	a	468.78	8.14126	YES	YES
96	a	486.87	1.01076	YES	YES
97	a	539.97	0.12275	YES	YES
98	a	540.29	0.50088	YES	YES
99	a	540.58	0.45980	YES	YES
100	a	544.91	0.05708	YES	YES
101	a	545.04	0.06020	YES	YES
102	a	545.85	0.01343	YES	YES
103	a	546.75	0.06220	YES	YES
104	a	547.12	0.00311	YES	YES
105	a	547.53	0.00827	YES	YES
106	a	561.22	4.51171	YES	YES
107	a	561.75	4.35039	YES	YES
108	a	572.52	0.98563	YES	YES
109	a	573.25	1.26809	YES	YES
110	a	574.00	1.09051	YES	YES
111	a	580.56	1.75695	YES	YES
112	a	581.20	0.99457	YES	YES
113	a	582.25	1.49323	YES	YES
114	a	586.15	0.43116	YES	YES
115	a	593.64	14.44990	YES	YES
116	a	594.03	14.70580	YES	YES
117	a	597.29	4.10394	YES	YES
118	a	731.50	11.58304	YES	YES
119	a	732.65	11.70608	YES	YES
120	a	768.84	59.83178	YES	YES
121	a	797.62	1.16015	YES	YES
122	a	798.06	3.54983	YES	YES
123	a	799.44	3.71847	YES	YES
124	a	803.54	2.74355	YES	YES
125	a	804.09	2.98561	YES	YES
126	a	804.54	3.16562	YES	YES
127	a	845.15	0.48774	YES	YES
128	a	889.88	6.12099	YES	YES
129	a	890.84	6.01671	YES	YES
130	a	919.74	1.16611	YES	YES
131	a	920.63	0.92566	YES	YES
132	a	921.10	0.90513	YES	YES
133	a	932.06	0.29898	YES	YES
134	a	933.24	0.43227	YES	YES
135	a	934.64	0.47987	YES	YES
136	a	970.01	10.02720	YES	YES
137	a	970.40	9.83268	YES	YES
138	a	978.28	12.21923	YES	YES
139	a	983.35	2.19427	YES	YES
140	a	984.16	1.63935	YES	YES
141	a	984.46	1.52390	YES	YES
142	a	989.78	2.56607	YES	YES
143	a	991.31	2.85872	YES	YES
144	a	991.59	1.33512	YES	YES
145	a	992.90	1.22146	YES	YES
146	a	993.87	0.73871	YES	YES
147	a	994.84	0.57919	YES	YES
148	a	999.62	0.33372	YES	YES
149	a	1000.73	0.19297	YES	YES
150	a	1001.14	0.84967	YES	YES
151	a	1002.77	21.48370	YES	YES
152	a	1004.20	21.07742	YES	YES
153	a	1007.89	0.85504	YES	YES
154	a	1009.03	0.71906	YES	YES
155	a	1009.63	0.47147	YES	YES
156	a	1011.75	0.08334	YES	YES
157	a	1026.59	1.41216	YES	YES
158	a	1044.45	2.24647	YES	YES
159	a	1044.68	2.44275	YES	YES
160	a	1045.60	1.55993	YES	YES
161	a	1047.39	1.18534	YES	YES
162	a	1047.68	0.68582	YES	YES
163	a	1048.28	0.80678	YES	YES
164	a	1053.73	13.23338	YES	YES
165	a	1054.16	13.08255	YES	YES
166	a	1070.96	0.36054	YES	YES
167	a	1071.17	0.40058	YES	YES
168	a	1071.84	0.29747	YES	YES
169	a	1080.42	37.26636	YES	YES
170	a	1101.20	2.45295	YES	YES
171	a	1102.29	1.83897	YES	YES
172	a	1104.74	6.24446	YES	YES

173	a	1137.13	7.73280	YES	YES
174	a	1137.92	7.16111	YES	YES
175	a	1161.39	0.00243	YES	YES
176	a	1162.55	0.16349	YES	YES
177	a	1163.12	0.16674	YES	YES
178	a	1166.20	0.02222	YES	YES
179	a	1167.01	0.07843	YES	YES
180	a	1167.35	0.08968	YES	YES
181	a	1199.78	2.16077	YES	YES
182	a	1200.33	2.09099	YES	YES
183	a	1215.52	0.69564	YES	YES
184	a	1239.14	0.52715	YES	YES
185	a	1239.92	0.51690	YES	YES
186	a	1267.64	1.49940	YES	YES
187	a	1268.50	22.40515	YES	YES
188	a	1277.21	10.06304	YES	YES
189	a	1277.53	10.09235	YES	YES
190	a	1316.72	2.85897	YES	YES
191	a	1329.06	0.20472	YES	YES
192	a	1329.83	0.15097	YES	YES
193	a	1337.16	0.44140	YES	YES
194	a	1337.59	0.27777	YES	YES
195	a	1338.05	0.33738	YES	YES
196	a	1340.68	0.42799	YES	YES
197	a	1341.38	0.75356	YES	YES
198	a	1341.81	1.00975	YES	YES
199	a	1342.82	2.30504	YES	YES
200	a	1343.57	5.30307	YES	YES
201	a	1344.55	3.09122	YES	YES
202	a	1345.16	2.46408	YES	YES
203	a	1346.06	1.78150	YES	YES
204	a	1346.46	4.14944	YES	YES
205	a	1349.50	0.95576	YES	YES
206	a	1350.01	0.30815	YES	YES
207	a	1351.41	0.32571	YES	YES
208	a	1356.72	15.05204	YES	YES
209	a	1364.18	5.26891	YES	YES
210	a	1365.83	4.71086	YES	YES
211	a	1382.28	0.35046	YES	YES
212	a	1384.29	2.65274	YES	YES
213	a	1385.17	3.33817	YES	YES
214	a	1385.51	2.29728	YES	YES
215	a	1386.22	0.49916	YES	YES
216	a	1386.95	0.74998	YES	YES
217	a	1388.24	8.52855	YES	YES
218	a	1389.34	6.81069	YES	YES
219	a	1393.32	2.56363	YES	YES
220	a	1394.61	20.73703	YES	YES
221	a	1394.63	18.74494	YES	YES
222	a	1395.53	5.57683	YES	YES
223	a	1398.44	3.98591	YES	YES
224	a	1399.18	4.07638	YES	YES
225	a	1401.17	4.01402	YES	YES
226	a	1402.53	8.15185	YES	YES
227	a	1403.33	19.36155	YES	YES
228	a	1403.66	30.15045	YES	YES
229	a	1404.72	10.58366	YES	YES
230	a	1405.30	6.31354	YES	YES
231	a	1405.58	9.91502	YES	YES
232	a	1407.28	0.69535	YES	YES
233	a	1407.85	1.77709	YES	YES
234	a	1409.25	6.70924	YES	YES
235	a	1410.62	10.44552	YES	YES
236	a	1411.25	9.68379	YES	YES
237	a	1411.89	7.61150	YES	YES
238	a	1414.03	25.26110	YES	YES
239	a	1414.51	12.32104	YES	YES
240	a	1414.81	11.95279	YES	YES
241	a	1415.30	30.26748	YES	YES
242	a	1416.39	14.72662	YES	YES
243	a	1417.30	2.77948	YES	YES
244	a	1417.79	4.26693	YES	YES
245	a	1418.17	7.72311	YES	YES
246	a	1420.47	18.95784	YES	YES
247	a	1421.59	5.41039	YES	YES
248	a	1422.73	11.45231	YES	YES
249	a	1423.68	1.43442	YES	YES
250	a	1424.23	13.98989	YES	YES

251	a	1424.86	19.66531	YES	YES
252	a	1425.28	5.55022	YES	YES
253	a	1426.42	6.57703	YES	YES
254	a	1426.64	5.96869	YES	YES
255	a	1439.77	7.53561	YES	YES
256	a	1439.86	8.02034	YES	YES
257	a	1440.87	0.73091	YES	YES
258	a	1441.63	4.75641	YES	YES
259	a	1443.93	4.98837	YES	YES
260	a	1444.33	4.59152	YES	YES
261	a	1448.86	19.14821	YES	YES
262	a	1451.58	0.35113	YES	YES
263	a	1452.60	0.77817	YES	YES
264	a	1452.79	0.73475	YES	YES
265	a	1486.95	2.02161	YES	YES
266	a	1488.20	7.16815	YES	YES
267	a	1488.29	7.37952	YES	YES
268	a	1496.72	5.87365	YES	YES
269	a	1497.43	5.71798	YES	YES
270	a	1497.71	8.12472	YES	YES
271	a	2940.51	23.53576	YES	YES
272	a	2941.04	33.18002	YES	YES
273	a	2942.04	34.21237	YES	YES
274	a	2942.70	49.06591	YES	YES
275	a	2943.22	23.28465	YES	YES
276	a	2943.77	8.98424	YES	YES
277	a	2947.70	3.69410	YES	YES
278	a	2947.87	20.78292	YES	YES
279	a	2948.07	16.32750	YES	YES
280	a	2949.62	48.63790	YES	YES
281	a	2949.78	47.56259	YES	YES
282	a	2950.36	57.31929	YES	YES
283	a	2951.88	21.10782	YES	YES
284	a	2951.92	28.92872	YES	YES
285	a	2952.40	24.66795	YES	YES
286	a	2953.92	19.99256	YES	YES
287	a	2954.03	28.37624	YES	YES
288	a	2954.29	52.82663	YES	YES
289	a	2961.23	27.30799	YES	YES
290	a	2961.44	25.77674	YES	YES
291	a	2961.54	34.17383	YES	YES
292	a	2986.78	6.09396	YES	YES
293	a	2987.12	5.72220	YES	YES
294	a	2989.83	68.84160	YES	YES
295	a	3016.43	8.51411	YES	YES
296	a	3016.59	8.22329	YES	YES
297	a	3016.69	13.34589	YES	YES
298	a	3017.00	13.24327	YES	YES
299	a	3017.35	12.02551	YES	YES
300	a	3017.53	4.47175	YES	YES
301	a	3022.34	2.02804	YES	YES
302	a	3022.41	11.78910	YES	YES
303	a	3022.56	9.97332	YES	YES
304	a	3025.72	12.00284	YES	YES
305	a	3026.07	6.81573	YES	YES
306	a	3026.28	7.06269	YES	YES
307	a	3034.80	8.06808	YES	YES
308	a	3035.18	7.30460	YES	YES
309	a	3036.43	3.59367	YES	YES
310	a	3041.30	3.82317	YES	YES
311	a	3041.55	4.04623	YES	YES
312	a	3041.66	4.10060	YES	YES
313	a	3049.55	0.17286	YES	YES
314	a	3050.39	0.93019	YES	YES
315	a	3051.80	11.56878	YES	YES
316	a	3052.06	7.67997	YES	YES
317	a	3052.36	5.45879	YES	YES
318	a	3052.83	16.55881	YES	YES
319	a	3053.02	12.93741	YES	YES
320	a	3053.51	11.10721	YES	YES
321	a	3054.55	9.84067	YES	YES
322	a	3059.86	6.72973	YES	YES
323	a	3060.02	7.31396	YES	YES
324	a	3060.93	7.14134	YES	YES
325	a	3064.48	6.88476	YES	YES
326	a	3064.77	6.73293	YES	YES
327	a	3065.31	6.15411	YES	YES
328	a	3075.76	6.01482	YES	YES

329	a	3076.54	6.83172	YES	YES
330	a	3076.70	4.14728	YES	YES
331	a	3087.00	5.76237	YES	YES
332	a	3087.21	2.88616	YES	YES
333	a	3087.30	2.38460	YES	YES
334	a	3096.86	0.56396	YES	YES
335	a	3097.38	0.52847	YES	YES
336	a	3097.70	0.42321	YES	YES

$[(Me_3TACN)Ga(AlCp^*)_3]^+$



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

Symmetry: c1

Cartesian coordinates in Ångström:

N	-1.9751311	2.3906802	15.6502623
C	-2.5332876	1.1287076	16.1464637
N	-0.4928810	3.0375719	13.2193151
C	-0.1492538	2.6036198	11.8613955
N	-2.5348033	4.8715451	14.2157350
C	-3.7925823	5.5613973	13.9120488
C	-0.4975961	2.3844818	15.6326623
H	-0.0971589	1.6113448	16.3236674
H	-0.1206584	3.3495917	16.0234474
C	0.0617599	2.1249959	14.2322463
H	1.1772242	2.1692862	14.2650780
H	-0.2128284	1.0999204	13.9154600
C	-0.1903015	4.4657925	13.4477559
H	0.5588717	4.8337045	12.7135072
H	0.2878886	4.5868416	14.4391305
C	-1.4403841	5.3431545	13.3517880
H	-1.1660126	6.4035003	13.5702077
H	-1.8253993	5.3151531	12.3137593
C	-2.2236513	4.8784175	15.6602893
H	-1.1504635	5.1101017	15.8047552
H	-2.7726102	5.6939754	16.1790286
C	-2.5740103	3.5491890	16.3325896
H	-3.6710437	3.4019205	16.2972272
H	-2.2844178	3.5920479	17.4103529
H	-0.6471198	3.2591631	11.1233389
H	-0.5363824	1.5809193	11.6961726
H	0.9502949	2.6186841	11.6823067
H	-3.6285836	1.1286677	15.9929288
H	-2.3088908	0.9667012	17.2257150
H	-2.1262068	0.2846872	15.5596753
H	-3.7292330	6.6557095	14.1117945
H	-4.6108906	5.1281763	14.5162958
H	-4.0532551	5.3942646	12.8503936
H	-5.6782579	3.0685298	17.0925397
H	-2.4503333	6.1189487	10.3818322
H	0.1215511	-0.9453258	13.2280480
H	-1.0663708	-1.0161588	14.5658004
H	-1.4065339	4.7015041	10.0548961
H	-5.7909449	4.3799647	15.8787882
C	-0.7818687	-1.4693260	13.5951228
C	-2.2988083	5.2572795	9.7036134
C	-6.3201146	3.5028623	16.3020482
Ga	-2.8686512	2.6130175	13.4111958
H	-2.0388881	5.6772167	8.7083412
H	-0.4773772	-2.5157137	13.8113816
H	-7.2280041	3.8949257	16.8084922
H	-5.5396121	0.9290840	17.2939585
H	-4.4471579	6.6792142	10.9595338
H	0.3147446	-0.5004355	11.1309719
C	-6.1289844	0.2978331	16.6014900
C	-5.2944537	6.0926098	10.5553478
C	-0.4979305	-0.8191593	10.4503847
C	-3.5226944	4.3934377	9.6169836
C	-1.8952493	-1.4327939	12.5897481
C	-6.6853520	2.4876396	15.2591473
H	-3.0328475	-2.6261036	14.8402055
H	-1.6000806	3.0181727	8.1329174
H	-7.7330423	4.8849459	14.2883669

H	-5.7748225	6.7176422	9.7723695
H	-6.9876732	-0.1025391	17.1819348
H	-0.1227355	-1.7036366	9.8922383
C	-6.6045609	1.0617597	15.4008224
C	-4.8551040	4.7732954	9.9914737
C	-1.7614517	-1.1493080	11.1892094
Al	-5.3557911	1.6814904	13.4851302
Al	-3.3504470	0.3562541	12.0961094
Al	-4.2927838	2.8011153	11.1776212
H	-5.5020437	-0.5729230	16.3206001
H	-6.0405172	5.9719739	11.3671790
H	-0.6496082	-0.0133473	9.7033947
C	-3.8183018	-2.2130066	14.1782612
C	-2.4064690	2.3334162	8.4595467
C	-7.6037158	4.1534612	13.4672962
C	-3.2571711	-1.8253314	12.8399455
C	-3.5830391	3.0937972	9.0014539
C	-7.3197880	2.7781428	14.0003295
H	-4.6038014	-2.9874681	14.0775180
H	-2.6917508	1.7199000	7.5825592
H	-8.5329718	4.1687803	12.8646631
H	-4.2771472	-1.3484805	14.7075801
H	-1.9692844	1.6420681	9.2140753
H	-6.7841086	4.5284986	12.8147692
C	-7.1845510	0.4677322	14.2285951
C	-5.7412539	3.7081219	9.6125534
C	-3.0405759	-1.3619009	10.5712638
C	-3.9648603	-1.7873177	11.5883969
C	-4.9580807	2.6721496	8.9933938
C	-7.6346421	1.5268122	13.3650680
H	-6.6069638	-1.6224049	14.3861166
H	-7.6020766	4.2207438	10.6131459
H	-2.7920553	-0.4939851	8.5935253
C	-7.4485572	-0.9956104	14.0354653
C	-7.2384743	3.7592071	9.6757195
C	-3.3091102	-1.3329797	9.0963903
C	-5.3998267	-2.1566326	11.3467191
C	-5.5135030	1.4023309	8.4161237
C	-8.3414279	1.3271346	12.0555893
H	-5.8327008	-2.6780936	12.2196819
H	-4.7642858	0.8844209	7.7901264
H	-8.7956073	2.2685209	11.6966056
H	-8.3468957	-1.3071732	14.6110432
H	-7.6416856	4.3670027	8.8370654
H	-2.9489864	-2.2693066	8.6179040
H	-7.6360323	-1.2432674	12.9750855
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H	-4.3884245	-1.2458475	8.8764664
H	-6.0366285	-1.2672210	11.1472878
H	-5.8341670	0.6859717	9.2037537
H	-7.6563421	0.9681733	11.2568688
H	-5.4953922	-2.8319606	10.4730840
H	-9.1541523	0.5797079	12.1520220
H	-6.3968019	1.6073875	7.7787870

SCF energy GEOOPT = -4341.229891963 H

ZPE = 2492. kJ/mol

FREEH energy = 2653.10 kJ/mol

FREEH entropy = 1.36149 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	17.67	0.13559	YES YES
8	a	32.32	0.12444	YES YES
9	a	33.20	0.08002	YES YES
10	a	37.57	0.01051	YES YES
11	a	41.31	0.01297	YES YES
12	a	46.95	0.01033	YES YES
13	a	51.22	0.39554	YES YES
14	a	56.62	0.20247	YES YES
15	a	60.18	0.32714	YES YES

16	a	66.08	0.17514	YES	YES
17	a	70.78	0.13457	YES	YES
18	a	72.48	0.09941	YES	YES
19	a	77.06	0.35900	YES	YES
20	a	84.56	0.83971	YES	YES
21	a	89.61	0.02684	YES	YES
22	a	94.21	0.04523	YES	YES
23	a	95.70	0.56476	YES	YES
24	a	97.72	0.08627	YES	YES
25	a	101.14	0.22275	YES	YES
26	a	106.30	0.02154	YES	YES
27	a	109.57	0.73139	YES	YES
28	a	117.10	0.04783	YES	YES
29	a	119.43	0.23901	YES	YES
30	a	123.18	2.98660	YES	YES
31	a	127.77	0.16180	YES	YES
32	a	130.38	0.52675	YES	YES
33	a	133.12	1.83702	YES	YES
34	a	138.58	1.35395	YES	YES
35	a	140.57	0.24544	YES	YES
36	a	144.15	0.28953	YES	YES
37	a	148.33	0.75535	YES	YES
38	a	150.17	1.34633	YES	YES
39	a	154.04	0.04714	YES	YES
40	a	156.70	0.16709	YES	YES
41	a	157.60	14.91668	YES	YES
42	a	159.33	23.79223	YES	YES
43	a	163.95	1.57780	YES	YES
44	a	165.73	0.77627	YES	YES
45	a	166.87	0.14738	YES	YES
46	a	172.93	1.80705	YES	YES
47	a	174.64	1.46456	YES	YES
48	a	176.57	3.06310	YES	YES
49	a	179.45	0.62141	YES	YES
50	a	179.79	0.24147	YES	YES
51	a	181.85	0.05313	YES	YES
52	a	189.36	0.79029	YES	YES
53	a	190.88	0.72347	YES	YES
54	a	201.66	2.17632	YES	YES
55	a	203.04	1.02550	YES	YES
56	a	204.50	0.78581	YES	YES
57	a	225.42	34.50723	YES	YES
58	a	225.77	9.51783	YES	YES
59	a	228.10	11.72433	YES	YES
60	a	235.24	2.74116	YES	YES
61	a	237.18	10.74522	YES	YES
62	a	239.08	1.58680	YES	YES
63	a	240.61	6.15795	YES	YES
64	a	247.20	1.88845	YES	YES
65	a	255.13	1.37380	YES	YES
66	a	265.88	1.44491	YES	YES
67	a	266.08	1.70641	YES	YES
68	a	268.03	0.59209	YES	YES
69	a	276.66	0.21919	YES	YES
70	a	276.94	0.32743	YES	YES
71	a	277.66	0.30372	YES	YES
72	a	278.75	0.57901	YES	YES
73	a	279.39	0.57100	YES	YES
74	a	279.70	0.51031	YES	YES
75	a	280.74	0.66536	YES	YES
76	a	286.38	1.41694	YES	YES
77	a	288.90	1.18956	YES	YES
78	a	289.36	1.84664	YES	YES
79	a	302.84	1.69202	YES	YES
80	a	305.84	1.55273	YES	YES
81	a	343.75	8.32177	YES	YES
82	a	344.51	24.19593	YES	YES
83	a	345.37	30.52406	YES	YES
84	a	361.42	5.15222	YES	YES
85	a	362.37	11.52534	YES	YES
86	a	365.29	38.96523	YES	YES
87	a	368.34	37.07902	YES	YES
88	a	371.80	57.13129	YES	YES
89	a	372.95	65.87298	YES	YES
90	a	395.24	286.24027	YES	YES
91	a	396.09	289.88602	YES	YES
92	a	403.18	11.50384	YES	YES
93	a	431.81	0.18243	YES	YES

94	a	432.10	0.32736	YES	YES
95	a	464.10	30.57838	YES	YES
96	a	475.63	34.05474	YES	YES
97	a	541.88	0.16656	YES	YES
98	a	542.37	0.45303	YES	YES
99	a	542.62	0.36740	YES	YES
100	a	545.20	0.02740	YES	YES
101	a	545.58	0.03179	YES	YES
102	a	546.00	0.06913	YES	YES
103	a	547.27	0.00598	YES	YES
104	a	547.45	0.00958	YES	YES
105	a	548.01	0.02665	YES	YES
106	a	554.12	5.32625	YES	YES
107	a	554.99	5.31845	YES	YES
108	a	575.48	0.70335	YES	YES
109	a	576.81	1.73609	YES	YES
110	a	577.27	1.67127	YES	YES
111	a	578.54	1.11605	YES	YES
112	a	578.96	1.09782	YES	YES
113	a	579.83	1.63302	YES	YES
114	a	580.50	0.39411	YES	YES
115	a	593.97	12.72742	YES	YES
116	a	594.32	12.92941	YES	YES
117	a	597.24	6.40167	YES	YES
118	a	735.72	13.18999	YES	YES
119	a	736.88	13.25819	YES	YES
120	a	757.21	83.44637	YES	YES
121	a	797.80	1.22178	YES	YES
122	a	798.30	3.16277	YES	YES
123	a	798.92	3.07666	YES	YES
124	a	804.53	3.15693	YES	YES
125	a	805.70	3.33015	YES	YES
126	a	806.20	3.24488	YES	YES
127	a	847.72	1.32942	YES	YES
128	a	884.86	6.07999	YES	YES
129	a	885.38	5.95196	YES	YES
130	a	920.76	0.86115	YES	YES
131	a	922.37	0.64942	YES	YES
132	a	922.75	0.58407	YES	YES
133	a	931.49	0.61866	YES	YES
134	a	932.83	0.88425	YES	YES
135	a	934.72	0.86901	YES	YES
136	a	970.17	12.82650	YES	YES
137	a	970.78	12.50309	YES	YES
138	a	980.74	21.85366	YES	YES
139	a	984.61	2.12337	YES	YES
140	a	985.42	1.20350	YES	YES
141	a	986.09	1.28848	YES	YES
142	a	991.09	2.06360	YES	YES
143	a	992.27	1.64859	YES	YES
144	a	992.76	1.11806	YES	YES
145	a	994.52	0.71280	YES	YES
146	a	994.90	1.09369	YES	YES
147	a	996.18	1.36394	YES	YES
148	a	1000.91	0.37757	YES	YES
149	a	1002.19	0.29618	YES	YES
150	a	1002.47	0.40243	YES	YES
151	a	1007.32	1.00193	YES	YES
152	a	1009.10	1.11338	YES	YES
153	a	1009.43	0.93777	YES	YES
154	a	1015.66	22.71505	YES	YES
155	a	1016.32	22.59863	YES	YES
156	a	1023.00	0.22443	YES	YES
157	a	1026.06	2.31318	YES	YES
158	a	1045.31	1.78567	YES	YES
159	a	1045.44	1.94783	YES	YES
160	a	1046.11	0.62569	YES	YES
161	a	1047.81	2.50353	YES	YES
162	a	1048.68	1.50487	YES	YES
163	a	1049.22	1.19435	YES	YES
164	a	1063.18	12.03599	YES	YES
165	a	1063.97	12.52074	YES	YES
166	a	1070.93	0.25698	YES	YES
167	a	1071.75	0.30712	YES	YES
168	a	1072.32	0.29336	YES	YES
169	a	1096.82	37.55542	YES	YES
170	a	1103.84	1.73496	YES	YES
171	a	1104.28	1.72938	YES	YES

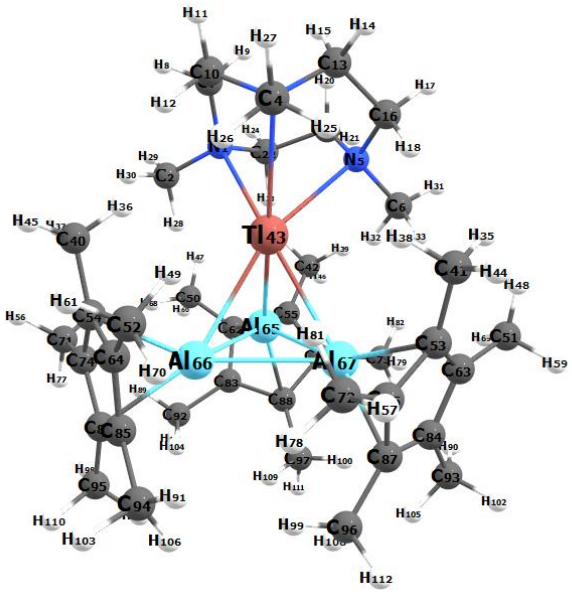
172	a	1107.31	0.88232	YES	YES
173	a	1140.93	11.30628	YES	YES
174	a	1141.97	11.24821	YES	YES
175	a	1162.86	0.00537	YES	YES
176	a	1164.01	0.19963	YES	YES
177	a	1164.41	0.21184	YES	YES
178	a	1166.29	0.01986	YES	YES
179	a	1167.37	0.13148	YES	YES
180	a	1167.79	0.15986	YES	YES
181	a	1215.14	3.44089	YES	YES
182	a	1215.43	3.55543	YES	YES
183	a	1230.00	1.40643	YES	YES
184	a	1242.37	2.05569	YES	YES
185	a	1243.04	1.92324	YES	YES
186	a	1268.30	5.57784	YES	YES
187	a	1281.79	11.83219	YES	YES
188	a	1289.46	10.11453	YES	YES
189	a	1289.93	10.00618	YES	YES
190	a	1321.84	3.46193	YES	YES
191	a	1335.40	1.05062	YES	YES
192	a	1335.49	1.12949	YES	YES
193	a	1337.47	0.61118	YES	YES
194	a	1338.06	0.76668	YES	YES
195	a	1338.79	0.88263	YES	YES
196	a	1340.11	0.55474	YES	YES
197	a	1341.04	0.39994	YES	YES
198	a	1341.23	1.37206	YES	YES
199	a	1343.14	1.33396	YES	YES
200	a	1344.52	2.63895	YES	YES
201	a	1344.83	2.43990	YES	YES
202	a	1345.97	3.12229	YES	YES
203	a	1346.75	1.57817	YES	YES
204	a	1347.78	5.68362	YES	YES
205	a	1350.44	1.05513	YES	YES
206	a	1351.06	0.37067	YES	YES
207	a	1352.83	0.44359	YES	YES
208	a	1358.16	19.42754	YES	YES
209	a	1366.13	6.20726	YES	YES
210	a	1367.73	6.55147	YES	YES
211	a	1383.18	0.65492	YES	YES
212	a	1385.64	5.86505	YES	YES
213	a	1385.95	3.58878	YES	YES
214	a	1386.74	1.95221	YES	YES
215	a	1386.95	1.10705	YES	YES
216	a	1387.84	1.93034	YES	YES
217	a	1390.06	3.80335	YES	YES
218	a	1390.91	4.74726	YES	YES
219	a	1393.22	1.23894	YES	YES
220	a	1394.60	13.62225	YES	YES
221	a	1394.78	9.56343	YES	YES
222	a	1394.93	20.52656	YES	YES
223	a	1397.99	5.32652	YES	YES
224	a	1398.36	5.42398	YES	YES
225	a	1400.70	3.74977	YES	YES
226	a	1402.61	12.96692	YES	YES
227	a	1403.40	5.45174	YES	YES
228	a	1403.49	5.98364	YES	YES
229	a	1404.97	15.56442	YES	YES
230	a	1405.79	12.83604	YES	YES
231	a	1406.51	6.33884	YES	YES
232	a	1407.16	14.30256	YES	YES
233	a	1407.90	6.88766	YES	YES
234	a	1409.07	1.65975	YES	YES
235	a	1412.43	2.21682	YES	YES
236	a	1412.45	3.73332	YES	YES
237	a	1413.43	10.66892	YES	YES
238	a	1414.25	19.80039	YES	YES
239	a	1414.56	20.28767	YES	YES
240	a	1414.91	36.36880	YES	YES
241	a	1415.56	6.50827	YES	YES
242	a	1416.00	4.25663	YES	YES
243	a	1418.40	0.25236	YES	YES
244	a	1419.21	1.73589	YES	YES
245	a	1419.69	26.69188	YES	YES
246	a	1420.48	5.99993	YES	YES
247	a	1420.88	0.52899	YES	YES
248	a	1421.45	3.57808	YES	YES
249	a	1421.97	7.95735	YES	YES

250	a	1425.30	16.40472	YES	YES
251	a	1425.63	14.66891	YES	YES
252	a	1428.76	5.24435	YES	YES
253	a	1429.65	11.93001	YES	YES
254	a	1430.19	11.81995	YES	YES
255	a	1440.15	3.92386	YES	YES
256	a	1441.09	11.13971	YES	YES
257	a	1441.42	11.08516	YES	YES
258	a	1443.75	0.45026	YES	YES
259	a	1444.35	0.60032	YES	YES
260	a	1444.55	0.74168	YES	YES
261	a	1448.31	8.18201	YES	YES
262	a	1451.30	1.02510	YES	YES
263	a	1452.14	0.92107	YES	YES
264	a	1452.47	0.91084	YES	YES
265	a	1487.46	3.83963	YES	YES
266	a	1488.52	7.03247	YES	YES
267	a	1488.81	7.24299	YES	YES
268	a	1496.05	6.09276	YES	YES
269	a	1496.42	5.75487	YES	YES
270	a	1496.84	11.02257	YES	YES
271	a	2914.66	36.32457	YES	YES
272	a	2914.83	34.98198	YES	YES
273	a	2914.98	60.84230	YES	YES
274	a	2927.61	60.79058	YES	YES
275	a	2927.67	60.04741	YES	YES
276	a	2928.15	32.03919	YES	YES
277	a	2938.74	33.47125	YES	YES
278	a	2940.13	24.56805	YES	YES
279	a	2940.31	49.84960	YES	YES
280	a	2948.80	63.26989	YES	YES
281	a	2949.98	5.61350	YES	YES
282	a	2950.14	5.15842	YES	YES
283	a	2955.09	18.11094	YES	YES
284	a	2955.33	20.19403	YES	YES
285	a	2955.80	20.87676	YES	YES
286	a	2957.04	24.15267	YES	YES
287	a	2957.13	25.76938	YES	YES
288	a	2957.36	45.55214	YES	YES
289	a	2963.15	23.87668	YES	YES
290	a	2963.25	27.42614	YES	YES
291	a	2963.47	31.36061	YES	YES
292	a	2968.67	16.99142	YES	YES
293	a	2969.05	15.83349	YES	YES
294	a	2971.22	100.81077	YES	YES
295	a	3020.53	5.04136	YES	YES
296	a	3021.15	5.17523	YES	YES
297	a	3021.90	5.90533	YES	YES
298	a	3022.68	15.21175	YES	YES
299	a	3022.74	13.01448	YES	YES
300	a	3022.90	11.71527	YES	YES
301	a	3025.42	4.66825	YES	YES
302	a	3025.54	4.58083	YES	YES
303	a	3026.00	4.53023	YES	YES
304	a	3026.28	4.42057	YES	YES
305	a	3026.33	8.97868	YES	YES
306	a	3027.74	14.14796	YES	YES
307	a	3027.80	0.71649	YES	YES
308	a	3028.36	7.54462	YES	YES
309	a	3028.49	7.52970	YES	YES
310	a	3041.73	1.27704	YES	YES
311	a	3041.98	1.21225	YES	YES
312	a	3044.13	1.18097	YES	YES
313	a	3044.36	3.30462	YES	YES
314	a	3044.47	3.49515	YES	YES
315	a	3044.64	2.87117	YES	YES
316	a	3045.26	2.61385	YES	YES
317	a	3045.34	3.25754	YES	YES
318	a	3047.07	34.09524	YES	YES
319	a	3057.96	8.90857	YES	YES
320	a	3058.51	10.08599	YES	YES
321	a	3058.77	15.62838	YES	YES
322	a	3059.20	5.00945	YES	YES
323	a	3059.42	9.73561	YES	YES
324	a	3059.90	8.78078	YES	YES
325	a	3063.21	5.66879	YES	YES
326	a	3063.39	5.68859	YES	YES
327	a	3063.51	5.91610	YES	YES

328	a	3078.53	6.98227	YES	YES
329	a	3078.72	7.17895	YES	YES
330	a	3078.83	2.71829	YES	YES
331	a	3082.54	0.90619	YES	YES
332	a	3083.02	1.13471	YES	YES
333	a	3083.73	1.05147	YES	YES
334	a	3088.70	4.53464	YES	YES
335	a	3088.96	2.69971	YES	YES
336	a	3089.69	3.04091	YES	YES

$end

$[(Me_3TACN)Tl(AlCp^*)_3]^+$



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

Symmetry: c1

Cartesian coordinates in Ångström:

N	-1.7616164	2.3349738	15.7603429
C	-2.1943790	1.0078813	16.1918982
N	0.0449262	3.3577620	13.5877543
C	0.7091420	3.0765772	12.3167057
N	-2.4464156	4.8881717	14.2803994
C	-3.7020654	5.4795318	13.8260328
C	-0.3217471	2.5647414	15.9536870
H	0.1012921	1.8347932	16.6790252
H	-0.1633233	3.5549171	16.4247176
C	0.5008649	2.4681639	14.6613089
H	1.5770126	2.6425425	14.9185536
H	0.4387351	1.4303603	14.2709800
C	0.0484986	4.7896074	13.9259124
H	0.8493701	5.3256310	13.3687156
H	0.3137185	4.9151644	14.9939179
C	-1.2795399	5.5021811	13.6364564
H	-1.1636718	6.5790669	13.9218595
H	-1.4710487	5.4865403	12.5434329
C	-2.3707172	4.7870947	15.7471881
H	-1.3792390	5.1400955	16.0931984
H	-3.1011094	5.4779787	16.2245870
C	-2.6437728	3.3801215	16.2894074
H	-3.6790752	3.0870523	16.0152622
H	-2.6081103	3.4246386	17.4085299
H	0.2731747	3.7039245	11.5143534
H	0.5502747	2.0166713	12.0322328
H	1.8093047	3.2685603	12.3519198
H	-3.2284792	0.8215480	15.8343510
H	-2.1739591	0.8893539	17.3027698
H	-1.5440969	0.2337745	15.7441121
H	-3.8144701	6.5466278	14.1376163
H	-4.5568267	4.8970281	14.2221329
H	-3.7673340	5.4226788	12.7230381
H	-5.6826730	3.2286686	17.1153447
H	-2.4252266	5.8307661	10.4293774
H	-0.7238617	-0.0879664	13.2484967
H	-1.2262136	-1.4490559	14.2966857
H	-1.6029945	4.2434043	10.3063375
H	-5.8826358	4.5298288	15.9047611
C	-0.9971411	-1.1664634	13.2522156
C	-2.3192608	4.9257734	9.8009632
C	-6.3613750	3.6294692	16.3385180
Tl	-2.5409201	2.4046172	13.0862974
H	-1.8487789	5.2412347	8.8463192
H	-0.0927759	-1.7305517	12.9430529
H	-7.2798043	3.9725241	16.8607307
H	-5.3670531	1.0663049	17.2619888
H	-4.3736188	6.6264207	10.8405171
H	-0.6458400	0.3020528	10.5866421
C	-6.0763689	0.4476124	16.6785198
C	-5.2766343	6.0977929	10.4808204
C	-0.9820606	-0.6664962	10.1577499
C	-3.6400447	4.2570407	9.5604704
C	-2.1514282	-1.4519443	12.3390811
C	-6.6915617	2.5964658	15.2997562
H	-3.0594622	-3.1459594	14.5334809
H	-2.2648174	2.5337435	7.4572533
H	-8.5990338	4.3071581	13.1034082
H	-5.7631974	6.7580174	9.7320752

H	-6.9080597	0.1732950	17.3621053
H	-0.1134088	-1.3573561	10.1919387
C	-6.5825678	1.1692691	15.4638047
C	-4.9437282	4.7643224	9.8787590
C	-2.1447315	-1.2310015	10.9177195
Al	-5.2811722	1.7535267	13.6179577
Al	-3.8277099	0.0530917	11.8444485
Al	-4.5995914	2.7394934	11.0269111
H	-5.5555817	-0.4929826	16.4088019
H	-5.9783726	6.0106562	11.3355768
H	-1.2258540	-0.4938886	9.0936067
C	-3.8018509	-2.4509126	14.0909488
C	-2.6753488	2.1310029	8.4072938
C	-7.5373788	4.2022289	13.4062849
C	-3.4058554	-2.0501699	12.6990766
C	-3.8011828	2.9795365	8.9157276
C	-7.2652731	2.8554960	14.0090994
H	-4.7794361	-2.9673153	14.1011801
H	-3.0074810	1.0946490	8.2110522
H	-6.9160398	4.3705567	12.4987329
H	-3.8801948	-1.5737991	14.7691328
H	-1.8401710	2.0806274	9.1349451
H	-7.3130282	5.0198704	14.1166854
C	-7.0897235	0.5480979	14.2734195
C	-5.9141008	3.7946490	9.4458745
C	-3.4026869	-1.6811697	10.3955970
C	-4.1898682	-2.1816241	11.4988286
C	-5.2069888	2.6909703	8.8425677
C	-7.4989707	1.5902029	13.3645402
H	-6.5269184	-1.5170234	14.6163609
H	-7.7590649	4.4943958	10.3692334
H	-3.2615913	-1.0275956	8.3277409
C	-7.2523134	-0.9210632	14.0319790
C	-7.3999876	4.0041499	9.4435126
C	-3.8038671	-1.7628906	8.9526723
C	-5.5240838	-2.8561091	11.3522916
C	-5.8361766	1.4833091	8.2126783
C	-8.1111183	1.3788532	12.0108164
H	-5.9922885	-3.0598549	12.3325742
H	-5.1693062	0.6026962	8.2702900
H	-8.0384770	2.2909247	11.3919557
H	-8.2695588	-1.2595645	14.3230698
H	-7.6947058	4.6605901	8.5965690
H	-3.5786306	-2.7691311	8.5388615
H	-7.1169772	-1.1746177	12.9632496
H	-7.9537622	3.0544016	9.3210535
H	-4.8894091	-1.5933187	8.8136199
H	-6.2398125	-2.2524812	10.7578100
H	-6.7895542	1.2113530	8.7070091
H	-7.6098479	0.5589977	11.4564379
H	-5.4139564	-3.8306574	10.8312816
H	-9.1867417	1.1134051	12.0894528
H	-6.0593478	1.6599242	7.1392001

SCF energy GEOOPT = -2589.014461531 H

ZPE = 2484. kJ/mol

FREEH energy = 2649.11 kJ/mol

FREEH entropy = 1.44928 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	3.45	0.04445	YES YES
8	a	17.63	0.28221	YES YES
9	a	23.04	0.02492	YES YES
10	a	25.00	0.04578	YES YES
11	a	33.46	0.01127	YES YES
12	a	34.54	0.03475	YES YES
13	a	41.01	0.15767	YES YES
14	a	42.17	0.13848	YES YES
15	a	45.12	0.13693	YES YES
16	a	48.02	0.13782	YES YES

17	a	55.96	0.06783	YES	YES
18	a	58.05	0.13856	YES	YES
19	a	64.32	0.13585	YES	YES
20	a	68.70	0.14103	YES	YES
21	a	76.64	0.18702	YES	YES
22	a	76.70	0.07238	YES	YES
23	a	77.74	0.19798	YES	YES
24	a	80.95	0.91480	YES	YES
25	a	86.33	1.67258	YES	YES
26	a	88.89	0.26990	YES	YES
27	a	91.00	0.24483	YES	YES
28	a	93.37	1.00418	YES	YES
29	a	96.34	0.42910	YES	YES
30	a	98.68	1.64040	YES	YES
31	a	102.74	0.34568	YES	YES
32	a	104.41	17.72402	YES	YES
33	a	113.48	0.72266	YES	YES
34	a	115.12	0.98122	YES	YES
35	a	120.08	0.62930	YES	YES
36	a	124.78	0.08467	YES	YES
37	a	134.88	0.58870	YES	YES
38	a	135.13	0.47890	YES	YES
39	a	136.00	1.01833	YES	YES
40	a	139.62	0.53150	YES	YES
41	a	143.55	0.20624	YES	YES
42	a	149.05	0.27599	YES	YES
43	a	151.33	0.49251	YES	YES
44	a	161.44	0.12901	YES	YES
45	a	161.51	0.33789	YES	YES
46	a	164.06	0.06994	YES	YES
47	a	169.43	1.38337	YES	YES
48	a	172.34	2.00967	YES	YES
49	a	173.67	1.00789	YES	YES
50	a	176.33	0.28750	YES	YES
51	a	178.84	0.09595	YES	YES
52	a	179.71	0.45784	YES	YES
53	a	183.14	0.51534	YES	YES
54	a	185.71	0.76385	YES	YES
55	a	187.25	0.73758	YES	YES
56	a	190.77	0.35382	YES	YES
57	a	203.79	5.16838	YES	YES
58	a	215.39	5.42647	YES	YES
59	a	216.83	1.06051	YES	YES
60	a	222.69	5.03529	YES	YES
61	a	223.79	9.99445	YES	YES
62	a	226.51	5.15974	YES	YES
63	a	243.71	0.67308	YES	YES
64	a	244.99	0.11854	YES	YES
65	a	246.10	0.25596	YES	YES
66	a	253.81	0.13349	YES	YES
67	a	263.74	1.19052	YES	YES
68	a	264.89	0.42476	YES	YES
69	a	268.22	0.05231	YES	YES
70	a	269.25	0.16128	YES	YES
71	a	273.17	2.00930	YES	YES
72	a	274.52	2.23117	YES	YES
73	a	278.70	0.04815	YES	YES
74	a	279.77	0.48045	YES	YES
75	a	280.91	1.12894	YES	YES
76	a	283.59	2.20684	YES	YES
77	a	285.12	0.16351	YES	YES
78	a	289.35	2.37181	YES	YES
79	a	290.19	0.40359	YES	YES
80	a	292.40	2.49203	YES	YES
81	a	347.01	2.13388	YES	YES
82	a	348.33	2.81038	YES	YES
83	a	353.63	24.38326	YES	YES
84	a	355.34	79.74801	YES	YES
85	a	357.69	39.30598	YES	YES
86	a	361.72	14.33605	YES	YES
87	a	369.07	16.74973	YES	YES
88	a	374.64	44.42440	YES	YES
89	a	383.03	15.20994	YES	YES
90	a	392.70	8.27592	YES	YES
91	a	402.94	276.94118	YES	YES
92	a	412.25	254.79709	YES	YES
93	a	429.41	0.04455	YES	YES
94	a	430.68	0.06066	YES	YES

95	a	462.93	96.59989	YES	YES
96	a	471.31	1.45591	YES	YES
97	a	542.25	0.17769	YES	YES
98	a	542.74	0.07317	YES	YES
99	a	543.57	0.03376	YES	YES
100	a	544.55	0.05592	YES	YES
101	a	544.94	0.09654	YES	YES
102	a	546.07	0.13046	YES	YES
103	a	546.65	5.59226	YES	YES
104	a	547.37	0.73801	YES	YES
105	a	547.99	5.21885	YES	YES
106	a	548.05	0.35958	YES	YES
107	a	549.08	0.08416	YES	YES
108	a	571.69	0.28678	YES	YES
109	a	574.81	0.27401	YES	YES
110	a	575.92	1.99243	YES	YES
111	a	577.80	1.85049	YES	YES
112	a	580.84	1.46012	YES	YES
113	a	582.47	0.25074	YES	YES
114	a	587.00	1.22140	YES	YES
115	a	592.86	9.36075	YES	YES
116	a	593.51	7.44498	YES	YES
117	a	594.82	6.26642	YES	YES
118	a	737.64	15.31450	YES	YES
119	a	740.88	11.38746	YES	YES
120	a	745.81	83.17190	YES	YES
121	a	796.61	2.11474	YES	YES
122	a	798.02	1.81246	YES	YES
123	a	800.98	2.97044	YES	YES
124	a	803.24	2.51206	YES	YES
125	a	805.10	4.27999	YES	YES
126	a	806.82	3.32867	YES	YES
127	a	846.74	2.28828	YES	YES
128	a	875.56	5.31803	YES	YES
129	a	876.09	4.35480	YES	YES
130	a	918.39	0.23880	YES	YES
131	a	919.70	1.32815	YES	YES
132	a	926.89	0.58093	YES	YES
133	a	928.10	1.40106	YES	YES
134	a	932.60	1.19976	YES	YES
135	a	937.08	0.20494	YES	YES
136	a	971.08	11.31898	YES	YES
137	a	971.78	10.00290	YES	YES
138	a	981.71	28.16817	YES	YES
139	a	985.83	4.98044	YES	YES
140	a	986.89	4.23531	YES	YES
141	a	988.38	1.48376	YES	YES
142	a	991.10	4.38902	YES	YES
143	a	992.31	0.77026	YES	YES
144	a	992.82	2.68875	YES	YES
145	a	995.70	1.38080	YES	YES
146	a	996.93	0.29858	YES	YES
147	a	997.34	1.54880	YES	YES
148	a	997.40	1.25890	YES	YES
149	a	998.61	0.48997	YES	YES
150	a	998.80	0.10242	YES	YES
151	a	1002.45	0.33382	YES	YES
152	a	1004.49	0.38609	YES	YES
153	a	1006.34	0.04617	YES	YES
154	a	1020.50	27.54852	YES	YES
155	a	1022.09	22.79020	YES	YES
156	a	1024.00	10.39752	YES	YES
157	a	1031.31	0.34733	YES	YES
158	a	1045.98	1.91925	YES	YES
159	a	1047.05	1.08846	YES	YES
160	a	1048.13	0.95382	YES	YES
161	a	1048.86	0.43837	YES	YES
162	a	1050.10	2.71574	YES	YES
163	a	1051.25	1.12559	YES	YES
164	a	1068.83	12.04409	YES	YES
165	a	1070.80	1.77315	YES	YES
166	a	1073.10	10.70664	YES	YES
167	a	1074.48	0.98382	YES	YES
168	a	1076.08	0.60895	YES	YES
169	a	1099.43	18.38446	YES	YES
170	a	1104.81	2.11346	YES	YES
171	a	1106.82	1.24874	YES	YES
172	a	1118.63	8.72062	YES	YES

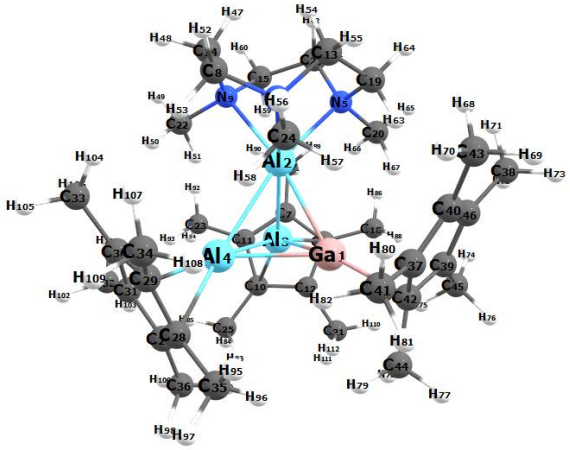
173	a	1142.73	18.57852	YES	YES
174	a	1144.85	19.94728	YES	YES
175	a	1163.43	0.13204	YES	YES
176	a	1164.69	0.09761	YES	YES
177	a	1165.18	0.45560	YES	YES
178	a	1166.44	0.20667	YES	YES
179	a	1166.93	0.24792	YES	YES
180	a	1169.67	0.11512	YES	YES
181	a	1220.25	4.20069	YES	YES
182	a	1223.48	3.66772	YES	YES
183	a	1237.92	1.51042	YES	YES
184	a	1244.54	5.17738	YES	YES
185	a	1246.81	7.30458	YES	YES
186	a	1267.84	3.07143	YES	YES
187	a	1291.57	6.31423	YES	YES
188	a	1298.63	8.43320	YES	YES
189	a	1299.88	9.73426	YES	YES
190	a	1323.61	1.82276	YES	YES
191	a	1336.31	2.23480	YES	YES
192	a	1337.01	2.00942	YES	YES
193	a	1338.05	0.24643	YES	YES
194	a	1339.63	3.71511	YES	YES
195	a	1339.74	1.72704	YES	YES
196	a	1340.59	3.78261	YES	YES
197	a	1340.75	2.55404	YES	YES
198	a	1341.17	4.57094	YES	YES
199	a	1342.25	7.26799	YES	YES
200	a	1343.73	1.58810	YES	YES
201	a	1345.44	1.29370	YES	YES
202	a	1345.89	4.09731	YES	YES
203	a	1346.85	5.22701	YES	YES
204	a	1348.35	1.52485	YES	YES
205	a	1349.26	1.73934	YES	YES
206	a	1351.38	2.09864	YES	YES
207	a	1351.59	0.25317	YES	YES
208	a	1356.02	20.15680	YES	YES
209	a	1363.19	7.01947	YES	YES
210	a	1365.74	5.17403	YES	YES
211	a	1381.80	0.37636	YES	YES
212	a	1384.10	0.86565	YES	YES
213	a	1386.58	3.55648	YES	YES
214	a	1388.42	0.44279	YES	YES
215	a	1389.13	7.17588	YES	YES
216	a	1390.14	6.22233	YES	YES
217	a	1390.69	7.95291	YES	YES
218	a	1392.12	0.96328	YES	YES
219	a	1393.36	0.67943	YES	YES
220	a	1395.68	5.32309	YES	YES
221	a	1396.16	3.20400	YES	YES
222	a	1396.61	2.01579	YES	YES
223	a	1397.53	2.71913	YES	YES
224	a	1398.64	0.60791	YES	YES
225	a	1399.57	7.37717	YES	YES
226	a	1400.54	12.03459	YES	YES
227	a	1401.55	5.73255	YES	YES
228	a	1401.96	5.20215	YES	YES
229	a	1402.29	9.40433	YES	YES
230	a	1403.43	16.35528	YES	YES
231	a	1404.99	1.57390	YES	YES
232	a	1405.51	4.42018	YES	YES
233	a	1406.97	16.63594	YES	YES
234	a	1407.69	12.84531	YES	YES
235	a	1408.77	16.22846	YES	YES
236	a	1409.35	11.88682	YES	YES
237	a	1409.81	2.70015	YES	YES
238	a	1411.33	3.20358	YES	YES
239	a	1412.56	1.85302	YES	YES
240	a	1413.78	10.07292	YES	YES
241	a	1414.50	6.62341	YES	YES
242	a	1415.04	38.30647	YES	YES
243	a	1415.42	15.68628	YES	YES
244	a	1415.62	11.99068	YES	YES
245	a	1416.61	15.37382	YES	YES
246	a	1417.09	21.69526	YES	YES
247	a	1417.67	43.54826	YES	YES
248	a	1419.67	20.35736	YES	YES
249	a	1421.41	8.35332	YES	YES
250	a	1423.35	2.82534	YES	YES

251	a	1425.13	5.94974	YES	YES
252	a	1430.56	2.21941	YES	YES
253	a	1431.52	10.27954	YES	YES
254	a	1432.36	12.43463	YES	YES
255	a	1434.88	7.57300	YES	YES
256	a	1435.25	9.58093	YES	YES
257	a	1441.68	2.63414	YES	YES
258	a	1445.45	1.78710	YES	YES
259	a	1446.23	0.31229	YES	YES
260	a	1447.04	3.09458	YES	YES
261	a	1448.40	1.66709	YES	YES
262	a	1453.34	1.15700	YES	YES
263	a	1454.23	4.46090	YES	YES
264	a	1455.53	1.43711	YES	YES
265	a	1482.53	3.72831	YES	YES
266	a	1483.08	8.40007	YES	YES
267	a	1487.30	11.46586	YES	YES
268	a	1494.90	6.85008	YES	YES
269	a	1499.81	10.56491	YES	YES
270	a	1500.70	10.59699	YES	YES
271	a	2870.49	61.67150	YES	YES
272	a	2876.92	56.58459	YES	YES
273	a	2877.25	102.19000	YES	YES
274	a	2894.42	85.32984	YES	YES
275	a	2895.94	70.72734	YES	YES
276	a	2898.19	89.93174	YES	YES
277	a	2935.97	24.75825	YES	YES
278	a	2937.80	24.30090	YES	YES
279	a	2948.76	3.08792	YES	YES
280	a	2948.95	44.81608	YES	YES
281	a	2950.32	23.23151	YES	YES
282	a	2951.92	37.53182	YES	YES
283	a	2953.46	56.77708	YES	YES
284	a	2957.73	19.84618	YES	YES
285	a	2958.14	99.06489	YES	YES
286	a	2958.84	40.42248	YES	YES
287	a	2959.25	18.51270	YES	YES
288	a	2959.29	16.29294	YES	YES
289	a	2960.69	28.99199	YES	YES
290	a	2961.21	29.53041	YES	YES
291	a	2961.42	14.71764	YES	YES
292	a	2962.00	26.01984	YES	YES
293	a	2965.04	10.67418	YES	YES
294	a	2965.11	28.35657	YES	YES
295	a	2991.16	1.28927	YES	YES
296	a	2992.22	3.88812	YES	YES
297	a	3001.22	8.82570	YES	YES
298	a	3003.99	0.48486	YES	YES
299	a	3007.95	15.12625	YES	YES
300	a	3010.23	16.13936	YES	YES
301	a	3016.08	4.29755	YES	YES
302	a	3018.70	9.05910	YES	YES
303	a	3019.58	7.21312	YES	YES
304	a	3023.27	8.40613	YES	YES
305	a	3024.51	5.65009	YES	YES
306	a	3024.62	6.84931	YES	YES
307	a	3026.07	4.97317	YES	YES
308	a	3026.12	7.34702	YES	YES
309	a	3026.19	11.69620	YES	YES
310	a	3028.44	7.72800	YES	YES
311	a	3029.23	8.15700	YES	YES
312	a	3030.51	5.24172	YES	YES
313	a	3030.70	7.29832	YES	YES
314	a	3033.61	39.50419	YES	YES
315	a	3033.87	4.41951	YES	YES
316	a	3034.16	5.62792	YES	YES
317	a	3040.04	3.22603	YES	YES
318	a	3043.17	3.50820	YES	YES
319	a	3053.27	8.27673	YES	YES
320	a	3056.66	8.26556	YES	YES
321	a	3058.43	9.15868	YES	YES
322	a	3063.57	6.83558	YES	YES
323	a	3065.19	8.03857	YES	YES
324	a	3066.32	4.71236	YES	YES
325	a	3067.00	5.31895	YES	YES
326	a	3068.74	5.66031	YES	YES
327	a	3069.42	2.33490	YES	YES
328	a	3069.50	6.87718	YES	YES

329	a	3071.29	6.28658	YES	YES
330	a	3072.57	5.62512	YES	YES
331	a	3074.37	5.69896	YES	YES
332	a	3074.65	3.22480	YES	YES
333	a	3076.58	4.18869	YES	YES
334	a	3077.15	10.77451	YES	YES
335	a	3081.24	1.57747	YES	YES
336	a	3088.26	0.93035	YES	YES

$end

$[(Me_3TACN)Al(GaCp^*)(AlCp^*)_2]^+$



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

Symmetry: c1

Cartesian coordinates in Ångström:

Ga	5.1317366	12.3515620	6.1876601
Al	2.9229371	12.3896471	4.8984543
Al	3.1710179	10.9146025	7.1561028
Al	3.1657783	13.6672464	7.2815169
N	3.1455287	11.0934422	3.1523661
N	2.9620686	13.9173099	3.3289643
C	2.1470935	8.7884391	7.1435270
C	1.6004782	14.4980232	3.3862090
N	0.8226870	12.3036741	4.2577421
C	2.8017417	9.8179954	9.1215894
C	1.6731728	9.5433579	8.2720644
C	3.9704399	9.2438715	8.5127079
C	3.2883227	13.2906252	2.0153613
C	0.5374611	13.4040199	3.2908187
C	0.7196715	10.9487998	3.6589430
C	3.5668562	8.6091379	7.2891842
C	1.2868241	8.1806458	6.0742705
C	4.4715850	7.8310805	6.3764112
C	3.9495015	11.9343503	2.2291640
C	3.9196832	9.8971929	3.5533517
C	5.3596890	9.2985420	9.0797871
C	-0.0416319	12.4086213	5.4538779
C	0.2496069	9.9135379	8.5727116
C	3.9899853	14.9176473	3.6925116
C	2.7593923	10.4567806	10.4760436
C	1.8079711	10.7206952	2.6115698
C	3.2305014	14.5993096	9.3687046
C	3.9622680	15.4784757	8.4995889
C	3.0472314	16.0176331	7.5337855
C	1.7511299	15.4550349	7.7902555
C	1.8614753	14.5725246	8.9247084
C	0.7211496	13.8400045	9.5696115
C	0.4758170	15.8289564	7.0932769
C	3.3644546	17.0779978	6.5206044
C	5.4159402	15.8110790	8.6556942
C	3.8369261	13.8801633	10.5365594
C	7.2006614	13.5928992	4.9132798
C	7.3958023	10.5411885	2.7144598
C	7.3767896	11.2649840	5.2128024
C	7.1892483	12.9707450	3.6493423
C	7.2133240	15.0632621	5.2143661
C	7.2748104	12.5418908	5.9348154
C	7.1929553	13.6473859	2.3063212
C	7.8931440	12.7648573	7.3020179
C	7.6697840	9.9469397	5.8663619
C	7.2923505	11.5374814	3.8344193
H	0.5002325	12.9874619	2.2661858
H	-0.4653976	13.8389617	3.4791241
H	-1.1074340	12.2321300	5.1918592
H	0.0741095	13.4117603	5.9007370
H	0.2966459	11.6734581	6.2086015
H	1.4441696	15.2637353	2.5934489
H	1.5207516	15.0116076	4.3664407
H	2.3640231	13.1936533	1.4140878
H	3.9672197	13.9453188	1.4321775
H	3.9902047	15.7654733	2.9741715
H	4.9793070	14.4248768	3.7106888
H	3.7881340	15.2867827	4.7124928
H	0.8520110	10.2307638	4.4916674
H	-0.2885528	10.7727756	3.2213641
H	1.7966219	9.6582528	2.2924694

H 1.6030654 11.3127560 1.6990081

H 4.9350875 12.0733303 2.7215393

H 4.1181799 11.4217428 1.2562246

H 4.1476253 9.2598709 2.6724335

H 3.3407205 9.3214492 4.2957414

H 4.8602643 10.2257120 4.0368030

H 6.4679222 13.1996879 1.5911071

H 8.1858846 13.5619122 1.8131401

H 6.9666936 14.7297181 2.3777359

H 6.6392381 10.7075752 1.9171108

H 7.2763548 9.4993059 3.0717534

H 8.3848977 10.5956670 2.2086993

H 7.4082275 9.0899152 5.2136554

H 7.1188617 9.8238488 6.8201392

H 8.7505570 9.8433058 6.1102944

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H 7.6550205 11.9429089 8.0074687

H 7.5370756 13.7059783 7.7671666

H 7.0783981 15.6756651 4.3010002

H 8.1730666 15.3829909 5.6758926

H 6.4115835 15.3493716 5.9287586

H 3.6995530 10.9900503 10.7088568

H 2.6108215 9.6883697 11.2649079

H 1.9253921 11.1784714 10.5677518

H 3.9288600 7.4423331 5.4939875

H 4.9002452 6.9514703 6.9005292

H 5.3244474 8.4374857 6.0121048

H 1.7820269 8.1693824 5.0821380

H 0.3213194 8.7134402 5.9681772

H 1.0394359 7.1242178 6.3134330

H -0.3938853 9.8508919 7.6732649

H 0.1674039 10.9437783 8.9730263

H -0.1927914 9.2340066 9.3320656

H 5.8167681 16.3438760 7.7730808

H 6.0312844 14.9008757 8.8064952

H 5.5813701 16.4652931 9.5380280

H 4.3194976 14.5985001 11.2307506

H 4.6211045 13.1602972 10.2161893

H 3.0800651 13.3192683 11.1133274

H 0.0288046 13.4039075 8.8209733

H 0.1213019 14.5153989 10.2155657

H 1.0806926 13.0109130 10.2075638

H 0.6118437 15.9609829 5.9999191

H 0.0760839 16.7917502 7.4780641

H -0.3179604 15.0726122 7.2497514

H 2.6646013 17.0616257 5.6621628

H 4.3948350 16.9835406 6.1241124

H 3.2872409 18.0898099 6.9737621

H 6.0600395 8.6755624 8.4928650

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H 5.7641126 10.3346623 9.0870166

SCF energy GEOOPT = -4341.237202990 H

ZPE = 2493. kJ/mol

FREEH energy = 2652.12 kJ/mol

FREEH entropy = 1.35856 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	7.24	0.13655	YES YES
8	a	28.06	0.21852	YES YES
9	a	33.97	0.09189	YES YES
10	a	40.77	0.47444	YES YES
11	a	44.45	0.26075	YES YES
12	a	48.76	0.17223	YES YES
13	a	50.74	0.10975	YES YES
14	a	58.30	0.09478	YES YES
15	a	63.25	0.24740	YES YES
16	a	64.19	0.77339	YES YES
17	a	68.25	0.10764	YES YES
18	a	71.20	0.24615	YES YES

19	a	71.79	0.67632	YES	YES
20	a	75.47	0.42944	YES	YES
21	a	79.69	0.24513	YES	YES
22	a	91.03	0.12206	YES	YES
23	a	95.84	1.46214	YES	YES
24	a	100.73	0.25353	YES	YES
25	a	102.61	0.12238	YES	YES
26	a	109.26	0.06482	YES	YES
27	a	112.35	0.19861	YES	YES
28	a	115.05	0.32915	YES	YES
29	a	118.38	0.19978	YES	YES
30	a	119.38	0.16894	YES	YES
31	a	123.60	0.47919	YES	YES
32	a	126.76	0.10172	YES	YES
33	a	128.56	0.05205	YES	YES
34	a	134.44	0.26777	YES	YES
35	a	138.09	0.17656	YES	YES
36	a	139.53	0.31019	YES	YES
37	a	143.10	0.34691	YES	YES
38	a	148.40	0.48143	YES	YES
39	a	149.61	0.15723	YES	YES
40	a	160.16	1.15173	YES	YES
41	a	162.75	0.34884	YES	YES
42	a	164.70	0.36927	YES	YES
43	a	167.84	0.95373	YES	YES
44	a	170.75	0.01429	YES	YES
45	a	173.41	0.01625	YES	YES
46	a	174.98	0.35838	YES	YES
47	a	177.95	0.12600	YES	YES
48	a	182.15	0.74328	YES	YES
49	a	182.28	0.72896	YES	YES
50	a	186.10	0.42500	YES	YES
51	a	190.94	0.55083	YES	YES
52	a	205.77	0.80831	YES	YES
53	a	209.50	1.35746	YES	YES
54	a	217.84	0.27212	YES	YES
55	a	221.17	2.20352	YES	YES
56	a	229.63	3.75378	YES	YES
57	a	230.82	1.12947	YES	YES
58	a	237.32	1.45331	YES	YES
59	a	238.61	1.44871	YES	YES
60	a	244.61	2.63384	YES	YES
61	a	255.13	19.46505	YES	YES
62	a	258.47	2.00083	YES	YES
63	a	260.17	21.69594	YES	YES
64	a	261.19	2.12218	YES	YES
65	a	263.68	1.40554	YES	YES
66	a	267.01	20.73673	YES	YES
67	a	271.79	0.93245	YES	YES
68	a	272.59	3.64733	YES	YES
69	a	273.36	1.13704	YES	YES
70	a	275.38	0.35036	YES	YES
71	a	278.74	0.31793	YES	YES
72	a	279.96	0.69017	YES	YES
73	a	280.17	1.42966	YES	YES
74	a	288.47	3.71631	YES	YES
75	a	289.49	1.01230	YES	YES
76	a	289.75	0.93093	YES	YES
77	a	294.53	9.29651	YES	YES
78	a	306.46	7.06836	YES	YES
79	a	328.44	5.74169	YES	YES
80	a	331.33	7.70375	YES	YES
81	a	343.73	59.85051	YES	YES
82	a	346.23	12.77893	YES	YES
83	a	349.00	16.35645	YES	YES
84	a	352.00	19.62660	YES	YES
85	a	364.17	14.61553	YES	YES
86	a	371.80	5.65270	YES	YES
87	a	377.65	121.93418	YES	YES
88	a	392.34	81.00121	YES	YES
89	a	393.88	18.64947	YES	YES
90	a	401.09	219.78032	YES	YES
91	a	402.21	215.04327	YES	YES
92	a	424.17	24.77805	YES	YES
93	a	441.86	1.36882	YES	YES
94	a	444.19	0.86552	YES	YES
95	a	471.67	15.32468	YES	YES
96	a	486.99	39.80083	YES	YES

97	a	527.37	0.31346	YES	YES
98	a	538.44	0.64480	YES	YES
99	a	541.52	0.05669	YES	YES
100	a	542.19	0.17940	YES	YES
101	a	542.67	0.02147	YES	YES
102	a	544.20	0.28753	YES	YES
103	a	545.64	0.04357	YES	YES
104	a	547.47	0.07315	YES	YES
105	a	548.57	0.05344	YES	YES
106	a	561.74	3.95129	YES	YES
107	a	563.04	4.08659	YES	YES
108	a	578.36	1.95132	YES	YES
109	a	580.52	0.75594	YES	YES
110	a	584.67	1.29145	YES	YES
111	a	586.49	0.79602	YES	YES
112	a	586.78	0.79708	YES	YES
113	a	589.83	5.81136	YES	YES
114	a	591.98	12.52460	YES	YES
115	a	594.70	7.99604	YES	YES
116	a	619.52	22.13220	YES	YES
117	a	637.38	0.60852	YES	YES
118	a	730.87	11.75810	YES	YES
119	a	735.90	11.53464	YES	YES
120	a	772.84	53.73045	YES	YES
121	a	791.76	4.49096	YES	YES
122	a	795.36	1.62495	YES	YES
123	a	796.47	1.59225	YES	YES
124	a	799.42	3.50316	YES	YES
125	a	801.77	2.09855	YES	YES
126	a	803.39	2.95695	YES	YES
127	a	844.85	0.33123	YES	YES
128	a	891.47	5.41307	YES	YES
129	a	893.30	4.71611	YES	YES
130	a	911.99	8.67143	YES	YES
131	a	918.17	1.16877	YES	YES
132	a	919.33	0.44125	YES	YES
133	a	924.66	1.19943	YES	YES
134	a	929.59	0.83579	YES	YES
135	a	936.07	0.65322	YES	YES
136	a	970.01	11.50211	YES	YES
137	a	973.03	10.00080	YES	YES
138	a	977.18	11.55495	YES	YES
139	a	981.04	8.42352	YES	YES
140	a	983.73	4.16505	YES	YES
141	a	984.77	3.13368	YES	YES
142	a	985.94	5.15529	YES	YES
143	a	989.23	3.29115	YES	YES
144	a	990.33	0.40308	YES	YES
145	a	991.95	1.12463	YES	YES
146	a	992.55	1.85474	YES	YES
147	a	995.08	3.49695	YES	YES
148	a	995.56	4.31053	YES	YES
149	a	997.25	0.75605	YES	YES
150	a	999.16	18.93444	YES	YES
151	a	1000.56	3.63028	YES	YES
152	a	1004.02	8.46044	YES	YES
153	a	1004.25	6.41842	YES	YES
154	a	1004.97	2.82328	YES	YES
155	a	1006.34	0.18791	YES	YES
156	a	1013.11	0.87893	YES	YES
157	a	1027.73	1.94268	YES	YES
158	a	1040.16	6.12182	YES	YES
159	a	1042.18	0.77937	YES	YES
160	a	1046.19	1.65451	YES	YES
161	a	1047.60	3.26381	YES	YES
162	a	1048.22	1.19107	YES	YES
163	a	1049.42	1.19655	YES	YES
164	a	1050.99	10.86433	YES	YES
165	a	1054.41	15.13036	YES	YES
166	a	1070.69	0.73654	YES	YES
167	a	1072.42	1.81262	YES	YES
168	a	1073.84	1.50661	YES	YES
169	a	1075.58	32.58730	YES	YES
170	a	1100.36	2.05131	YES	YES
171	a	1104.90	2.54444	YES	YES
172	a	1109.29	6.17357	YES	YES
173	a	1137.63	7.06334	YES	YES
174	a	1140.27	6.23130	YES	YES

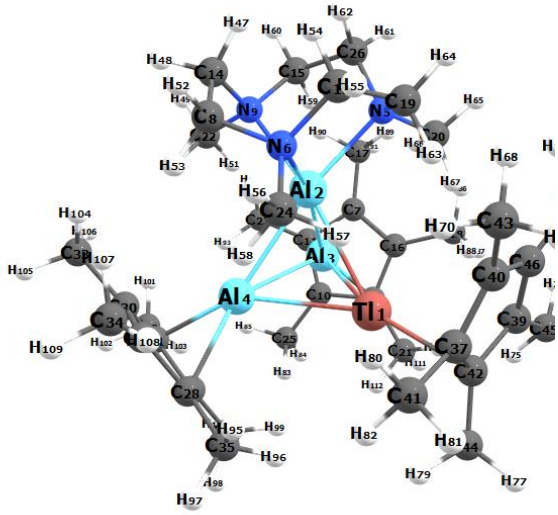
175	a	1151.46	3.70179	YES	YES
176	a	1156.78	0.41355	YES	YES
177	a	1164.30	0.19312	YES	YES
178	a	1166.22	0.12679	YES	YES
179	a	1166.98	0.20776	YES	YES
180	a	1168.00	0.14609	YES	YES
181	a	1195.99	1.46765	YES	YES
182	a	1197.91	1.81336	YES	YES
183	a	1213.79	1.34056	YES	YES
184	a	1236.04	0.22882	YES	YES
185	a	1240.84	0.54249	YES	YES
186	a	1265.19	12.13661	YES	YES
187	a	1267.29	10.82564	YES	YES
188	a	1274.60	11.11005	YES	YES
189	a	1275.45	8.16312	YES	YES
190	a	1313.71	2.36183	YES	YES
191	a	1326.12	1.78795	YES	YES
192	a	1327.89	1.56381	YES	YES
193	a	1328.11	7.96308	YES	YES
194	a	1329.76	21.09128	YES	YES
195	a	1337.27	1.65621	YES	YES
196	a	1337.63	3.61031	YES	YES
197	a	1338.64	0.14683	YES	YES
198	a	1340.22	0.95444	YES	YES
199	a	1340.76	0.42389	YES	YES
200	a	1341.28	0.26489	YES	YES
201	a	1342.92	0.65919	YES	YES
202	a	1343.72	10.84301	YES	YES
203	a	1344.48	1.09446	YES	YES
204	a	1345.79	1.82181	YES	YES
205	a	1346.72	0.97794	YES	YES
206	a	1348.71	0.21461	YES	YES
207	a	1350.41	0.16149	YES	YES
208	a	1354.09	11.63514	YES	YES
209	a	1360.86	4.07573	YES	YES
210	a	1362.42	15.09354	YES	YES
211	a	1369.10	4.72931	YES	YES
212	a	1370.87	1.98356	YES	YES
213	a	1382.86	3.68983	YES	YES
214	a	1383.64	2.62368	YES	YES
215	a	1386.08	5.22911	YES	YES
216	a	1387.38	1.16224	YES	YES
217	a	1389.15	0.97225	YES	YES
218	a	1391.79	3.46327	YES	YES
219	a	1392.25	2.02873	YES	YES
220	a	1392.94	0.62095	YES	YES
221	a	1395.55	0.24358	YES	YES
222	a	1397.04	1.57505	YES	YES
223	a	1397.63	4.54158	YES	YES
224	a	1398.73	9.72298	YES	YES
225	a	1399.19	10.38680	YES	YES
226	a	1400.76	6.74493	YES	YES
227	a	1401.21	7.61300	YES	YES
228	a	1402.32	7.62174	YES	YES
229	a	1402.79	20.97214	YES	YES
230	a	1403.66	0.85044	YES	YES
231	a	1404.58	2.30766	YES	YES
232	a	1404.92	3.10618	YES	YES
233	a	1406.20	18.04736	YES	YES
234	a	1406.64	27.20825	YES	YES
235	a	1407.18	13.15749	YES	YES
236	a	1407.88	2.57538	YES	YES
237	a	1409.08	7.06815	YES	YES
238	a	1410.54	6.55372	YES	YES
239	a	1411.06	3.29796	YES	YES
240	a	1412.51	30.94223	YES	YES
241	a	1413.04	18.04983	YES	YES
242	a	1413.91	6.69091	YES	YES
243	a	1414.88	2.32324	YES	YES
244	a	1415.65	37.74694	YES	YES
245	a	1417.79	3.82326	YES	YES
246	a	1418.25	3.67770	YES	YES
247	a	1419.15	4.21506	YES	YES
248	a	1420.23	4.38347	YES	YES
249	a	1421.42	15.02233	YES	YES
250	a	1422.56	13.07578	YES	YES
251	a	1423.59	34.59485	YES	YES
252	a	1424.90	28.20547	YES	YES

253	a	1426.77	30.85787	YES	YES
254	a	1427.81	3.89426	YES	YES
255	a	1430.38	15.36723	YES	YES
256	a	1431.46	5.90283	YES	YES
257	a	1436.99	1.91779	YES	YES
258	a	1438.60	2.31569	YES	YES
259	a	1441.53	0.45316	YES	YES
260	a	1443.37	3.98596	YES	YES
261	a	1448.35	12.41049	YES	YES
262	a	1449.78	11.19834	YES	YES
263	a	1452.61	2.16328	YES	YES
264	a	1453.59	0.38227	YES	YES
265	a	1488.06	6.16254	YES	YES
266	a	1491.14	7.04689	YES	YES
267	a	1492.25	6.71725	YES	YES
268	a	1496.90	9.20237	YES	YES
269	a	1498.02	0.70340	YES	YES
270	a	1547.49	4.32023	YES	YES
271	a	2935.78	46.88152	YES	YES
272	a	2939.45	50.55891	YES	YES
273	a	2940.02	32.50667	YES	YES
274	a	2941.63	28.14483	YES	YES
275	a	2943.90	67.55479	YES	YES
276	a	2945.54	14.16951	YES	YES
277	a	2948.11	8.63348	YES	YES
278	a	2948.28	30.15977	YES	YES
279	a	2950.39	16.19158	YES	YES
280	a	2950.98	53.77423	YES	YES
281	a	2951.12	35.28571	YES	YES
282	a	2952.23	34.54956	YES	YES
283	a	2953.35	21.68442	YES	YES
284	a	2953.79	34.87597	YES	YES
285	a	2955.96	32.41511	YES	YES
286	a	2956.93	18.13775	YES	YES
287	a	2958.14	27.76900	YES	YES
288	a	2958.73	31.43339	YES	YES
289	a	2959.59	25.54027	YES	YES
290	a	2962.41	26.06602	YES	YES
291	a	2966.57	24.18975	YES	YES
292	a	2990.68	8.14376	YES	YES
293	a	2991.06	17.43677	YES	YES
294	a	2991.96	8.99149	YES	YES
295	a	2995.08	58.14272	YES	YES
296	a	2996.41	6.19036	YES	YES
297	a	3000.82	8.80923	YES	YES
298	a	3011.45	4.74727	YES	YES
299	a	3011.78	10.46001	YES	YES
300	a	3014.52	7.07837	YES	YES
301	a	3017.77	10.71367	YES	YES
302	a	3018.61	7.92616	YES	YES
303	a	3019.48	11.22874	YES	YES
304	a	3021.77	9.48375	YES	YES
305	a	3022.47	7.95076	YES	YES
306	a	3024.35	6.07068	YES	YES
307	a	3028.05	1.57349	YES	YES
308	a	3028.92	8.59673	YES	YES
309	a	3029.73	4.53329	YES	YES
310	a	3035.57	5.93603	YES	YES
311	a	3038.30	3.54907	YES	YES
312	a	3039.63	5.30963	YES	YES
313	a	3043.44	22.46276	YES	YES
314	a	3044.03	1.22440	YES	YES
315	a	3045.21	3.78810	YES	YES
316	a	3045.41	13.55561	YES	YES
317	a	3045.78	9.09652	YES	YES
318	a	3048.22	0.39924	YES	YES
319	a	3049.26	5.71168	YES	YES
320	a	3049.82	10.20782	YES	YES
321	a	3050.02	7.83651	YES	YES
322	a	3052.85	8.31256	YES	YES
323	a	3053.40	9.92941	YES	YES
324	a	3056.11	4.38826	YES	YES
325	a	3056.35	8.70302	YES	YES
326	a	3056.67	12.73828	YES	YES
327	a	3066.63	6.11444	YES	YES
328	a	3066.81	5.63690	YES	YES
329	a	3067.23	7.04840	YES	YES
330	a	3069.85	6.26941	YES	YES

331	a	3072.17	4.82948	YES	YES
332	a	3080.69	5.95717	YES	YES
333	a	3084.53	3.89811	YES	YES
334	a	3096.34	1.51946	YES	YES
335	a	3099.94	2.30917	YES	YES
336	a	3103.80	5.55604	YES	YES

$end

[(Me$_3$TACN)Al(TlCp*)(AlCp*)$_2$]$^+$



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

Symmetry: c1

Cartesian coordinates in Ångström:

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Al	-0.1503629	0.2673434	-1.6279653
Al	-1.4664514	-1.4876126	0.0317032
Al	-1.6340872	1.2639883	0.4365182
N	1.1746062	-0.7727769	-3.0335547
N	0.8289554	1.9956211	-2.5629032
C	-2.0503057	-3.5873615	-0.7893497
C	-0.3054486	2.6510655	-3.2544964
N	-1.3815004	0.4085409	-3.4097251
C	-2.8639373	-2.8340165	1.2576986
C	-3.1922898	-2.9972306	-0.1328223
C	-1.5127923	-3.2805267	1.4510578
C	1.9189760	1.5480544	-3.4756826
C	-1.0415832	1.6600362	-4.1560192
C	-1.0380801	-0.8324415	-4.1558436
C	-1.0156200	-3.7620025	0.1896021
C	-1.9996370	-4.0212856	-2.2252919
C	0.3452120	-4.3616534	-0.0149134
C	2.3498825	0.1304894	-3.1176193
C	1.5625942	-2.0646407	-2.4256535
C	-0.7656428	-3.2867136	2.7516082
C	-2.8105150	0.3955465	-3.0199856
C	-4.5210103	-2.6917800	-0.7636408
C	1.3731506	2.8481859	-1.4817633
C	-3.7694184	-2.3360922	2.3428928
C	0.4733173	-0.9716995	-4.3318871
C	-2.6498235	1.9931517	2.3473733
C	-1.6310235	2.9540000	2.0100005
C	-1.9967443	3.5732759	0.7675242
C	-3.2112455	2.9617651	0.3071129
C	-3.6218333	1.9866673	1.2886484
C	-4.8802206	1.1710363	1.2268687
C	-3.9909222	3.3637882	-0.9111534
C	-1.2984313	4.7294537	0.1155640
C	-0.4327843	3.2705897	2.8567590
C	-2.6399195	1.1493728	3.5875717
C	3.5347028	1.1633325	1.2637673
C	4.7631882	-1.6607666	-0.9169019
C	3.5094721	-1.1835791	1.3105135
C	4.1340693	0.6794624	0.0724340
C	3.4730974	2.5930289	1.7212688
C	3.1289016	0.0125252	2.0569001
C	4.8375316	1.5186998	-0.9592249
C	2.8819566	0.0449956	3.5469668
C	3.4400517	-2.5883915	1.8391030
C	4.1144245	-0.7630112	0.0992597
H	-0.4223601	1.3998627	-5.0353568
H	-1.9607248	2.1320269	-4.5588205
H	-3.4667981	0.3375851	-3.9148617
H	-3.0419699	1.3089619	-2.4434843
H	-2.9953058	-0.4711692	-2.3558320
H	0.0226773	3.5395919	-3.8394147
H	-0.9908123	3.0082322	-2.4576613
H	1.5695158	1.6083790	-4.5245233
H	2.7921080	2.2274110	-3.4019236
H	1.7869514	3.7937579	-1.8930580
H	2.1577126	2.2873454	-0.9389609
H	0.5673467	3.0678500	-0.7598266
H	-1.4218503	-1.6761999	-3.5481149
H	-1.5522745	-0.8655790	-5.1421991

H	0.7048044	-1.9709500	-4.7551573
H	0.8498344	-0.2364238	-5.0684969
H	2.8151806	0.1268332	-2.1084788
H	3.1025288	-0.2477069	-3.8441217
H	2.3097730	-2.5912943	-3.0567461
H	0.6627505	-2.6914997	-2.3006799
H	1.9870545	-1.8752723	-1.4207452
H	4.8310609	1.0563336	-1.9692534
H	5.9111109	1.6649683	-0.7044213
H	4.4048617	2.5370503	-1.0491314
H	4.6453674	-1.2926883	-1.9584437
H	4.3573039	-2.6921726	-0.8826690
H	5.8598309	-1.7484816	-0.7487995
H	3.4031167	-3.3396305	1.0239078
H	2.5508738	-2.7541575	2.4814247
H	4.3280360	-2.8414913	2.4610000
H	3.8419890	0.0499141	4.1100242
H	2.3072124	-0.8357475	3.8984896
H	2.3227158	0.9500996	3.8609006
H	3.3620717	3.3039398	0.8753877
H	4.3966692	2.8973699	2.2633171
H	2.6266022	2.7712755	2.4143342
H	-3.2668810	-1.5878996	2.9874482
H	-4.0903157	-3.1706233	3.0011196
H	-4.6858436	-1.8730980	1.9319399
H	0.5252356	-4.6296800	-1.0730247
H	0.4613593	-5.2917380	0.5789713
H	1.1549499	-3.6730533	0.3052767
H	-0.9800247	-3.9439180	-2.6530840
H	-2.6830661	-3.4242438	-2.8618584
H	-2.3106458	-5.0820383	-2.3366129
H	-4.4318569	-2.5238350	-1.8553181
H	-4.9873880	-1.7877775	-0.3239060
H	-5.2370936	-3.5297674	-0.6252993
H	0.3833753	3.7267705	2.2635754
H	-0.0226610	2.3594838	3.3374749
H	-0.6887440	3.9832768	3.6695496
H	-2.5424861	1.7779699	4.4957068
H	-1.7880191	0.4330466	3.5900555
H	-3.5714856	0.5626214	3.6890964
H	-5.0726901	0.7806926	0.2063450
H	-5.7655256	1.7750732	1.5175890
H	-4.8326475	0.3020722	1.9080144
H	-3.3315982	3.6660881	-1.7508478
H	-4.6486167	4.2341322	-0.6981837
H	-4.6499889	2.5483620	-1.2685650
H	-1.3301196	4.6767212	-0.9915153
H	-0.2379420	4.8046801	0.4244690
H	-1.7825287	5.6888594	0.3987359
H	0.3289952	-3.2220923	2.5929583
H	-0.9611732	-4.2183805	3.3242744
H	-1.0602919	-2.4348666	3.3960747

SCF energy GEOOPT = -2589.015516359 H

ZPE = 2488. kJ/mol

FREEH energy = 2649.62 kJ/mol

FREEH entropy = 1.39584 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	12.00	0.24805	YES YES
8	a	19.60	0.02415	YES YES
9	a	24.64	0.01845	YES YES
10	a	31.24	0.64467	YES YES
11	a	33.94	0.21529	YES YES
12	a	39.29	0.19534	YES YES
13	a	43.65	0.32816	YES YES
14	a	49.57	0.21487	YES YES
15	a	52.86	0.28937	YES YES
16	a	57.77	0.16779	YES YES
17	a	60.70	0.04518	YES YES

18	a	63.75	0.20427	YES	YES
19	a	66.73	0.05588	YES	YES
20	a	72.29	0.90261	YES	YES
21	a	76.80	0.34338	YES	YES
22	a	82.49	0.43513	YES	YES
23	a	87.97	0.15205	YES	YES
24	a	90.14	0.06633	YES	YES
25	a	94.07	0.72105	YES	YES
26	a	95.04	0.13190	YES	YES
27	a	99.93	0.27074	YES	YES
28	a	107.66	0.28592	YES	YES
29	a	108.90	0.34641	YES	YES
30	a	112.92	0.09760	YES	YES
31	a	118.75	0.06036	YES	YES
32	a	119.80	0.17445	YES	YES
33	a	122.38	0.67502	YES	YES
34	a	124.66	0.76212	YES	YES
35	a	125.00	0.11900	YES	YES
36	a	129.84	0.10558	YES	YES
37	a	136.14	4.11759	YES	YES
38	a	145.19	0.69024	YES	YES
39	a	146.50	0.27444	YES	YES
40	a	153.77	0.29384	YES	YES
41	a	159.75	0.34150	YES	YES
42	a	162.62	0.24029	YES	YES
43	a	164.79	0.20573	YES	YES
44	a	166.02	0.00503	YES	YES
45	a	168.23	0.79094	YES	YES
46	a	169.34	0.22401	YES	YES
47	a	172.85	0.01629	YES	YES
48	a	174.75	0.71893	YES	YES
49	a	176.81	0.55755	YES	YES
50	a	179.16	0.05202	YES	YES
51	a	185.04	1.50290	YES	YES
52	a	198.68	0.54552	YES	YES
53	a	209.25	1.73185	YES	YES
54	a	211.11	1.36347	YES	YES
55	a	215.24	0.97656	YES	YES
56	a	220.75	0.12969	YES	YES
57	a	224.75	0.37642	YES	YES
58	a	228.17	13.76151	YES	YES
59	a	232.90	17.99606	YES	YES
60	a	234.67	42.75975	YES	YES
61	a	254.40	1.20453	YES	YES
62	a	255.93	0.48314	YES	YES
63	a	258.45	0.46063	YES	YES
64	a	258.89	0.18994	YES	YES
65	a	262.63	1.00486	YES	YES
66	a	264.55	0.29316	YES	YES
67	a	266.66	0.19196	YES	YES
68	a	269.80	0.35650	YES	YES
69	a	271.81	0.34821	YES	YES
70	a	273.76	4.68619	YES	YES
71	a	275.66	0.14369	YES	YES
72	a	276.38	0.70941	YES	YES
73	a	279.74	0.15939	YES	YES
74	a	280.59	1.02104	YES	YES
75	a	283.80	1.53789	YES	YES
76	a	284.12	0.31929	YES	YES
77	a	289.14	9.87696	YES	YES
78	a	294.95	6.38589	YES	YES
79	a	322.70	52.45391	YES	YES
80	a	327.50	4.24719	YES	YES
81	a	327.98	7.08802	YES	YES
82	a	330.10	13.32454	YES	YES
83	a	347.29	121.04243	YES	YES
84	a	356.16	17.80716	YES	YES
85	a	364.03	13.85700	YES	YES
86	a	367.87	10.80657	YES	YES
87	a	377.56	7.93411	YES	YES
88	a	393.46	26.72171	YES	YES
89	a	395.08	78.81611	YES	YES
90	a	398.18	83.89429	YES	YES
91	a	399.65	308.54785	YES	YES
92	a	422.88	28.18340	YES	YES
93	a	438.21	1.39254	YES	YES
94	a	442.12	3.56946	YES	YES
95	a	465.48	82.97296	YES	YES

96	a	475.99	37.44071	YES	YES
97	a	533.11	0.10730	YES	YES
98	a	536.73	0.09999	YES	YES
99	a	541.48	0.14663	YES	YES
100	a	542.50	0.05537	YES	YES
101	a	542.70	0.01152	YES	YES
102	a	543.52	0.06895	YES	YES
103	a	544.22	0.16842	YES	YES
104	a	545.40	0.30162	YES	YES
105	a	547.12	0.07310	YES	YES
106	a	560.20	3.64700	YES	YES
107	a	562.56	4.60276	YES	YES
108	a	578.47	0.35605	YES	YES
109	a	578.78	0.61671	YES	YES
110	a	583.55	1.29970	YES	YES
111	a	584.04	0.58164	YES	YES
112	a	586.53	0.76866	YES	YES
113	a	590.70	9.44084	YES	YES
114	a	592.13	13.53466	YES	YES
115	a	594.02	4.50732	YES	YES
116	a	610.17	8.06852	YES	YES
117	a	637.85	0.22549	YES	YES
118	a	728.12	14.24175	YES	YES
119	a	735.75	11.14016	YES	YES
120	a	770.18	58.43675	YES	YES
121	a	793.25	5.57860	YES	YES
122	a	796.74	1.77616	YES	YES
123	a	797.51	1.44381	YES	YES
124	a	798.86	3.91918	YES	YES
125	a	801.30	4.29578	YES	YES
126	a	803.08	0.32538	YES	YES
127	a	845.35	0.49807	YES	YES
128	a	890.42	5.04532	YES	YES
129	a	893.25	5.15797	YES	YES
130	a	912.05	6.56265	YES	YES
131	a	919.45	0.27189	YES	YES
132	a	920.19	0.06221	YES	YES
133	a	923.32	1.00654	YES	YES
134	a	926.91	0.20846	YES	YES
135	a	931.58	0.95919	YES	YES
136	a	969.55	13.75665	YES	YES
137	a	970.30	9.09942	YES	YES
138	a	975.94	14.62857	YES	YES
139	a	978.85	21.19254	YES	YES
140	a	982.62	8.96276	YES	YES
141	a	985.22	5.51652	YES	YES
142	a	985.83	2.59465	YES	YES
143	a	989.15	2.07736	YES	YES
144	a	989.82	6.04953	YES	YES
145	a	993.72	0.12039	YES	YES
146	a	994.42	0.86713	YES	YES
147	a	995.27	8.70820	YES	YES
148	a	996.92	0.11650	YES	YES
149	a	997.45	1.37132	YES	YES
150	a	998.05	2.33723	YES	YES
151	a	998.57	16.42748	YES	YES
152	a	999.51	1.02818	YES	YES
153	a	1001.41	14.95269	YES	YES
154	a	1002.03	0.92651	YES	YES
155	a	1005.61	0.18719	YES	YES
156	a	1010.38	2.19043	YES	YES
157	a	1026.47	1.90436	YES	YES
158	a	1040.10	3.87035	YES	YES
159	a	1041.65	1.01074	YES	YES
160	a	1045.95	1.79546	YES	YES
161	a	1047.15	5.45737	YES	YES
162	a	1048.39	4.17265	YES	YES
163	a	1049.09	2.94724	YES	YES
164	a	1050.09	1.22711	YES	YES
165	a	1052.25	13.22544	YES	YES
166	a	1071.83	1.15835	YES	YES
167	a	1072.09	0.80668	YES	YES
168	a	1074.30	34.16124	YES	YES
169	a	1075.05	1.17670	YES	YES
170	a	1102.04	1.64780	YES	YES
171	a	1102.82	1.15304	YES	YES
172	a	1107.66	7.12177	YES	YES
173	a	1136.92	5.69263	YES	YES

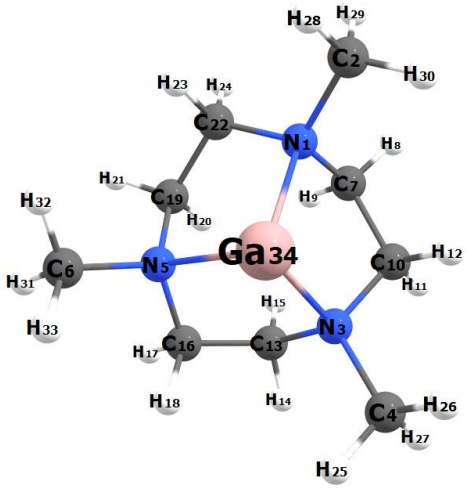
174	a	1138.29	7.61984	YES	YES
175	a	1150.39	8.85185	YES	YES
176	a	1156.21	2.69316	YES	YES
177	a	1164.46	0.26535	YES	YES
178	a	1164.78	0.12429	YES	YES
179	a	1165.63	0.02780	YES	YES
180	a	1167.03	0.28685	YES	YES
181	a	1193.20	1.16867	YES	YES
182	a	1197.50	2.05075	YES	YES
183	a	1211.76	1.08873	YES	YES
184	a	1237.43	0.09367	YES	YES
185	a	1241.14	0.04573	YES	YES
186	a	1264.41	11.93178	YES	YES
187	a	1267.75	10.55297	YES	YES
188	a	1273.54	10.12128	YES	YES
189	a	1275.13	7.10827	YES	YES
190	a	1314.13	1.71274	YES	YES
191	a	1326.66	0.81822	YES	YES
192	a	1327.48	0.60786	YES	YES
193	a	1333.26	1.86917	YES	YES
194	a	1335.81	28.51358	YES	YES
195	a	1338.06	1.11225	YES	YES
196	a	1339.05	0.59748	YES	YES
197	a	1340.21	2.63187	YES	YES
198	a	1340.81	2.12008	YES	YES
199	a	1342.30	5.07969	YES	YES
200	a	1343.03	7.06288	YES	YES
201	a	1343.48	8.85078	YES	YES
202	a	1344.31	2.19975	YES	YES
203	a	1345.80	12.82368	YES	YES
204	a	1346.17	4.04026	YES	YES
205	a	1348.09	2.77319	YES	YES
206	a	1349.63	0.10306	YES	YES
207	a	1350.91	1.17721	YES	YES
208	a	1355.37	10.36727	YES	YES
209	a	1362.27	3.85476	YES	YES
210	a	1366.36	5.11606	YES	YES
211	a	1369.56	21.73541	YES	YES
212	a	1373.63	1.54790	YES	YES
213	a	1383.24	0.60375	YES	YES
214	a	1384.54	0.80285	YES	YES
215	a	1387.73	6.08377	YES	YES
216	a	1388.37	1.32799	YES	YES
217	a	1389.29	2.93592	YES	YES
218	a	1389.55	3.61600	YES	YES
219	a	1391.77	5.17947	YES	YES
220	a	1392.97	4.20179	YES	YES
221	a	1393.81	4.97447	YES	YES
222	a	1396.12	1.71313	YES	YES
223	a	1397.71	9.68670	YES	YES
224	a	1398.69	6.26839	YES	YES
225	a	1399.02	6.96049	YES	YES
226	a	1400.67	11.73834	YES	YES
227	a	1400.95	1.09947	YES	YES
228	a	1402.24	2.46908	YES	YES
229	a	1402.59	5.85520	YES	YES
230	a	1403.23	11.47832	YES	YES
231	a	1404.86	8.79124	YES	YES
232	a	1405.68	0.80488	YES	YES
233	a	1406.22	9.41085	YES	YES
234	a	1407.52	6.54845	YES	YES
235	a	1408.00	7.28035	YES	YES
236	a	1408.08	15.31560	YES	YES
237	a	1408.88	36.20691	YES	YES
238	a	1410.67	8.92769	YES	YES
239	a	1411.18	21.94137	YES	YES
240	a	1411.43	1.86307	YES	YES
241	a	1412.55	4.99590	YES	YES
242	a	1412.96	14.07013	YES	YES
243	a	1413.53	11.44323	YES	YES
244	a	1414.96	16.57774	YES	YES
245	a	1415.26	39.10156	YES	YES
246	a	1416.47	15.97859	YES	YES
247	a	1417.51	40.13702	YES	YES
248	a	1418.09	18.39365	YES	YES
249	a	1420.46	11.91202	YES	YES
250	a	1421.57	3.65064	YES	YES
251	a	1422.97	5.86261	YES	YES

252	a	1424.16	42.91311	YES	YES
253	a	1425.40	33.52265	YES	YES
254	a	1426.60	5.63253	YES	YES
255	a	1430.07	10.79894	YES	YES
256	a	1434.18	4.06026	YES	YES
257	a	1437.03	2.68018	YES	YES
258	a	1439.71	1.20734	YES	YES
259	a	1444.46	0.38896	YES	YES
260	a	1447.84	12.43775	YES	YES
261	a	1449.19	16.19839	YES	YES
262	a	1451.10	1.13975	YES	YES
263	a	1453.54	1.05281	YES	YES
264	a	1455.39	1.99010	YES	YES
265	a	1471.85	0.52455	YES	YES
266	a	1484.41	6.86991	YES	YES
267	a	1486.30	5.63371	YES	YES
268	a	1496.25	7.52418	YES	YES
269	a	1497.73	9.62631	YES	YES
270	a	1514.55	2.25411	YES	YES
271	a	2934.65	92.98917	YES	YES
272	a	2934.92	35.58451	YES	YES
273	a	2935.44	19.45638	YES	YES
274	a	2937.12	54.44573	YES	YES
275	a	2938.01	58.97253	YES	YES
276	a	2938.67	43.38803	YES	YES
277	a	2944.49	25.70493	YES	YES
278	a	2948.30	12.97237	YES	YES
279	a	2948.39	31.69712	YES	YES
280	a	2950.50	44.57008	YES	YES
281	a	2951.16	26.91609	YES	YES
282	a	2951.73	31.38270	YES	YES
283	a	2954.82	31.93842	YES	YES
284	a	2955.87	29.10031	YES	YES
285	a	2956.94	13.14882	YES	YES
286	a	2957.01	29.96499	YES	YES
287	a	2957.87	32.78902	YES	YES
288	a	2958.77	21.16724	YES	YES
289	a	2959.60	22.81168	YES	YES
290	a	2960.24	22.40156	YES	YES
291	a	2965.49	23.42923	YES	YES
292	a	2989.98	10.21827	YES	YES
293	a	2991.49	10.14880	YES	YES
294	a	2992.40	30.65427	YES	YES
295	a	2995.59	12.19008	YES	YES
296	a	2996.41	30.96491	YES	YES
297	a	2998.32	9.25081	YES	YES
298	a	3001.40	7.67848	YES	YES
299	a	3007.14	8.69519	YES	YES
300	a	3009.06	3.78136	YES	YES
301	a	3011.07	5.76519	YES	YES
302	a	3015.56	14.03948	YES	YES
303	a	3021.38	0.86654	YES	YES
304	a	3021.47	15.73702	YES	YES
305	a	3022.51	10.59592	YES	YES
306	a	3026.39	16.16285	YES	YES
307	a	3026.91	8.25023	YES	YES
308	a	3029.06	5.50948	YES	YES
309	a	3029.93	3.90503	YES	YES
310	a	3030.14	5.10586	YES	YES
311	a	3030.25	3.92348	YES	YES
312	a	3032.28	7.39449	YES	YES
313	a	3035.13	9.63360	YES	YES
314	a	3036.37	11.77063	YES	YES
315	a	3037.89	2.57982	YES	YES
316	a	3039.61	16.88764	YES	YES
317	a	3041.10	9.57670	YES	YES
318	a	3045.46	3.50323	YES	YES
319	a	3047.29	5.11026	YES	YES
320	a	3047.90	1.55607	YES	YES
321	a	3048.78	13.86878	YES	YES
322	a	3050.69	8.50361	YES	YES
323	a	3052.15	3.87703	YES	YES
324	a	3053.52	8.46721	YES	YES
325	a	3054.10	13.05311	YES	YES
326	a	3056.96	4.59828	YES	YES
327	a	3057.44	6.52739	YES	YES
328	a	3058.35	5.38635	YES	YES
329	a	3060.22	8.03775	YES	YES

330	a	3065.26	7.89762	YES	YES
331	a	3073.97	7.18418	YES	YES
332	a	3075.17	4.44580	YES	YES
333	a	3080.50	3.28420	YES	YES
334	a	3090.13	2.58460	YES	YES
335	a	3094.28	3.05506	YES	YES
336	a	3094.97	2.03401	YES	YES

$end

[Ga(Me$_3$TACN)]$^+$



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

Symmetry: c1

Cartesian coordinates in Ångström:

N	-1.9923808	2.3811235	15.6405954
C	-2.5359373	1.1101549	16.1640775
N	-0.5061701	3.0245541	13.2076149
C	-0.1330903	2.6007095	11.8416141
N	-2.5491627	4.8634074	14.2015143
C	-3.8083074	5.5815207	13.9123135
C	-0.5048808	2.3788173	15.6267656
H	-0.1095025	1.6115172	16.3254685
H	-0.1346726	3.3472158	16.0137719
C	0.0612377	2.1141416	14.2306197
H	1.1743133	2.1763379	14.2604994
H	-0.1882424	1.0791992	13.9158999
C	-0.1975823	4.4608839	13.4415008
H	0.5580218	4.8213624	12.7117949
H	0.2756456	4.5754899	14.4352232
C	-1.4419637	5.3448383	13.3414580
H	-1.1707119	6.4004912	13.5775089
H	-1.8194967	5.3423769	12.2975263
C	-2.2315591	4.8735552	15.6547891
H	-1.1572685	5.1009369	15.7922408
H	-2.7748416	5.6955966	16.1669994
C	-2.5847462	3.5494766	16.3344417
H	-3.6856020	3.4064260	16.3253812
H	-2.2791193	3.5862101	17.4063023
H	-0.6098806	3.2672957	11.0981193
H	-0.4939223	1.5703530	11.6554534
H	0.9688103	2.6277986	11.6910494
H	-3.6361584	1.0914200	16.0389670
H	-2.2948961	0.9745252	17.2416384
H	-2.1147653	0.2591035	15.5958713
H	-3.7160937	6.6703186	14.1211740
H	-4.6270375	5.1689155	14.5319569
H	-4.0843302	5.4438878	12.8486540
Ga	-2.8333464	2.6369690	13.4392351

SCF energy GEOOPT = -2444.271803112 H

ZPE = 789.1 kJ/mol

FREEH energy = 826.54 kJ/mol

FREEH entropy = 0.47660 kJ/mol/K

$vibrational spectrum

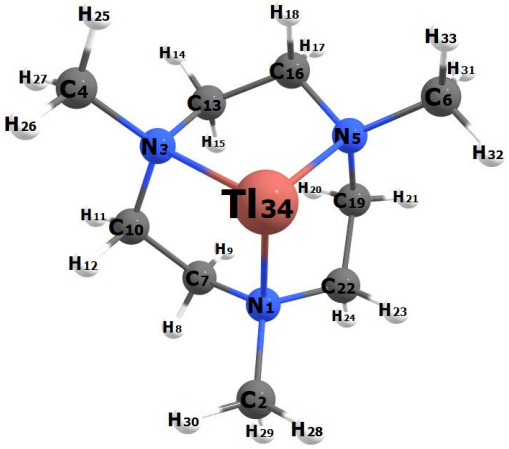
# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		-0.00	0.00000	- -
2		-0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	133.90	0.45466	YES YES
8	a	134.88	0.45991	YES YES
9	a	153.10	1.52703	YES YES
10	a	153.62	1.53864	YES YES
11	a	176.42	0.32310	YES YES
12	a	194.35	0.28531	YES YES
13	a	195.96	0.28475	YES YES
14	a	240.94	2.50288	YES YES
15	a	251.01	0.41563	YES YES
16	a	251.61	0.41584	YES YES
17	a	254.86	0.58708	YES YES
18	a	273.12	0.08904	YES YES

19	a	305.04	2.79625	YES	YES
20	a	305.47	2.77967	YES	YES
21	a	372.03	15.04947	YES	YES
22	a	372.39	15.10183	YES	YES
23	a	386.81	3.56945	YES	YES
24	a	430.46	0.92896	YES	YES
25	a	431.04	0.92629	YES	YES
26	a	445.69	9.18233	YES	YES
27	a	488.08	24.35159	YES	YES
28	a	553.19	6.48687	YES	YES
29	a	553.64	6.48398	YES	YES
30	a	579.52	0.00331	YES	YES
31	a	727.46	23.48299	YES	YES
32	a	727.80	23.48644	YES	YES
33	a	766.57	41.65705	YES	YES
34	a	843.09	0.32908	YES	YES
35	a	881.87	5.71446	YES	YES
36	a	882.07	5.68762	YES	YES
37	a	965.15	10.64127	YES	YES
38	a	965.48	10.51882	YES	YES
39	a	975.77	7.52168	YES	YES
40	a	1002.70	47.24938	YES	YES
41	a	1003.38	47.68501	YES	YES
42	a	1007.05	0.18551	YES	YES
43	a	1024.06	0.04002	YES	YES
44	a	1053.76	15.84323	YES	YES
45	a	1053.99	15.77639	YES	YES
46	a	1081.08	33.71421	YES	YES
47	a	1103.62	4.97362	YES	YES
48	a	1103.99	4.94696	YES	YES
49	a	1109.98	5.18824	YES	YES
50	a	1134.53	16.97050	YES	YES
51	a	1135.21	17.26413	YES	YES
52	a	1199.73	3.58644	YES	YES
53	a	1199.93	3.59606	YES	YES
54	a	1215.62	0.25770	YES	YES
55	a	1239.11	2.02338	YES	YES
56	a	1239.48	1.98071	YES	YES
57	a	1267.11	14.53937	YES	YES
58	a	1273.31	2.02349	YES	YES
59	a	1281.99	12.10976	YES	YES
60	a	1282.49	11.99441	YES	YES
61	a	1316.41	1.93480	YES	YES
62	a	1333.22	2.80892	YES	YES
63	a	1333.81	2.62273	YES	YES
64	a	1357.54	1.99598	YES	YES
65	a	1364.54	3.17353	YES	YES
66	a	1365.32	3.04267	YES	YES
67	a	1394.53	10.97117	YES	YES
68	a	1396.24	2.70309	YES	YES
69	a	1396.53	2.69376	YES	YES
70	a	1414.82	2.17327	YES	YES
71	a	1415.42	2.17697	YES	YES
72	a	1420.24	0.23827	YES	YES
73	a	1420.55	2.62844	YES	YES
74	a	1421.78	33.65995	YES	YES
75	a	1425.71	5.84857	YES	YES
76	a	1425.85	5.32593	YES	YES
77	a	1427.54	0.71310	YES	YES
78	a	1435.65	9.56163	YES	YES
79	a	1437.48	36.12063	YES	YES
80	a	1437.58	36.46301	YES	YES
81	a	1450.25	8.82195	YES	YES
82	a	2937.87	25.84361	YES	YES
83	a	2938.00	25.29751	YES	YES
84	a	2938.21	15.09205	YES	YES
85	a	2947.29	47.50428	YES	YES
86	a	2947.30	47.53089	YES	YES
87	a	2947.72	0.36564	YES	YES
88	a	2984.40	7.07187	YES	YES
89	a	2984.59	6.99467	YES	YES
90	a	2986.97	34.73423	YES	YES
91	a	3009.31	7.38755	YES	YES
92	a	3009.74	2.88413	YES	YES
93	a	3009.94	0.65117	YES	YES
94	a	3044.83	8.61044	YES	YES
95	a	3044.95	8.82789	YES	YES
96	a	3045.53	7.63932	YES	YES

97	a	3045.91	0.21950	YES	YES
98	a	3045.97	0.81640	YES	YES
99	a	3051.65	18.55274	YES	YES
100	a	3078.85	0.44766	YES	YES
101	a	3079.07	5.48986	YES	YES
102	a	3079.26	5.07692	YES	YES

$end

[Tl(Me$_3$TACN)]$^+$



C	-2.6057035	3.5201738	16.3148024
H	-3.7074978	3.3777597	16.3057995
H	-2.3111445	3.5849946	17.3909082
H	-0.4724554	3.2634660	11.0462512
H	-0.3225448	1.5665063	11.6044237
H	1.0893515	2.6759709	11.7232804
H	-3.6109121	1.0449233	16.2096226
H	-2.2171904	1.0002359	17.3471164
H	-2.0973299	0.2108713	15.7330018
H	-3.6580943	6.7713932	14.1859838
H	-4.6479333	5.3124898	14.5528952
H	-4.0975225	5.6198019	12.8747330
Tl	-3.0863940	2.4639868	13.2387709

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

Symmetry: c1

SCF energy GEOOPT = -692.0725466709 H

ZPE = 786.1 kJ/mol

FREEH energy = 824.77 kJ/mol

FREEH entropy = 0.49836 kJ/mol/K

Cartesian coordinates in Ångström:

N	-2.0084003	2.3332952	15.6658536
C	-2.5053853	1.0865544	16.2738268
N	-0.4856781	3.0116219	13.1564066
C	-0.0194209	2.6109115	11.8173627
N	-2.5947815	4.8960336	14.1947269
C	-3.8073339	5.6941190	13.9417160
C	-0.5274790	2.3620524	15.5993956
H	-0.0943972	1.6041098	16.2869608
H	-0.1614817	3.3348607	15.9802575
C	0.0370824	2.1028568	14.1993009
H	1.1523359	2.1488838	14.2549713
H	-0.2125224	1.0668507	13.8852036
C	-0.2294559	4.4476131	13.4226965
H	0.5235587	4.8452344	12.7087921
H	0.2370300	4.5586702	14.4204016
C	-1.4779102	5.3300707	13.3282363
H	-1.1811422	6.3849911	13.5475562
H	-1.8550070	5.3276854	12.2832945
C	-2.2569067	4.8490814	15.6377238
H	-1.1802375	5.0696748	15.7704426
H	-2.7847361	5.6592154	16.1853150

$vibrational spectrum

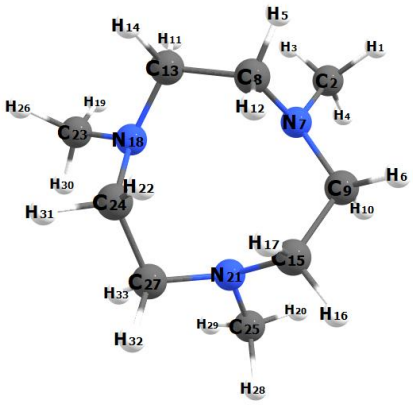
#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1			-0.00	0.00000	-	-
2			-0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	106.20	0.43580	YES	YES
8		a	107.02	0.45206	YES	YES
9		a	131.34	1.28990	YES	YES
10		a	134.42	0.13822	YES	YES
11		a	135.22	0.15211	YES	YES
12		a	163.60	2.96124	YES	YES
13		a	183.02	0.16201	YES	YES
14		a	184.56	0.16167	YES	YES
15		a	256.00	0.43004	YES	YES
16		a	256.62	0.43211	YES	YES
17		a	259.12	0.04599	YES	YES

18	a	274.11	0.03112	YES	YES
19	a	298.66	1.23529	YES	YES
20	a	299.20	1.22737	YES	YES
21	a	364.61	10.49833	YES	YES
22	a	365.22	10.59940	YES	YES
23	a	373.48	8.62655	YES	YES
24	a	405.43	13.93006	YES	YES
25	a	428.79	0.27334	YES	YES
26	a	429.15	0.24489	YES	YES
27	a	474.29	4.17387	YES	YES
28	a	551.06	6.77362	YES	YES
29	a	551.58	6.74886	YES	YES
30	a	571.80	0.02056	YES	YES
31	a	733.56	20.36344	YES	YES
32	a	734.08	20.44343	YES	YES
33	a	753.71	42.63871	YES	YES
34	a	842.90	0.89017	YES	YES
35	a	874.04	4.54073	YES	YES
36	a	874.24	4.67208	YES	YES
37	a	968.56	7.21892	YES	YES
38	a	968.67	7.26819	YES	YES
39	a	978.80	9.10455	YES	YES
40	a	1008.88	52.26465	YES	YES
41	a	1009.84	53.13935	YES	YES
42	a	1013.27	0.53730	YES	YES
43	a	1025.92	0.35665	YES	YES
44	a	1063.73	15.65035	YES	YES
45	a	1063.95	15.76916	YES	YES
46	a	1090.33	30.75647	YES	YES
47	a	1106.87	5.18498	YES	YES
48	a	1107.97	5.20554	YES	YES
49	a	1111.19	1.00693	YES	YES
50	a	1134.46	23.44126	YES	YES
51	a	1135.17	23.87514	YES	YES
52	a	1204.83	5.31198	YES	YES
53	a	1205.05	5.28095	YES	YES
54	a	1221.42	0.30126	YES	YES
55	a	1243.07	4.99729	YES	YES
56	a	1243.63	5.06858	YES	YES
57	a	1267.27	9.82230	YES	YES
58	a	1282.40	2.58856	YES	YES
59	a	1290.81	11.30290	YES	YES
60	a	1291.29	11.11724	YES	YES
61	a	1318.67	1.22277	YES	YES
62	a	1338.67	7.26390	YES	YES
63	a	1339.15	7.13911	YES	YES
64	a	1357.97	3.10597	YES	YES
65	a	1363.95	3.11047	YES	YES
66	a	1364.86	3.06865	YES	YES
67	a	1394.75	14.03609	YES	YES
68	a	1395.17	5.17429	YES	YES
69	a	1395.79	4.86316	YES	YES
70	a	1414.58	1.26240	YES	YES
71	a	1415.58	1.24530	YES	YES
72	a	1420.64	2.21421	YES	YES
73	a	1420.98	15.14952	YES	YES
74	a	1421.19	14.83657	YES	YES
75	a	1428.48	3.49226	YES	YES
76	a	1429.05	3.34577	YES	YES
77	a	1430.27	0.72554	YES	YES
78	a	1440.09	10.81541	YES	YES
79	a	1441.25	28.06305	YES	YES
80	a	1441.46	28.12045	YES	YES
81	a	1449.93	3.40386	YES	YES
82	a	2911.34	40.40128	YES	YES
83	a	2911.45	40.56732	YES	YES
84	a	2911.90	26.62580	YES	YES
85	a	2928.38	67.17559	YES	YES
86	a	2928.49	66.86333	YES	YES
87	a	2928.97	3.54522	YES	YES
88	a	2976.27	10.28506	YES	YES
89	a	2976.34	10.30492	YES	YES
90	a	2978.87	41.83944	YES	YES
91	a	2994.46	8.78106	YES	YES
92	a	2995.22	6.48206	YES	YES
93	a	2995.46	1.76856	YES	YES
94	a	3028.00	7.06468	YES	YES
95	a	3028.15	6.46721	YES	YES

96	a	3028.39	6.31594	YES	YES
97	a	3038.02	6.78091	YES	YES
98	a	3038.34	6.77491	YES	YES
99	a	3045.09	21.23808	YES	YES
100	a	3069.35	1.87410	YES	YES
101	a	3069.55	9.49550	YES	YES
102	a	3070.03	7.85966	YES	YES

$end

Me_3TACN



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

Symmetry: c1

Cartesian coordinates in Ångström:

H	3.4762254	6.1389685	3.1947332
C	2.4226585	6.5088258	3.3433677
H	2.0846067	6.1418850	4.3352369
H	2.4632131	7.6165261	3.4021778
H	2.0173381	4.0569218	2.7106312
H	2.5726681	6.3172441	0.4474763
N	1.4991462	6.0963995	2.3147571
C	1.1694114	4.6831008	2.3313860
C	1.6890629	6.7208899	1.0217011
H	1.9169822	7.7933111	1.2062025
H	0.1421047	4.6032964	4.2392307
H	1.0062953	4.3311869	1.2921482
C	-0.0778158	4.3562628	3.1778133
H	-0.2312741	3.2385841	3.1518396
C	0.4504023	6.6349397	0.1067682
H	0.6961576	7.1531192	-0.8555671
H	0.2834951	5.5767950	-0.1813003
N	-1.2514004	5.1152063	2.7975829
H	-1.8723136	5.5040562	4.7688445
H	-0.0862951	9.1573465	0.6820911
N	-0.7550352	7.1627666	0.7190138
H	-1.0083266	4.3527190	0.8576423
C	-2.2934797	5.1851870	3.7925888
C	-1.7272363	4.9701052	1.4342445
C	-0.9962210	8.5612484	0.4599735
H	-2.8392793	4.2142004	3.9601362
C	-1.9309755	6.3170408	0.7111337
H	-1.2914575	8.7908247	-0.6025748
H	-1.8037611	8.9409769	1.1201322
H	-3.0533568	5.9411588	3.5030236
H	-2.6912218	4.4016646	1.3823370
H	-2.3270035	6.0989338	-0.3227929
H	-2.7400642	6.8763480	1.2293811

SCF energy GEOOPT = -519.4917522946 H

ZPE = 772.0 kJ/mol

FREEH energy = 807.98 kJ/mol

FREEH entropy = 0.47460 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	64.50	0.05304	YES YES
8	a	64.84	0.05504	YES YES
9	a	75.22	0.97618	YES YES
10	a	167.73	0.71844	YES YES
11	a	168.08	0.70509	YES YES
12	a	205.47	1.36900	YES YES
13	a	206.16	1.30112	YES YES
14	a	208.60	0.12763	YES YES
15	a	232.19	1.13723	YES YES
16	a	233.01	1.13059	YES YES
17	a	256.51	0.06337	YES YES
18	a	317.91	2.91426	YES YES
19	a	328.16	1.71961	YES YES

20	a	328.63	1.73681	YES	YES
21	a	391.69	1.12683	YES	YES
22	a	420.93	0.01048	YES	YES
23	a	421.85	0.00566	YES	YES
24	a	447.37	0.88946	YES	YES
25	a	539.25	10.07590	YES	YES
26	a	540.40	10.00902	YES	YES
27	a	572.10	1.20947	YES	YES
28	a	743.01	7.69639	YES	YES
29	a	743.85	7.82828	YES	YES
30	a	746.81	11.54143	YES	YES
31	a	851.48	0.15648	YES	YES
32	a	872.48	7.01495	YES	YES
33	a	872.77	6.92744	YES	YES
34	a	964.55	16.89188	YES	YES
35	a	964.72	16.88924	YES	YES
36	a	980.44	2.83193	YES	YES
37	a	1014.51	0.00684	YES	YES
38	a	1036.11	38.95962	YES	YES
39	a	1036.50	39.73745	YES	YES
40	a	1048.36	1.52314	YES	YES
41	a	1072.35	15.03592	YES	YES
42	a	1072.76	14.78251	YES	YES
43	a	1099.90	2.16523	YES	YES
44	a	1100.07	2.41279	YES	YES
45	a	1100.74	27.35078	YES	YES
46	a	1141.72	27.37941	YES	YES
47	a	1157.86	49.99640	YES	YES
48	a	1158.04	49.68994	YES	YES
49	a	1228.27	5.93142	YES	YES
50	a	1228.41	6.36862	YES	YES
51	a	1241.31	1.11150	YES	YES
52	a	1262.75	37.15958	YES	YES
53	a	1263.08	37.00437	YES	YES
54	a	1275.78	0.43636	YES	YES
55	a	1300.26	7.28160	YES	YES
56	a	1310.02	9.90495	YES	YES
57	a	1310.69	9.29768	YES	YES
58	a	1339.34	9.69959	YES	YES
59	a	1347.39	28.09612	YES	YES
60	a	1348.03	60.46562	YES	YES
61	a	1348.86	58.42259	YES	YES
62	a	1358.33	34.38991	YES	YES
63	a	1358.85	35.23902	YES	YES
64	a	1387.78	0.92038	YES	YES
65	a	1388.13	0.85741	YES	YES
66	a	1388.38	0.70625	YES	YES
67	a	1406.22	9.64214	YES	YES
68	a	1406.49	10.32572	YES	YES
69	a	1411.35	39.28114	YES	YES
70	a	1413.76	4.94850	YES	YES
71	a	1414.32	5.21540	YES	YES
72	a	1427.98	0.66014	YES	YES
73	a	1432.99	5.76876	YES	YES
74	a	1433.46	6.22710	YES	YES
75	a	1434.94	3.70595	YES	YES
76	a	1440.71	15.33738	YES	YES
77	a	1441.06	15.23608	YES	YES
78	a	1448.79	4.35793	YES	YES
79	a	2776.24	102.17148	YES	YES
80	a	2776.36	101.62692	YES	YES
81	a	2776.77	110.85842	YES	YES
82	a	2800.39	315.37456	YES	YES
83	a	2800.55	314.26162	YES	YES
84	a	2803.82	2.22420	YES	YES
85	a	2868.51	110.83700	YES	YES
86	a	2869.10	110.13405	YES	YES
87	a	2872.52	128.88640	YES	YES
88	a	2973.10	7.76182	YES	YES
89	a	2973.21	6.81578	YES	YES
90	a	2974.42	2.09751	YES	YES
91	a	2976.30	9.67611	YES	YES
92	a	2976.50	9.03869	YES	YES
93	a	2977.41	109.40577	YES	YES
94	a	3002.60	21.36040	YES	YES
95	a	3003.30	21.29849	YES	YES
96	a	3012.34	68.61041	YES	YES
97	a	3030.88	8.87199	YES	YES

98	a	3031.47	35.14299	YES	YES
99	a	3031.72	36.55099	YES	YES

$e

S-5 Overview on crystal data

S-Table 4: Summary of crystallographic data for the molecular structures

Compound	Compound 1A	Compound 1B	Compound 3
CCDC number	2193060	2193049	
Empirical formula	$C_{52.45}H_{49.31}Al_4F_{38.14}GaO_4$	$C_{92}H_{90}Al_8F_{72}Ga_2O_8$	$C_{48.10}H_{46.39}Al_4F_{36.73}InO_4$
Formula weight	1645.91	3046.75	1609.11
Temperature [K]	120(2)	100(2)	100(2)
Crystal system	triclinic	monoclinic	triclinic
Space group (number)	$P\bar{1}$ (2)	$P2_1/c$ (14)	$P\bar{1}$ (2)
a [Å]	16.445(6)	44.352(11)	22.327(6)
b [Å]	16.685(6)	18.147(4)	26.903(8)
c [Å]	28.346(9)	30.839(7)	29.692(9)
α [°]	80.473(15)	90	88.983(7)
β [°]	83.826(10)	102.490(9)	70.929(9)
γ [°]	60.715(9)	90	70.884(7)
Volume [Å^3]	6687(4)	24234(9)	15847(8)
Z	4	8	10
ρ_{calc} [gcm^{-3}]	1.635	1.670	1.686
μ [mm^{-1}]	0.613	0.664	0.577
F(000)	3289	12159	7986
Crystal size [mm^3]	0.151×0.101×0.039	0.399×0.202×0.074	0.256×0.109×0.098
Crystal colour	orange	yellow	yellow
Crystal shape	plate	plate	plate
Radiation	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)
2Θ range [°]	2.82 to 56.01 (0.76 Å)	2.62 to 59.29 (0.72 Å)	2.87 to 61.23 (0.70 Å)
Index ranges	-21 ≤ h ≤ 21 -21 ≤ k ≤ 21 -37 ≤ l ≤ 37	−61 ≤ h ≤ 60 −23 ≤ k ≤ 25 −42 ≤ l ≤ 42	−31 ≤ h ≤ 31 −38 ≤ k ≤ 38 −42 ≤ l ≤ 42
Reflections collected	335017	525980	891645
Independent reflections	32094 R_{int} = 0.0632 R_{sigma} = 0.0353	66650 R_{int} = 0.0542 R_{sigma} = 0.0394	97222 R_{int} = 0.0598 R_{sigma} = 0.0350
Completeness to Θ = 25.242°	100.0 %	100.0 %	99.9 %
Data / Restraints / Parameters	32094/71606/3886	66650/125086/4996	97222/352965/8649
Goodness-of-fit on F^2	1.025	1.018	1.025
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0553 wR_2 = 0.1514	R_1 = 0.0415 wR_2 = 0.0942	R_1 = 0.0622 wR_2 = 0.1666
Final *R* indexes [all data]	R_1 = 0.0861 wR_2 = 0.1746	R_1 = 0.0727 wR_2 = 0.1072	R_1 = 0.0911 wR_2 = 0.1920
Largest peak/hole [eÅ^{-3}]	1.21/-1.15	0.96/-0.88	2.47/-1.36

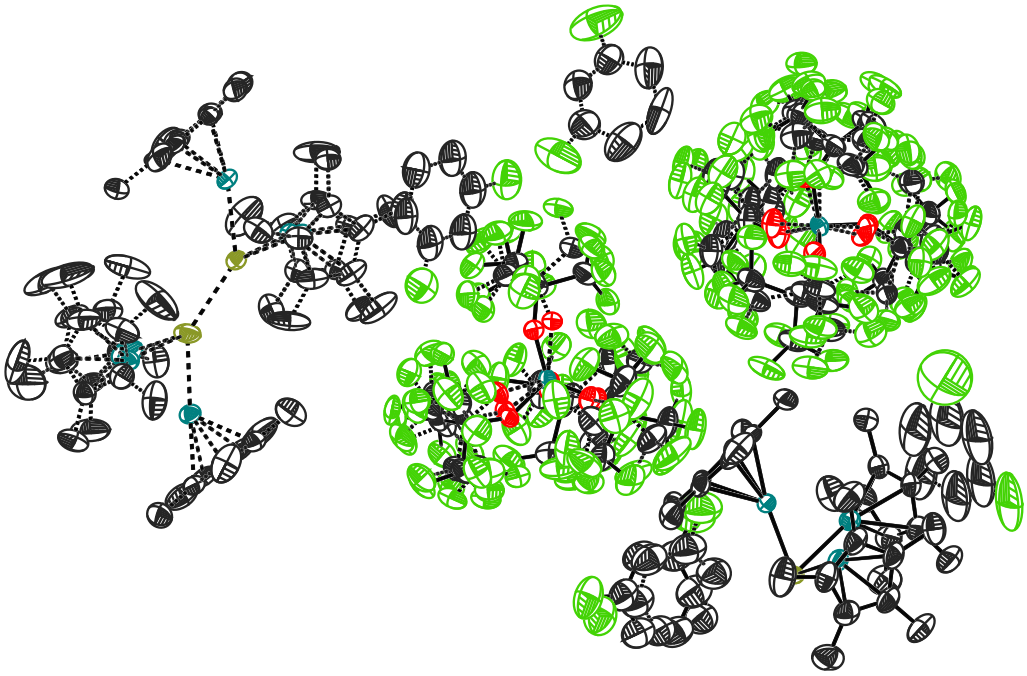
S-Table 5: Summary of crystallographic data for the molecular structures

Compound	Compound 3	Compound 4	Compound 5
CCDC number		2193851	2194404
Empirical formula	$C_{48.13}H_{46.42}Al_4F_{36.71}O_4Tl$	$C_{55}H_{66}Al_5F_{36}N_3O_4$	$C_{56.88}H_{67.67}Al_4F_{36.06}GaN_3O_{3.97}$
Formula weight	1698.63	1652.00	1719.55
Temperature [K]	100(2)	100(2)	100(2)
Crystal system	triclinic	monoclinic	triclinic
Space group (number)	$P\overline{1}$ (2)	$P2_1/c$ (14)	$P\overline{1}$ (2)
a [Å]	22.345(17)	21.369(8)	10.927(6)
b [Å]	26.95(3)	17.024(3)	17.637(11)
c [Å]	29.77(2)	21.581(7)	19.087(10)
α [°]	88.88(3)	90	94.601(14)
β [°]	70.81(5)	116.118(16)	97.945(15)
γ [°]	70.94(5)	90	98.66(3)
Volume [Å^3]	15925(24)	7049(4)	3582(4)
Z	10	4	2
ρ_{calc} [gcm^{-3}]	1.771	1.557	1.594
μ [mm^{-1}]	2.739	0.219	0.573
F(000)	8306	3352	1738
Crystal size [mm^3]	0.232×0.198×0.156	0.412×0.244×0.108	0.426×0.170×0.056
Crystal colour	yellow	yellow	yellow
Crystal shape	block	block	plate
Radiation	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)	MoK_α (λ=0.71073 Å)
2Θ range [°]	1.46 to 55.06 (0.77 Å)	3.18 to 55.13 (0.77 Å)	2.17 to 56.72 (0.75 Å)
Index ranges	−29 ≤ h ≤ 29 −34 ≤ k ≤ 35 −38 ≤ l ≤ 38	−27 ≤ h ≤ 27 −22 ≤ k ≤ 22 −28 ≤ l ≤ 28	−14 ≤ h ≤ 14 −23 ≤ k ≤ 23 −25 ≤ l ≤ 25
Reflections collected	299768	179713	70915
Independent reflections	73155 R_{int} = 0.0682 R_{sigma} = 0.0706	16215 R_{int} = 0.0522 R_{sigma} = 0.0223	17881 R_{int} = 0.0442 R_{sigma} = 0.0452
Completeness to Θ = 25.242°	100.0 %	99.9 %	100.0 %
Data / Restraints / Parameters	73155/322897/8254	16215/4026/946	17881/13768/1616
Goodness-of-fit on F^2	1.031	1.026	1.052
Final *R* indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0583 wR_2 = 0.1410	R_1 = 0.0357 wR_2 = 0.0841	R_1 = 0.0609 wR_2 = 0.1469
Final *R* indexes [all data]	R_1 = 0.1018 wR_2 = 0.1631	R_1 = 0.0523 wR_2 = 0.0940	R_1 = 0.0869 wR_2 = 0.1617
Largest peak/hole [eÅ^{-3}]	3.60/-1.51	0.37/-0.32	1.30/-0.59

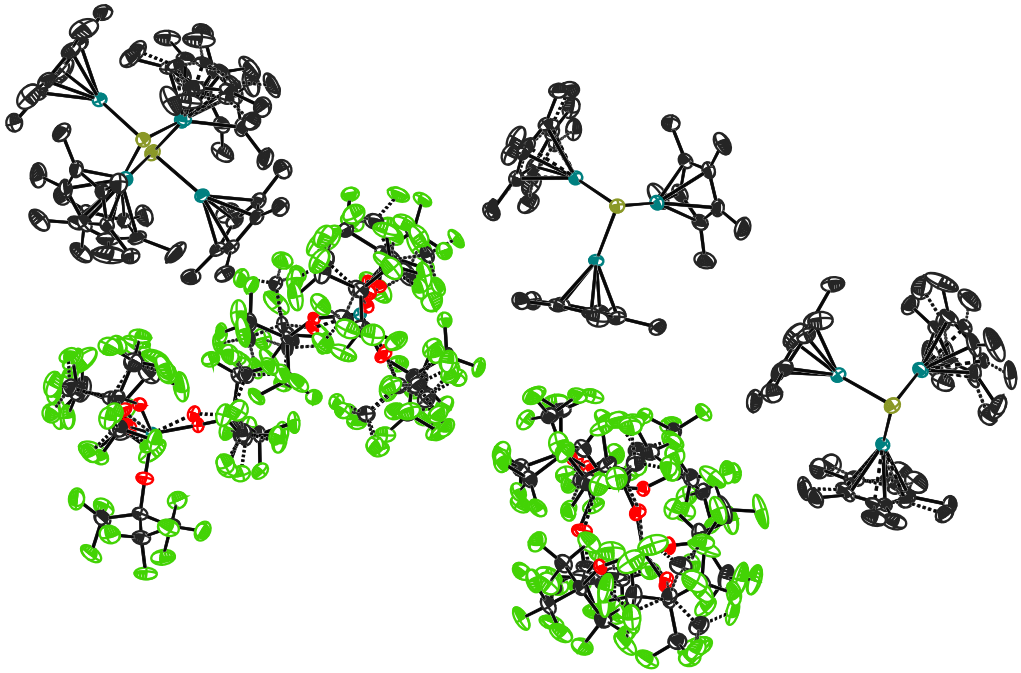
S-Table 6: Summary of crystallographic data for the molecular structures

Compound	Compound 6
CCDC number	2194403
Empirical formula	$C_{55}H_{66}Al_4F_{36}GaN_3O_4$
Formula weight	1694.57
Temperature [K]	100(2)
Crystal system	triclinic
Space group (number)	$P\bar{1}$ (2)
a [Å]	17.181(7)
b [Å]	21.399(6)
c [Å]	21.691(5)
α [°]	117.464(12)
β [°]	90.245(14)
γ [°]	90.863(16)
Volume [Å^3]	7075(4)
Z	4
ρ_{calc} [gcm^{-3}]	1.591
μ [mm^{-1}]	0.579
F(000)	3424
Crystal size [mm^3]	0.180×0.127×0.126
Crystal colour	yellow
Crystal shape	block
Radiation	MoK_α (λ=0.71073 Å)
2Θ range [°]	3.16 to 52.87 (0.80 Å)
Index ranges	−21 ≤ h ≤ 21 −26 ≤ k ≤ 23 0 ≤ l ≤ 27
Reflections collected	28962
Independent reflections	28962 R_{int} = 0.0372 R_{sigma} = 0.0802
Completeness to Θ = 25.242°	96.3 %
Data / Restraints / Parameters	28962/39668/2783
Goodness-of-fit on F^2	1.051
Final *R* indexes [*I*≥2σ(*I*)]	R_1 = 0.0743 wR_2 = 0.1716
Final *R* indexes [all data]	R_1 = 0.1249 wR_2 = 0.2022
Largest peak/hole [eÅ^{-3}]	1.05/-0.72

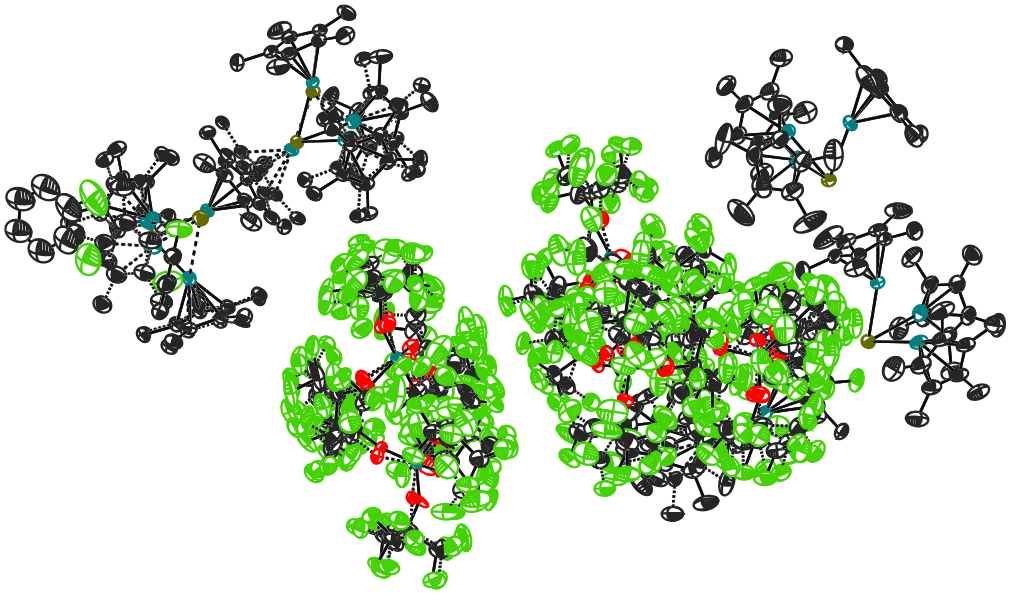
Pictures of the asymmetric units



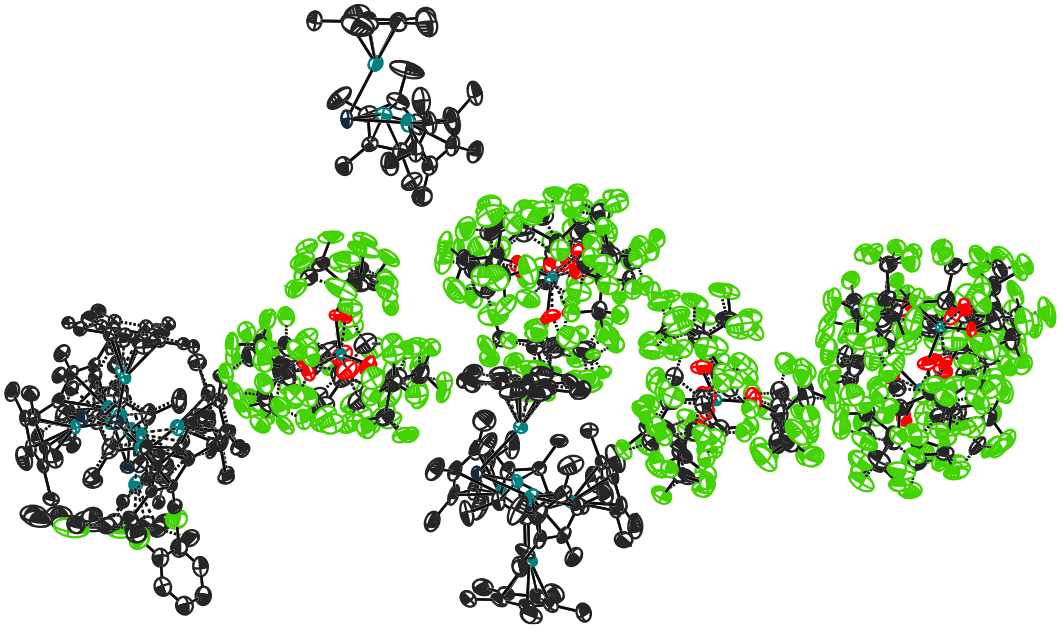
S-Figure 69: Asymmetric unit of the molecular structure of compound 1A. Hydrogen atoms were omitted for clarity. Thermal displacement of the ellipsoids was set at 50 % probability.



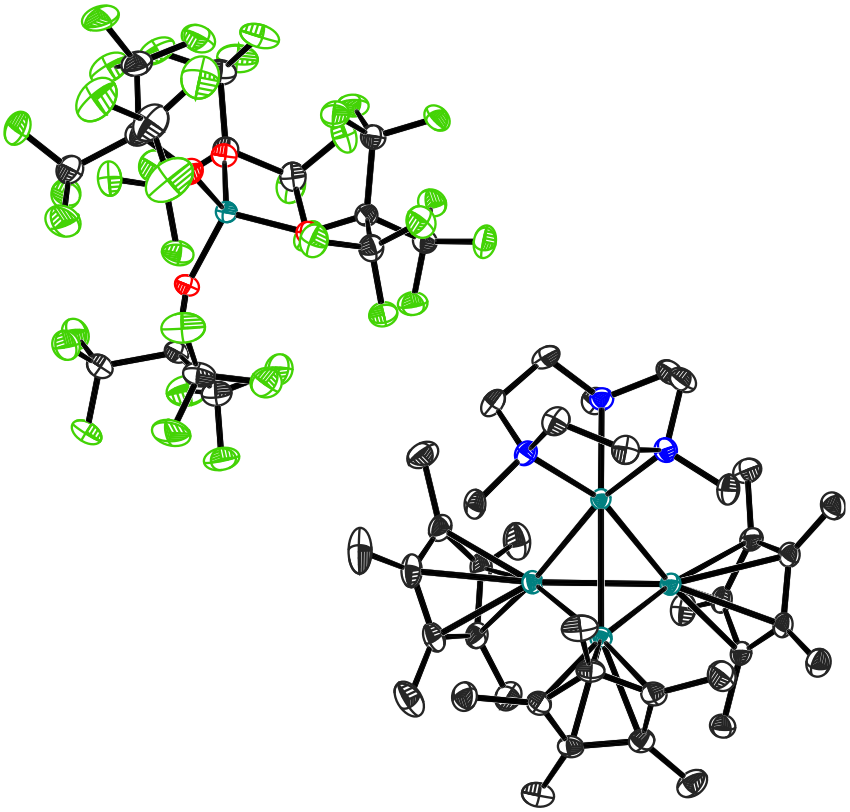
S-Figure 70: Asymmetric unit of the molecular structure of compound 1B. Hydrogen atoms were omitted for clarity. Thermal displacement of the ellipsoids was set at 50 % probability.



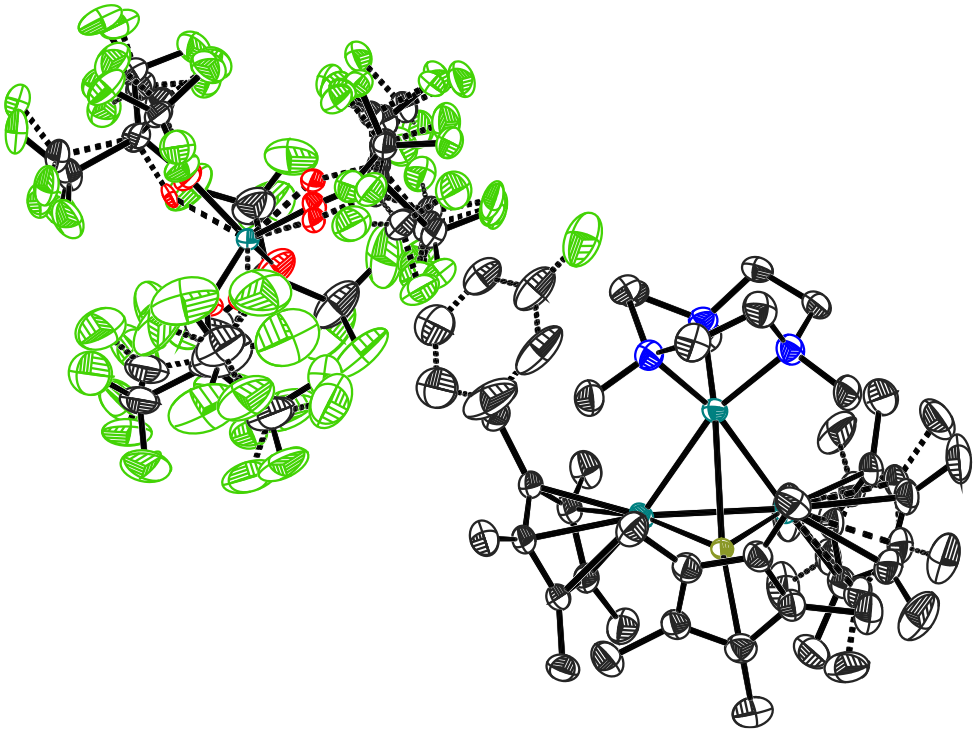
S-Figure 71: Asymmetric unit of the molecular structure of compound 2. Hydrogen atoms were omitted for clarity. Thermal displacement of the ellipsoids was set at 50 % probability.



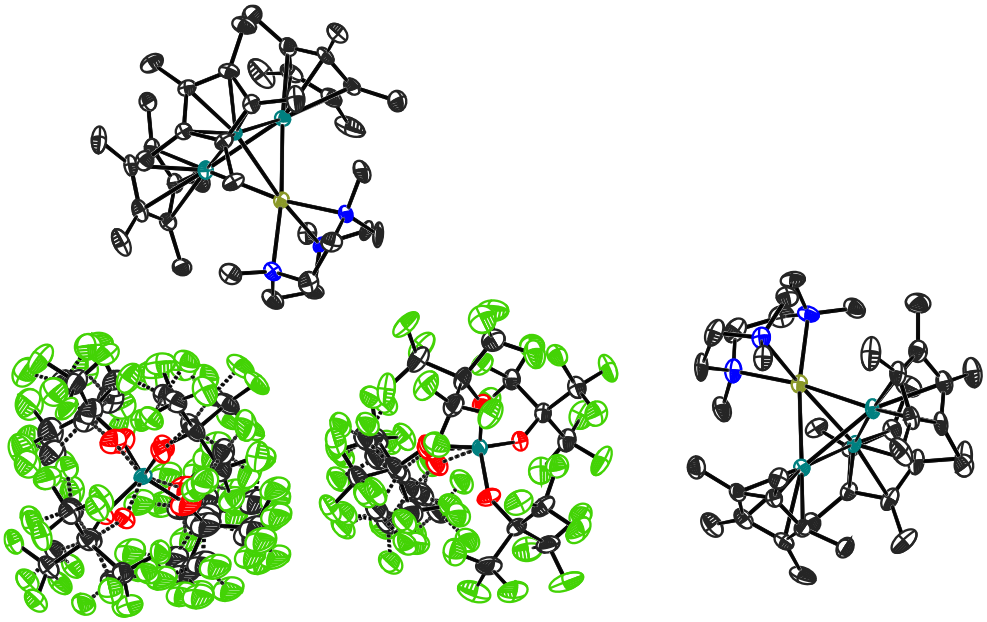
S-Figure 72: Asymmetric unit of the molecular structure of compound 3. Hydrogen atoms were omitted for clarity. Thermal displacement of the ellipsoids was set at 50 % probability.



S-Figure 73: Asymmetric unit of the molecular structure of compound 4. Hydrogen atoms were omitted for clarity. Thermal displacement of the ellipsoids was set at 50 % probability.



S-Figure 74: Asymmetric unit of the molecular structure of compound 5. Hydrogen atoms were omitted for clarity. Thermal displacement of the ellipsoids was set at 50 % probability.



S-Figure 75: Asymmetric unit of the molecular structure of compound 6. Hydrogen atoms were omitted for clarity. Thermal displacement of the ellipsoids was set at 50 % probability.

Tables of bond distances and angles

S-Table 7 Bond lengths and angles for **1A**

Atom–Atom	Length [Å]
Ga3–Al6	2.498(5)
Ga3–Al7	2.508(7)
Ga3–Al8	2.509(9)
Ga3–Ga2	2.7893(14)
Al6–C4_19	2.168(14)
Al6–C3_19	2.188(11)
Al6–C5_19	2.207(12)
Al6–C1_19	2.221(11)
Al6–C2_19	2.221(10)
Al7–C2_21	2.132(14)
Al7–C1_21	2.193(13)
Al7–C3_21	2.223(16)
Al7–C5_21	2.261(15)
Al7–C4_21	2.275(17)
Al8–C1_23	2.082(18)
Al8–C5_23	2.15(2)
Al8–C2_23	2.214(16)
Al8–C4_23	2.26(2)
Al8–C3_23	2.310(17)
Ga1–Al3	2.5152(12)
Ga1–Al1	2.5159(13)
Ga1–Al2	2.5294(12)
Ga1–Ga1$^{\#1}$	2.8599(9)
Al1–C2_28	2.193(3)
Al1–C1_28	2.201(3)
Al1–C3_28	2.208(4)
Al1–C4_28	2.225(4)
Al1–C5_28	2.227(3)
Al2–C4_27	2.210(3)
Al2–C1_27	2.212(3)
Al2–C5_27	2.212(3)
Al2–C2_27	2.216(3)
Al2–C3_27	2.222(4)
Al3–C4_24	2.199(3)
Al3–C5_24	2.201(3)
Al3–C3_24	2.220(3)
Al3–C2_24	2.223(3)
Al3–C1_24	2.231(3)
Ga2–Al10	2.506(7)
Ga2–Al11	2.522(9)
Ga2–Al9	2.524(2)
Al9–C1_18	2.200(6)
Al9–C2_18	2.213(6)
Al9–C5_18	2.225(7)
Al9–C3_18	2.225(9)
Al9–C4_18	2.237(9)
Al10–C3_20	2.157(17)
Al10–C4_20	2.173(13)
Al10–C2_20	2.193(15)
Al10–C5_20	2.244(13)
Al10–C1_20	2.267(14)
Al11–C2_22	2.146(16)
Al11–C3_22	2.20(2)
Al11–C1_22	2.233(17)
Al11–C4_22	2.31(2)
Al11–C5_22	2.347(19)
Al4–O1_33	1.63(2)
Al4–O1_14	1.63(2)
Al4–O1_26	1.64(3)
Al4–O1_35	1.70(2)
Al4–O1_8	1.706(4)
Al4–O1_15	1.71(2)
Al4–O1_36	1.72(3)
Al4–O1_7	1.728(9)
Al4–O1_5	1.728(2)
Al4–O1_6	1.747(7)
Al4–O1_17	1.77(2)
Al5–O1_10	1.619(16)
Al5–O1_13	1.654(13)
Al5–O1_2	1.663(4)
Al5–O1_11	1.708(6)
Al5–O1_32	1.72(3)
Al5–O1_3	1.740(8)
Al5–O1_1	1.769(6)
Al5–O1_4	1.776(10)
Al5–O1_12	1.846(7)
O1_1–C1_1	1.356(7)
C1_1–C3_1	1.536(8)
C1_1–C4_1	1.557(8)
C1_1–C2_1	1.564(8)
C2_1–F1_1	1.324(8)
C2_1–F2_1	1.331(8)
C2_1–F3_1	1.343(8)
C3_1–F6_1	1.311(8)
C3_1–F5_1	1.346(7)
C3_1–F4_1	1.349(9)
C4_1–F9_1	1.322(8)
C4_1–F7_1	1.336(8)
C4_1–F8_1	1.342(8)
O1_2–C1_2	1.346(7)
C1_2–C4_2	1.552(8)
C1_2–C3_2	1.553(7)
C1_2–C2_2	1.558(8)
C2_2–F3_2	1.316(8)
C2_2–F2_2	1.336(7)
C2_2–F1_2	1.338(7)
C3_2–F4_2	1.321(7)
C3_2–F5_2	1.331(7)
C3_2–F6_2	1.335(7)
C4_2–F9_2	1.330(9)
C4_2–F8_2	1.332(8)
C4_2–F7_2	1.334(9)
O1_3–C1_3	1.353(7)
C1_3–C3_3	1.530(7)
C1_3–C2_3	1.556(8)

C1_3–C4_3	1.557(8)	C2_7–F2_7	1.340(7)
C2_3–F3_3	1.330(8)	C3_7–F4_7	1.328(8)
C2_3–F1_3	1.332(8)	C3_7–F5_7	1.336(7)
C2_3–F2_3	1.339(7)	C3_7–F6_7	1.342(7)
C3_3–F4_3	1.334(6)	C4_7–F7_7	1.328(7)
C3_3–F6_3	1.335(7)	C4_7–F9_7	1.336(7)
C3_3–F5_3	1.359(8)	C4_7–F8_7	1.340(7)
C4_3–F9_3	1.306(7)	O1_8–C1_8	1.348(5)
C4_3–F8_3	1.329(6)	C1_8–C3_8	1.527(5)
C4_3–F7_3	1.366(8)	C1_8–C4_8	1.529(6)
O1_4–C1_4	1.348(8)	C1_8–C2_8	1.554(6)
C1_4–C3_4	1.549(7)	C2_8–F3_8	1.309(6)
C1_4–C2_4	1.553(8)	C2_8–F1_8	1.337(5)
C1_4–C4_4	1.555(8)	C2_8–F2_8	1.344(5)
C2_4–F1_4	1.327(7)	C3_8–F6_8	1.337(5)
C2_4–F3_4	1.329(7)	C3_8–F5_8	1.342(6)
C2_4–F2_4	1.335(6)	C3_8–F4_8	1.354(6)
C3_4–F4_4	1.316(7)	C4_8–F9_8	1.320(5)
C3_4–F5_4	1.336(8)	C4_8–F8_8	1.327(5)
C3_4–F6_4	1.336(6)	C4_8–F7_8	1.403(6)
C4_4–F7_4	1.322(8)	O1_10–C1_10	1.352(12)
C4_4–F9_4	1.325(8)	C1_10–C3_10	1.531(11)
C4_4–F8_4	1.341(8)	C1_10–C2_10	1.543(10)
O1_5–C1_5	1.356(4)	C1_10–C4_10	1.554(10)
C1_5–C2_5	1.543(5)	C2_10–F3_10	1.318(10)
C1_5–C3_5	1.551(5)	C2_10–F1_10	1.332(11)
C1_5–C4_5	1.553(5)	C2_10–F2_10	1.340(8)
C2_5–F3_5	1.298(5)	C3_10–F5_10	1.330(11)
C2_5–F1_5	1.352(5)	C3_10–F6_10	1.331(11)
C2_5–F2_5	1.352(4)	C3_10–F4_10	1.333(11)
C3_5–F5_5	1.325(5)	C4_10–F8_10	1.321(10)
C3_5–F4_5	1.328(4)	C4_10–F9_10	1.325(10)
C3_5–F6_5	1.339(4)	C4_10–F7_10	1.345(10)
C4_5–F7_5	1.328(5)	O1_11–C1_11	1.363(11)
C4_5–F8_5	1.331(4)	C1_11–C4_11	1.540(11)
C4_5–F9_5	1.337(5)	C1_11–C2_11	1.542(11)
O1_6–C1_6	1.351(5)	C1_11–C3_11	1.555(11)
C1_6–C2_6	1.545(6)	C2_11–F3_11	1.324(10)
C1_6–C3_6	1.549(6)	C2_11–F1_11	1.332(11)
C1_6–C4_6	1.557(6)	C2_11–F2_11	1.340(10)
C2_6–F1_6	1.324(5)	C3_11–F6_11	1.322(11)
C2_6–F2_6	1.335(7)	C3_11–F4_11	1.340(12)
C2_6–F3_6	1.350(6)	C3_11–F5_11	1.346(11)
C3_6–F4_6	1.325(6)	C4_11–F8_11	1.329(10)
C3_6–F5_6	1.335(6)	C4_11–F9_11	1.334(10)
C3_6–F6_6	1.357(7)	C4_11–F7_11	1.354(10)
C4_6–F7_6	1.327(5)	O1_12–C1_12	1.350(11)
C4_6–F9_6	1.327(6)	C1_12–C4_12	1.545(11)
C4_6–F8_6	1.353(6)	C1_12–C3_12	1.551(11)
O1_7–C1_7	1.348(7)	C1_12–C2_12	1.554(11)
C1_7–C2_7	1.551(7)	C2_12–F3_12	1.324(10)
C1_7–C4_7	1.551(7)	C2_12–F2_12	1.328(10)
C1_7–C3_7	1.560(7)	C2_12–F1_12	1.335(10)
C2_7–F3_7	1.330(7)	C3_12–F5_12	1.325(12)
C2_7–F1_7	1.332(7)	C3_12–F6_12	1.325(12)

C3_12–F4_12	1.329(12)	C6_18–H6C_18	0.9800
C4_12–F9_12	1.322(12)	C7_18–H7A_18	0.9800
C4_12–F7_12	1.339(11)	C7_18–H7B_18	0.9800
C4_12–F8_12	1.343(11)	C7_18–H7C_18	0.9800
O1_13–C1_13	1.356(11)	C8_18–H8A_18	0.9800
C1_13–C3_13	1.541(10)	C8_18–H8B_18	0.9800
C1_13–C2_13	1.545(11)	C8_18–H8C_18	0.9800
C1_13–C4_13	1.554(10)	C9_18–H9A_18	0.9800
C2_13–F1_13	1.325(11)	C9_18–H9B_18	0.9800
C2_13–F3_13	1.327(10)	C9_18–H9C_18	0.9800
C2_13–F2_13	1.339(10)	C10_18–H10A_18	0.9800
C3_13–F4_13	1.330(10)	C10_18–H10B_18	0.9800
C3_13–F6_13	1.344(9)	C10_18–H10C_18	0.9800
C3_13–F5_13	1.352(11)	C1_19–C2_19	1.416(10)
C4_13–F9_13	1.317(10)	C1_19–C5_19	1.421(10)
C4_13–F8_13	1.319(9)	C1_19–C10_19	1.512(10)
C4_13–F7_13	1.344(10)	C2_19–C3_19	1.422(9)
O1_14–C1_14	1.353(13)	C2_19–C9_19	1.498(10)
C1_14–C2_14	1.544(12)	C3_19–C4_19	1.434(9)
C1_14–C4_14	1.552(12)	C3_19–C8_19	1.502(10)
C1_14–C3_14	1.560(12)	C4_19–C5_19	1.425(10)
C2_14–F1_14	1.328(12)	C4_19–C7_19	1.515(10)
C2_14–F3_14	1.330(13)	C5_19–C6_19	1.517(10)
C2_14–F2_14	1.340(13)	C6_19–H6A_19	0.9800
C3_14–F6_14	1.328(13)	C6_19–H6B_19	0.9800
C3_14–F4_14	1.332(12)	C6_19–H6C_19	0.9800
C3_14–F5_14	1.341(12)	C7_19–H7A_19	0.9800
C4_14–F7_14	1.329(12)	C7_19–H7B_19	0.9800
C4_14–F9_14	1.332(12)	C7_19–H7C_19	0.9800
C4_14–F8_14	1.335(13)	C8_19–H8A_19	0.9800
O1_15–C1_15	1.355(13)	C8_19–H8B_19	0.9800
C1_15–C3_15	1.545(12)	C8_19–H8C_19	0.9800
C1_15–C2_15	1.551(12)	C9_19–H9A_19	0.9800
C1_15–C4_15	1.563(12)	C9_19–H9B_19	0.9800
C2_15–F2_15	1.339(13)	C9_19–H9C_19	0.9800
C2_15–F3_15	1.343(13)	C10_19–H10A_19	0.9800
C2_15–F1_15	1.344(13)	C10_19–H10B_19	0.9800
C3_15–F5_15	1.333(12)	C10_19–H10C_19	0.9800
C3_15–F4_15	1.335(12)	C1_20–C2_20	1.400(11)
C3_15–F6_15	1.346(13)	C1_20–C5_20	1.430(10)
C4_15–F8_15	1.323(12)	C1_20–C10_20	1.489(11)
C4_15–F9_15	1.327(12)	C2_20–C3_20	1.440(10)
C4_15–F7_15	1.344(12)	C2_20–C9_20	1.505(10)
C1_18–C5_18	1.414(9)	C3_20–C4_20	1.424(9)
C1_18–C2_18	1.429(8)	C3_20–C8_20	1.479(10)
C1_18–C10_18	1.484(9)	C4_20–C5_20	1.400(9)
C2_18–C3_18	1.423(9)	C4_20–C7_20	1.497(9)
C2_18–C9_18	1.493(9)	C5_20–C6_20	1.501(9)
C3_18–C4_18	1.421(9)	C6_20–H6A_20	0.9800
C3_18–C8_18	1.498(10)	C6_20–H6B_20	0.9800
C4_18–C5_18	1.414(10)	C6_20–H6C_20	0.9800
C4_18–C7_18	1.507(10)	C7_20–H7A_20	0.9800
C5_18–C6_18	1.516(9)	C7_20–H7B_20	0.9800
C6_18–H6A_18	0.9800	C7_20–H7C_20	0.9800
C6_18–H6B_18	0.9800	C8_20–H8A_20	0.9800

C8_20–H8B_20	0.9800	C10_22–H10A_22	0.9800
C8_20–H8C_20	0.9800	C10_22–H10B_22	0.9800
C9_20–H9A_20	0.9800	C10_22–H10C_22	0.9800
C9_20–H9B_20	0.9800	C1_23–C2_23	1.407(9)
C9_20–H9C_20	0.9800	C1_23–C5_23	1.423(10)
C10_20–H10A_20	0.9800	C1_23–C10_23	1.501(10)
C10_20–H10B_20	0.9800	C2_23–C3_23	1.418(10)
C10_20–H10C_20	0.9800	C2_23–C9_23	1.515(10)
C1_21–C5_21	1.403(11)	C3_23–C4_23	1.423(10)
C1_21–C2_21	1.435(10)	C3_23–C8_23	1.498(10)
C1_21–C10_21	1.510(11)	C4_23–C5_23	1.408(10)
C2_21–C3_21	1.406(9)	C4_23–C7_23	1.512(10)
C2_21–C9_21	1.474(10)	C5_23–C6_23	1.516(11)
C3_21–C4_21	1.413(10)	C6_23–H6A_23	0.9800
C3_21–C8_21	1.509(10)	C6_23–H6B_23	0.9800
C4_21–C5_21	1.417(11)	C6_23–H6C_23	0.9800
C4_21–C7_21	1.480(11)	C7_23–H7A_23	0.9800
C5_21–C6_21	1.510(11)	C7_23–H7B_23	0.9800
C6_21–H6A_21	0.9800	C7_23–H7C_23	0.9800
C6_21–H6B_21	0.9800	C8_23–H8A_23	0.9800
C6_21–H6C_21	0.9800	C8_23–H8B_23	0.9800
C7_21–H7A_21	0.9800	C8_23–H8C_23	0.9800
C7_21–H7B_21	0.9800	C9_23–H9A_23	0.9800
C7_21–H7C_21	0.9800	C9_23–H9B_23	0.9800
C8_21–H8A_21	0.9800	C9_23–H9C_23	0.9800
C8_21–H8B_21	0.9800	C10_23–H10A_23	0.9800
C8_21–H8C_21	0.9800	C10_23–H10B_23	0.9800
C9_21–H9A_21	0.9800	C10_23–H10C_23	0.9800
C9_21–H9B_21	0.9800	O1_17–C1_17	1.361(13)
C9_21–H9C_21	0.9800	C1_17–C3_17	1.533(12)
C10_21–H10A_21	0.9800	C1_17–C4_17	1.545(12)
C10_21–H10B_21	0.9800	C1_17–C2_17	1.552(12)
C10_21–H10C_21	0.9800	C2_17–F3_17	1.324(13)
C1_22–C5_22	1.414(10)	C2_17–F2_17	1.350(13)
C1_22–C2_22	1.420(10)	C2_17–F1_17	1.360(13)
C1_22–C10_22	1.510(10)	C3_17–F4_17	1.333(13)
C2_22–C3_22	1.422(9)	C3_17–F6_17	1.345(13)
C2_22–C9_22	1.506(10)	C3_17–F5_17	1.379(13)
C3_22–C4_22	1.414(10)	C4_17–F8_17	1.329(13)
C3_22–C8_22	1.508(10)	C4_17–F9_17	1.336(13)
C4_22–C5_22	1.417(10)	C4_17–F7_17	1.348(13)
C4_22–C7_22	1.514(10)	O1_26–C1_26	1.348(14)
C5_22–C6_22	1.498(11)	C1_26–C4_26	1.537(13)
C6_22–H6A_22	0.9800	C1_26–C2_26	1.547(13)
C6_22–H6B_22	0.9800	C1_26–C3_26	1.563(13)
C6_22–H6C_22	0.9800	C2_26–F1_26	1.326(14)
C7_22–H7A_22	0.9800	C2_26–F2_26	1.330(14)
C7_22–H7B_22	0.9800	C2_26–F3_26	1.351(14)
C7_22–H7C_22	0.9800	C3_26–F6_26	1.337(14)
C8_22–H8A_22	0.9800	C3_26–F4_26	1.338(14)
C8_22–H8B_22	0.9800	C3_26–F5_26	1.346(14)
C8_22–H8C_22	0.9800	C4_26–F9_26	1.329(14)
C9_22–H9A_22	0.9800	C4_26–F8_26	1.337(14)
C9_22–H9B_22	0.9800	C4_26–F7_26	1.346(14)
C9_22–H9C_22	0.9800	C1_24–C2_24	1.410(4)

C1_24–C5_24	1.427(4)	C3_28–C8_28	1.507(5)
C1_24–C10_24	1.490(4)	C4_28–C5_28	1.415(5)
C2_24–C3_24	1.418(4)	C4_28–C7_28	1.508(5)
C2_24–C9_24	1.505(4)	C5_28–C6_28	1.503(5)
C3_24–C4_24	1.408(4)	C6_28–H6A_28	0.9800
C3_24–C8_24	1.510(4)	C6_28–H6B_28	0.9800
C4_24–C5_24	1.428(4)	C6_28–H6C_28	0.9800
C4_24–C7_24	1.507(4)	C7_28–H7A_28	0.9800
C5_24–C6_24	1.499(4)	C7_28–H7B_28	0.9800
C6_24–H6A_24	0.9800	C7_28–H7C_28	0.9800
C6_24–H6B_24	0.9800	C8_28–H8A_28	0.9800
C6_24–H6C_24	0.9800	C8_28–H8B_28	0.9800
C7_24–H7A_24	0.9800	C8_28–H8C_28	0.9800
C7_24–H7B_24	0.9800	C9_28–H9A_28	0.9800
C7_24–H7C_24	0.9800	C9_28–H9B_28	0.9800
C8_24–H8A_24	0.9800	C9_28–H9C_28	0.9800
C8_24–H8B_24	0.9800	C10_28–H10A_28	0.9800
C8_24–H8C_24	0.9800	C10_28–H10B_28	0.9800
C9_24–H9A_24	0.9800	C10_28–H10C_28	0.9800
C9_24–H9B_24	0.9800	C1_30–C6_30	1.343(10)
C9_24–H9C_24	0.9800	C1_30–C2_30	1.363(11)
C10_24–H10A_24	0.9800	C1_30–F1_30	1.381(10)
C10_24–H10B_24	0.9800	C2_30–C3_30	1.342(10)
C10_24–H10C_24	0.9800	C2_30–H2_30	0.9500
C1_27–C5_27	1.408(5)	C3_30–C4_30	1.340(10)
C1_27–C2_27	1.419(5)	C3_30–F2_30	1.353(9)
C1_27–C10_27	1.493(5)	C4_30–C5_30	1.422(11)
C2_27–C3_27	1.404(5)	C4_30–H4_30	0.9500
C2_27–C9_27	1.504(5)	C5_30–C6_30	1.420(11)
C3_27–C4_27	1.447(5)	C5_30–H5_30	0.9500
C3_27–C8_27	1.486(5)	C6_30–H6_30	0.9500
C4_27–C5_27	1.420(5)	C1_16–C6_16	1.267(11)
C4_27–C7_27	1.503(5)	C1_16–C2_16	1.298(12)
C5_27–C6_27	1.509(5)	C1_16–F1_16	1.304(11)
C6_27–H6A_27	0.9800	C2_16–C3_16	1.294(12)
C6_27–H6B_27	0.9800	C2_16–H2_16	0.9500
C6_27–H6C_27	0.9800	C3_16–C4_16	1.317(12)
C7_27–H7A_27	0.9800	C3_16–F2_16	1.329(12)
C7_27–H7B_27	0.9800	C4_16–C5_16	1.488(13)
C7_27–H7C_27	0.9800	C4_16–H4_16	0.9500
C8_27–H8A_27	0.9800	C5_16–C6_16	1.515(13)
C8_27–H8B_27	0.9800	C5_16–H5_16	0.9500
C8_27–H8C_27	0.9800	C6_16–H6_16	0.9500
C9_27–H9A_27	0.9800	C1_31–C6_31	1.339(13)
C9_27–H9B_27	0.9800	C1_31–F1_31	1.346(12)
C9_27–H9C_27	0.9800	C1_31–C2_31	1.355(13)
C10_27–H10A_27	0.9800	C2_31–C3_31	1.357(13)
C10_27–H10B_27	0.9800	C2_31–H2_31	0.9500
C10_27–H10C_27	0.9800	C3_31–C4_31	1.319(14)
C1_28–C2_28	1.421(5)	C3_31–F2_31	1.341(13)
C1_28–C5_28	1.423(5)	C4_31–C5_31	1.456(14)
C1_28–C10_28	1.502(5)	C4_31–H4_31	0.9500
C2_28–C3_28	1.426(5)	C5_31–C6_31	1.452(13)
C2_28–C9_28	1.503(5)	C5_31–H5_31	0.9500
C3_28–C4_28	1.415(5)	C6_31–H6_31	0.9500

O1_32–C1_32	1.354(14)
C1_32–C3_32	1.545(12)
C1_32–C2_32	1.548(13)
C1_32–C4_32	1.553(13)
C2_32–F2_32	1.332(14)
C2_32–F3_32	1.333(13)
C2_32–F1_32	1.337(13)
C3_32–F5_32	1.327(13)
C3_32–F6_32	1.335(13)
C3_32–F4_32	1.339(13)
C4_32–F7_32	1.331(13)
C4_32–F9_32	1.332(13)
C4_32–F8_32	1.337(14)
O1_33–C1_33	1.358(14)
C1_33–C2_33	1.537(13)
C1_33–C3_33	1.543(13)
C1_33–C4_33	1.556(13)
C2_33–F3_33	1.326(13)
C2_33–F1_33	1.331(13)
C2_33–F2_33	1.340(14)
C3_33–F4_33	1.338(14)
C3_33–F6_33	1.340(13)
C3_33–F5_33	1.341(14)
C4_33–F9_33	1.316(14)
C4_33–F8_33	1.322(14)
C4_33–F7_33	1.332(14)
O1_35–C1_35	1.359(14)
C1_35–C2_35	1.544(12)
C1_35–C3_35	1.551(13)
C1_35–C4_35	1.555(13)
C2_35–F3_35	1.333(13)
C2_35–F1_35	1.335(13)
C2_35–F2_35	1.335(13)
C3_35–F5_35	1.329(14)
C3_35–F6_35	1.331(14)
C3_35–F4_35	1.335(14)
C4_35–F9_35	1.330(14)
C4_35–F8_35	1.332(13)
C4_35–F7_35	1.334(14)
O1_36–C1_36	1.344(14)
C1_36–C4_36	1.544(13)
C1_36–C2_36	1.550(13)
C1_36–C3_36	1.556(13)
C2_36–F3_36	1.329(14)
C2_36–F1_36	1.334(14)
C2_36–F2_36	1.344(14)
C3_36–F4_36	1.334(14)
C3_36–F6_36	1.335(14)
C3_36–F5_36	1.346(14)
C4_36–F9_36	1.332(14)
C4_36–F7_36	1.333(14)
C4_36–F8_36	1.338(14)
C1_37–C6_37	1.327(15)
C1_37–C2_37	1.335(15)
C1_37–F1_37	1.346(14)
C2_37–C3_37	1.340(15)
C2_37–H2_37	0.9500
C3_37–C4_37	1.327(15)
C3_37–F2_37	1.344(15)
C4_37–C5_37	1.462(16)
C4_37–H4_37	0.9500
C5_37–C6_37	1.464(15)
C5_37–H5_37	0.9500
C6_37–H6_37	0.9500
C1_41–F1_41	1.315(13)
C1_41–C2_41	1.344(14)
C1_41–C6_41	1.346(14)
C2_41–C3_41	1.330(14)
C2_41–H2_41	0.9500
C3_41–F2_41	1.299(14)
C3_41–C4_41	1.308(15)
C4_41–C5_41	1.472(15)
C4_41–H4_41	0.9500
C5_41–C6_41	1.527(14)
C5_41–H5_41	0.9500
C6_41–H6_41	0.9500

Atom–Atom–Atom	**Angle [°]**
Al6–Ga3–Al7	75.48(13)
Al6–Ga3–Al8	74.02(13)
Al7–Ga3–Al8	75.9(3)
Al6–Ga3–Ga2	137.13(9)
Al7–Ga3–Ga2	122.21(16)
Al8–Ga3–Ga2	144.23(15)
C4_19–Al6–C3_19	38.4(3)
C4_19–Al6–C5_19	38.0(3)
C3_19–Al6–C5_19	62.9(4)
C4_19–Al6–C1_19	63.6(4)
C3_19–Al6–C1_19	62.6(3)
C5_19–Al6–C1_19	37.4(3)
C4_19–Al6–C2_19	63.8(4)
C3_19–Al6–C2_19	37.6(3)
C5_19–Al6–C2_19	62.6(4)
C1_19–Al6–C2_19	37.2(3)
C4_19–Al6–Ga3	160.1(3)
C3_19–Al6–Ga3	160.9(3)
C5_19–Al6–Ga3	133.5(3)
C1_19–Al6–Ga3	122.2(3)
C2_19–Al6–Ga3	133.5(3)
C2_21–Al7–C1_21	38.7(3)
C2_21–Al7–C3_21	37.6(3)
C1_21–Al7–C3_21	63.6(4)
C2_21–Al7–C5_21	61.5(4)
C1_21–Al7–C5_21	36.7(3)
C3_21–Al7–C5_21	60.9(4)
C2_21–Al7–C4_21	62.0(5)
C1_21–Al7–C4_21	62.6(5)
C3_21–Al7–C4_21	36.6(4)
C5_21–Al7–C4_21	36.4(3)
C2_21–Al7–Ga3	136.5(4)

C1_21–Al7–Ga3	117.7(4)	C4_24–Al3–C5_24	37.89(12)
C3_21–Al7–Ga3	169.5(4)	C4_24–Al3–C3_24	37.15(10)
C5_21–Al7–Ga3	127.0(4)	C5_24–Al3–C3_24	62.38(11)
C4_21–Al7–Ga3	153.9(4)	C4_24–Al3–C2_24	62.32(10)
C1_23–Al8–C5_23	39.3(4)	C5_24–Al3–C2_24	62.12(10)
C1_23–Al8–C2_23	38.1(4)	C3_24–Al3–C2_24	37.23(9)
C5_23–Al8–C2_23	63.4(5)	C4_24–Al3–C1_24	62.94(11)
C1_23–Al8–C4_23	63.4(5)	C5_24–Al3–C1_24	37.55(11)
C5_23–Al8–C4_23	37.1(4)	C3_24–Al3–C1_24	62.26(10)
C2_23–Al8–C4_23	61.8(5)	C2_24–Al3–C1_24	36.92(10)
C1_23–Al8–C3_23	62.4(5)	C4_24–Al3–Ga1	163.79(9)
C5_23–Al8–C3_23	61.7(5)	C5_24–Al3–Ga1	158.28(10)
C2_23–Al8–C3_23	36.5(3)	C3_24–Al3–Ga1	132.98(8)
C4_23–Al8–C3_23	36.3(4)	C2_24–Al3–Ga1	118.57(8)
C1_23–Al8–Ga3	133.4(4)	C1_24–Al3–Ga1	128.70(8)
C5_23–Al8–Ga3	114.7(5)	Al10–Ga2–Al11	75.8(3)
C2_23–Al8–Ga3	169.0(4)	Al10–Ga2–Al9	76.14(11)
C4_23–Al8–Ga3	124.1(5)	Al11–Ga2–Al9	76.98(12)
C3_23–Al8–Ga3	153.7(5)	Al10–Ga2–Ga3	118.13(15)
Al3–Ga1–Al1	75.64(3)	Al11–Ga2–Ga3	138.53(14)
Al3–Ga1–Al2	74.76(3)	Al9–Ga2–Ga3	142.28(8)
Al1–Ga1–Al2	75.01(4)	C1_18–Al9–C2_18	37.8(2)
Al3–Ga1–Ga1	130.13(3)	C1_18–Al9–C5_18	37.3(2)
Al1–Ga1–Ga1	140.82(3)	C2_18–Al9–C5_18	62.8(2)
Al2–Ga1–Ga1	134.28(3)	C1_18–Al9–C3_18	62.4(3)
C2_28–Al1–C1_28	37.73(13)	C2_18–Al9–C3_18	37.4(2)
C2_28–Al1–C3_28	37.83(14)	C5_18–Al9–C3_18	62.2(3)
C1_28–Al1–C3_28	62.88(14)	C1_18–Al9–C4_18	62.0(3)
C2_28–Al1–C4_28	62.72(14)	C2_18–Al9–C4_18	62.4(3)
C1_28–Al1–C4_28	62.55(14)	C5_18–Al9–C4_18	36.9(3)
C3_28–Al1–C4_28	37.23(13)	C3_18–Al9–C4_18	37.1(3)
C2_28–Al1–C5_28	62.69(13)	C1_18–Al9–Ga2	166.3(2)
C1_28–Al1–C5_28	37.50(13)	C2_18–Al9–Ga2	152.6(2)
C3_28–Al1–C5_28	62.26(13)	C5_18–Al9–Ga2	130.3(2)
C4_28–Al1–C5_28	37.06(13)	C3_18–Al9–Ga2	121.0(3)
C2_28–Al1–Ga1	160.78(10)	C4_18–Al9–Ga2	111.7(3)
C1_28–Al1–Ga1	161.48(10)	C3_20–Al10–C4_20	38.4(3)
C3_28–Al1–Ga1	131.01(10)	C3_20–Al10–C2_20	38.7(4)
C4_28–Al1–Ga1	119.19(10)	C4_20–Al10–C2_20	63.4(4)
C5_28–Al1–Ga1	131.76(10)	C3_20–Al10–C5_20	62.6(4)
C4_27–Al2–C1_27	61.93(14)	C4_20–Al10–C5_20	36.9(3)
C4_27–Al2–C5_27	37.47(14)	C2_20–Al10–C5_20	61.5(4)
C1_27–Al2–C5_27	37.11(12)	C3_20–Al10–C1_20	63.2(5)
C4_27–Al2–C2_27	62.25(13)	C4_20–Al10–C1_20	62.7(4)
C1_27–Al2–C2_27	37.39(12)	C2_20–Al10–C1_20	36.5(4)
C5_27–Al2–C2_27	62.63(13)	C5_20–Al10–C1_20	37.0(3)
C4_27–Al2–C3_27	38.12(14)	C3_20–Al10–Ga2	160.4(4)
C1_27–Al2–C3_27	62.30(14)	C4_20–Al10–Ga2	130.0(4)
C5_27–Al2–C3_27	63.31(14)	C2_20–Al10–Ga2	160.9(4)
C2_27–Al2–C3_27	36.88(13)	C5_20–Al10–Ga2	119.0(4)
C4_27–Al2–Ga1	116.55(11)	C1_20–Al10–Ga2	131.3(4)
C1_27–Al2–Ga1	164.22(10)	C2_22–Al11–C3_22	38.2(4)
C5_27–Al2–Ga1	131.52(10)	C2_22–Al11–C1_22	37.8(4)
C2_27–Al2–Ga1	157.90(10)	C3_22–Al11–C1_22	62.4(5)
C3_27–Al2–Ga1	127.47(11)	C2_22–Al11–C4_22	61.8(5)

C3_22–Al11–C4_22	36.5(4)	F9_1–C4_1–F7_1	108.2(6)
C1_22–Al11–C4_22	60.3(5)	F9_1–C4_1–F8_1	108.2(7)
C2_22–Al11–C5_22	61.4(5)	F7_1–C4_1–F8_1	107.6(7)
C3_22–Al11–C5_22	60.7(5)	F9_1–C4_1–C1_1	110.8(6)
C1_22–Al11–C5_22	35.9(4)	F7_1–C4_1–C1_1	110.1(6)
C4_22–Al11–C5_22	35.4(3)	F8_1–C4_1–C1_1	111.8(6)
C2_22–Al11–Ga2	159.8(5)	C1_2–O1_2–Al5	146.6(4)
C3_22–Al11–Ga2	124.8(5)	O1_2–C1_2–C4_2	110.6(5)
C1_22–Al11–Ga2	158.5(4)	O1_2–C1_2–C3_2	110.5(5)
C4_22–Al11–Ga2	111.7(5)	C4_2–C1_2–C3_2	110.0(6)
C5_22–Al11–Ga2	125.8(4)	O1_2–C1_2–C2_2	107.0(5)
O1_33–Al4–O1_14	116.0(15)	C4_2–C1_2–C2_2	110.2(6)
O1_26–Al4–O1_35	101(2)	C3_2–C1_2–C2_2	108.6(5)
O1_33–Al4–O1_15	97.4(13)	F3_2–C2_2–F2_2	109.2(7)
O1_14–Al4–O1_15	101.9(15)	F3_2–C2_2–F1_2	106.9(6)
O1_8–Al4–O1_7	109.9(4)	F2_2–C2_2–F1_2	106.8(5)
O1_8–Al4–O1_5	105.9(2)	F3_2–C2_2–C1_2	111.4(6)
O1_7–Al4–O1_5	111.1(4)	F2_2–C2_2–C1_2	112.5(6)
O1_8–Al4–O1_6	111.8(4)	F1_2–C2_2–C1_2	109.9(5)
O1_7–Al4–O1_6	108.7(4)	F4_2–C3_2–F5_2	107.6(5)
O1_5–Al4–O1_6	109.4(3)	F4_2–C3_2–F6_2	107.0(6)
O1_33–Al4–O1_17	115.0(14)	F5_2–C3_2–F6_2	108.2(5)
O1_14–Al4–O1_17	119.7(15)	F4_2–C3_2–C1_2	110.2(5)
O1_15–Al4–O1_17	101.3(13)	F5_2–C3_2–C1_2	111.5(5)
O1_10–Al5–O1_13	113.0(10)	F6_2–C3_2–C1_2	112.0(5)
O1_10–Al5–O1_11	114.3(10)	F9_2–C4_2–F8_2	106.9(7)
O1_13–Al5–O1_11	114.0(6)	F9_2–C4_2–F7_2	107.4(9)
O1_2–Al5–O1_3	116.7(4)	F8_2–C4_2–F7_2	107.5(7)
O1_2–Al5–O1_1	110.6(3)	F9_2–C4_2–C1_2	111.5(7)
O1_3–Al5–O1_1	104.6(4)	F8_2–C4_2–C1_2	111.9(7)
O1_2–Al5–O1_4	109.3(4)	F7_2–C4_2–C1_2	111.4(7)
O1_3–Al5–O1_4	106.1(5)	C1_3–O1_3–Al5	147.9(6)
O1_1–Al5–O1_4	109.1(6)	O1_3–C1_3–C3_3	112.3(6)
O1_10–Al5–O1_12	107.7(9)	O1_3–C1_3–C2_3	107.2(6)
O1_13–Al5–O1_12	102.7(8)	C3_3–C1_3–C2_3	110.4(6)
O1_11–Al5–O1_12	103.9(4)	O1_3–C1_3–C4_3	109.2(6)
C1_1–O1_1–Al5	144.4(5)	C3_3–C1_3–C4_3	110.1(5)
O1_1–C1_1–C3_1	112.7(6)	C2_3–C1_3–C4_3	107.4(5)
O1_1–C1_1–C4_1	110.4(6)	F3_3–C2_3–F1_3	108.2(6)
C3_1–C1_1–C4_1	109.6(6)	F3_3–C2_3–F2_3	108.3(6)
O1_1–C1_1–C2_1	107.0(6)	F1_3–C2_3–F2_3	108.1(6)
C3_1–C1_1–C2_1	109.2(6)	F3_3–C2_3–C1_3	110.6(5)
C4_1–C1_1–C2_1	107.7(6)	F1_3–C2_3–C1_3	110.6(6)
F1_1–C2_1–F2_1	108.2(7)	F2_3–C2_3–C1_3	111.0(6)
F1_1–C2_1–F3_1	109.1(8)	F4_3–C3_3–F6_3	107.6(5)
F2_1–C2_1–F3_1	107.6(6)	F4_3–C3_3–F5_3	107.5(6)
F1_1–C2_1–C1_1	109.2(7)	F6_3–C3_3–F5_3	108.2(6)
F2_1–C2_1–C1_1	112.8(7)	F4_3–C3_3–C1_3	110.8(5)
F3_1–C2_1–C1_1	109.9(5)	F6_3–C3_3–C1_3	112.7(6)
F6_1–C3_1–F5_1	104.9(6)	F5_3–C3_3–C1_3	109.9(6)
F6_1–C3_1–F4_1	109.7(8)	F9_3–C4_3–F8_3	107.8(5)
F5_1–C3_1–F4_1	106.9(8)	F9_3–C4_3–F7_3	107.5(5)
F6_1–C3_1–C1_1	114.5(6)	F8_3–C4_3–F7_3	107.6(5)
F5_1–C3_1–C1_1	110.9(6)	F9_3–C4_3–C1_3	112.3(5)
F4_1–C3_1–C1_1	109.7(7)	F8_3–C4_3–C1_3	112.4(5)

F7_3–C4_3–C1_3	109.0(5)	O1_6–C1_6–C4_6	107.4(5)
C1_4–O1_4–Al5	146.9(10)	C2_6–C1_6–C4_6	108.6(4)
O1_4–C1_4–C3_4	111.8(8)	C3_6–C1_6–C4_6	108.7(4)
O1_4–C1_4–C2_4	111.1(7)	F1_6–C2_6–F2_6	107.3(5)
C3_4–C1_4–C2_4	109.2(5)	F1_6–C2_6–F3_6	108.1(4)
O1_4–C1_4–C4_4	106.5(7)	F2_6–C2_6–F3_6	106.2(5)
C3_4–C1_4–C4_4	108.9(5)	F1_6–C2_6–C1_6	110.9(4)
C2_4–C1_4–C4_4	109.2(5)	F2_6–C2_6–C1_6	114.3(5)
F1_4–C2_4–F3_4	106.6(5)	F3_6–C2_6–C1_6	109.8(4)
F1_4–C2_4–F2_4	108.2(5)	F4_6–C3_6–F5_6	108.6(5)
F3_4–C2_4–F2_4	108.7(5)	F4_6–C3_6–F6_6	106.9(5)
F1_4–C2_4–C1_4	111.3(5)	F5_6–C3_6–F6_6	108.1(5)
F3_4–C2_4–C1_4	110.5(5)	F4_6–C3_6–C1_6	111.2(4)
F2_4–C2_4–C1_4	111.3(5)	F5_6–C3_6–C1_6	110.6(4)
F4_4–C3_4–F5_4	108.0(6)	F6_6–C3_6–C1_6	111.4(5)
F4_4–C3_4–F6_4	107.4(5)	F7_6–C4_6–F9_6	108.8(4)
F5_4–C3_4–F6_4	106.2(6)	F7_6–C4_6–F8_6	107.1(4)
F4_4–C3_4–C1_4	111.2(5)	F9_6–C4_6–F8_6	107.4(5)
F5_4–C3_4–C1_4	110.9(5)	F7_6–C4_6–C1_6	111.0(4)
F6_4–C3_4–C1_4	112.9(5)	F9_6–C4_6–C1_6	110.7(4)
F7_4–C4_4–F9_4	108.0(6)	F8_6–C4_6–C1_6	111.7(5)
F7_4–C4_4–F8_4	108.3(6)	C1_7–O1_7–Al4	143.1(8)
F9_4–C4_4–F8_4	107.7(6)	O1_7–C1_7–C2_7	111.3(6)
F7_4–C4_4–C1_4	111.3(6)	O1_7–C1_7–C4_7	107.8(6)
F9_4–C4_4–C1_4	109.6(6)	C2_7–C1_7–C4_7	108.6(5)
F8_4–C4_4–C1_4	111.8(6)	O1_7–C1_7–C3_7	109.5(6)
C1_5–O1_5–Al4	148.0(3)	C2_7–C1_7–C3_7	110.8(5)
O1_5–C1_5–C2_5	107.6(3)	C4_7–C1_7–C3_7	108.8(5)
O1_5–C1_5–C3_5	108.7(3)	F3_7–C2_7–F1_7	107.8(7)
C2_5–C1_5–C3_5	109.8(3)	F3_7–C2_7–F2_7	107.7(7)
O1_5–C1_5–C4_5	112.1(3)	F1_7–C2_7–F2_7	107.3(7)
C2_5–C1_5–C4_5	109.3(3)	F3_7–C2_7–C1_7	110.0(6)
C3_5–C1_5–C4_5	109.4(3)	F1_7–C2_7–C1_7	110.6(6)
F3_5–C2_5–F1_5	108.9(4)	F2_7–C2_7–C1_7	113.2(7)
F3_5–C2_5–F2_5	107.7(4)	F4_7–C3_7–F5_7	108.7(6)
F1_5–C2_5–F2_5	105.3(3)	F4_7–C3_7–F6_7	106.5(6)
F3_5–C2_5–C1_5	112.2(3)	F5_7–C3_7–F6_7	106.1(7)
F1_5–C2_5–C1_5	109.8(3)	F4_7–C3_7–C1_7	111.9(6)
F2_5–C2_5–C1_5	112.7(3)	F5_7–C3_7–C1_7	111.2(6)
F5_5–C3_5–F4_5	107.7(3)	F6_7–C3_7–C1_7	112.2(7)
F5_5–C3_5–F6_5	106.5(3)	F7_7–C4_7–F9_7	106.5(6)
F4_5–C3_5–F6_5	108.0(3)	F7_7–C4_7–F8_7	108.3(6)
F5_5–C3_5–C1_5	111.1(3)	F9_7–C4_7–F8_7	107.2(6)
F4_5–C3_5–C1_5	110.8(3)	F7_7–C4_7–C1_7	110.9(6)
F6_5–C3_5–C1_5	112.6(3)	F9_7–C4_7–C1_7	110.6(6)
F7_5–C4_5–F8_5	107.3(3)	F8_7–C4_7–C1_7	113.1(6)
F7_5–C4_5–F9_5	106.2(4)	C1_8–O1_8–Al4	150.1(4)
F8_5–C4_5–F9_5	108.8(3)	O1_8–C1_8–C3_8	111.6(4)
F7_5–C4_5–C1_5	111.1(3)	O1_8–C1_8–C4_8	109.9(4)
F8_5–C4_5–C1_5	112.6(3)	C3_8–C1_8–C4_8	110.5(4)
F9_5–C4_5–C1_5	110.6(3)	O1_8–C1_8–C2_8	106.8(4)
C1_6–O1_6–Al4	146.6(7)	C3_8–C1_8–C2_8	109.3(4)
O1_6–C1_6–C2_6	111.8(5)	C4_8–C1_8–C2_8	108.7(4)
O1_6–C1_6–C3_6	110.5(5)	F3_8–C2_8–F1_8	107.9(4)
C2_6–C1_6–C3_6	109.8(4)	F3_8–C2_8–F2_8	108.1(4)

F1_8–C2_8–F2_8	107.4(4)	F6_11–C3_11–F5_11	109.0(10)
F3_8–C2_8–C1_8	111.5(4)	F4_11–C3_11–F5_11	109.1(12)
F1_8–C2_8–C1_8	110.3(3)	F6_11–C3_11–C1_11	112.8(9)
F2_8–C2_8–C1_8	111.4(4)	F4_11–C3_11–C1_11	109.9(11)
F6_8–C3_8–F5_8	106.9(4)	F5_11–C3_11–C1_11	110.8(8)
F6_8–C3_8–F4_8	107.1(4)	F8_11–C4_11–F9_11	107.9(8)
F5_8–C3_8–F4_8	107.2(4)	F8_11–C4_11–F7_11	108.1(8)
F6_8–C3_8–C1_8	113.8(4)	F9_11–C4_11–F7_11	106.3(9)
F5_8–C3_8–C1_8	111.7(4)	F8_11–C4_11–C1_11	113.2(8)
F4_8–C3_8–C1_8	109.9(4)	F9_11–C4_11–C1_11	110.9(8)
F9_8–C4_8–F8_8	108.1(4)	F7_11–C4_11–C1_11	110.2(8)
F9_8–C4_8–F7_8	105.6(4)	C1_12–O1_12–Al5	150.2(7)
F8_8–C4_8–F7_8	106.4(4)	O1_12–C1_12–C4_12	109.5(9)
F9_8–C4_8–C1_8	112.5(4)	O1_12–C1_12–C3_12	110.7(9)
F8_8–C4_8–C1_8	114.7(4)	C4_12–C1_12–C3_12	110.0(9)
F7_8–C4_8–C1_8	109.1(4)	O1_12–C1_12–C2_12	107.9(8)
C1_10–O1_10–Al5	152(2)	C4_12–C1_12–C2_12	110.9(9)
O1_10–C1_10–C3_10	109.0(12)	C3_12–C1_12–C2_12	107.7(9)
O1_10–C1_10–C2_10	109.8(11)	F3_12–C2_12–F2_12	109.8(9)
C3_10–C1_10–C2_10	110.2(8)	F3_12–C2_12–F1_12	106.5(8)
O1_10–C1_10–C4_10	109.6(13)	F2_12–C2_12–F1_12	107.5(8)
C3_10–C1_10–C4_10	109.3(8)	F3_12–C2_12–C1_12	110.9(8)
C2_10–C1_10–C4_10	108.9(8)	F2_12–C2_12–C1_12	112.0(8)
F3_10–C2_10–F1_10	106.5(9)	F1_12–C2_12–C1_12	109.8(8)
F3_10–C2_10–F2_10	109.9(9)	F5_12–C3_12–F6_12	107.2(11)
F1_10–C2_10–F2_10	106.4(8)	F5_12–C3_12–F4_12	109.8(15)
F3_10–C2_10–C1_10	112.1(8)	F6_12–C3_12–F4_12	106.2(12)
F1_10–C2_10–C1_10	109.3(9)	F5_12–C3_12–C1_12	111.6(11)
F2_10–C2_10–C1_10	112.3(7)	F6_12–C3_12–C1_12	112.4(10)
F5_10–C3_10–F6_10	105.3(9)	F4_12–C3_12–C1_12	109.5(12)
F5_10–C3_10–F4_10	106.9(9)	F9_12–C4_12–F7_12	107.7(12)
F6_10–C3_10–F4_10	107.2(9)	F9_12–C4_12–F8_12	107.9(12)
F5_10–C3_10–C1_10	111.3(8)	F7_12–C4_12–F8_12	106.2(10)
F6_10–C3_10–C1_10	113.1(9)	F9_12–C4_12–C1_12	111.8(12)
F4_10–C3_10–C1_10	112.5(9)	F7_12–C4_12–C1_12	110.6(9)
F8_10–C4_10–F9_10	109.3(8)	F8_12–C4_12–C1_12	112.3(9)
F8_10–C4_10–F7_10	106.6(7)	C1_13–O1_13–Al5	157.8(14)
F9_10–C4_10–F7_10	106.7(8)	O1_13–C1_13–C3_13	109.7(10)
F8_10–C4_10–C1_10	112.8(8)	O1_13–C1_13–C2_13	110.3(11)
F9_10–C4_10–C1_10	110.3(7)	C3_13–C1_13–C2_13	110.5(8)
F7_10–C4_10–C1_10	110.9(7)	O1_13–C1_13–C4_13	109.1(9)
C1_11–O1_11–Al5	143.8(7)	C3_13–C1_13–C4_13	108.9(8)
O1_11–C1_11–C4_11	108.5(8)	C2_13–C1_13–C4_13	108.2(8)
O1_11–C1_11–C2_11	112.0(8)	F1_13–C2_13–F3_13	107.9(8)
C4_11–C1_11–C2_11	108.4(8)	F1_13–C2_13–F2_13	109.8(9)
O1_11–C1_11–C3_11	110.8(8)	F3_13–C2_13–F2_13	108.8(8)
C4_11–C1_11–C3_11	108.4(8)	F1_13–C2_13–C1_13	109.7(8)
C2_11–C1_11–C3_11	108.6(8)	F3_13–C2_13–C1_13	109.5(8)
F3_11–C2_11–F1_11	106.4(11)	F2_13–C2_13–C1_13	111.2(8)
F3_11–C2_11–F2_11	107.0(9)	F4_13–C3_13–F6_13	106.2(8)
F1_11–C2_11–F2_11	106.6(11)	F4_13–C3_13–F5_13	108.6(10)
F3_11–C2_11–C1_11	109.2(8)	F6_13–C3_13–F5_13	110.6(10)
F1_11–C2_11–C1_11	114.5(11)	F4_13–C3_13–C1_13	110.9(8)
F2_11–C2_11–C1_11	112.6(9)	F6_13–C3_13–C1_13	110.9(8)
F6_11–C3_11–F4_11	105.1(12)	F5_13–C3_13–C1_13	109.5(9)

F9_13–C4_13–F8_13	106.6(8)
F9_13–C4_13–F7_13	109.9(9)
F8_13–C4_13–F7_13	108.6(8)
F9_13–C4_13–C1_13	110.9(7)
F8_13–C4_13–C1_13	112.9(8)
F7_13–C4_13–C1_13	107.8(8)
C1_14–O1_14–Al4	154(3)
O1_14–C1_14–C2_14	111.0(15)
O1_14–C1_14–C4_14	110.0(17)
C2_14–C1_14–C4_14	108.8(10)
O1_14–C1_14–C3_14	108.3(16)
C2_14–C1_14–C3_14	109.7(11)
C4_14–C1_14–C3_14	109.0(10)
F1_14–C2_14–F3_14	108.5(13)
F1_14–C2_14–F2_14	109.2(16)
F3_14–C2_14–F2_14	107.9(17)
F1_14–C2_14–C1_14	110.2(11)
F3_14–C2_14–C1_14	111.1(11)
F2_14–C2_14–C1_14	109.9(16)
F6_14–C3_14–F4_14	108.5(15)
F6_14–C3_14–F5_14	111.6(16)
F4_14–C3_14–F5_14	110.1(13)
F6_14–C3_14–C1_14	110.9(15)
F4_14–C3_14–C1_14	107.0(11)
F5_14–C3_14–C1_14	108.8(11)
F7_14–C4_14–F9_14	108.6(12)
F7_14–C4_14–F8_14	108.3(17)
F9_14–C4_14–F8_14	109.5(18)
F7_14–C4_14–C1_14	110.7(10)
F9_14–C4_14–C1_14	109.7(13)
F8_14–C4_14–C1_14	110.0(16)
C1_15–O1_15–Al4	154(2)
O1_15–C1_15–C3_15	112.8(15)
O1_15–C1_15–C2_15	108.5(14)
C3_15–C1_15–C2_15	111.6(11)
O1_15–C1_15–C4_15	105.7(13)
C3_15–C1_15–C4_15	107.2(11)
C2_15–C1_15–C4_15	111.0(12)
F2_15–C2_15–F3_15	112.3(16)
F2_15–C2_15–F1_15	106.6(15)
F3_15–C2_15–F1_15	107.8(15)
F2_15–C2_15–C1_15	109.6(14)
F3_15–C2_15–C1_15	108.7(14)
F1_15–C2_15–C1_15	111.8(14)
F5_15–C3_15–F4_15	108.2(15)
F5_15–C3_15–F6_15	107.0(15)
F4_15–C3_15–F6_15	106.0(15)
F5_15–C3_15–C1_15	111.2(14)
F4_15–C3_15–C1_15	112.6(14)
F6_15–C3_15–C1_15	111.5(15)
F8_15–C4_15–F9_15	109.4(14)
F8_15–C4_15–F7_15	107.4(15)
F9_15–C4_15–F7_15	108.5(13)
F8_15–C4_15–C1_15	113.3(14)
F9_15–C4_15–C1_15	108.2(12)
F7_15–C4_15–C1_15	110.0(13)
C5_18–C1_18–C2_18	108.8(6)
C5_18–C1_18–C10_18	125.4(7)
C2_18–C1_18–C10_18	125.6(7)
C5_18–C1_18–Al9	72.3(4)
C2_18–C1_18–Al9	71.6(3)
C10_18–C1_18–Al9	126.2(4)
C3_18–C2_18–C1_18	106.9(6)
C3_18–C2_18–C9_18	126.0(7)
C1_18–C2_18–C9_18	127.0(7)
C3_18–C2_18–Al9	71.8(4)
C1_18–C2_18–Al9	70.6(3)
C9_18–C2_18–Al9	124.9(4)
C4_18–C3_18–C2_18	108.3(7)
C4_18–C3_18–C8_18	125.7(10)
C2_18–C3_18–C8_18	126.0(10)
C4_18–C3_18–Al9	71.9(5)
C2_18–C3_18–Al9	70.9(4)
C8_18–C3_18–Al9	122.9(11)
C5_18–C4_18–C3_18	108.3(7)
C5_18–C4_18–C7_18	126.6(10)
C3_18–C4_18–C7_18	125.1(10)
C5_18–C4_18–Al9	71.1(4)
C3_18–C4_18–Al9	71.0(5)
C7_18–C4_18–Al9	122.7(9)
C4_18–C5_18–C1_18	107.7(6)
C4_18–C5_18–C6_18	126.1(9)
C1_18–C5_18–C6_18	126.1(9)
C4_18–C5_18–Al9	72.0(5)
C1_18–C5_18–Al9	70.4(3)
C6_18–C5_18–Al9	125.1(4)
C5_18–C6_18–H6A_18	109.5
C5_18–C6_18–H6B_18	109.5
H6A_18–C6_18–H6B_18	109.5
C5_18–C6_18–H6C_18	109.5
H6A_18–C6_18–H6C_18	109.5
H6B_18–C6_18–H6C_18	109.5
C4_18–C7_18–H7A_18	109.5
C4_18–C7_18–H7B_18	109.5
H7A_18–C7_18–H7B_18	109.5
C4_18–C7_18–H7C_18	109.5
H7A_18–C7_18–H7C_18	109.5
H7B_18–C7_18–H7C_18	109.5
C3_18–C8_18–H8A_18	109.5
C3_18–C8_18–H8B_18	109.5
H8A_18–C8_18–H8B_18	109.5
C3_18–C8_18–H8C_18	109.5

H8A_18–C8_18–H8C_18	109.5
H8B_18–C8_18–H8C_18	109.5
C2_18–C9_18–H9A_18	109.5
C2_18–C9_18–H9B_18	109.5
H9A_18–C9_18–H9B_18	109.5
C2_18–C9_18–H9C_18	109.5
H9A_18–C9_18–H9C_18	109.5
H9B_18–C9_18–H9C_18	109.5
C1_18–C10_18–H10A_18	109.5
C1_18–C10_18–H10B_18	109.5
H10A_18–C10_18–H10B_18	109.5
C1_18–C10_18–H10C_18	109.5
H10A_18–C10_18–H10C_18	109.5
H10B_18–C10_18–H10C_18	109.5
C2_19–C1_19–C5_19	108.3(7)
C2_19–C1_19–C10_19	128.3(12)
C5_19–C1_19–C10_19	123.4(12)
C2_19–C1_19–Al6	71.4(5)
C5_19–C1_19–Al6	70.7(6)
C10_19–C1_19–Al6	124.8(10)
C1_19–C2_19–C3_19	107.7(7)
C1_19–C2_19–C9_19	126.6(11)
C3_19–C2_19–C9_19	125.7(11)
C1_19–C2_19–Al6	71.4(5)
C3_19–C2_19–Al6	69.9(5)
C9_19–C2_19–Al6	123.8(11)
C2_19–C3_19–C4_19	108.7(7)
C2_19–C3_19–C8_19	126.7(9)
C4_19–C3_19–C8_19	124.5(9)
C2_19–C3_19–Al6	72.5(5)
C4_19–C3_19–Al6	70.0(7)
C8_19–C3_19–Al6	125.4(8)
C5_19–C4_19–C3_19	106.6(7)
C5_19–C4_19–C7_19	126.9(9)
C3_19–C4_19–C7_19	126.4(9)
C5_19–C4_19–Al6	72.5(7)
C3_19–C4_19–Al6	71.5(6)
C7_19–C4_19–Al6	121.9(12)
C1_19–C5_19–C4_19	108.6(7)
C1_19–C5_19–C6_19	126.9(10)
C4_19–C5_19–C6_19	124.4(10)
C1_19–C5_19–Al6	71.8(6)
C4_19–C5_19–Al6	69.5(7)
C6_19–C5_19–Al6	125.2(11)
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
C2_20–C1_20–C5_20	106.5(8)
C2_20–C1_20–C10_20	129.4(11)
C5_20–C1_20–C10_20	124.0(10)
C2_20–C1_20–Al10	68.9(6)
C5_20–C1_20–Al10	70.6(6)
C10_20–C1_20–Al10	125.7(9)
C1_20–C2_20–C3_20	109.5(8)

C1_20–C2_20–C9_20	123.3(11)
C3_20–C2_20–C9_20	127.1(12)
C1_20–C2_20–Al10	74.6(6)
C3_20–C2_20–Al10	69.3(6)
C9_20–C2_20–Al10	125.8(10)
C4_20–C3_20–C2_20	106.4(7)
C4_20–C3_20–C8_20	124.5(9)
C2_20–C3_20–C8_20	129.1(10)
C4_20–C3_20–Al10	71.4(7)
C2_20–C3_20–Al10	72.0(6)
C8_20–C3_20–Al10	122.0(10)
C5_20–C4_20–C3_20	108.1(7)
C5_20–C4_20–C7_20	124.5(7)
C3_20–C4_20–C7_20	127.2(8)
C5_20–C4_20–Al10	74.3(6)
C3_20–C4_20–Al10	70.2(7)
C7_20–C4_20–Al10	124.9(8)
C4_20–C5_20–C1_20	109.4(7)
C4_20–C5_20–C6_20	127.9(8)
C1_20–C5_20–C6_20	122.6(8)
C4_20–C5_20–Al10	68.8(6)
C1_20–C5_20–Al10	72.4(6)
C6_20–C5_20–Al10	126.9(8)
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	104.8(8)
C5_21–C1_21–C10_21	129.3(11)
C2_21–C1_21–C10_21	125.9(11)
C5_21–C1_21–Al7	74.3(7)
C2_21–C1_21–Al7	68.4(6)
C10_21–C1_21–Al7	121.1(9)
C3_21–C2_21–C1_21	110.0(8)
C3_21–C2_21–C9_21	127.4(9)
C1_21–C2_21–C9_21	122.3(9)
C3_21–C2_21–Al7	74.7(6)
C1_21–C2_21–Al7	72.9(6)
C9_21–C2_21–Al7	124.1(9)
C2_21–C3_21–C4_21	107.5(8)
C2_21–C3_21–C8_21	123.9(9)
C4_21–C3_21–C8_21	128.6(9)
C2_21–C3_21–Al7	67.7(5)
C4_21–C3_21–Al7	73.7(7)
C8_21–C3_21–Al7	125.2(10)
C3_21–C4_21–C5_21	106.9(8)
C3_21–C4_21–C7_21	123.7(10)
C5_21–C4_21–C7_21	128.6(11)
C3_21–C4_21–Al7	69.7(7)
C5_21–C4_21–Al7	71.2(7)
C7_21–C4_21–Al7	131.9(11)
C1_21–C5_21–C4_21	110.8(8)
C1_21–C5_21–C6_21	127.3(12)
C4_21–C5_21–C6_21	122.0(12)
C1_21–C5_21–Al7	69.0(7)
C4_21–C5_21–Al7	72.4(8)
C6_21–C5_21–Al7	125.5(10)
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	108.6(8)
C5_22–C1_22–C10_22	127.0(10)
C2_22–C1_22–C10_22	124.3(10)
C5_22–C1_22–Al11	76.5(8)
C2_22–C1_22–Al11	67.8(6)
C10_22–C1_22–Al11	125.2(10)
C1_22–C2_22–C3_22	107.5(8)
C1_22–C2_22–C9_22	127.3(9)
C3_22–C2_22–C9_22	124.9(10)
C1_22–C2_22–Al11	74.4(6)
C3_22–C2_22–Al11	72.8(7)
C9_22–C2_22–Al11	123.3(10)
C4_22–C3_22–C2_22	107.8(8)
C4_22–C3_22–C8_22	123.8(10)
C2_22–C3_22–C8_22	128.4(11)
C4_22–C3_22–Al11	76.0(10)
C2_22–C3_22–Al11	69.0(6)
C8_22–C3_22–Al11	121.8(11)
C3_22–C4_22–C5_22	108.7(8)
C3_22–C4_22–C7_22	127.3(10)
C5_22–C4_22–C7_22	124.0(10)
C3_22–C4_22–Al11	67.5(9)
C5_22–C4_22–Al11	73.8(10)
C7_22–C4_22–Al11	127.3(14)
C1_22–C5_22–C4_22	107.4(9)
C1_22–C5_22–C6_22	124.7(11)
C4_22–C5_22–C6_22	127.9(11)
C1_22–C5_22–Al11	67.7(7)
C4_22–C5_22–Al11	70.7(10)
C6_22–C5_22–Al11	127.7(13)
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
C2_23–C1_23–C5_23	108.3(8)
C2_23–C1_23–C10_23	125.5(10)
C5_23–C1_23–C10_23	126.0(10)
C2_23–C1_23–Al8	76.0(7)
C5_23–C1_23–Al8	72.9(11)
C10_23–C1_23–Al8	120.5(12)
C1_23–C2_23–C3_23	107.8(8)
C1_23–C2_23–C9_23	124.6(9)
C3_23–C2_23–C9_23	127.4(10)
C1_23–C2_23–Al8	65.9(6)
C3_23–C2_23–Al8	75.4(6)
C9_23–C2_23–Al8	127.3(11)
C2_23–C3_23–C4_23	108.0(8)
C2_23–C3_23–C8_23	125.8(10)
C4_23–C3_23–C8_23	126.1(10)
C2_23–C3_23–Al8	68.1(6)
C4_23–C3_23–Al8	70.0(8)
C8_23–C3_23–Al8	130.6(10)
C5_23–C4_23–C3_23	107.9(9)
C5_23–C4_23–C7_23	129.2(12)
C3_23–C4_23–C7_23	122.8(12)
C5_23–C4_23–Al8	67.1(11)
C3_23–C4_23–Al8	73.7(8)
C7_23–C4_23–Al8	125.0(13)
C4_23–C5_23–C1_23	107.8(9)
C4_23–C5_23–C6_23	125.3(11)
C1_23–C5_23–C6_23	126.6(11)
C4_23–C5_23–Al8	75.7(11)
C1_23–C5_23–Al8	67.8(10)
C6_23–C5_23–Al8	118.0(16)
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
C1_17–O1_17–Al4	148(2)
O1_17–C1_17–C3_17	114.1(15)
O1_17–C1_17–C4_17	109.2(13)
C3_17–C1_17–C4_17	108.9(11)
O1_17–C1_17–C2_17	108.3(14)
C3_17–C1_17–C2_17	109.8(11)
C4_17–C1_17–C2_17	106.1(11)
F3_17–C2_17–F2_17	104.3(13)
F3_17–C2_17–F1_17	112.5(14)
F2_17–C2_17–F1_17	113.1(14)
F3_17–C2_17–C1_17	111.4(12)
F2_17–C2_17–C1_17	109.6(12)
F1_17–C2_17–C1_17	106.0(12)
F4_17–C3_17–F6_17	105.0(13)
F4_17–C3_17–F5_17	106.5(14)
F6_17–C3_17–F5_17	112.2(14)
F4_17–C3_17–C1_17	113.4(12)
F6_17–C3_17–C1_17	113.4(12)
F5_17–C3_17–C1_17	106.3(12)
F8_17–C4_17–F9_17	108.5(15)
F8_17–C4_17–F7_17	107.7(16)
F9_17–C4_17–F7_17	106.0(16)
F8_17–C4_17–C1_17	112.5(13)

F9_17–C4_17–C1_17	112.7(14)	C4_24–C5_24–Al3	70.97(16)
F7_17–C4_17–C1_17	109.1(13)	C6_24–C5_24–Al3	128.0(2)
C1_26–O1_26–Al4	153(4)	C5_24–C6_24–H6A_24	109.5
O1_26–C1_26–C4_26	110.4(19)	C5_24–C6_24–H6B_24	109.5
O1_26–C1_26–C2_26	110(2)	H6A_24–C6_24–H6B_24	109.5
C4_26–C1_26–C2_26	113.5(15)		
O1_26–C1_26–C3_26	109(2)	C5_24–C6_24–H6C_24	109.5
C4_26–C1_26–C3_26	108.0(14)	H6A_24–C6_24–H6C_24	109.5
C2_26–C1_26–C3_26	104.8(14)		
F1_26–C2_26–F2_26	110.4(19)	H6B_24–C6_24–H6C_24	109.5
F1_26–C2_26–F3_26	105(2)		
F2_26–C2_26–F3_26	110(2)	C4_24–C7_24–H7A_24	109.5
F1_26–C2_26–C1_26	114.7(18)	C4_24–C7_24–H7B_24	109.5
F2_26–C2_26–C1_26	110.6(17)	H7A_24–C7_24–H7B_24	109.5
F3_26–C2_26–C1_26	106.0(18)		
F6_26–C3_26–F4_26	106.2(19)	C4_24–C7_24–H7C_24	109.5
F6_26–C3_26–F5_26	107(2)	H7A_24–C7_24–H7C_24	109.5
F4_26–C3_26–F5_26	112(2)		
F6_26–C3_26–C1_26	110.5(19)	H7B_24–C7_24–H7C_24	109.5
F4_26–C3_26–C1_26	112.6(18)		
F5_26–C3_26–C1_26	107.9(17)	C3_24–C8_24–H8A_24	109.5
F9_26–C4_26–F8_26	107.7(19)	C3_24–C8_24–H8B_24	109.5
F9_26–C4_26–F7_26	110(2)	H8A_24–C8_24–H8B_24	109.5
F8_26–C4_26–F7_26	103.4(19)		
F9_26–C4_26–C1_26	116.8(19)	C3_24–C8_24–H8C_24	109.5
F8_26–C4_26–C1_26	113.6(19)	H8A_24–C8_24–H8C_24	109.5
F7_26–C4_26–C1_26	104.7(16)		
C2_24–C1_24–C5_24	107.1(2)	H8B_24–C8_24–H8C_24	109.5
C2_24–C1_24–C10_24	126.6(3)		
C5_24–C1_24–C10_24	126.3(3)	C2_24–C9_24–H9A_24	109.5
C2_24–C1_24–Al3	71.24(14)	C2_24–C9_24–H9B_24	109.5
C5_24–C1_24–Al3	70.08(15)	H9A_24–C9_24–H9B_24	109.5
C10_24–C1_24–Al3	125.3(2)		
C1_24–C2_24–C3_24	108.9(2)	C2_24–C9_24–H9C_24	109.5
C1_24–C2_24–C9_24	125.8(3)	H9A_24–C9_24–H9C_24	109.5
C3_24–C2_24–C9_24	125.4(2)		
C1_24–C2_24–Al3	71.84(15)	H9B_24–C9_24–H9C_24	109.5
C3_24–C2_24–Al3	71.24(14)		
C9_24–C2_24–Al3	123.3(2)	C1_24–C10_24–H10A_24	109.5
C4_24–C3_24–C2_24	108.1(2)		
C4_24–C3_24–C8_24	127.1(3)	C1_24–C10_24–H10B_24	109.5
C2_24–C3_24–C8_24	124.7(3)		
C4_24–C3_24–Al3	70.62(15)	H10A_24–C10_24–H10B_24	109.5
C2_24–C3_24–Al3	71.53(14)		
C8_24–C3_24–Al3	124.2(2)	C1_24–C10_24–H10C_24	109.5
C3_24–C4_24–C5_24	107.7(2)		
C3_24–C4_24–C7_24	126.5(3)	H10A_24–C10_24–H10C_24	109.5
C5_24–C4_24–C7_24	125.8(3)		
C3_24–C4_24–Al3	72.23(15)	H10B_24–C10_24–H10C_24	109.5
C5_24–C4_24–Al3	71.14(16)		
C7_24–C4_24–Al3	123.8(2)	C5_27–C1_27–C2_27	109.0(3)
C1_24–C5_24–C4_24	108.2(2)	C5_27–C1_27–C10_27	125.9(3)
C1_24–C5_24–C6_24	126.4(3)	C2_27–C1_27–C10_27	124.9(3)
C4_24–C5_24–C6_24	125.1(3)	C5_27–C1_27–Al2	71.45(19)
C1_24–C5_24–Al3	72.37(15)	C2_27–C1_27–Al2	71.48(17)

C10_27–C1_27–Al2	126.5(3)	H9A_27–C9_27–H9B_27	109.5
C3_27–C2_27–C1_27	108.7(3)	C2_27–C9_27–H9C_27	109.5
C3_27–C2_27–C9_27	127.5(3)	H9A_27–C9_27–H9C_27	109.5
C1_27–C2_27–C9_27	123.5(3)	H9B_27–C9_27–H9C_27	109.5
C3_27–C2_27–Al2	71.78(18)	C1_27–C10_27–H10A_27	109.5
C1_27–C2_27–Al2	71.14(18)	C1_27–C10_27–H10B_27	109.5
C9_27–C2_27–Al2	127.8(2)	H10A_27–C10_27–H10B_27	109.5
C2_27–C3_27–C4_27	106.7(3)	C1_27–C10_27–H10C_27	109.5
C2_27–C3_27–C8_27	127.1(4)	H10A_27–C10_27–H10C_27	109.5
C4_27–C3_27–C8_27	126.2(4)	H10B_27–C10_27–H10C_27	109.5
C2_27–C3_27–Al2	71.34(19)	C2_28–C1_28–C5_28	107.9(3)
C4_27–C3_27–Al2	70.47(19)	C2_28–C1_28–C10_28	124.8(4)
C8_27–C3_27–Al2	125.2(3)	C5_28–C1_28–C10_28	127.0(3)
C5_27–C4_27–C3_27	108.5(3)	C2_28–C1_28–Al1	70.83(17)
C5_27–C4_27–C7_27	125.4(4)	C5_28–C1_28–Al1	72.24(18)
C3_27–C4_27–C7_27	126.1(4)	C10_28–C1_28–Al1	127.9(3)
C5_27–C4_27–Al2	71.37(19)	C1_28–C2_28–C3_28	107.7(3)
C3_27–C4_27–Al2	71.41(18)	C1_28–C2_28–C9_28	124.9(4)
C7_27–C4_27–Al2	122.6(3)	C3_28–C2_28–C9_28	127.2(4)
C1_27–C5_27–C4_27	107.1(3)	C1_28–C2_28–Al1	71.44(18)
C1_27–C5_27–C6_27	126.5(4)	C3_28–C2_28–Al1	71.65(18)
C4_27–C5_27–C6_27	126.3(3)	C9_28–C2_28–Al1	125.2(3)
C1_27–C5_27–Al2	71.43(18)	C4_28–C3_28–C2_28	108.0(3)
C4_27–C5_27–Al2	71.17(19)	C4_28–C3_28–C8_28	125.7(4)
C6_27–C5_27–Al2	124.6(3)	C2_28–C3_28–C8_28	126.2(4)
C5_27–C6_27–H6A_27	109.5	C4_28–C3_28–Al1	72.0(2)
C5_27–C6_27–H6B_27	109.5	C2_28–C3_28–Al1	70.5(2)
H6A_27–C6_27–H6B_27	109.5	C8_28–C3_28–Al1	123.7(3)
C5_27–C6_27–H6C_27	109.5	C3_28–C4_28–C5_28	108.2(3)
H6A_27–C6_27–H6C_27	109.5	C3_28–C4_28–C7_28	126.1(4)
H6B_27–C6_27–H6C_27	109.5	C5_28–C4_28–C7_28	125.7(4)
C4_27–C7_27–H7A_27	109.5	C3_28–C4_28–Al1	70.7(2)
C4_27–C7_27–H7B_27	109.5	C5_28–C4_28–Al1	71.6(2)
H7A_27–C7_27–H7B_27	109.5	C7_28–C4_28–Al1	124.2(3)
C4_27–C7_27–H7C_27	109.5	C4_28–C5_28–C1_28	108.1(3)
H7A_27–C7_27–H7C_27	109.5	C4_28–C5_28–C6_28	126.2(4)
H7B_27–C7_27–H7C_27	109.5	C1_28–C5_28–C6_28	125.7(4)
C3_27–C8_27–H8A_27	109.5	C4_28–C5_28–Al1	71.38(18)
C3_27–C8_27–H8B_27	109.5	C1_28–C5_28–Al1	70.26(17)
H8A_27–C8_27–H8B_27	109.5	C6_28–C5_28–Al1	125.3(3)
C3_27–C8_27–H8C_27	109.5	C5_28–C6_28–H6A_28	109.5
H8A_27–C8_27–H8C_27	109.5	C5_28–C6_28–H6B_28	109.5
H8B_27–C8_27–H8C_27	109.5	H6A_28–C6_28–H6B_28	109.5
C2_27–C9_27–H9A_27	109.5	C5_28–C6_28–H6C_28	109.5
C2_27–C9_27–H9B_27	109.5		

H6A_28–C6_28–H6C_28	109.5
H6B_28–C6_28–H6C_28	109.5
C4_28–C7_28–H7A_28	109.5
C4_28–C7_28–H7B_28	109.5
H7A_28–C7_28–H7B_28	109.5
C4_28–C7_28–H7C_28	109.5
H7A_28–C7_28–H7C_28	109.5
H7B_28–C7_28–H7C_28	109.5
C3_28–C8_28–H8A_28	109.5
C3_28–C8_28–H8B_28	109.5
H8A_28–C8_28–H8B_28	109.5
C3_28–C8_28–H8C_28	109.5
H8A_28–C8_28–H8C_28	109.5
H8B_28–C8_28–H8C_28	109.5
C2_28–C9_28–H9A_28	109.5
C2_28–C9_28–H9B_28	109.5
H9A_28–C9_28–H9B_28	109.5
C2_28–C9_28–H9C_28	109.5
H9A_28–C9_28–H9C_28	109.5
H9B_28–C9_28–H9C_28	109.5
C1_28–C10_28–H10A_28	109.5
C1_28–C10_28–H10B_28	109.5
H10A_28–C10_28–H10B_28	109.5
C1_28–C10_28–H10C_28	109.5
H10A_28–C10_28–H10C_28	109.5
H10B_28–C10_28–H10C_28	109.5
C6_30–C1_30–C2_30	123.7(9)
C6_30–C1_30–F1_30	118.6(10)
C2_30–C1_30–F1_30	117.6(9)
C3_30–C2_30–C1_30	117.5(9)
C3_30–C2_30–H2_30	121.2
C1_30–C2_30–H2_30	121.2
C4_30–C3_30–C2_30	125.0(9)
C4_30–C3_30–F2_30	114.2(8)
C2_30–C3_30–F2_30	120.7(8)
C3_30–C4_30–C5_30	116.6(9)
C3_30–C4_30–H4_30	121.7
C5_30–C4_30–H4_30	121.7
C6_30–C5_30–C4_30	119.9(9)
C6_30–C5_30–H5_30	120.1
C4_30–C5_30–H5_30	120.1
C1_30–C6_30–C5_30	117.2(10)
C1_30–C6_30–H6_30	121.4
C5_30–C6_30–H6_30	121.4
C6_16–C1_16–C2_16	125.5(11)
C6_16–C1_16–F1_16	119.6(11)
C2_16–C1_16–F1_16	114.8(10)
C3_16–C2_16–C1_16	123.3(12)
C3_16–C2_16–H2_16	118.3
C1_16–C2_16–H2_16	118.3
C2_16–C3_16–C4_16	123.0(12)
C2_16–C3_16–F2_16	133.0(12)
C4_16–C3_16–F2_16	103.9(12)
C3_16–C4_16–C5_16	115.1(11)
C3_16–C4_16–H4_16	122.5
C5_16–C4_16–H4_16	122.5
C4_16–C5_16–C6_16	116.3(10)
C4_16–C5_16–H5_16	121.8
C6_16–C5_16–H5_16	121.8
C1_16–C6_16–C5_16	114.6(11)
C1_16–C6_16–H6_16	122.7
C5_16–C6_16–H6_16	122.7
C6_31–C1_31–F1_31	114.3(13)
C6_31–C1_31–C2_31	127.8(13)
F1_31–C1_31–C2_31	117.6(13)
C1_31–C2_31–C3_31	114.2(14)
C1_31–C2_31–H2_31	122.9
C3_31–C2_31–H2_31	122.9
C4_31–C3_31–F2_31	114.4(13)
C4_31–C3_31–C2_31	126.5(14)
F2_31–C3_31–C2_31	119.1(13)
C3_31–C4_31–C5_31	118.3(14)
C3_31–C4_31–H4_31	120.9
C5_31–C4_31–H4_31	120.9
C6_31–C5_31–C4_31	116.8(13)
C6_31–C5_31–H5_31	121.6
C4_31–C5_31–H5_31	121.6
C1_31–C6_31–C5_31	116.1(13)
C1_31–C6_31–H6_31	121.9
C5_31–C6_31–H6_31	121.9
C1_32–O1_32–Al5	155(3)
O1_32–C1_32–C3_32	108.7(16)
O1_32–C1_32–C2_32	109.3(17)
C3_32–C1_32–C2_32	111.7(12)
O1_32–C1_32–C4_32	111.5(17)
C3_32–C1_32–C4_32	108.5(12)
C2_32–C1_32–C4_32	107.2(12)
F2_32–C2_32–F3_32	109.1(18)
F2_32–C2_32–F1_32	106.7(18)
F3_32–C2_32–F1_32	107.5(16)
F2_32–C2_32–C1_32	110.0(17)
F3_32–C2_32–C1_32	112.4(13)
F1_32–C2_32–C1_32	111.1(14)

F5_32–C3_32–F6_32	109.3(18)	F4_35–C3_35–C1_35	110.9(14)
F5_32–C3_32–F4_32	108.2(16)	F9_35–C4_35–F8_35	108.5(18)
F6_32–C3_32–F4_32	104.5(16)	F9_35–C4_35–F7_35	105.4(17)
F5_32–C3_32–C1_32	112.1(17)	F8_35–C4_35–F7_35	108.7(17)
F6_32–C3_32–C1_32	111.2(15)	F9_35–C4_35–C1_35	109.6(15)
F4_32–C3_32–C1_32	111.2(13)	F8_35–C4_35–C1_35	112.4(16)
F7_32–C4_32–F9_32	108.2(16)	F7_35–C4_35–C1_35	111.9(15)
F7_32–C4_32–F8_32	108.4(18)	C1_36–O1_36–Al4	148(3)
F9_32–C4_32–F8_32	104.6(17)	O1_36–C1_36–C4_36	112.5(18)
F7_32–C4_32–C1_32	111.0(14)	O1_36–C1_36–C2_36	110.7(19)
F9_32–C4_32–C1_32	110.6(13)	C4_36–C1_36–C2_36	109.2(14)
F8_32–C4_32–C1_32	113.8(17)	O1_36–C1_36–C3_36	107.9(18)
C1_33–O1_33–Al4	147(2)	C4_36–C1_36–C3_36	109.9(14)
O1_33–C1_33–C2_33	112.6(15)	C2_36–C1_36–C3_36	106.4(14)
O1_33–C1_33–C3_33	110.1(16)	F3_36–C2_36–F1_36	105.3(19)
C2_33–C1_33–C3_33	112.2(13)	F3_36–C2_36–F2_36	110(2)
O1_33–C1_33–C4_33	106.7(15)	F1_36–C2_36–F2_36	110(2)
C2_33–C1_33–C4_33	108.3(13)	F3_36–C2_36–C1_36	112.2(17)
C3_33–C1_33–C4_33	106.7(12)	F1_36–C2_36–C1_36	111.8(18)
F3_33–C2_33–F1_33	107.1(17)	F2_36–C2_36–C1_36	107.6(17)
F3_33–C2_33–F2_33	106.4(17)	F4_36–C3_36–F6_36	107.1(19)
F1_33–C2_33–F2_33	108.8(18)	F4_36–C3_36–F5_36	109(2)
F3_33–C2_33–C1_33	110.6(15)	F6_36–C3_36–F5_36	107(2)
F1_33–C2_33–C1_33	112.9(16)	F4_36–C3_36–C1_36	114.6(19)
F2_33–C2_33–C1_33	110.7(16)	F6_36–C3_36–C1_36	111.3(18)
F4_33–C3_33–F6_33	108.0(17)	F5_36–C3_36–C1_36	108.0(17)
F4_33–C3_33–F5_33	106.2(18)	F9_36–C4_36–F7_36	105.9(19)
F6_33–C3_33–F5_33	105.8(16)	F9_36–C4_36–F8_36	109.6(19)
F4_33–C3_33–C1_33	109.9(15)	F7_36–C4_36–F8_36	105.0(19)
F6_33–C3_33–C1_33	115.8(16)	F9_36–C4_36–C1_36	113.6(17)
F5_33–C3_33–C1_33	110.5(15)	F7_36–C4_36–C1_36	110.4(17)
F9_33–C4_33–F8_33	109.3(18)	F8_36–C4_36–C1_36	111.9(17)
F9_33–C4_33–F7_33	109.0(18)	C6_37–C1_37–C2_37	124.7(17)
F8_33–C4_33–F7_33	110(2)	C6_37–C1_37–F1_37	118.4(18)
F9_33–C4_33–C1_33	112.6(16)	C2_37–C1_37–F1_37	116.9(17)
F8_33–C4_33–C1_33	111.4(17)	C1_37–C2_37–C3_37	118.2(18)
F7_33–C4_33–C1_33	104.4(15)	C1_37–C2_37–H2_37	120.9
C1_35–O1_35–Al4	149(2)	C3_37–C2_37–H2_37	120.9
O1_35–C1_35–C2_35	110.1(15)	C4_37–C3_37–C2_37	125.7(17)
O1_35–C1_35–C3_35	108.2(16)	C4_37–C3_37–F2_37	118.9(17)
C2_35–C1_35–C3_35	112.2(12)	C2_37–C3_37–F2_37	115.4(17)
O1_35–C1_35–C4_35	108.9(16)	C3_37–C4_37–C5_37	116.8(17)
C2_35–C1_35–C4_35	109.7(12)	C3_37–C4_37–H4_37	121.6
C3_35–C1_35–C4_35	107.6(12)	C5_37–C4_37–H4_37	121.6
F3_35–C2_35–F1_35	106.7(18)	C4_37–C5_37–C6_37	116.8(17)
F3_35–C2_35–F2_35	107.5(18)	C4_37–C5_37–H5_37	121.6
F1_35–C2_35–F2_35	108.3(18)	C6_37–C5_37–H5_37	121.6
F3_35–C2_35–C1_35	113.9(16)	C1_37–C6_37–C5_37	117.8(17)
F1_35–C2_35–C1_35	110.7(15)	C1_37–C6_37–H6_37	121.1
F2_35–C2_35–C1_35	109.5(15)	C5_37–C6_37–H6_37	121.1
F5_35–C3_35–F6_35	108.5(19)	F1_41–C1_41–C2_41	116.6(15)
F5_35–C3_35–F4_35	107.3(18)	F1_41–C1_41–C6_41	125.0(16)
F6_35–C3_35–F4_35	108.4(18)	C2_41–C1_41–C6_41	118.3(14)
F5_35–C3_35–C1_35	109.5(16)	C3_41–C2_41–C1_41	111.0(17)
F6_35–C3_35–C1_35	112.1(16)	C3_41–C2_41–H2_41	124.5

C1_41–C2_41–H2_41	124.5
F2_41–C3_41–C4_41	107.8(17)
F2_41–C3_41–C2_41	111.7(17)
C4_41–C3_41–C2_41	140.2(19)
C3_41–C4_41–C5_41	111.1(15)
C3_41–C4_41–H4_41	124.5
C5_41–C4_41–H4_41	124.5
C4_41–C5_41–C6_41	108.6(15)
C4_41–C5_41–H5_41	125.7
C6_41–C5_41–H5_41	125.7
C1_41–C6_41–C5_41	128.4(15)
C1_41–C6_41–H6_41	115.8
C5_41–C6_41–H6_41	115.8

Symmetry transformations used to generate equivalent atoms:
#1: 2-X, -Y, -Z;

S-Table 8: Bond lengths and angles for 2A

Atom–Atom	Length [Å]
Ga1–Al2	2.5306(8)
Ga1–Al3	2.5364(9)
Ga1–Al1	2.5392(7)
Ga2–Al4	2.5219(9)
Ga2–Al6	2.5266(7)
Ga2–Al5	2.5350(9)
Ga3–Al7	2.5299(8)
Ga3–Al9	2.5341(7)
Ga3–Al8	2.5341(7)
Ga4–Al11	2.5206(7)
Ga4–Al10	2.5263(9)
Ga4–Al12	2.5483(8)
Al1–C3_21	2.204(2)
Al1–C2_21	2.216(2)
Al1–C4_21	2.219(2)
Al1–C5_21	2.222(2)
Al1–C1_21	2.227(2)
Al6–C2_19	2.202(2)
Al6–C1_19	2.205(2)
Al6–C3_19	2.212(2)
Al6–C4_19	2.217(2)
Al6–C5_19	2.219(2)
Al7–C2_24	2.200(2)
Al7–C1_24	2.215(2)
Al7–C3_24	2.216(2)
Al7–C5_24	2.226(2)
Al7–C4_24	2.229(2)
Al8–C5_42	2.12(2)
Al8–C4_42	2.155(18)
Al8–C1_42	2.17(2)
Al8–C4_23	2.197(3)
Al8–C5_23	2.216(4)
Al8–C3_23	2.226(3)
Al8–C1_23	2.239(3)
Al8–C2_23	2.250(3)
Al8–C3_42	2.309(14)
Al8–C2_42	2.313(18)
Al9–C4_25	2.201(2)
Al9–C5_25	2.210(2)
Al9–C3_25	2.213(2)
Al9–C1_25	2.2145(19)
Al9–C2_25	2.229(2)
Al10–C4_41	2.133(6)
Al10–C3_41	2.149(5)
Al10–C5_41	2.161(8)
Al10–C2_41	2.189(4)
Al10–C1_41	2.193(5)
Al10–C3_38	2.229(8)
Al10–C2_38	2.248(10)
Al10–C4_38	2.271(7)
Al10–C1_38	2.322(9)
Al10–C5_38	2.334(6)
Al11–C2_27	2.193(2)
Al11–C1_27	2.206(2)
Al11–C3_27	2.213(2)
Al11–C4_27	2.230(2)
Al11–C5_27	2.234(2)
Al12–C4_40	2.19(3)
Al12–C5_40	2.199(19)
Al12–C5_26	2.207(11)
Al12–C4_26	2.216(16)
Al12–C1_26	2.220(9)
Al12–C3_26	2.220(10)
Al12–C2_26	2.223(9)
Al12–C1_40	2.228(13)
Al12–C3_40	2.258(15)
Al12–C2_40	2.267(13)
Al13–O1_31	1.653(11)
Al13–O1_28	1.675(17)
Al13–O1_30	1.691(15)
Al13–O1_10	1.693(5)
Al13–O1_36	1.693(16)
Al13–O1_9	1.7317(19)
Al13–O1_12	1.733(4)
Al13–O1_11	1.747(3)
Al13–O1_29	1.833(13)
Al14–O1_35	1.670(11)
Al14–O1_34	1.693(12)
Al14–O1_15	1.7195(15)
Al14–O1_14	1.7219(16)
Al14–O1_16	1.726(2)
Al14–O1_13	1.7276(14)
Al15–O1_39	1.65(2)
Al15–O1_8	1.7221(14)
Al15–O1_7	1.7231(14)
Al15–O1_5	1.7268(14)
Al15–O1_6	1.735(3)
Al16–O1_4	1.683(13)
Al16–O1_33	1.696(19)
Al16–O1_2	1.7173(14)
Al16–O1_3	1.7223(14)
Al16–O1_1	1.745(13)
Al16–O1_32	1.775(14)
Al2–C4_20	2.209(2)
Al2–C5_20	2.211(2)
Al2–C3_20	2.219(2)
Al2–C1_20	2.225(2)
Al2–C2_20	2.237(2)
Al3–C2_22	2.202(2)
Al3–C1_22	2.212(2)
Al3–C3_22	2.216(2)
Al3–C4_22	2.231(2)
Al3–C5_22	2.232(2)
Al4–C4_18	2.162(4)
Al4–C3_18	2.174(9)
Al4–C3_37	2.196(9)
Al4–C2_18	2.204(7)

Al4–C5_18	2.216(3)	C2_4–F1_4	1.329(8)
Al4–C1_18	2.232(3)	C2_4–F2_4	1.341(6)
Al4–C4_37	2.25(3)	C3_4–F4_4	1.324(10)
Al4–C5_37	2.34(2)	C3_4–F5_4	1.326(7)
Al4–C2_37	2.344(9)	C3_4–F6_4	1.354(8)
Al4–C1_37	2.447(9)	C4_4–F9_4	1.328(10)
Al5–C1_17	2.204(2)	C4_4–F7_4	1.338(5)
Al5–C5_17	2.216(2)	C4_4–F8_4	1.339(7)
Al5–C2_17	2.220(2)	O1_5–C1_5	1.351(2)
Al5–C4_17	2.222(2)	C1_5–C2_5	1.550(3)
Al5–C3_17	2.232(2)	C1_5–C4_5	1.553(3)
O1_1–C1_1	1.353(8)	C1_5–C3_5	1.556(3)
C1_1–C2_1	1.538(7)	C2_5–F1_5	1.329(3)
C1_1–C3_1	1.543(7)	C2_5–F3_5	1.333(3)
C1_1–C4_1	1.549(6)	C2_5–F2_5	1.336(2)
C2_1–F2_1	1.324(8)	C3_5–F4_5	1.314(3)
C2_1–F3_1	1.328(7)	C3_5–F5_5	1.334(3)
C2_1–F1_1	1.338(6)	C3_5–F6_5	1.338(2)
C3_1–F6_1	1.326(7)	C4_5–F7_5	1.326(3)
C3_1–F4_1	1.329(8)	C4_5–F9_5	1.330(2)
C3_1–F5_1	1.332(5)	C4_5–F8_5	1.339(2)
C4_1–F9_1	1.258(7)	O1_6–C1_6	1.353(3)
C4_1–F7_1	1.333(7)	C1_6–C4_6	1.551(4)
C4_1–F8_1	1.338(7)	C1_6–C3_6	1.553(4)
O1_2–C1_2	1.348(2)	C1_6–C2_6	1.557(4)
C1_2–C3_2	1.548(3)	C2_6–F3_6	1.311(4)
C1_2–C2_2	1.548(4)	C2_6–F2_6	1.328(3)
C1_2–C4_2	1.556(3)	C2_6–F1_6	1.332(3)
C2_2–F3_2	1.322(3)	C3_6–F4_6	1.315(4)
C2_2–F1_2	1.340(3)	C3_6–F6_6	1.334(3)
C2_2–F2_2	1.349(3)	C3_6–F5_6	1.343(5)
C3_2–F4_2	1.323(3)	C4_6–F9_6	1.324(5)
C3_2–F5_2	1.334(3)	C4_6–F8_6	1.330(4)
C3_2–F6_2	1.345(2)	C4_6–F7_6	1.338(3)
C4_2–F9_2	1.335(3)	O1_7–C1_7	1.347(2)
C4_2–F8_2	1.342(3)	C1_7–C2_7	1.551(3)
C4_2–F7_2	1.343(4)	C1_7–C3_7	1.552(3)
O1_3–C1_3	1.349(2)	C1_7–C4_7	1.561(3)
C1_3–C3_3	1.551(3)	C2_7–F3_7	1.320(2)
C1_3–C2_3	1.552(3)	C2_7–F1_7	1.334(3)
C1_3–C4_3	1.557(3)	C2_7–F2_7	1.349(2)
C2_3–F3_3	1.313(3)	C3_7–F4_7	1.322(3)
C2_3–F1_3	1.330(3)	C3_7–F5_7	1.338(3)
C2_3–F2_3	1.340(2)	C3_7–F6_7	1.342(3)
C3_3–F4_3	1.313(3)	C4_7–F9_7	1.323(3)
C3_3–F6_3	1.332(3)	C4_7–F7_7	1.334(3)
C3_3–F5_3	1.340(3)	C4_7–F8_7	1.336(2)
C4_3–F9_3	1.327(3)	O1_8–C1_8	1.347(2)
C4_3–F7_3	1.333(3)	C1_8–C4_8	1.549(3)
C4_3–F8_3	1.335(3)	C1_8–C2_8	1.551(3)
O1_4–C1_4	1.355(9)	C1_8–C3_8	1.561(3)
C1_4–C4_4	1.549(8)	C2_8–F3_8	1.325(3)
C1_4–C3_4	1.558(8)	C2_8–F1_8	1.334(3)
C1_4–C2_4	1.560(8)	C2_8–F2_8	1.339(3)
C2_4–F3_4	1.325(9)	C3_8–F4_8	1.328(3)

C3_8–F6_8	1.330(3)	C4_12–F7_12	1.333(5)
C3_8–F5_8	1.339(3)	C4_12–F8_12	1.333(3)
C4_8–F7_8	1.330(3)	O1_13–C1_13	1.348(2)
C4_8–F9_8	1.333(2)	C1_13–C4_13	1.550(3)
C4_8–F8_8	1.338(3)	C1_13–C3_13	1.551(3)
O1_9–C1_9	1.344(3)	C1_13–C2_13	1.551(3)
C1_9–C2_9	1.547(3)	C2_13–F2_13	1.328(3)
C1_9–C3_9	1.553(3)	C2_13–F3_13	1.332(3)
C1_9–C4_9	1.553(3)	C2_13–F1_13	1.341(3)
C2_9–F1_9	1.330(3)	C3_13–F4_13	1.321(3)
C2_9–F3_9	1.336(3)	C3_13–F5_13	1.333(3)
C2_9–F2_9	1.336(3)	C3_13–F6_13	1.340(3)
C3_9–F5_9	1.324(3)	C4_13–F9_13	1.317(3)
C3_9–F4_9	1.330(3)	C4_13–F7_13	1.339(3)
C3_9–F6_9	1.349(3)	C4_13–F8_13	1.342(2)
C4_9–F9_9	1.315(3)	O1_14–C1_14	1.350(3)
C4_9–F7_9	1.326(3)	C1_14–C4_14	1.552(3)
C4_9–F8_9	1.348(3)	C1_14–C3_14	1.556(3)
O1_10–C1_10	1.356(5)	C1_14–C2_14	1.561(3)
C1_10–C2_10	1.536(5)	C2_14–F3_14	1.325(3)
C1_10–C3_10	1.550(5)	C2_14–F1_14	1.332(3)
C1_10–C4_10	1.554(4)	C2_14–F2_14	1.338(3)
C2_10–F1_10	1.311(5)	C3_14–F4_14	1.322(3)
C2_10–F3_10	1.336(4)	C3_14–F5_14	1.335(3)
C2_10–F2_10	1.345(5)	C3_14–F6_14	1.337(3)
C3_10–F4_10	1.305(6)	C4_14–F9_14	1.321(3)
C3_10–F5_10	1.316(5)	C4_14–F8_14	1.333(3)
C3_10–F6_10	1.348(4)	C4_14–F7_14	1.338(3)
C4_10–F9_10	1.315(4)	O1_15–C1_15	1.351(2)
C4_10–F7_10	1.326(4)	C1_15–C4_15	1.536(3)
C4_10–F8_10	1.344(3)	C1_15–C3_15	1.541(3)
O1_11–C1_11	1.349(4)	C1_15–C2_15	1.559(3)
C1_11–C3_11	1.548(4)	C2_15–F3_15	1.307(3)
C1_11–C4_11	1.552(4)	C2_15–F2_15	1.346(3)
C1_11–C2_11	1.563(4)	C2_15–F1_15	1.351(3)
C2_11–F2_11	1.318(3)	C3_15–F4_15	1.335(3)
C2_11–F3_11	1.325(3)	C3_15–F6_15	1.341(3)
C2_11–F1_11	1.342(3)	C3_15–F5_15	1.344(4)
C3_11–F5_11	1.321(3)	C4_15–F9_15	1.325(3)
C3_11–F4_11	1.335(3)	C4_15–F8_15	1.343(3)
C3_11–F6_11	1.341(3)	C4_15–F7_15	1.361(4)
C4_11–F9_11	1.310(4)	O1_16–C1_16	1.345(3)
C4_11–F8_11	1.342(3)	C1_16–C2_16	1.548(4)
C4_11–F7_11	1.347(3)	C1_16–C4_16	1.552(4)
O1_12–C1_12	1.354(5)	C1_16–C3_16	1.560(4)
C1_12–C2_12	1.549(5)	C2_16–F3_16	1.323(4)
C1_12–C3_12	1.552(4)	C2_16–F1_16	1.329(4)
C1_12–C4_12	1.560(4)	C2_16–F2_16	1.341(4)
C2_12–F3_12	1.317(5)	C3_16–F5_16	1.314(4)
C2_12–F2_12	1.333(4)	C3_16–F4_16	1.336(4)
C2_12–F1_12	1.339(5)	C3_16–F6_16	1.346(3)
C3_12–F4_12	1.330(4)	C4_16–F9_16	1.325(4)
C3_12–F6_12	1.334(5)	C4_16–F7_16	1.328(4)
C3_12–F5_12	1.335(4)	C4_16–F8_16	1.345(3)
C4_12–F9_12	1.321(3)	C1_17–C5_17	1.421(3)

C1_17–C2_17	1.428(3)	C3_19–C8_19	1.502(3)
C1_17–C10_17	1.503(3)	C4_19–C5_19	1.420(3)
C2_17–C3_17	1.422(3)	C4_19–C7_19	1.505(3)
C2_17–C9_17	1.501(3)	C5_19–C6_19	1.499(3)
C3_17–C4_17	1.411(3)	C6_19–H6A_19	0.9800
C3_17–C8_17	1.510(3)	C6_19–H6B_19	0.9800
C4_17–C5_17	1.428(3)	C6_19–H6C_19	0.9800
C4_17–C7_17	1.507(3)	C7_19–H7A_19	0.9800
C5_17–C6_17	1.501(3)	C7_19–H7B_19	0.9800
C6_17–H6A_17	0.9800	C7_19–H7C_19	0.9800
C6_17–H6B_17	0.9800	C8_19–H8A_19	0.9800
C6_17–H6C_17	0.9800	C8_19–H8B_19	0.9800
C7_17–H7A_17	0.9800	C8_19–H8C_19	0.9800
C7_17–H7B_17	0.9800	C9_19–H9A_19	0.9800
C7_17–H7C_17	0.9800	C9_19–H9B_19	0.9800
C8_17–H8A_17	0.9800	C9_19–H9C_19	0.9800
C8_17–H8B_17	0.9800	C10_19–H10A_19	0.9800
C8_17–H8C_17	0.9800	C10_19–H10B_19	0.9800
C9_17–H9A_17	0.9800	C10_19–H10C_19	0.9800
C9_17–H9B_17	0.9800	C1_20–C5_20	1.415(4)
C9_17–H9C_17	0.9800	C1_20–C2_20	1.418(3)
C10_17–H10A_17	0.9800	C1_20–C10_20	1.505(4)
C10_17–H10B_17	0.9800	C2_20–C3_20	1.424(3)
C10_17–H10C_17	0.9800	C2_20–C9_20	1.501(4)
C1_18–C2_18	1.420(5)	C3_20–C4_20	1.420(3)
C1_18–C5_18	1.428(5)	C3_20–C8_20	1.501(3)
C1_18–C10_18	1.512(5)	C4_20–C5_20	1.427(4)
C2_18–C3_18	1.426(5)	C4_20–C7_20	1.501(4)
C2_18–C9_18	1.504(6)	C5_20–C6_20	1.508(4)
C3_18–C4_18	1.413(6)	C6_20–H6A_20	0.9800
C3_18–C8_18	1.511(5)	C6_20–H6B_20	0.9800
C4_18–C5_18	1.418(6)	C6_20–H6C_20	0.9800
C4_18–C7_18	1.508(5)	C7_20–H7A_20	0.9800
C5_18–C6_18	1.504(5)	C7_20–H7B_20	0.9800
C6_18–H6A_18	0.9800	C7_20–H7C_20	0.9800
C6_18–H6B_18	0.9800	C8_20–H8A_20	0.9800
C6_18–H6C_18	0.9800	C8_20–H8B_20	0.9800
C7_18–H7A_18	0.9800	C8_20–H8C_20	0.9800
C7_18–H7B_18	0.9800	C9_20–H9A_20	0.9800
C7_18–H7C_18	0.9800	C9_20–H9B_20	0.9800
C8_18–H8A_18	0.9800	C9_20–H9C_20	0.9800
C8_18–H8B_18	0.9800	C10_20–H10A_20	0.9800
C8_18–H8C_18	0.9800	C10_20–H10B_20	0.9800
C9_18–H9A_18	0.9800	C10_20–H10C_20	0.9800
C9_18–H9B_18	0.9800	C1_21–C5_21	1.416(3)
C9_18–H9C_18	0.9800	C1_21–C2_21	1.418(3)
C10_18–H10A_18	0.9800	C1_21–C10_21	1.506(3)
C10_18–H10B_18	0.9800	C2_21–C3_21	1.420(3)
C10_18–H10C_18	0.9800	C2_21–C9_21	1.503(3)
C1_19–C5_19	1.425(3)	C3_21–C4_21	1.411(3)
C1_19–C2_19	1.431(3)	C3_21–C8_21	1.503(3)
C1_19–C10_19	1.501(3)	C4_21–C5_21	1.416(3)
C2_19–C3_19	1.425(3)	C4_21–C7_21	1.504(3)
C2_19–C9_19	1.499(3)	C5_21–C6_21	1.504(3)
C3_19–C4_19	1.417(3)	C6_21–H6A_21	0.9800

C6_21–H6B_21	0.9800	C8_23–H8A_23	0.9800
C6_21–H6C_21	0.9800	C8_23–H8B_23	0.9800
C7_21–H7A_21	0.9800	C8_23–H8C_23	0.9800
C7_21–H7B_21	0.9800	C9_23–H9A_23	0.9800
C7_21–H7C_21	0.9800	C9_23–H9B_23	0.9800
C8_21–H8A_21	0.9800	C9_23–H9C_23	0.9800
C8_21–H8B_21	0.9800	C10_23–H10A_23	0.9800
C8_21–H8C_21	0.9800	C10_23–H10B_23	0.9800
C9_21–H9A_21	0.9800	C10_23–H10C_23	0.9800
C9_21–H9B_21	0.9800	C1_24–C5_24	1.420(3)
C9_21–H9C_21	0.9800	C1_24–C2_24	1.423(3)
C10_21–H10A_21	0.9800	C1_24–C10_24	1.503(3)
C10_21–H10B_21	0.9800	C2_24–C3_24	1.419(3)
C10_21–H10C_21	0.9800	C2_24–C9_24	1.511(3)
C1_22–C2_22	1.420(3)	C3_24–C4_24	1.426(3)
C1_22–C5_22	1.432(3)	C3_24–C8_24	1.503(3)
C1_22–C10_22	1.500(3)	C4_24–C5_24	1.412(3)
C2_22–C3_22	1.425(3)	C4_24–C7_24	1.509(3)
C2_22–C9_22	1.502(3)	C5_24–C6_24	1.504(3)
C3_22–C4_22	1.414(3)	C6_24–H6A_24	0.9800
C3_22–C8_22	1.504(3)	C6_24–H6B_24	0.9800
C4_22–C5_22	1.413(3)	C6_24–H6C_24	0.9800
C4_22–C7_22	1.510(3)	C7_24–H7A_24	0.9800
C5_22–C6_22	1.503(3)	C7_24–H7B_24	0.9800
C6_22–H6A_22	0.9800	C7_24–H7C_24	0.9800
C6_22–H6B_22	0.9800	C8_24–H8A_24	0.9800
C6_22–H6C_22	0.9800	C8_24–H8B_24	0.9800
C7_22–H7A_22	0.9800	C8_24–H8C_24	0.9800
C7_22–H7B_22	0.9800	C9_24–H9A_24	0.9800
C7_22–H7C_22	0.9800	C9_24–H9B_24	0.9800
C8_22–H8A_22	0.9800	C9_24–H9C_24	0.9800
C8_22–H8B_22	0.9800	C10_24–H10A_24	0.9800
C8_22–H8C_22	0.9800	C10_24–H10B_24	0.9800
C9_22–H9A_22	0.9800	C10_24–H10C_24	0.9800
C9_22–H9B_22	0.9800	C1_25–C2_25	1.424(3)
C9_22–H9C_22	0.9800	C1_25–C5_25	1.425(3)
C10_22–H10A_22	0.9800	C1_25–C10_25	1.498(3)
C10_22–H10B_22	0.9800	C2_25–C3_25	1.427(3)
C10_22–H10C_22	0.9800	C2_25–C9_25	1.501(3)
C1_23–C2_23	1.417(3)	C3_25–C4_25	1.426(3)
C1_23–C5_23	1.425(4)	C3_25–C8_25	1.503(3)
C1_23–C10_23	1.504(4)	C4_25–C5_25	1.426(3)
C2_23–C3_23	1.421(4)	C4_25–C7_25	1.500(3)
C2_23–C9_23	1.512(4)	C5_25–C6_25	1.500(3)
C3_23–C4_23	1.443(4)	C6_25–H6A_25	0.9800
C3_23–C8_23	1.497(4)	C6_25–H6B_25	0.9800
C4_23–C5_23	1.421(4)	C6_25–H6C_25	0.9800
C4_23–C7_23	1.504(4)	C7_25–H7A_25	0.9800
C5_23–C6_23	1.504(4)	C7_25–H7B_25	0.9800
C6_23–H6A_23	0.9800	C7_25–H7C_25	0.9800
C6_23–H6B_23	0.9800	C8_25–H8A_25	0.9800
C6_23–H6C_23	0.9800	C8_25–H8B_25	0.9800
C7_23–H7A_23	0.9800	C8_25–H8C_25	0.9800
C7_23–H7B_23	0.9800	C9_25–H9A_25	0.9800
C7_23–H7C_23	0.9800	C9_25–H9B_25	0.9800

C9_25–H9C_25	0.9800	C1_29–C2_29	1.545(10)
C10_25–H10A_25	0.9800	C1_29–C4_29	1.547(9)
C10_25–H10B_25	0.9800	C1_29–C3_29	1.566(9)
C10_25–H10C_25	0.9800	C2_29–F2_29	1.332(10)
C1_26–C2_26	1.409(6)	C2_29–F3_29	1.350(10)
C1_26–C5_26	1.426(6)	C2_29–F1_29	1.357(9)
C1_26–C10_26	1.513(7)	C3_29–F5_29	1.321(8)
C2_26–C3_26	1.425(7)	C3_29–F6_29	1.332(8)
C2_26–C9_26	1.508(7)	C3_29–F4_29	1.339(8)
C3_26–C4_26	1.423(7)	C4_29–F7_29	1.314(10)
C3_26–C8_26	1.503(7)	C4_29–F9_29	1.324(9)
C4_26–C5_26	1.413(7)	C4_29–F8_29	1.343(10)
C4_26–C7_26	1.503(7)	O1_30–C1_30	1.358(12)
C5_26–C6_26	1.493(6)	C1_30–C4_30	1.548(11)
C6_26–H6A_26	0.9800	C1_30–C2_30	1.548(11)
C6_26–H6B_26	0.9800	C1_30–C3_30	1.560(11)
C6_26–H6C_26	0.9800	C2_30–F2_30	1.340(12)
C7_26–H7A_26	0.9800	C2_30–F1_30	1.348(12)
C7_26–H7B_26	0.9800	C2_30–F3_30	1.351(12)
C7_26–H7C_26	0.9800	C3_30–F4_30	1.321(11)
C8_26–H8A_26	0.9800	C3_30–F6_30	1.335(11)
C8_26–H8B_26	0.9800	C3_30–F5_30	1.341(11)
C8_26–H8C_26	0.9800	C4_30–F7_30	1.312(11)
C9_26–H9A_26	0.9800	C4_30–F9_30	1.319(11)
C9_26–H9B_26	0.9800	C4_30–F8_30	1.344(12)
C9_26–H9C_26	0.9800	O1_31–C1_31	1.345(11)
C10_26–H10A_26	0.9800	C1_31–C3_31	1.556(10)
C10_26–H10B_26	0.9800	C1_31–C2_31	1.560(10)
C10_26–H10C_26	0.9800	C1_31–C4_31	1.575(10)
C1_27–C2_27	1.423(3)	C2_31–F2_31	1.326(9)
C1_27–C5_27	1.430(3)	C2_31–F3_31	1.347(10)
C1_27–C10_27	1.502(3)	C2_31–F1_31	1.353(9)
C2_27–C3_27	1.421(3)	C3_31–F5_31	1.292(10)
C2_27–C9_27	1.501(3)	C3_31–F4_31	1.313(9)
C3_27–C4_27	1.426(3)	C3_31–F6_31	1.350(8)
C3_27–C8_27	1.501(3)	C4_31–F9_31	1.306(10)
C4_27–C5_27	1.416(3)	C4_31–F7_31	1.315(11)
C4_27–C7_27	1.504(3)	C4_31–F8_31	1.340(10)
C5_27–C6_27	1.500(3)	O1_32–C1_32	1.352(10)
C6_27–H6A_27	0.9800	C1_32–C3_32	1.544(9)
C6_27–H6B_27	0.9800	C1_32–C4_32	1.549(9)
C6_27–H6C_27	0.9800	C1_32–C2_32	1.553(9)
C7_27–H7A_27	0.9800	C2_32–F3_32	1.317(10)
C7_27–H7B_27	0.9800	C2_32–F1_32	1.321(8)
C7_27–H7C_27	0.9800	C2_32–F2_32	1.337(7)
C8_27–H8A_27	0.9800	C3_32–F4_32	1.327(11)
C8_27–H8B_27	0.9800	C3_32–F5_32	1.332(7)
C8_27–H8C_27	0.9800	C3_32–F6_32	1.343(8)
C9_27–H9A_27	0.9800	C4_32–F9_32	1.332(11)
C9_27–H9B_27	0.9800	C4_32–F7_32	1.336(7)
C9_27–H9C_27	0.9800	C4_32–F8_32	1.338(9)
C10_27–H10A_27	0.9800	O1_33–C1_33	1.355(11)
C10_27–H10B_27	0.9800	C1_33–C2_33	1.535(10)
C10_27–H10C_27	0.9800	C1_33–C3_33	1.545(10)
O1_29–C1_29	1.349(11)	C1_33–C4_33	1.555(10)

C2_33–F1_33	1.327(9)	C4_37–C5_37	1.418(12)
C2_33–F3_33	1.331(11)	C4_37–C7_37	1.510(12)
C2_33–F2_33	1.357(9)	C5_37–C6_37	1.522(11)
C3_33–F6_33	1.325(11)	C6_37–H6A_37	0.9800
C3_33–F4_33	1.328(10)	C6_37–H6B_37	0.9800
C3_33–F5_33	1.334(9)	C6_37–H6C_37	0.9800
C4_33–F9_33	1.274(10)	C7_37–H7A_37	0.9800
C4_33–F7_33	1.306(8)	C7_37–H7B_37	0.9800
C4_33–F8_33	1.342(10)	C7_37–H7C_37	0.9800
O1_34–C1_34	1.363(13)	C8_37–H8A_37	0.9800
C1_34–C4_34	1.536(12)	C8_37–H8B_37	0.9800
C1_34–C2_34	1.551(12)	C8_37–H8C_37	0.9800
C1_34–C3_34	1.553(12)	C9_37–H9A_37	0.9800
C2_34–F2_34	1.321(13)	C9_37–H9B_37	0.9800
C2_34–F1_34	1.323(13)	C9_37–H9C_37	0.9800
C2_34–F3_34	1.326(13)	C10_37–H10A_37	0.9800
C3_34–F6_34	1.326(13)	C10_37–H10B_37	0.9800
C3_34–F5_34	1.327(13)	C10_37–H10C_37	0.9800
C3_34–F4_34	1.328(13)	O1_39–C1_39	1.359(13)
C4_34–F9_34	1.333(12)	C1_39–C4_39	1.544(12)
C4_34–F8_34	1.334(12)	C1_39–C2_39	1.547(12)
C4_34–F7_34	1.341(12)	C1_39–C3_39	1.551(12)
O1_35–C1_35	1.365(12)	C2_39–F1_39	1.325(12)
C1_35–C4_35	1.538(12)	C2_39–F3_39	1.328(13)
C1_35–C3_35	1.548(12)	C2_39–F2_39	1.342(13)
C1_35–C2_35	1.552(12)	C3_39–F4_39	1.311(13)
C2_35–F1_35	1.333(12)	C3_39–F6_39	1.328(12)
C2_35–F2_35	1.333(12)	C3_39–F5_39	1.339(12)
C2_35–F3_35	1.337(12)	C4_39–F9_39	1.290(12)
C3_35–F6_35	1.325(12)	C4_39–F8_39	1.335(12)
C3_35–F4_35	1.334(13)	C4_39–F7_39	1.344(13)
C3_35–F5_35	1.336(13)	C1_41–C5_41	1.419(6)
C4_35–F9_35	1.329(13)	C1_41–C2_41	1.425(6)
C4_35–F7_35	1.333(13)	C1_41–C10_41	1.500(6)
C4_35–F8_35	1.337(13)	C2_41–C3_41	1.414(7)
O1_36–C1_36	1.353(13)	C2_41–C9_41	1.516(7)
C1_36–C4_36	1.547(12)	C3_41–C4_41	1.432(8)
C1_36–C2_36	1.557(12)	C3_41–C8_41	1.505(6)
C1_36–C3_36	1.561(12)	C4_41–C5_41	1.413(8)
C2_36–F2_36	1.340(12)	C4_41–C7_41	1.495(7)
C2_36–F1_36	1.341(12)	C5_41–C6_41	1.510(7)
C2_36–F3_36	1.342(12)	C6_41–H6A_41	0.9800
C3_36–F5_36	1.331(13)	C6_41–H6B_41	0.9800
C3_36–F6_36	1.335(12)	C6_41–H6C_41	0.9800
C3_36–F4_36	1.337(13)	C7_41–H7A_41	0.9800
C4_36–F9_36	1.329(13)	C7_41–H7B_41	0.9800
C4_36–F8_36	1.336(13)	C7_41–H7C_41	0.9800
C4_36–F7_36	1.337(13)	C8_41–H8A_41	0.9800
C1_37–C5_37	1.417(11)	C8_41–H8B_41	0.9800
C1_37–C2_37	1.419(10)	C8_41–H8C_41	0.9800
C1_37–C10_37	1.521(10)	C9_41–H9A_41	0.9800
C2_37–C3_37	1.411(10)	C9_41–H9B_41	0.9800
C2_37–C9_37	1.506(10)	C9_41–H9C_41	0.9800
C3_37–C4_37	1.431(12)	C10_41–H10A_41	0.9800
C3_37–C8_37	1.503(10)	C10_41–H10B_41	0.9800

C10_41–H10C_41	0.9800
C1_38–C5_38	1.412(8)
C1_38–C2_38	1.425(9)
C1_38–C10_38	1.504(9)
C2_38–C3_38	1.403(10)
C2_38–C9_38	1.493(9)
C3_38–C4_38	1.420(9)
C3_38–C8_38	1.495(9)
C4_38–C5_38	1.413(7)
C4_38–C7_38	1.520(9)
C5_38–C6_38	1.489(7)
C6_38–H6A_38	0.9800
C6_38–H6B_38	0.9800
C6_38–H6C_38	0.9800
C7_38–H7A_38	0.9800
C7_38–H7B_38	0.9800
C7_38–H7C_38	0.9800
C8_38–H8A_38	0.9800
C8_38–H8B_38	0.9800
C8_38–H8C_38	0.9800
C9_38–H9A_38	0.9800
C9_38–H9B_38	0.9800
C9_38–H9C_38	0.9800
C10_38–H10A_38	0.9800
C10_38–H10B_38	0.9800
C10_38–H10C_38	0.9800
O1_28–C1_28	1.356(13)
C1_28–C3_28	1.551(12)
C1_28–C4_28	1.552(12)
C1_28–C2_28	1.555(12)
C2_28–F2_28	1.326(12)
C2_28–F1_28	1.327(12)
C2_28–F3_28	1.343(12)
C3_28–F4_28	1.334(12)
C3_28–F6_28	1.341(12)
C3_28–F5_28	1.342(12)
C4_28–F8_28	1.324(13)
C4_28–F9_28	1.327(13)
C4_28–F7_28	1.342(13)
C1_40–C2_40	1.416(9)
C1_40–C5_40	1.420(9)
C1_40–C10_40	1.518(9)
C2_40–C3_40	1.424(9)
C2_40–C9_40	1.511(10)
C3_40–C4_40	1.420(10)
C3_40–C8_40	1.512(10)
C4_40–C5_40	1.423(10)
C4_40–C7_40	1.514(10)
C5_40–C6_40	1.495(10)
C6_40–H6A_40	0.9800
C6_40–H6B_40	0.9800
C6_40–H6C_40	0.9800
C7_40–H7A_40	0.9800
C7_40–H7B_40	0.9800
C7_40–H7C_40	0.9800
C8_40–H8A_40	0.9800
C8_40–H8B_40	0.9800
C8_40–H8C_40	0.9800
C9_40–H9A_40	0.9800
C9_40–H9B_40	0.9800
C9_40–H9C_40	0.9800
C10_40–H10A_40	0.9800
C10_40–H10B_40	0.9800
C10_40–H10C_40	0.9800
C1_42–C2_42	1.419(12)
C1_42–C5_42	1.423(12)
C1_42–C10_42	1.504(13)
C2_42–C3_42	1.414(12)
C2_42–C9_42	1.509(12)
C3_42–C4_42	1.417(12)
C3_42–C8_42	1.513(12)
C4_42–C5_42	1.416(12)
C4_42–C7_42	1.507(12)
C5_42–C6_42	1.494(12)
C6_42–H6A_42	0.9800
C6_42–H6B_42	0.9800
C6_42–H6C_42	0.9800
C7_42–H7A_42	0.9800
C7_42–H7B_42	0.9800
C7_42–H7C_42	0.9800
C8_42–H8A_42	0.9800
C8_42–H8B_42	0.9800
C8_42–H8C_42	0.9800
C9_42–H9A_42	0.9800
C9_42–H9B_42	0.9800
C9_42–H9C_42	0.9800
C10_42–H10A_42	0.9800
C10_42–H10B_42	0.9800
C10_42–H10C_42	0.9800

Atom–Atom–Atom	**Angle [°]**
Al2–Ga1–Al3	75.22(3)
Al2–Ga1–Al1	74.86(3)
Al3–Ga1–Al1	76.25(2)
Al4–Ga2–Al6	73.77(3)
Al4–Ga2–Al5	73.51(2)
Al6–Ga2–Al5	75.91(2)
Al7–Ga3–Al9	76.31(2)
Al7–Ga3–Al8	75.44(2)
Al9–Ga3–Al8	76.07(3)
Al11–Ga4–Al10	75.66(2)
Al11–Ga4–Al12	76.96(3)
Al10–Ga4–Al12	73.62(2)
C3_21–Al1–C2_21	37.47(8)
C3_21–Al1–C4_21	37.22(8)
C2_21–Al1–C4_21	62.30(8)
C3_21–Al1–C5_21	62.19(8)
C2_21–Al1–C5_21	62.15(8)
C4_21–Al1–C5_21	37.20(9)
C3_21–Al1–C1_21	62.30(8)

C2_21–Al1–C1_21	37.21(8)	C4_42–Al8–C2_42	61.5(5)
C4_21–Al1–C1_21	62.16(9)	C1_42–Al8–C2_42	36.7(4)
C5_21–Al1–C1_21	37.13(9)	C3_42–Al8–C2_42	35.6(4)
C3_21–Al1–Ga1	173.64(6)	C5_42–Al8–Ga3	127.5(5)
C2_21–Al1–Ga1	148.27(7)	C4_42–Al8–Ga3	140.2(5)
C4_21–Al1–Ga1	141.94(7)	C1_42–Al8–Ga3	136.0(5)
C5_21–Al1–Ga1	121.22(6)	C4_23–Al8–Ga3	166.62(10)
C1_21–Al1–Ga1	123.86(6)	C5_23–Al8–Ga3	133.67(10)
C2_19–Al6–C1_19	37.91(8)	C3_23–Al8–Ga3	155.07(9)
C2_19–Al6–C3_19	37.66(8)	C1_23–Al8–Ga3	117.04(8)
C1_19–Al6–C3_19	63.04(8)	C2_23–Al8–Ga3	126.25(8)
C2_19–Al6–C4_19	62.66(8)	C3_42–Al8–Ga3	162.6(3)
C1_19–Al6–C4_19	62.69(8)	C2_42–Al8–Ga3	157.6(4)
C3_19–Al6–C4_19	37.33(8)	C4_25–Al9–C5_25	37.72(7)
C2_19–Al6–C5_19	62.92(8)	C4_25–Al9–C3_25	37.70(8)
C1_19–Al6–C5_19	37.58(7)	C5_25–Al9–C3_25	62.92(8)
C3_19–Al6–C5_19	62.66(8)	C4_25–Al9–C1_25	62.84(7)
C4_19–Al6–C5_19	37.35(8)	C5_25–Al9–C1_25	37.58(7)
C2_19–Al6–Ga2	160.03(6)	C3_25–Al9–C1_25	62.63(7)
C1_19–Al6–Ga2	160.01(6)	C4_25–Al9–C2_25	62.85(7)
C3_19–Al6–Ga2	126.39(6)	C5_25–Al9–C2_25	62.78(8)
C4_19–Al6–Ga2	112.61(6)	C3_25–Al9–C2_25	37.47(7)
C5_19–Al6–Ga2	126.48(6)	C1_25–Al9–C2_25	37.38(8)
C2_24–Al7–C1_24	37.60(8)	C4_25–Al9–Ga3	159.08(6)
C2_24–Al7–C3_24	37.50(9)	C5_25–Al9–Ga3	127.75(6)
C1_24–Al7–C3_24	62.46(8)	C3_25–Al9–Ga3	162.78(6)
C2_24–Al7–C5_24	62.61(8)	C1_25–Al9–Ga3	116.01(6)
C1_24–Al7–C5_24	37.29(8)	C2_25–Al9–Ga3	130.43(6)
C3_24–Al7–C5_24	62.29(8)	C4_41–Al10–C3_41	39.1(2)
C2_24–Al7–C4_24	62.56(9)	C4_41–Al10–C5_41	38.4(2)
C1_24–Al7–C4_24	62.13(8)	C3_41–Al10–C5_41	65.1(2)
C3_24–Al7–C4_24	37.42(9)	C4_41–Al10–C2_41	63.8(2)
C5_24–Al7–C4_24	36.95(8)	C3_41–Al10–C2_41	38.04(18)
C2_24–Al7–Ga3	166.56(7)	C5_41–Al10–C2_41	64.0(2)
C1_24–Al7–Ga3	139.11(6)	C4_41–Al10–C1_41	63.5(2)
C3_24–Al7–Ga3	154.69(7)	C3_41–Al10–C1_41	64.08(16)
C5_24–Al7–Ga3	123.70(6)	C5_41–Al10–C1_41	38.02(18)
C4_24–Al7–Ga3	130.22(7)	C2_41–Al10–C1_41	37.95(15)
C5_42–Al8–C4_42	38.7(4)	C3_38–Al10–C2_38	36.5(3)
C5_42–Al8–C1_42	38.8(4)	C3_38–Al10–C4_38	36.8(2)
C4_42–Al8–C1_42	63.5(6)	C2_38–Al10–C4_38	60.3(3)
C4_23–Al8–C5_23	37.56(11)	C3_38–Al10–C1_38	61.1(3)
C4_23–Al8–C3_23	38.07(11)	C2_38–Al10–C1_38	36.3(3)
C5_23–Al8–C3_23	62.69(12)	C4_38–Al10–C1_38	60.2(3)
C4_23–Al8–C1_23	62.67(11)	C3_38–Al10–C5_38	60.2(2)
C5_23–Al8–C1_23	37.29(10)	C2_38–Al10–C5_38	59.2(3)
C3_23–Al8–C1_23	62.18(10)	C4_38–Al10–C5_38	35.71(19)
C4_23–Al8–C2_23	62.51(10)	C1_38–Al10–C5_38	35.3(2)
C5_23–Al8–C2_23	61.90(11)	C4_41–Al10–Ga4	129.00(15)
C3_23–Al8–C2_23	37.00(10)	C3_41–Al10–Ga4	119.85(13)
C1_23–Al8–C2_23	36.79(9)	C5_41–Al10–Ga4	155.85(15)
C5_42–Al8–C3_42	62.7(5)	C2_41–Al10–Ga4	135.96(14)
C4_42–Al8–C3_42	36.8(3)	C1_41–Al10–Ga4	165.69(14)
C1_42–Al8–C3_42	61.3(5)	C3_38–Al10–Ga4	157.9(3)
C5_42–Al8–C2_42	62.8(5)	C2_38–Al10–Ga4	165.3(3)

C4_38–Al10–Ga4	128.8(2)	O1_9–Al13–O1_11	107.63(15)
C1_38–Al10–Ga4	133.6(2)	O1_12–Al13–O1_11	108.2(2)
C5_38–Al10–Ga4	119.81(16)	O1_31–Al13–O1_29	105.2(7)
C2_27–Al11–C1_27	37.74(9)	O1_30–Al13–O1_29	107.2(8)
C2_27–Al11–C3_27	37.62(8)	O1_36–Al13–O1_29	110.0(9)
C1_27–Al11–C3_27	62.83(9)	O1_35–Al14–O1_34	105.7(9)
C2_27–Al11–C4_27	62.64(8)	O1_15–Al14–O1_14	107.50(8)
C1_27–Al11–C4_27	62.43(8)	O1_15–Al14–O1_16	113.38(11)
C3_27–Al11–C4_27	37.45(7)	O1_14–Al14–O1_16	107.24(11)
C2_27–Al11–C5_27	62.81(9)	O1_15–Al14–O1_13	108.12(7)
C1_27–Al11–C5_27	37.57(8)	O1_14–Al14–O1_13	112.06(8)
C3_27–Al11–C5_27	62.49(8)	O1_16–Al14–O1_13	108.62(8)
C4_27–Al11–C5_27	37.00(8)	O1_8–Al15–O1_7	111.57(7)
C2_27–Al11–Ga4	172.94(7)	O1_8–Al15–O1_5	108.51(7)
C1_27–Al11–Ga4	148.85(7)	O1_7–Al15–O1_5	107.41(7)
C3_27–Al11–Ga4	137.05(7)	O1_8–Al15–O1_6	107.79(13)
C4_27–Al11–Ga4	116.10(6)	O1_7–Al15–O1_6	107.54(11)
C5_27–Al11–Ga4	120.89(7)	O1_5–Al15–O1_6	114.07(14)
C4_40–Al12–C5_40	37.8(4)	O1_4–Al16–O1_2	114.6(7)
C5_26–Al12–C4_26	37.3(3)	O1_4–Al16–O1_3	107.4(7)
C5_26–Al12–C1_26	37.6(2)	O1_2–Al16–O1_3	107.46(7)
C4_26–Al12–C1_26	62.5(3)	O1_4–Al16–O1_1	110.1(8)
C5_26–Al12–C3_26	62.4(3)	O1_2–Al16–O1_1	105.6(6)
C4_26–Al12–C3_26	37.4(2)	O1_3–Al16–O1_1	111.7(6)
C1_26–Al12–C3_26	62.4(3)	O1_33–Al16–O1_32	102.7(11)
C5_26–Al12–C2_26	62.2(3)	C4_20–Al2–C5_20	37.67(10)
C4_26–Al12–C2_26	62.4(3)	C4_20–Al2–C3_20	37.41(8)
C1_26–Al12–C2_26	37.0(2)	C5_20–Al2–C3_20	62.26(8)
C3_26–Al12–C2_26	37.4(2)	C4_20–Al2–C1_20	62.60(11)
C4_40–Al12–C1_40	62.1(6)	C5_20–Al2–C1_20	37.20(12)
C5_40–Al12–C1_40	37.4(3)	C3_20–Al2–C1_20	62.00(8)
C4_40–Al12–C3_40	37.2(4)	C4_20–Al2–C2_20	62.68(9)
C5_40–Al12–C3_40	62.4(5)	C5_20–Al2–C2_20	62.24(10)
C1_40–Al12–C3_40	61.2(4)	C3_20–Al2–C2_20	37.27(8)
C4_40–Al12–C2_40	62.1(6)	C1_20–Al2–C2_20	37.05(9)
C5_40–Al12–C2_40	62.5(4)	C4_20–Al2–Ga1	158.16(7)
C1_40–Al12–C2_40	36.7(3)	C5_20–Al2–Ga1	128.58(7)
C3_40–Al12–C2_40	36.7(3)	C3_20–Al2–Ga1	164.36(6)
C4_40–Al12–Ga4	160.6(3)	C1_20–Al2–Ga1	118.23(8)
C5_40–Al12–Ga4	126.3(4)	C2_20–Al2–Ga1	132.75(7)
C5_26–Al12–Ga4	123.6(2)	C2_22–Al3–C1_22	37.54(8)
C4_26–Al12–Ga4	154.4(2)	C2_22–Al3–C3_22	37.62(8)
C1_26–Al12–Ga4	114.00(19)	C1_22–Al3–C3_22	62.40(8)
C3_26–Al12–Ga4	166.7(2)	C2_22–Al3–C4_22	62.68(8)
C2_26–Al12–Ga4	131.8(2)	C1_22–Al3–C4_22	62.45(9)
C1_40–Al12–Ga4	112.9(3)	C3_22–Al3–C4_22	37.08(8)
C3_40–Al12–Ga4	159.7(3)	C2_22–Al3–C5_22	62.63(8)
C2_40–Al12–Ga4	126.5(3)	C1_22–Al3–C5_22	37.58(9)
O1_31–Al13–O1_30	123.5(9)	C3_22–Al3–C5_22	61.84(9)
O1_31–Al13–O1_36	122.0(8)	C4_22–Al3–C5_22	36.91(9)
O1_30–Al13–O1_36	87.6(9)	C2_22–Al3–Ga1	163.78(7)
O1_10–Al13–O1_9	107.4(2)	C1_22–Al3–Ga1	158.60(7)
O1_10–Al13–O1_12	110.8(2)	C3_22–Al3–Ga1	134.17(6)
O1_9–Al13–O1_12	111.66(15)	C4_22–Al3–Ga1	120.28(6)
O1_10–Al13–O1_11	111.1(3)	C5_22–Al3–Ga1	130.43(7)

C4_18–Al4–C3_18	38.02(17)	F2_1–C2_1–C1_1	114.8(8)
C4_18–Al4–C2_18	63.38(18)	F3_1–C2_1–C1_1	110.0(5)
C3_18–Al4–C2_18	38.01(18)	F1_1–C2_1–C1_1	110.8(5)
C4_18–Al4–C5_18	37.78(15)	F6_1–C3_1–F4_1	108.0(7)
C3_18–Al4–C5_18	63.13(18)	F6_1–C3_1–F5_1	106.3(5)
C2_18–Al4–C5_18	62.73(17)	F4_1–C3_1–F5_1	107.0(5)
C4_18–Al4–C1_18	63.08(14)	F6_1–C3_1–C1_1	113.4(6)
C3_18–Al4–C1_18	63.03(18)	F4_1–C3_1–C1_1	111.0(6)
C2_18–Al4–C1_18	37.32(14)	F5_1–C3_1–C1_1	110.8(4)
C5_18–Al4–C1_18	37.46(13)	F9_1–C4_1–F7_1	100.9(5)
C3_37–Al4–C4_37	37.5(4)	F9_1–C4_1–F8_1	110.0(6)
C3_37–Al4–C5_37	61.2(5)	F7_1–C4_1–F8_1	106.9(5)
C4_37–Al4–C5_37	35.9(4)	F9_1–C4_1–C1_1	114.2(6)
C3_37–Al4–C2_37	36.0(3)	F7_1–C4_1–C1_1	111.1(4)
C4_37–Al4–C2_37	59.7(5)	F8_1–C4_1–C1_1	112.9(5)
C5_37–Al4–C2_37	58.8(4)	C1_2–O1_2–Al16	146.01(13)
C3_37–Al4–C1_37	59.0(3)	O1_2–C1_2–C3_2	106.90(16)
C4_37–Al4–C1_37	58.0(5)	O1_2–C1_2–C2_2	110.92(19)
C5_37–Al4–C1_37	34.3(3)	C3_2–C1_2–C2_2	109.65(18)
C2_37–Al4–C1_37	34.4(2)	O1_2–C1_2–C4_2	110.99(18)
C4_18–Al4–Ga2	157.63(14)	C3_2–C1_2–C4_2	109.9(2)
C3_18–Al4–Ga2	163.40(14)	C2_2–C1_2–C4_2	108.5(2)
C3_37–Al4–Ga2	128.5(3)	F3_2–C2_2–F1_2	108.2(2)
C2_18–Al4–Ga2	129.54(15)	F3_2–C2_2–F2_2	106.8(2)
C5_18–Al4–Ga2	125.90(12)	F1_2–C2_2–F2_2	108.0(2)
C1_18–Al4–Ga2	114.29(10)	F3_2–C2_2–C1_2	110.7(2)
C4_37–Al4–Ga2	135.8(4)	F1_2–C2_2–C1_2	110.9(2)
C5_37–Al4–Ga2	157.0(3)	F2_2–C2_2–C1_2	111.9(2)
C2_37–Al4–Ga2	142.9(3)	F4_2–C3_2–F5_2	108.84(18)
C1_37–Al4–Ga2	166.0(2)	F4_2–C3_2–F6_2	106.9(2)
C1_17–Al5–C5_17	37.50(8)	F5_2–C3_2–F6_2	107.85(18)
C1_17–Al5–C2_17	37.65(8)	F4_2–C3_2–C1_2	110.33(17)
C5_17–Al5–C2_17	62.59(8)	F5_2–C3_2–C1_2	110.57(19)
C1_17–Al5–C4_17	62.60(8)	F6_2–C3_2–C1_2	112.25(18)
C5_17–Al5–C4_17	37.54(9)	F9_2–C4_2–F8_2	106.8(2)
C2_17–Al5–C4_17	62.20(8)	F9_2–C4_2–F7_2	108.2(2)
C1_17–Al5–C3_17	62.55(8)	F8_2–C4_2–F7_2	107.9(2)
C5_17–Al5–C3_17	62.34(9)	F9_2–C4_2–C1_2	110.4(2)
C2_17–Al5–C3_17	37.25(8)	F8_2–C4_2–C1_2	112.4(2)
C4_17–Al5–C3_17	36.95(8)	F7_2–C4_2–C1_2	111.0(2)
C1_17–Al5–Ga2	152.43(6)	C1_3–O1_3–Al16	148.67(13)
C5_17–Al5–Ga2	125.03(6)	O1_3–C1_3–C3_3	109.12(16)
C2_17–Al5–Ga2	169.92(6)	O1_3–C1_3–C2_3	107.98(16)
C4_17–Al5–Ga2	118.81(7)	C3_3–C1_3–C2_3	109.52(17)
C3_17–Al5–Ga2	137.15(6)	O1_3–C1_3–C4_3	112.13(16)
C1_1–O1_1–Al16	145.0(13)	C3_3–C1_3–C4_3	108.90(17)
O1_1–C1_1–C2_1	112.2(9)	C2_3–C1_3–C4_3	109.15(17)
O1_1–C1_1–C3_1	107.4(9)	F3_3–C2_3–F1_3	107.97(18)
C2_1–C1_1–C3_1	109.0(5)	F3_3–C2_3–F2_3	107.89(19)
O1_1–C1_1–C4_1	110.2(9)	F1_3–C2_3–F2_3	107.07(18)
C2_1–C1_1–C4_1	109.3(5)	F3_3–C2_3–C1_3	111.14(18)
C3_1–C1_1–C4_1	108.6(5)	F1_3–C2_3–C1_3	110.02(18)
F2_1–C2_1–F3_1	109.5(9)	F2_3–C2_3–C1_3	112.56(17)
F2_1–C2_1–F1_1	104.4(7)	F4_3–C3_3–F6_3	108.85(18)
F3_1–C2_1–F1_1	107.0(5)	F4_3–C3_3–F5_3	107.6(2)

F6_3–C3_3–F5_3	107.21(18)	F7_5–C4_5–F8_5	107.74(17)
F4_3–C3_3–C1_3	110.43(18)	F9_5–C4_5–F8_5	107.12(17)
F6_3–C3_3–C1_3	112.47(18)	F7_5–C4_5–C1_5	111.29(17)
F5_3–C3_3–C1_3	110.12(17)	F9_5–C4_5–C1_5	110.74(16)
F9_3–C4_3–F7_3	107.2(2)	F8_5–C4_5–C1_5	112.49(17)
F9_3–C4_3–F8_3	108.0(2)	C1_6–O1_6–Al15	146.3(2)
F7_3–C4_3–F8_3	107.21(19)	O1_6–C1_6–C4_6	111.9(3)
F9_3–C4_3–C1_3	110.49(18)	O1_6–C1_6–C3_6	110.7(2)
F7_3–C4_3–C1_3	111.27(19)	C4_6–C1_6–C3_6	109.5(2)
F8_3–C4_3–C1_3	112.47(19)	O1_6–C1_6–C2_6	106.6(2)
C1_4–O1_4–Al16	150.6(14)	C4_6–C1_6–C2_6	109.1(2)
O1_4–C1_4–C4_4	109.9(10)	C3_6–C1_6–C2_6	108.9(2)
O1_4–C1_4–C3_4	110.2(10)	F3_6–C2_6–F2_6	108.4(3)
C4_4–C1_4–C3_4	108.9(5)	F3_6–C2_6–F1_6	105.4(3)
O1_4–C1_4–C2_4	110.2(9)	F2_6–C2_6–F1_6	107.3(2)
C4_4–C1_4–C2_4	108.6(5)	F3_6–C2_6–C1_6	111.7(2)
C3_4–C1_4–C2_4	108.9(5)	F2_6–C2_6–C1_6	113.2(2)
F3_4–C2_4–F1_4	107.6(7)	F1_6–C2_6–C1_6	110.4(2)
F3_4–C2_4–F2_4	107.2(7)	F4_6–C3_6–F6_6	108.8(3)
F1_4–C2_4–F2_4	107.7(5)	F4_6–C3_6–F5_6	106.7(3)
F3_4–C2_4–C1_4	110.5(6)	F6_6–C3_6–F5_6	108.5(3)
F1_4–C2_4–C1_4	111.1(5)	F4_6–C3_6–C1_6	110.3(3)
F2_4–C2_4–C1_4	112.6(5)	F6_6–C3_6–C1_6	112.3(2)
F4_4–C3_4–F5_4	107.1(7)	F5_6–C3_6–C1_6	110.1(3)
F4_4–C3_4–F6_4	106.2(9)	F9_6–C4_6–F8_6	108.3(3)
F5_4–C3_4–F6_4	108.3(6)	F9_6–C4_6–F7_6	107.4(3)
F4_4–C3_4–C1_4	112.5(9)	F8_6–C4_6–F7_6	106.8(2)
F5_4–C3_4–C1_4	111.2(5)	F9_6–C4_6–C1_6	110.6(3)
F6_4–C3_4–C1_4	111.3(7)	F8_6–C4_6–C1_6	112.8(3)
F9_4–C4_4–F7_4	106.8(7)	F7_6–C4_6–C1_6	110.7(2)
F9_4–C4_4–F8_4	107.6(10)	C1_7–O1_7–Al15	150.49(13)
F7_4–C4_4–F8_4	107.4(4)	O1_7–C1_7–C2_7	111.81(16)
F9_4–C4_4–C1_4	110.7(9)	O1_7–C1_7–C3_7	110.06(17)
F7_4–C4_4–C1_4	111.2(4)	C2_7–C1_7–C3_7	109.30(16)
F8_4–C4_4–C1_4	112.8(5)	O1_7–C1_7–C4_7	107.14(16)
C1_5–O1_5–Al15	146.99(13)	C2_7–C1_7–C4_7	109.29(17)
O1_5–C1_5–C2_5	110.99(16)	C3_7–C1_7–C4_7	109.18(17)
O1_5–C1_5–C4_5	111.23(16)	F3_7–C2_7–F1_7	107.39(18)
C2_5–C1_5–C4_5	108.43(17)	F3_7–C2_7–F2_7	107.53(17)
O1_5–C1_5–C3_5	107.71(16)	F1_7–C2_7–F2_7	106.80(17)
C2_5–C1_5–C3_5	109.44(17)	F3_7–C2_7–C1_7	111.05(16)
C4_5–C1_5–C3_5	109.01(16)	F1_7–C2_7–C1_7	111.04(17)
F1_5–C2_5–F3_5	107.51(19)	F2_7–C2_7–C1_7	112.76(17)
F1_5–C2_5–F2_5	107.56(19)	F4_7–C3_7–F5_7	107.56(19)
F3_5–C2_5–F2_5	107.41(18)	F4_7–C3_7–F6_7	107.14(19)
F1_5–C2_5–C1_5	110.81(18)	F5_7–C3_7–F6_7	106.89(17)
F3_5–C2_5–C1_5	110.91(18)	F4_7–C3_7–C1_7	111.70(17)
F2_5–C2_5–C1_5	112.44(18)	F5_7–C3_7–C1_7	110.83(18)
F4_5–C3_5–F5_5	107.33(18)	F6_7–C3_7–C1_7	112.45(19)
F4_5–C3_5–F6_5	108.03(18)	F9_7–C4_7–F7_7	107.45(18)
F5_5–C3_5–F6_5	107.05(17)	F9_7–C4_7–F8_7	107.91(19)
F4_5–C3_5–C1_5	111.24(17)	F7_7–C4_7–F8_7	107.77(18)
F5_5–C3_5–C1_5	110.71(18)	F9_7–C4_7–C1_7	110.32(17)
F6_5–C3_5–C1_5	112.25(18)	F7_7–C4_7–C1_7	110.67(18)
F7_5–C4_5–F9_5	107.23(17)	F8_7–C4_7–C1_7	112.53(17)

C1_8–O1_8–Al15	148.13(13)	C2_10–C1_10–C4_10	109.0(3)
O1_8–C1_8–C4_8	111.27(16)	C3_10–C1_10–C4_10	109.0(3)
O1_8–C1_8–C2_8	110.25(16)	F1_10–C2_10–F3_10	107.0(4)
C4_8–C1_8–C2_8	109.72(18)	F1_10–C2_10–F2_10	107.1(4)
O1_8–C1_8–C3_8	107.01(17)	F3_10–C2_10–F2_10	107.7(4)
C4_8–C1_8–C3_8	109.16(16)	F1_10–C2_10–C1_10	111.8(3)
C2_8–C1_8–C3_8	109.38(17)	F3_10–C2_10–C1_10	110.1(3)
F3_8–C2_8–F1_8	107.91(19)	F2_10–C2_10–C1_10	112.8(4)
F3_8–C2_8–F2_8	107.69(19)	F4_10–C3_10–F5_10	106.1(4)
F1_8–C2_8–F2_8	107.42(18)	F4_10–C3_10–F6_10	107.4(5)
F3_8–C2_8–C1_8	110.53(18)	F5_10–C3_10–F6_10	107.3(4)
F1_8–C2_8–C1_8	110.73(18)	F4_10–C3_10–C1_10	111.7(4)
F2_8–C2_8–C1_8	112.38(19)	F5_10–C3_10–C1_10	111.7(4)
F4_8–C3_8–F6_8	107.76(18)	F6_10–C3_10–C1_10	112.3(3)
F4_8–C3_8–F5_8	107.08(19)	F9_10–C4_10–F7_10	107.5(3)
F6_8–C3_8–F5_8	107.51(18)	F9_10–C4_10–F8_10	108.3(3)
F4_8–C3_8–C1_8	111.02(18)	F7_10–C4_10–F8_10	107.3(2)
F6_8–C3_8–C1_8	112.75(19)	F9_10–C4_10–C1_10	110.7(2)
F5_8–C3_8–C1_8	110.48(17)	F7_10–C4_10–C1_10	111.1(3)
F7_8–C4_8–F9_8	107.11(18)	F8_10–C4_10–C1_10	111.9(2)
F7_8–C4_8–F8_8	108.06(18)	C1_11–O1_11–Al13	147.1(3)
F9_8–C4_8–F8_8	107.11(18)	O1_11–C1_11–C3_11	110.3(3)
F7_8–C4_8–C1_8	111.27(18)	O1_11–C1_11–C4_11	107.4(3)
F9_8–C4_8–C1_8	110.46(16)	C3_11–C1_11–C4_11	110.0(2)
F8_8–C4_8–C1_8	112.57(18)	O1_11–C1_11–C2_11	111.9(3)
C1_9–O1_9–Al13	148.53(18)	C3_11–C1_11–C2_11	108.4(2)
O1_9–C1_9–C2_9	111.2(2)	C4_11–C1_11–C2_11	108.8(2)
O1_9–C1_9–C3_9	107.0(2)	F2_11–C2_11–F3_11	108.3(2)
C2_9–C1_9–C3_9	109.2(2)	F2_11–C2_11–F1_11	107.1(2)
O1_9–C1_9–C4_9	111.3(2)	F3_11–C2_11–F1_11	106.8(2)
C2_9–C1_9–C4_9	108.7(2)	F2_11–C2_11–C1_11	113.3(2)
C3_9–C1_9–C4_9	109.3(2)	F3_11–C2_11–C1_11	110.4(2)
F1_9–C2_9–F3_9	107.8(2)	F1_11–C2_11–C1_11	110.7(2)
F1_9–C2_9–F2_9	107.7(2)	F5_11–C3_11–F4_11	107.5(2)
F3_9–C2_9–F2_9	107.4(2)	F5_11–C3_11–F6_11	107.1(2)
F1_9–C2_9–C1_9	111.5(2)	F4_11–C3_11–F6_11	106.5(2)
F3_9–C2_9–C1_9	110.1(2)	F5_11–C3_11–C1_11	111.0(2)
F2_9–C2_9–C1_9	112.2(2)	F4_11–C3_11–C1_11	111.2(2)
F5_9–C3_9–F4_9	107.7(3)	F6_11–C3_11–C1_11	113.3(2)
F5_9–C3_9–F6_9	108.0(2)	F9_11–C4_11–F8_11	107.9(2)
F4_9–C3_9–F6_9	106.6(2)	F9_11–C4_11–F7_11	107.9(3)
F5_9–C3_9–C1_9	111.0(2)	F8_11–C4_11–F7_11	105.9(2)
F4_9–C3_9–C1_9	111.0(2)	F9_11–C4_11–C1_11	111.3(3)
F6_9–C3_9–C1_9	112.3(2)	F8_11–C4_11–C1_11	112.3(2)
F9_9–C4_9–F7_9	107.6(2)	F7_11–C4_11–C1_11	111.3(2)
F9_9–C4_9–F8_9	107.3(2)	C1_12–O1_12–Al13	147.0(4)
F7_9–C4_9–F8_9	107.0(2)	O1_12–C1_12–C2_12	110.4(3)
F9_9–C4_9–C1_9	110.9(2)	O1_12–C1_12–C3_12	107.5(3)
F7_9–C4_9–C1_9	111.4(2)	C2_12–C1_12–C3_12	109.9(3)
F8_9–C4_9–C1_9	112.4(2)	O1_12–C1_12–C4_12	111.4(3)
C1_10–O1_10–Al13	144.9(4)	C2_12–C1_12–C4_12	109.2(3)
O1_10–C1_10–C2_10	107.0(4)	C3_12–C1_12–C4_12	108.4(2)
O1_10–C1_10–C3_10	111.3(4)	F3_12–C2_12–F2_12	107.6(4)
C2_10–C1_10–C3_10	109.2(3)	F3_12–C2_12–F1_12	108.4(3)
O1_10–C1_10–C4_10	111.3(3)	F2_12–C2_12–F1_12	107.1(3)

F3_12–C2_12–C1_12	110.4(3)	F5_14–C3_14–F6_14	106.3(2)
F2_12–C2_12–C1_12	113.0(3)	F4_14–C3_14–C1_14	110.5(2)
F1_12–C2_12–C1_12	110.2(3)	F5_14–C3_14–C1_14	110.6(2)
F4_12–C3_12–F6_12	108.4(4)	F6_14–C3_14–C1_14	112.8(2)
F4_12–C3_12–F5_12	106.8(3)	F9_14–C4_14–F8_14	108.3(2)
F6_12–C3_12–F5_12	106.3(3)	F9_14–C4_14–F7_14	107.1(2)
F4_12–C3_12–C1_12	111.5(3)	F8_14–C4_14–F7_14	107.1(2)
F6_12–C3_12–C1_12	113.0(4)	F9_14–C4_14–C1_14	110.9(2)
F5_12–C3_12–C1_12	110.5(3)	F8_14–C4_14–C1_14	113.0(2)
F9_12–C4_12–F7_12	107.0(3)	F7_14–C4_14–C1_14	110.1(2)
F9_12–C4_12–F8_12	107.8(2)	C1_15–O1_15–Al14	149.24(14)
F7_12–C4_12–F8_12	107.5(3)	O1_15–C1_15–C4_15	109.33(18)
F9_12–C4_12–C1_12	110.2(2)	O1_15–C1_15–C3_15	112.36(17)
F7_12–C4_12–C1_12	111.5(3)	C4_15–C1_15–C3_15	109.4(2)
F8_12–C4_12–C1_12	112.6(3)	O1_15–C1_15–C2_15	108.46(18)
C1_13–O1_13–Al14	146.80(13)	C4_15–C1_15–C2_15	108.5(2)
O1_13–C1_13–C4_13	107.63(16)	C3_15–C1_15–C2_15	108.6(2)
O1_13–C1_13–C3_13	110.26(17)	F3_15–C2_15–F2_15	108.3(2)
C4_13–C1_13–C3_13	109.43(17)	F3_15–C2_15–F1_15	108.3(2)
O1_13–C1_13–C2_13	111.12(16)	F2_15–C2_15–F1_15	107.6(2)
C4_13–C1_13–C2_13	109.49(17)	F3_15–C2_15–C1_15	111.3(2)
C3_13–C1_13–C2_13	108.88(17)	F2_15–C2_15–C1_15	111.8(2)
F2_13–C2_13–F3_13	108.07(19)	F1_15–C2_15–C1_15	109.4(2)
F2_13–C2_13–F1_13	107.79(19)	F4_15–C3_15–F6_15	106.9(2)
F3_13–C2_13–F1_13	106.76(19)	F4_15–C3_15–F5_15	108.3(2)
F2_13–C2_13–C1_13	113.00(19)	F6_15–C3_15–F5_15	109.5(2)
F3_13–C2_13–C1_13	110.43(17)	F4_15–C3_15–C1_15	109.9(2)
F1_13–C2_13–C1_13	110.55(18)	F6_15–C3_15–C1_15	112.4(2)
F4_13–C3_13–F5_13	107.08(19)	F5_15–C3_15–C1_15	109.8(2)
F4_13–C3_13–F6_13	107.48(19)	F9_15–C4_15–F8_15	107.0(2)
F5_13–C3_13–F6_13	107.12(19)	F9_15–C4_15–F7_15	107.6(2)
F4_13–C3_13–C1_13	111.22(18)	F8_15–C4_15–F7_15	108.7(2)
F5_13–C3_13–C1_13	111.23(18)	F9_15–C4_15–C1_15	111.5(2)
F6_13–C3_13–C1_13	112.44(19)	F8_15–C4_15–C1_15	112.5(2)
F9_13–C4_13–F7_13	107.81(19)	F7_15–C4_15–C1_15	109.3(2)
F9_13–C4_13–F8_13	107.35(18)	C1_16–O1_16–Al14	150.0(2)
F7_13–C4_13–F8_13	106.95(18)	O1_16–C1_16–C2_16	111.4(2)
F9_13–C4_13–C1_13	111.48(17)	O1_16–C1_16–C4_16	110.3(2)
F7_13–C4_13–C1_13	110.63(18)	C2_16–C1_16–C4_16	109.0(2)
F8_13–C4_13–C1_13	112.38(18)	O1_16–C1_16–C3_16	107.1(2)
C1_14–O1_14–Al14	150.31(16)	C2_16–C1_16–C3_16	109.0(3)
O1_14–C1_14–C4_14	107.20(19)	C4_16–C1_16–C3_16	110.0(3)
O1_14–C1_14–C3_14	111.9(2)	F3_16–C2_16–F1_16	107.7(3)
C4_14–C1_14–C3_14	109.6(2)	F3_16–C2_16–F2_16	108.3(4)
O1_14–C1_14–C2_14	110.0(2)	F1_16–C2_16–F2_16	107.0(3)
C4_14–C1_14–C2_14	109.2(2)	F3_16–C2_16–C1_16	110.3(3)
C3_14–C1_14–C2_14	108.8(2)	F1_16–C2_16–C1_16	111.1(3)
F3_14–C2_14–F1_14	108.6(2)	F2_16–C2_16–C1_16	112.3(3)
F3_14–C2_14–F2_14	107.9(2)	F5_16–C3_16–F4_16	108.1(3)
F1_14–C2_14–F2_14	106.8(3)	F5_16–C3_16–F6_16	108.7(3)
F3_14–C2_14–C1_14	110.6(2)	F4_16–C3_16–F6_16	107.2(3)
F1_14–C2_14–C1_14	110.3(3)	F5_16–C3_16–C1_16	111.3(3)
F2_14–C2_14–C1_14	112.6(2)	F4_16–C3_16–C1_16	110.0(3)
F4_14–C3_14–F5_14	108.1(2)	F6_16–C3_16–C1_16	111.4(3)
F4_14–C3_14–F6_14	108.3(3)	F9_16–C4_16–F7_16	106.9(3)

F9_16–C4_16–F8_16	107.3(3)
F7_16–C4_16–F8_16	107.3(3)
F9_16–C4_16–C1_16	110.7(2)
F7_16–C4_16–C1_16	111.8(3)
F8_16–C4_16–C1_16	112.6(3)
C5_17–C1_17–C2_17	107.98(18)
C5_17–C1_17–C10_17	127.8(2)
C2_17–C1_17–C10_17	124.1(2)
C5_17–C1_17–Al5	71.70(12)
C2_17–C1_17–Al5	71.78(12)
C10_17–C1_17–Al5	125.26(15)
C3_17–C2_17–C1_17	107.86(19)
C3_17–C2_17–C9_17	127.2(2)
C1_17–C2_17–C9_17	124.75(19)
C3_17–C2_17–Al5	71.83(12)
C1_17–C2_17–Al5	70.57(12)
C9_17–C2_17–Al5	127.20(15)
C4_17–C3_17–C2_17	108.16(19)
C4_17–C3_17–C8_17	126.0(2)
C2_17–C3_17–C8_17	125.8(2)
C4_17–C3_17–Al5	71.14(13)
C2_17–C3_17–Al5	70.93(12)
C8_17–C3_17–Al5	126.41(17)
C3_17–C4_17–C5_17	108.35(19)
C3_17–C4_17–C7_17	125.4(2)
C5_17–C4_17–C7_17	126.2(2)
C3_17–C4_17–Al5	71.91(12)
C5_17–C4_17–Al5	71.01(12)
C7_17–C4_17–Al5	123.88(18)
C1_17–C5_17–C4_17	107.64(19)
C1_17–C5_17–C6_17	125.8(2)
C4_17–C5_17–C6_17	126.5(2)
C1_17–C5_17–Al5	70.80(12)
C4_17–C5_17–Al5	71.45(12)
C6_17–C5_17–Al5	122.71(17)
C5_17–C6_17–H6A_17	109.5
C5_17–C6_17–H6B_17	109.5
H6A_17–C6_17–H6B_17	109.5
C5_17–C6_17–H6C_17	109.5
H6A_17–C6_17–H6C_17	109.5
H6B_17–C6_17–H6C_17	109.5
C4_17–C7_17–H7A_17	109.5
C4_17–C7_17–H7B_17	109.5
H7A_17–C7_17–H7B_17	109.5
C4_17–C7_17–H7C_17	109.5
H7A_17–C7_17–H7C_17	109.5
H7B_17–C7_17–H7C_17	109.5
C3_17–C8_17–H8A_17	109.5
C3_17–C8_17–H8B_17	109.5
H8A_17–C8_17–H8B_17	109.5
C3_17–C8_17–H8C_17	109.5
H8A_17–C8_17–H8C_17	109.5
H8B_17–C8_17–H8C_17	109.5
C2_17–C9_17–H9A_17	109.5
C2_17–C9_17–H9B_17	109.5
H9A_17–C9_17–H9B_17	109.5
C2_17–C9_17–H9C_17	109.5
H9A_17–C9_17–H9C_17	109.5
H9B_17–C9_17–H9C_17	109.5
C1_17–C10_17–H10A_17	109.5
C1_17–C10_17–H10B_17	109.5
H10A_17–C10_17–H10B_17	109.5
C1_17–C10_17–H10C_17	109.5
H10A_17–C10_17–H10C_17	109.5
H10B_17–C10_17–H10C_17	109.5
C2_18–C1_18–C5_18	107.8(3)
C2_18–C1_18–C10_18	126.2(4)
C5_18–C1_18–C10_18	126.0(3)
C2_18–C1_18–Al4	70.3(3)
C5_18–C1_18–Al4	70.67(19)
C10_18–C1_18–Al4	123.7(2)
C1_18–C2_18–C3_18	108.1(4)
C1_18–C2_18–C9_18	125.2(4)
C3_18–C2_18–C9_18	126.7(5)
C1_18–C2_18–Al4	72.4(3)
C3_18–C2_18–Al4	69.9(4)
C9_18–C2_18–Al4	124.4(6)
C4_18–C3_18–C2_18	107.8(4)
C4_18–C3_18–C8_18	127.2(5)
C2_18–C3_18–C8_18	125.0(5)
C4_18–C3_18–Al4	70.5(4)
C2_18–C3_18–Al4	72.1(3)
C8_18–C3_18–Al4	123.8(5)
C3_18–C4_18–C5_18	108.6(3)
C3_18–C4_18–C7_18	123.5(5)
C5_18–C4_18–C7_18	127.6(4)
C3_18–C4_18–Al4	71.5(4)
C5_18–C4_18–Al4	73.2(2)
C7_18–C4_18–Al4	126.2(3)
C4_18–C5_18–C1_18	107.7(3)
C4_18–C5_18–C6_18	127.5(4)
C1_18–C5_18–C6_18	124.7(4)

C4_18–C5_18–Al4	69.0(2)
C1_18–C5_18–Al4	71.87(19)
C6_18–C5_18–Al4	124.5(2)
C5_18–C6_18–H6A_18	109.5
C5_18–C6_18–H6B_18	109.5
H6A_18–C6_18–H6B_18	109.5
C5_18–C6_18–H6C_18	109.5
H6A_18–C6_18–H6C_18	109.5
H6B_18–C6_18–H6C_18	109.5
C4_18–C7_18–H7A_18	109.5
C4_18–C7_18–H7B_18	109.5
H7A_18–C7_18–H7B_18	109.5
C4_18–C7_18–H7C_18	109.5
H7A_18–C7_18–H7C_18	109.5
H7B_18–C7_18–H7C_18	109.5
C3_18–C8_18–H8A_18	109.5
C3_18–C8_18–H8B_18	109.5
H8A_18–C8_18–H8B_18	109.5
C3_18–C8_18–H8C_18	109.5
H8A_18–C8_18–H8C_18	109.5
H8B_18–C8_18–H8C_18	109.5
C2_18–C9_18–H9A_18	109.5
C2_18–C9_18–H9B_18	109.5
H9A_18–C9_18–H9B_18	109.5
C2_18–C9_18–H9C_18	109.5
H9A_18–C9_18–H9C_18	109.5
H9B_18–C9_18–H9C_18	109.5
C1_18–C10_18–H10A_18	109.5
C1_18–C10_18–H10B_18	109.5
H10A_18–C10_18–H10B_18	109.5
C1_18–C10_18–H10C_18	109.5
H10A_18–C10_18–H10C_18	109.5
H10B_18–C10_18–H10C_18	109.5
C5_19–C1_19–C2_19	107.76(18)
C5_19–C1_19–C10_19	126.34(19)
C2_19–C1_19–C10_19	125.53(18)
C5_19–C1_19–Al6	71.74(11)
C2_19–C1_19–Al6	70.94(11)
C10_19–C1_19–Al6	128.22(14)
C3_19–C2_19–C1_19	107.90(18)
C3_19–C2_19–C9_19	126.1(2)
C1_19–C2_19–C9_19	125.6(2)
C3_19–C2_19–Al6	71.56(12)
C1_19–C2_19–Al6	71.15(11)
C9_19–C2_19–Al6	127.82(15)
C4_19–C3_19–C2_19	107.89(19)
C4_19–C3_19–C8_19	125.8(2)
C2_19–C3_19–C8_19	126.3(2)
C4_19–C3_19–Al6	71.53(12)
C2_19–C3_19–Al6	70.78(12)
C8_19–C3_19–Al6	125.31(17)
C3_19–C4_19–C5_19	108.55(18)
C3_19–C4_19–C7_19	126.2(2)
C5_19–C4_19–C7_19	125.2(2)
C3_19–C4_19–Al6	71.14(12)
C5_19–C4_19–Al6	71.38(12)
C7_19–C4_19–Al6	123.22(16)
C4_19–C5_19–C1_19	107.89(18)
C4_19–C5_19–C6_19	125.45(19)
C1_19–C5_19–C6_19	126.7(2)
C4_19–C5_19–Al6	71.27(11)
C1_19–C5_19–Al6	70.68(11)
C6_19–C5_19–Al6	123.86(15)
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	108.5(2)
C5_20–C1_20–C10_20	127.5(3)
C2_20–C1_20–C10_20	124.0(3)
C5_20–C1_20–Al2	70.84(15)
C2_20–C1_20–Al2	71.91(13)
C10_20–C1_20–Al2	123.49(19)
C1_20–C2_20–C3_20	107.3(2)
C1_20–C2_20–C9_20	125.6(2)
C3_20–C2_20–C9_20	127.1(2)
C1_20–C2_20–Al2	71.04(13)
C3_20–C2_20–Al2	70.68(12)
C9_20–C2_20–Al2	125.37(18)
C4_20–C3_20–C2_20	108.8(2)
C4_20–C3_20–C8_20	123.4(2)
C2_20–C3_20–C8_20	127.6(2)
C4_20–C3_20–Al2	70.94(12)
C2_20–C3_20–Al2	72.05(12)
C8_20–C3_20–Al2	127.08(15)
C3_20–C4_20–C5_20	107.1(2)
C3_20–C4_20–C7_20	124.6(2)
C5_20–C4_20–C7_20	128.1(2)
C3_20–C4_20–Al2	71.65(13)
C5_20–C4_20–Al2	71.22(14)
C7_20–C4_20–Al2	127.19(18)
C1_20–C5_20–C4_20	108.3(2)
C1_20–C5_20–C6_20	127.2(3)
C4_20–C5_20–C6_20	124.5(3)
C1_20–C5_20–Al2	71.96(14)
C4_20–C5_20–Al2	71.11(13)
C6_20–C5_20–Al2	123.92(19)
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	107.87(19)
C5_21–C1_21–C10_21	125.5(3)
C2_21–C1_21–C10_21	126.6(3)
C5_21–C1_21–Al1	71.23(12)
C2_21–C1_21–Al1	70.99(12)
C10_21–C1_21–Al1	124.18(19)
C1_21–C2_21–C3_21	107.78(19)
C1_21–C2_21–C9_21	126.8(2)
C3_21–C2_21–C9_21	125.1(2)
C1_21–C2_21–Al1	71.80(12)
C3_21–C2_21–Al1	70.78(12)
C9_21–C2_21–Al1	127.62(16)

C4_21–C3_21–C2_21	108.27(19)
C4_21–C3_21–C8_21	126.8(2)
C2_21–C3_21–C8_21	124.8(2)
C4_21–C3_21–Al1	71.97(12)
C2_21–C3_21–Al1	71.75(12)
C8_21–C3_21–Al1	124.65(15)
C3_21–C4_21–C5_21	107.86(19)
C3_21–C4_21–C7_21	126.3(3)
C5_21–C4_21–C7_21	125.7(3)
C3_21–C4_21–Al1	70.81(12)
C5_21–C4_21–Al1	71.52(13)
C7_21–C4_21–Al1	126.02(17)
C1_21–C5_21–C4_21	108.23(19)
C1_21–C5_21–C6_21	126.1(3)
C4_21–C5_21–C6_21	125.7(3)
C1_21–C5_21–Al1	71.64(13)
C4_21–C5_21–Al1	71.28(12)
C6_21–C5_21–Al1	124.39(18)
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
C2_22–C1_22–C5_22	107.8(2)
C2_22–C1_22–C10_22	124.9(2)
C5_22–C1_22–C10_22	126.9(2)
C2_22–C1_22–Al3	70.87(12)
C5_22–C1_22–Al3	71.98(12)
C10_22–C1_22–Al3	128.25(16)
C1_22–C2_22–C3_22	107.44(19)
C1_22–C2_22–C9_22	125.9(2)
C3_22–C2_22–C9_22	126.6(2)
C1_22–C2_22–Al3	71.59(12)
C3_22–C2_22–Al3	71.70(12)
C9_22–C2_22–Al3	124.24(15)
C4_22–C3_22–C2_22	108.7(2)
C4_22–C3_22–C8_22	124.6(2)
C2_22–C3_22–C8_22	126.8(2)
C4_22–C3_22–Al3	72.04(13)
C2_22–C3_22–Al3	70.67(11)
C8_22–C3_22–Al3	124.50(16)
C5_22–C4_22–C3_22	107.9(2)
C5_22–C4_22–C7_22	127.9(2)
C3_22–C4_22–C7_22	124.2(2)
C5_22–C4_22–Al3	71.59(13)
C3_22–C4_22–Al3	70.88(12)
C7_22–C4_22–Al3	123.17(16)
C4_22–C5_22–C1_22	108.1(2)
C4_22–C5_22–C6_22	126.3(3)
C1_22–C5_22–C6_22	125.5(3)
C4_22–C5_22–Al3	71.50(13)
C1_22–C5_22–Al3	70.44(12)
C6_22–C5_22–Al3	126.45(16)
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
C2_23–C1_23–C5_23	107.9(2)
C2_23–C1_23–C10_23	125.7(3)
C5_23–C1_23–C10_23	126.4(3)
C2_23–C1_23–Al8	72.02(16)
C5_23–C1_23–Al8	70.47(19)
C10_23–C1_23–Al8	123.5(2)
C1_23–C2_23–C3_23	108.7(2)
C1_23–C2_23–C9_23	125.1(3)
C3_23–C2_23–C9_23	126.1(3)
C1_23–C2_23–Al8	71.19(16)
C3_23–C2_23–Al8	70.59(15)
C9_23–C2_23–Al8	125.39(19)
C2_23–C3_23–C4_23	107.4(2)
C2_23–C3_23–C8_23	127.0(3)
C4_23–C3_23–C8_23	125.2(3)
C2_23–C3_23–Al8	72.41(15)
C4_23–C3_23–Al8	69.87(16)
C8_23–C3_23–Al8	128.5(2)
C5_23–C4_23–C3_23	107.6(2)
C5_23–C4_23–C7_23	126.5(3)
C3_23–C4_23–C7_23	125.8(3)
C5_23–C4_23–Al8	71.95(17)
C3_23–C4_23–Al8	72.06(16)
C7_23–C4_23–Al8	124.8(2)
C4_23–C5_23–C1_23	108.4(3)
C4_23–C5_23–C6_23	127.1(3)
C1_23–C5_23–C6_23	124.6(3)
C4_23–C5_23–Al8	70.49(17)
C1_23–C5_23–Al8	72.24(19)
C6_23–C5_23–Al8	124.3(3)
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_24–C1_24–C2_24	108.04(19)
C5_24–C1_24–C10_24	125.1(2)
C2_24–C1_24–C10_24	126.9(2)
C5_24–C1_24–Al7	71.80(12)
C2_24–C1_24–Al7	70.66(12)
C10_24–C1_24–Al7	124.27(16)
C3_24–C2_24–C1_24	107.84(19)
C3_24–C2_24–C9_24	125.8(2)
C1_24–C2_24–C9_24	126.4(2)
C3_24–C2_24–Al7	71.83(12)
C1_24–C2_24–Al7	71.74(12)
C9_24–C2_24–Al7	124.12(16)
C2_24–C3_24–C4_24	107.89(19)
C2_24–C3_24–C8_24	125.6(3)
C4_24–C3_24–C8_24	126.2(3)
C2_24–C3_24–Al7	70.67(12)
C4_24–C3_24–Al7	71.82(12)
C8_24–C3_24–Al7	127.77(17)
C5_24–C4_24–C3_24	108.08(19)
C5_24–C4_24–C7_24	125.5(2)
C3_24–C4_24–C7_24	126.4(2)
C5_24–C4_24–Al7	71.40(12)
C3_24–C4_24–Al7	70.76(12)
C7_24–C4_24–Al7	124.83(17)
C4_24–C5_24–C1_24	108.14(18)
C4_24–C5_24–C6_24	126.5(2)
C1_24–C5_24–C6_24	125.3(2)
C4_24–C5_24–Al7	71.64(12)
C1_24–C5_24–Al7	70.91(11)
C6_24–C5_24–Al7	125.32(15)
C5_24–C6_24–H6A_24	109.5
C5_24–C6_24–H6B_24	109.5
H6A_24–C6_24–H6B_24	109.5
C5_24–C6_24–H6C_24	109.5
H6A_24–C6_24–H6C_24	109.5
H6B_24–C6_24–H6C_24	109.5
C4_24–C7_24–H7A_24	109.5
C4_24–C7_24–H7B_24	109.5
H7A_24–C7_24–H7B_24	109.5
C4_24–C7_24–H7C_24	109.5
H7A_24–C7_24–H7C_24	109.5
H7B_24–C7_24–H7C_24	109.5
C3_24–C8_24–H8A_24	109.5
C3_24–C8_24–H8B_24	109.5
H8A_24–C8_24–H8B_24	109.5
C3_24–C8_24–H8C_24	109.5
H8A_24–C8_24–H8C_24	109.5
H8B_24–C8_24–H8C_24	109.5
C2_24–C9_24–H9A_24	109.5
C2_24–C9_24–H9B_24	109.5
H9A_24–C9_24–H9B_24	109.5
C2_24–C9_24–H9C_24	109.5
H9A_24–C9_24–H9C_24	109.5
H9B_24–C9_24–H9C_24	109.5
C1_24–C10_24–H10A_24	109.5
C1_24–C10_24–H10B_24	109.5
H10A_24–C10_24–H10B_24	109.5
C1_24–C10_24–H10C_24	109.5
H10A_24–C10_24–H10C_24	109.5
H10B_24–C10_24–H10C_24	109.5
C2_25–C1_25–C5_25	108.49(17)
C2_25–C1_25–C10_25	125.8(2)
C5_25–C1_25–C10_25	125.6(2)
C2_25–C1_25–Al9	71.86(11)
C5_25–C1_25–Al9	71.03(11)
C10_25–C1_25–Al9	125.76(14)
C1_25–C2_25–C3_25	107.65(17)
C1_25–C2_25–C9_25	125.60(19)
C3_25–C2_25–C9_25	126.7(2)
C1_25–C2_25–Al9	70.76(11)
C3_25–C2_25–Al9	70.67(11)
C9_25–C2_25–Al9	126.27(15)
C4_25–C3_25–C2_25	108.11(17)
C4_25–C3_25–C8_25	124.67(18)
C2_25–C3_25–C8_25	126.74(19)
C4_25–C3_25–Al9	70.69(11)
C2_25–C3_25–Al9	71.86(11)
C8_25–C3_25–Al9	129.30(15)
C5_25–C4_25–C3_25	108.06(17)
C5_25–C4_25–C7_25	126.9(2)
C3_25–C4_25–C7_25	124.78(19)
C5_25–C4_25–Al9	71.46(11)
C3_25–C4_25–Al9	71.61(11)
C7_25–C4_25–Al9	126.82(15)
C1_25–C5_25–C4_25	107.69(18)
C1_25–C5_25–C6_25	125.58(18)
C4_25–C5_25–C6_25	126.71(19)

C1_25–C5_25–Al9	71.39(11)
C4_25–C5_25–Al9	70.82(11)
C6_25–C5_25–Al9	124.37(14)
C5_25–C6_25–H6A_25	109.5
C5_25–C6_25–H6B_25	109.5
H6A_25–C6_25–H6B_25	109.5
C5_25–C6_25–H6C_25	109.5
H6A_25–C6_25–H6C_25	109.5
H6B_25–C6_25–H6C_25	109.5
C4_25–C7_25–H7A_25	109.5
C4_25–C7_25–H7B_25	109.5
H7A_25–C7_25–H7B_25	109.5
C4_25–C7_25–H7C_25	109.5
H7A_25–C7_25–H7C_25	109.5
H7B_25–C7_25–H7C_25	109.5
C3_25–C8_25–H8A_25	109.5
C3_25–C8_25–H8B_25	109.5
H8A_25–C8_25–H8B_25	109.5
C3_25–C8_25–H8C_25	109.5
H8A_25–C8_25–H8C_25	109.5
H8B_25–C8_25–H8C_25	109.5
C2_25–C9_25–H9A_25	109.5
C2_25–C9_25–H9B_25	109.5
H9A_25–C9_25–H9B_25	109.5
C2_25–C9_25–H9C_25	109.5
H9A_25–C9_25–H9C_25	109.5
H9B_25–C9_25–H9C_25	109.5
C1_25–C10_25–H10A_25	109.5
C1_25–C10_25–H10B_25	109.5
H10A_25–C10_25–H10B_25	109.5
C1_25–C10_25–H10C_25	109.5
H10A_25–C10_25–H10C_25	109.5
H10B_25–C10_25–H10C_25	109.5
C2_26–C1_26–C5_26	107.6(5)
C2_26–C1_26–C10_26	128.0(5)
C5_26–C1_26–C10_26	124.3(5)
C2_26–C1_26–Al12	71.6(4)
C5_26–C1_26–Al12	70.7(5)
C10_26–C1_26–Al12	123.7(5)
C1_26–C2_26–C3_26	108.5(5)
C1_26–C2_26–C9_26	124.8(6)
C3_26–C2_26–C9_26	126.6(6)
C1_26–C2_26–Al12	71.4(4)
C3_26–C2_26–Al12	71.2(4)
C9_26–C2_26–Al12	126.5(6)
C4_26–C3_26–C2_26	107.7(6)
C4_26–C3_26–C8_26	125.9(6)
C2_26–C3_26–C8_26	125.8(6)
C4_26–C3_26–Al12	71.2(7)
C2_26–C3_26–Al12	71.4(4)
C8_26–C3_26–Al12	129.9(6)
C5_26–C4_26–C3_26	107.9(6)
C5_26–C4_26–C7_26	127.4(6)
C3_26–C4_26–C7_26	124.6(6)
C5_26–C4_26–Al12	71.0(7)
C3_26–C4_26–Al12	71.4(6)
C7_26–C4_26–Al12	125.8(11)
C4_26–C5_26–C1_26	108.4(5)
C4_26–C5_26–C6_26	126.5(6)
C1_26–C5_26–C6_26	125.1(5)
C4_26–C5_26–Al12	71.7(8)
C1_26–C5_26–Al12	71.7(5)
C6_26–C5_26–Al12	120.8(7)
C5_26–C6_26–H6A_26	109.5
C5_26–C6_26–H6B_26	109.5
H6A_26–C6_26–H6B_26	109.5
C5_26–C6_26–H6C_26	109.5
H6A_26–C6_26–H6C_26	109.5
H6B_26–C6_26–H6C_26	109.5
C4_26–C7_26–H7A_26	109.5
C4_26–C7_26–H7B_26	109.5
H7A_26–C7_26–H7B_26	109.5
C4_26–C7_26–H7C_26	109.5
H7A_26–C7_26–H7C_26	109.5
H7B_26–C7_26–H7C_26	109.5
C3_26–C8_26–H8A_26	109.5
C3_26–C8_26–H8B_26	109.5
H8A_26–C8_26–H8B_26	109.5
C3_26–C8_26–H8C_26	109.5
H8A_26–C8_26–H8C_26	109.5
H8B_26–C8_26–H8C_26	109.5
C2_26–C9_26–H9A_26	109.5
C2_26–C9_26–H9B_26	109.5

H9A_26–C9_26–H9B_26	109.5
C2_26–C9_26–H9C_26	109.5
H9A_26–C9_26–H9C_26	109.5
H9B_26–C9_26–H9C_26	109.5
C1_26–C10_26–H10A_26	109.5
C1_26–C10_26–H10B_26	109.5
H10A_26–C10_26–H10B_26	109.5
C1_26–C10_26–H10C_26	109.5
H10A_26–C10_26–H10C_26	109.5
H10B_26–C10_26–H10C_26	109.5
C2_27–C1_27–C5_27	107.9(2)
C2_27–C1_27–C10_27	125.8(2)
C5_27–C1_27–C10_27	126.0(3)
C2_27–C1_27–Al11	70.62(12)
C5_27–C1_27–Al11	72.25(13)
C10_27–C1_27–Al11	127.21(17)
C3_27–C2_27–C1_27	108.19(19)
C3_27–C2_27–C9_27	126.1(2)
C1_27–C2_27–C9_27	125.7(2)
C3_27–C2_27–Al11	71.96(12)
C1_27–C2_27–Al11	71.63(12)
C9_27–C2_27–Al11	124.10(16)
C2_27–C3_27–C4_27	107.7(2)
C2_27–C3_27–C8_27	126.9(2)
C4_27–C3_27–C8_27	125.3(2)
C2_27–C3_27–Al11	70.42(12)
C4_27–C3_27–Al11	71.91(12)
C8_27–C3_27–Al11	125.13(17)
C5_27–C4_27–C3_27	108.46(19)
C5_27–C4_27–C7_27	127.3(2)
C3_27–C4_27–C7_27	124.3(2)
C5_27–C4_27–Al11	71.66(12)
C3_27–C4_27–Al11	70.64(12)
C7_27–C4_27–Al11	122.67(17)
C4_27–C5_27–C1_27	107.7(2)
C4_27–C5_27–C6_27	125.8(2)
C1_27–C5_27–C6_27	126.4(2)
C4_27–C5_27–Al11	71.34(13)
C1_27–C5_27–Al11	70.17(12)
C6_27–C5_27–Al11	123.60(17)
C5_27–C6_27–H6A_27	109.5
C5_27–C6_27–H6B_27	109.5
H6A_27–C6_27–H6B_27	109.5
C5_27–C6_27–H6C_27	109.5
H6A_27–C6_27–H6C_27	109.5
H6B_27–C6_27–H6C_27	109.5
C4_27–C7_27–H7A_27	109.5
C4_27–C7_27–H7B_27	109.5
H7A_27–C7_27–H7B_27	109.5
C4_27–C7_27–H7C_27	109.5
H7A_27–C7_27–H7C_27	109.5
H7B_27–C7_27–H7C_27	109.5
C3_27–C8_27–H8A_27	109.5
C3_27–C8_27–H8B_27	109.5
H8A_27–C8_27–H8B_27	109.5
C3_27–C8_27–H8C_27	109.5
H8A_27–C8_27–H8C_27	109.5
H8B_27–C8_27–H8C_27	109.5
C2_27–C9_27–H9A_27	109.5
C2_27–C9_27–H9B_27	109.5
H9A_27–C9_27–H9B_27	109.5
C2_27–C9_27–H9C_27	109.5
H9A_27–C9_27–H9C_27	109.5
H9B_27–C9_27–H9C_27	109.5
C1_27–C10_27–H10A_27	109.5
C1_27–C10_27–H10B_27	109.5
H10A_27–C10_27–H10B_27	109.5
C1_27–C10_27–H10C_27	109.5
H10A_27–C10_27–H10C_27	109.5
H10B_27–C10_27–H10C_27	109.5
C1_29–O1_29–Al13	146.2(13)
O1_29–C1_29–C2_29	109.2(9)
O1_29–C1_29–C4_29	108.4(10)
C2_29–C1_29–C4_29	110.5(7)
O1_29–C1_29–C3_29	112.5(8)
C2_29–C1_29–C3_29	107.5(6)
C4_29–C1_29–C3_29	108.8(6)
F2_29–C2_29–F3_29	114.7(10)
F2_29–C2_29–F1_29	107.4(8)
F3_29–C2_29–F1_29	103.4(9)
F2_29–C2_29–C1_29	111.4(7)
F3_29–C2_29–C1_29	110.0(9)

F1_29–C2_29–C1_29	109.4(7)	F4_31–C3_31–C1_31	110.6(7)
F5_29–C3_29–F6_29	107.6(6)	F6_31–C3_31–C1_31	112.3(7)
F5_29–C3_29–F4_29	107.0(6)	F9_31–C4_31–F7_31	105.6(9)
F6_29–C3_29–F4_29	108.2(6)	F9_31–C4_31–F8_31	110.1(10)
F5_29–C3_29–C1_29	111.7(5)	F7_31–C4_31–F8_31	112.7(10)
F6_29–C3_29–C1_29	111.8(6)	F9_31–C4_31–C1_31	110.5(9)
F4_29–C3_29–C1_29	110.3(6)	F7_31–C4_31–C1_31	109.3(8)
F7_29–C4_29–F9_29	106.2(8)	F8_31–C4_31–C1_31	108.6(8)
F7_29–C4_29–F8_29	108.0(10)	C1_32–O1_32–Al16	146.7(15)
F9_29–C4_29–F8_29	109.0(9)	O1_32–C1_32–C3_32	111.3(11)
F7_29–C4_29–C1_29	111.3(8)	O1_32–C1_32–C4_32	105.5(10)
F9_29–C4_29–C1_29	110.5(7)	C3_32–C1_32–C4_32	109.8(6)
F8_29–C4_29–C1_29	111.7(8)	O1_32–C1_32–C2_32	111.2(11)
C1_30–O1_30–Al13	157.6(15)	C3_32–C1_32–C2_32	109.5(6)
O1_30–C1_30–C4_30	110.1(11)	C4_32–C1_32–C2_32	109.4(6)
O1_30–C1_30–C2_30	108.4(12)	F3_32–C2_32–F1_32	107.8(8)
C4_30–C1_30–C2_30	111.4(9)	F3_32–C2_32–F2_32	108.2(9)
O1_30–C1_30–C3_30	109.1(12)	F1_32–C2_32–F2_32	106.7(6)
C4_30–C1_30–C3_30	108.1(8)	F3_32–C2_32–C1_32	110.9(9)
C2_30–C1_30–C3_30	109.7(9)	F1_32–C2_32–C1_32	111.4(5)
F2_30–C2_30–F1_30	105.7(11)	F2_32–C2_32–C1_32	111.7(6)
F2_30–C2_30–F3_30	108.5(11)	F4_32–C3_32–F5_32	107.5(9)
F1_30–C2_30–F3_30	108.5(11)	F4_32–C3_32–F6_32	107.1(11)
F2_30–C2_30–C1_30	112.0(10)	F5_32–C3_32–F6_32	107.3(7)
F1_30–C2_30–C1_30	110.2(10)	F4_32–C3_32–C1_32	111.3(10)
F3_30–C2_30–C1_30	111.6(10)	F5_32–C3_32–C1_32	111.0(5)
F4_30–C3_30–F6_30	107.4(10)	F6_32–C3_32–C1_32	112.3(7)
F4_30–C3_30–F5_30	107.5(10)	F9_32–C4_32–F7_32	108.0(9)
F6_30–C3_30–F5_30	107.1(10)	F9_32–C4_32–F8_32	109.0(12)
F4_30–C3_30–C1_30	112.2(10)	F7_32–C4_32–F8_32	106.6(6)
F6_30–C3_30–C1_30	111.6(10)	F9_32–C4_32–C1_32	109.6(10)
F5_30–C3_30–C1_30	110.8(9)	F7_32–C4_32–C1_32	110.8(5)
F7_30–C4_30–F9_30	109.2(11)	F8_32–C4_32–C1_32	112.7(8)
F7_30–C4_30–F8_30	105.3(14)	C1_33–O1_33–Al16	148(2)
F9_30–C4_30–F8_30	107.0(13)	O1_33–C1_33–C2_33	109.2(14)
F7_30–C4_30–C1_30	112.1(9)	O1_33–C1_33–C3_33	110.9(14)
F9_30–C4_30–C1_30	112.8(10)	C2_33–C1_33–C3_33	110.3(7)
F8_30–C4_30–C1_30	110.1(12)	O1_33–C1_33–C4_33	108.4(13)
C1_31–O1_31–Al13	147.5(11)	C2_33–C1_33–C4_33	109.5(7)
O1_31–C1_31–C3_31	110.7(9)	C3_33–C1_33–C4_33	108.4(7)
O1_31–C1_31–C2_31	107.4(8)	F1_33–C2_33–F3_33	109.9(8)
C3_31–C1_31–C2_31	108.6(7)	F1_33–C2_33–F2_33	109.2(7)
O1_31–C1_31–C4_31	110.0(9)	F3_33–C2_33–F2_33	105.0(9)
C3_31–C1_31–C4_31	109.5(7)	F1_33–C2_33–C1_33	111.0(6)
C2_31–C1_31–C4_31	110.6(7)	F3_33–C2_33–C1_33	109.1(9)
F2_31–C2_31–F3_31	109.4(8)	F2_33–C2_33–C1_33	112.3(8)
F2_31–C2_31–F1_31	106.5(8)	F6_33–C3_33–F4_33	108.0(12)
F3_31–C2_31–F1_31	110.2(8)	F6_33–C3_33–F5_33	105.3(11)
F2_31–C2_31–C1_31	111.3(8)	F4_33–C3_33–F5_33	110.7(7)
F3_31–C2_31–C1_31	109.9(7)	F6_33–C3_33–C1_33	112.3(11)
F1_31–C2_31–C1_31	109.5(7)	F4_33–C3_33–C1_33	109.2(9)
F5_31–C3_31–F4_31	104.2(8)	F5_33–C3_33–C1_33	111.3(7)
F5_31–C3_31–F6_31	109.6(8)	F9_33–C4_33–F7_33	100.8(7)
F4_31–C3_31–F6_31	108.4(8)	F9_33–C4_33–F8_33	110.1(10)
F5_31–C3_31–C1_31	111.3(7)	F7_33–C4_33–F8_33	109.5(8)

F9_33–C4_33–C1_33	113.7(8)	O1_36–C1_36–C2_36	108.3(12)
F7_33–C4_33–C1_33	111.5(6)	C4_36–C1_36–C2_36	109.6(11)
F8_33–C4_33–C1_33	110.8(9)	O1_36–C1_36–C3_36	112.3(13)
C1_34–O1_34–Al14	150.9(12)	C4_36–C1_36–C3_36	107.3(11)
O1_34–C1_34–C4_34	111.6(11)	C2_36–C1_36–C3_36	109.0(11)
O1_34–C1_34–C2_34	108.3(11)	F2_36–C2_36–F1_36	111.9(14)
C4_34–C1_34–C2_34	109.8(11)	F2_36–C2_36–F3_36	103.8(13)
O1_34–C1_34–C3_34	108.3(12)	F1_36–C2_36–F3_36	112.9(14)
C4_34–C1_34–C3_34	110.1(11)	F2_36–C2_36–C1_36	110.6(12)
C2_34–C1_34–C3_34	108.8(12)	F1_36–C2_36–C1_36	108.5(12)
F2_34–C2_34–F1_34	112.2(18)	F3_36–C2_36–C1_36	109.0(11)
F2_34–C2_34–F3_34	107.7(14)	F5_36–C3_36–F6_36	112.5(14)
F1_34–C2_34–F3_34	100.9(16)	F5_36–C3_36–F4_36	111.2(14)
F2_34–C2_34–C1_34	112.1(13)	F6_36–C3_36–F4_36	106.4(13)
F1_34–C2_34–C1_34	112.7(17)	F5_36–C3_36–C1_36	105.1(12)
F3_34–C2_34–C1_34	110.6(12)	F6_36–C3_36–C1_36	111.0(12)
F6_34–C3_34–F5_34	108.1(16)	F4_36–C3_36–C1_36	110.8(11)
F6_34–C3_34–F4_34	107.0(18)	F9_36–C4_36–F8_36	109.3(17)
F5_34–C3_34–F4_34	107.3(16)	F9_36–C4_36–F7_36	110.2(16)
F6_34–C3_34–C1_34	111.5(16)	F8_36–C4_36–F7_36	107.8(16)
F5_34–C3_34–C1_34	111.5(13)	F9_36–C4_36–C1_36	109.6(14)
F4_34–C3_34–C1_34	111.2(15)	F8_36–C4_36–C1_36	110.9(15)
F9_34–C4_34–F8_34	108.6(13)	F7_36–C4_36–C1_36	108.9(14)
F9_34–C4_34–F7_34	105.2(13)	C5_37–C1_37–C2_37	108.3(8)
F8_34–C4_34–F7_34	106.3(13)	C5_37–C1_37–C10_37	124.0(9)
F9_34–C4_34–C1_34	110.7(11)	C2_37–C1_37–C10_37	127.6(9)
F8_34–C4_34–C1_34	113.7(12)	C5_37–C1_37–Al4	68.6(10)
F7_34–C4_34–C1_34	111.8(12)	C2_37–C1_37–Al4	68.8(5)
C1_35–O1_35–Al14	150.3(12)	C10_37–C1_37–Al4	129.0(6)
O1_35–C1_35–C4_35	112.0(12)	C3_37–C2_37–C1_37	108.4(7)
O1_35–C1_35–C3_35	107.6(11)	C3_37–C2_37–C9_37	128.5(10)
C4_35–C1_35–C3_35	109.9(12)	C1_37–C2_37–C9_37	123.1(10)
O1_35–C1_35–C2_35	109.2(11)	C3_37–C2_37–Al4	66.3(4)
C4_35–C1_35–C2_35	108.7(11)	C1_37–C2_37–Al4	76.8(5)
C3_35–C1_35–C2_35	109.4(11)	C9_37–C2_37–Al4	124.0(7)
F1_35–C2_35–F2_35	105.8(13)	C2_37–C3_37–C4_37	107.2(8)
F1_35–C2_35–F3_35	108.9(14)	C2_37–C3_37–C8_37	128.3(11)
F2_35–C2_35–F3_35	110.1(14)	C4_37–C3_37–C8_37	124.4(11)
F1_35–C2_35–C1_35	110.6(12)	C2_37–C3_37–Al4	77.7(4)
F2_35–C2_35–C1_35	112.5(13)	C4_37–C3_37–Al4	73.2(11)
F3_35–C2_35–C1_35	108.9(11)	C8_37–C3_37–Al4	117.0(8)
F6_35–C3_35–F4_35	106.9(15)	C5_37–C4_37–C3_37	108.4(9)
F6_35–C3_35–F5_35	107.4(17)	C5_37–C4_37–C7_37	124.1(13)
F4_35–C3_35–F5_35	110.9(16)	C3_37–C4_37–C7_37	127.0(13)
F6_35–C3_35–C1_35	114.1(16)	C5_37–C4_37–Al4	75.5(11)
F4_35–C3_35–C1_35	110.8(12)	C3_37–C4_37–Al4	69.2(9)
F5_35–C3_35–C1_35	106.6(15)	C7_37–C4_37–Al4	115.0(18)
F9_35–C4_35–F7_35	107.8(16)	C1_37–C5_37–C4_37	107.3(9)
F9_35–C4_35–F8_35	106.9(18)	C1_37–C5_37–C6_37	124.0(11)
F7_35–C4_35–F8_35	105.4(18)	C4_37–C5_37–C6_37	127.9(12)
F9_35–C4_35–C1_35	112.5(15)	C1_37–C5_37–Al4	77.0(9)
F7_35–C4_35–C1_35	111.3(15)	C4_37–C5_37–Al4	68.6(11)
F8_35–C4_35–C1_35	112.6(17)	C6_37–C5_37–Al4	128.1(15)
C1_36–O1_36–Al13	150.6(15)	C5_37–C6_37–H6A_37	109.5
O1_36–C1_36–C4_36	110.3(13)	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
C1_39–O1_39–Al15	156(2)
O1_39–C1_39–C4_39	109.7(15)
O1_39–C1_39–C2_39	109.7(15)
C4_39–C1_39–C2_39	111.8(11)
O1_39–C1_39–C3_39	108.4(14)
C4_39–C1_39–C3_39	106.7(10)
C2_39–C1_39–C3_39	110.4(11)
F1_39–C2_39–F3_39	109.4(16)
F1_39–C2_39–F2_39	104.9(14)
F3_39–C2_39–F2_39	107.1(18)
F1_39–C2_39–C1_39	111.5(11)
F3_39–C2_39–C1_39	112.0(15)
F2_39–C2_39–C1_39	111.7(16)
F4_39–C3_39–F6_39	109.9(16)
F4_39–C3_39–F5_39	103.8(15)
F6_39–C3_39–F5_39	104.0(12)
F4_39–C3_39–C1_39	113.7(15)
F6_39–C3_39–C1_39	114.2(12)
F5_39–C3_39–C1_39	110.3(11)
F9_39–C4_39–F8_39	110.1(15)
F9_39–C4_39–F7_39	101.7(16)
F8_39–C4_39–F7_39	106.9(16)
F9_39–C4_39–C1_39	116.4(14)
F8_39–C4_39–C1_39	111.4(12)
F7_39–C4_39–C1_39	109.5(14)
C5_41–C1_41–C2_41	108.4(5)
C5_41–C1_41–C10_41	127.7(5)
C2_41–C1_41–C10_41	123.8(5)
C5_41–C1_41–Al10	69.8(4)
C2_41–C1_41–Al10	70.9(3)
C10_41–C1_41–Al10	128.6(4)
C3_41–C2_41–C1_41	108.5(5)
C3_41–C2_41–C9_41	123.6(6)
C1_41–C2_41–C9_41	128.0(6)
C3_41–C2_41–Al10	69.4(3)
C1_41–C2_41–Al10	71.2(3)
C9_41–C2_41–Al10	126.6(4)
C2_41–C3_41–C4_41	106.7(4)
C2_41–C3_41–C8_41	126.2(7)
C4_41–C3_41–C8_41	127.0(7)
C2_41–C3_41–Al10	72.5(2)
C4_41–C3_41–Al10	69.9(3)
C8_41–C3_41–Al10	123.1(4)
C5_41–C4_41–C3_41	109.3(4)
C5_41–C4_41–C7_41	125.8(7)
C3_41–C4_41–C7_41	124.9(6)
C5_41–C4_41–Al10	71.9(4)
C3_41–C4_41–Al10	71.1(3)
C7_41–C4_41–Al10	122.7(4)
C4_41–C5_41–C1_41	107.1(5)
C4_41–C5_41–C6_41	130.7(6)
C1_41–C5_41–C6_41	122.1(5)
C4_41–C5_41–Al10	69.7(4)
C1_41–C5_41–Al10	72.2(3)
C6_41–C5_41–Al10	125.7(5)
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
C5_38–C1_38–C2_38	106.0(7)
C5_38–C1_38–C10_38	122.8(7)
C2_38–C1_38–C10_38	131.2(7)
C5_38–C1_38–Al10	72.8(4)
C2_38–C1_38–Al10	69.0(4)
C10_38–C1_38–Al10	123.7(6)
C3_38–C2_38–C1_38	109.9(7)
C3_38–C2_38–C9_38	127.2(9)
C1_38–C2_38–C9_38	122.9(9)
C3_38–C2_38–Al10	71.0(4)
C1_38–C2_38–Al10	74.7(4)
C9_38–C2_38–Al10	123.6(6)
C2_38–C3_38–C4_38	107.0(6)
C2_38–C3_38–C8_38	127.8(10)
C4_38–C3_38–C8_38	124.9(10)
C2_38–C3_38–Al10	72.5(4)
C4_38–C3_38–Al10	73.2(4)
C8_38–C3_38–Al10	124.1(6)
C5_38–C4_38–C3_38	107.9(6)
C5_38–C4_38–C7_38	125.5(8)
C3_38–C4_38–C7_38	126.6(8)
C5_38–C4_38–Al10	74.6(4)
C3_38–C4_38–Al10	70.0(4)
C7_38–C4_38–Al10	122.0(5)
C1_38–C5_38–C4_38	109.2(6)
C1_38–C5_38–C6_38	127.1(7)
C4_38–C5_38–C6_38	123.7(7)
C1_38–C5_38–Al10	71.9(5)
C4_38–C5_38–Al10	69.7(4)
C6_38–C5_38–Al10	124.3(4)
C5_38–C6_38–H6A_38	109.5
C5_38–C6_38–H6B_38	109.5
H6A_38–C6_38–H6B_38	109.5
C5_38–C6_38–H6C_38	109.5
H6A_38–C6_38–H6C_38	109.5
H6B_38–C6_38–H6C_38	109.5
C4_38–C7_38–H7A_38	109.5
C4_38–C7_38–H7B_38	109.5
H7A_38–C7_38–H7B_38	109.5
C4_38–C7_38–H7C_38	109.5
H7A_38–C7_38–H7C_38	109.5
H7B_38–C7_38–H7C_38	109.5
C3_38–C8_38–H8A_38	109.5
C3_38–C8_38–H8B_38	109.5
H8A_38–C8_38–H8B_38	109.5
C3_38–C8_38–H8C_38	109.5
H8A_38–C8_38–H8C_38	109.5
H8B_38–C8_38–H8C_38	109.5
C2_38–C9_38–H9A_38	109.5
C2_38–C9_38–H9B_38	109.5
H9A_38–C9_38–H9B_38	109.5
C2_38–C9_38–H9C_38	109.5
H9A_38–C9_38–H9C_38	109.5
H9B_38–C9_38–H9C_38	109.5
C1_38–C10_38–H10A_38	109.5
C1_38–C10_38–H10B_38	109.5

H10A_38–C10_38–H10B_38	109.5
C1_38–C10_38–H10C_38	109.5
H10A_38–C10_38–H10C_38	109.5
H10B_38–C10_38–H10C_38	109.5
C1_28–O1_28–Al13	151.2(15)
O1_28–C1_28–C3_28	108.9(12)
O1_28–C1_28–C4_28	109.4(13)
C3_28–C1_28–C4_28	109.3(11)
O1_28–C1_28–C2_28	109.9(13)
C3_28–C1_28–C2_28	108.8(10)
C4_28–C1_28–C2_28	110.5(11)
F2_28–C2_28–F1_28	107.2(13)
F2_28–C2_28–F3_28	111.7(13)
F1_28–C2_28–F3_28	108.5(14)
F2_28–C2_28–C1_28	110.9(12)
F1_28–C2_28–C1_28	109.3(11)
F3_28–C2_28–C1_28	109.1(12)
F4_28–C3_28–F6_28	107.5(13)
F4_28–C3_28–F5_28	111.3(14)
F6_28–C3_28–F5_28	106.6(13)
F4_28–C3_28–C1_28	110.9(12)
F6_28–C3_28–C1_28	110.9(12)
F5_28–C3_28–C1_28	109.6(12)
F8_28–C4_28–F9_28	104.7(14)
F8_28–C4_28–F7_28	107.0(15)
F9_28–C4_28–F7_28	109.6(15)
F8_28–C4_28–C1_28	113.0(13)
F9_28–C4_28–C1_28	112.3(14)
F7_28–C4_28–C1_28	110.0(14)
C2_40–C1_40–C5_40	109.6(8)
C2_40–C1_40–C10_40	125.2(8)
C5_40–C1_40–C10_40	125.2(8)
C2_40–C1_40–Al12	73.1(5)
C5_40–C1_40–Al12	70.2(9)
C10_40–C1_40–Al12	121.5(8)
C1_40–C2_40–C3_40	107.0(8)
C1_40–C2_40–C9_40	128.5(8)
C3_40–C2_40–C9_40	124.4(8)
C1_40–C2_40–Al12	70.2(5)
C3_40–C2_40–Al12	71.3(5)
C9_40–C2_40–Al12	125.5(8)
C4_40–C3_40–C2_40	108.1(8)
C4_40–C3_40–C8_40	124.2(9)
C2_40–C3_40–C8_40	127.5(9)
C4_40–C3_40–Al12	69.0(11)
C2_40–C3_40–Al12	72.0(5)
C8_40–C3_40–Al12	129.0(10)
C3_40–C4_40–C5_40	108.6(9)
C3_40–C4_40–C7_40	126.5(9)
C5_40–C4_40–C7_40	124.4(9)
C3_40–C4_40–Al12	73.9(10)
C5_40–C4_40–Al12	71.3(12)
C7_40–C4_40–Al12	126.4(17)
C1_40–C5_40–C4_40	106.7(8)
C1_40–C5_40–C6_40	124.8(8)
C4_40–C5_40–C6_40	128.5(9)
C1_40–C5_40–Al12	72.4(8)
C4_40–C5_40–Al12	70.9(13)
C6_40–C5_40–Al12	123.2(12)
C5_40–C6_40–H6A_40	109.5
C5_40–C6_40–H6B_40	109.5
H6A_40–C6_40–H6B_40	109.5
C5_40–C6_40–H6C_40	109.5
H6A_40–C6_40–H6C_40	109.5
H6B_40–C6_40–H6C_40	109.5
C4_40–C7_40–H7A_40	109.5
C4_40–C7_40–H7B_40	109.5
H7A_40–C7_40–H7B_40	109.5
C4_40–C7_40–H7C_40	109.5
H7A_40–C7_40–H7C_40	109.5
H7B_40–C7_40–H7C_40	109.5
C3_40–C8_40–H8A_40	109.5
C3_40–C8_40–H8B_40	109.5
H8A_40–C8_40–H8B_40	109.5
C3_40–C8_40–H8C_40	109.5
H8A_40–C8_40–H8C_40	109.5
H8B_40–C8_40–H8C_40	109.5
C2_40–C9_40–H9A_40	109.5
C2_40–C9_40–H9B_40	109.5
H9A_40–C9_40–H9B_40	109.5
C2_40–C9_40–H9C_40	109.5
H9A_40–C9_40–H9C_40	109.5
H9B_40–C9_40–H9C_40	109.5
C1_40–C10_40–H10A_40	109.5
C1_40–C10_40–H10B_40	109.5
H10A_40–C10_40–H10B_40	109.5
C1_40–C10_40–H10C_40	109.5
H10A_40–C10_40–H10C_40	109.5

H10B_40–C10_40–H10C_40	109.5
C2_42–C1_42–C5_42	109.0(11)
C2_42–C1_42–C10_42	124.3(16)
C5_42–C1_42–C10_42	126.6(16)
C2_42–C1_42–Al8	77.2(8)
C5_42–C1_42–Al8	68.6(11)
C10_42–C1_42–Al8	122.4(15)
C3_42–C2_42–C1_42	107.5(11)
C3_42–C2_42–C9_42	125.8(13)
C1_42–C2_42–C9_42	126.7(13)
C3_42–C2_42–Al8	72.0(7)
C1_42–C2_42–Al8	66.1(8)
C9_42–C2_42–Al8	128.1(12)
C2_42–C3_42–C4_42	107.8(10)
C2_42–C3_42–C8_42	123.9(13)
C4_42–C3_42–C8_42	128.2(13)
C2_42–C3_42–Al8	72.3(7)
C4_42–C3_42–Al8	65.7(9)
C8_42–C3_42–Al8	131.0(10)
C5_42–C4_42–C3_42	109.2(10)
C5_42–C4_42–C7_42	124.2(14)
C3_42–C4_42–C7_42	126.6(14)
C5_42–C4_42–Al8	69.1(11)
C3_42–C4_42–Al8	77.5(9)
C7_42–C4_42–Al8	121.3(13)
C4_42–C5_42–C1_42	106.4(10)
C4_42–C5_42–C6_42	129.0(15)
C1_42–C5_42–C6_42	124.5(14)
C4_42–C5_42–Al8	72.1(11)
C1_42–C5_42–Al8	72.6(12)
C6_42–C5_42–Al8	118.0(15)
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

S-Table 9: Bond lengths and angles for **2**

Atom–Atom	Length [Å]
Al16–O1_44	1.621(6)
Al16–O1_67	1.64(2)
Al16–O1_12	1.716(10)
Al16–O1_10	1.719(4)
Al16–O1_29	1.720(10)
Al16–O1_23	1.724(7)
Al16–O1_11	1.742(3)
Al16–O1_9	1.764(4)
Al17–O1_30	1.585(7)
Al17–O1_15	1.685(3)
Al17–O1_13	1.702(6)
Al17–O1_20	1.717(3)
Al17–O1_31	1.727(12)
Al17–O1_64	1.736(19)
Al17–O1_24	1.770(6)
Al17–O1_25	1.783(6)
Al17–O1_14	1.805(7)
Al18–O1_38	1.596(15)
Al18–O1_22	1.610(7)
Al18–O1_32	1.635(15)
Al18–O1_63	1.66(2)
Al18–O1_51	1.680(14)
Al18–O1_16	1.718(11)
Al18–O1_33	1.718(17)
Al18–O1_65	1.73(2)
Al18–O1_28	1.733(19)
Al18–O1_17	1.749(7)
Al18–O1_27	1.781(8)
Al18–O1_21	1.803(10)
Al19–O1_8	1.626(7)
Al19–O1_26	1.649(10)
Al19–O1_42	1.665(19)
Al19–O1_5	1.693(4)
Al19–O1_6	1.700(4)
Al19–O1_7	1.751(9)
Al19–O1_46	1.757(7)
Al19–O1_43	1.797(6)
Al20–O1_50	1.667(11)
Al20–O1_37	1.678(11)
Al20–O1_4	1.691(7)
Al20–O1_36	1.697(10)
Al20–O1_35	1.70(2)
Al20–O1_1	1.709(4)
Al20–O1_2	1.711(7)
Al20–O1_62	1.72(2)
Al20–O1_34	1.761(9)
Al20–O1_3	1.781(8)
Al20–O1_61	1.809(10)
In1–Al3	2.7417(11)
In1–Al2	2.7492(12)
In1–Al1	2.7672(14)
Al2–C5_52	2.228(3)
Al2–C1_52	2.232(3)
Al2–C2_52	2.249(4)
Al2–C4_52	2.254(4)
Al2–C3_52	2.265(4)
Al3–C1_40	2.187(4)
Al3–C5_40	2.210(4)
Al3–C2_40	2.217(3)
Al3–C4_40	2.241(4)
Al3–C3_40	2.255(4)
Al1–C4_53	2.167(6)
Al1–C3_53	2.193(5)
Al1–C5_53	2.200(10)
Al1–C2_53	2.223(5)
Al1–C3_49	2.229(12)
Al1–C4_49	2.24(2)
Al1–C1_53	2.237(5)
Al1–C2_49	2.318(12)
Al1–C5_49	2.398(15)
Al1–C1_49	2.432(11)
O1_1–C1_1	1.336(5)
C1_1–C2_1	1.535(7)
C1_1–C4_1	1.543(7)
C1_1–C3_1	1.559(8)
C2_1–F3_1	1.299(7)
C2_1–F2_1	1.331(7)
C2_1–F1_1	1.336(8)
C3_1–F4_1	1.311(7)
C3_1–F5_1	1.333(7)
C3_1–F6_1	1.350(6)
C4_1–F7_1	1.308(9)
C4_1–F8_1	1.343(7)
C4_1–F9_1	1.352(8)
O1_2–C1_2	1.351(7)
C1_2–C3_2	1.543(9)
C1_2–C2_2	1.551(9)
C1_2–C4_2	1.552(8)
C2_2–F3_2	1.325(9)
C2_2–F1_2	1.339(9)
C2_2–F2_2	1.344(8)
C3_2–F4_2	1.319(9)
C3_2–F5_2	1.338(8)
C3_2–F6_2	1.353(7)
C4_2–F9_2	1.328(7)
C4_2–F7_2	1.338(9)
C4_2–F8_2	1.348(9)
O1_3–C1_3	1.357(9)
C1_3–C4_3	1.548(9)
C1_3–C2_3	1.559(10)
C1_3–C3_3	1.561(9)
C2_3–F3_3	1.310(9)
C2_3–F1_3	1.332(9)
C2_3–F2_3	1.340(10)
C3_3–F6_3	1.304(9)
C3_3–F4_3	1.323(9)
C3_3–F5_3	1.340(9)

C4_3–F9_3	1.318(10)	O1_8–C1_8	1.371(10)
C4_3–F8_3	1.330(9)	C1_8–C3_8	1.526(10)
C4_3–F7_3	1.346(10)	C1_8–C2_8	1.537(10)
O1_4–C1_4	1.353(8)	C1_8–C4_8	1.553(10)
C1_4–C3_4	1.550(9)	C2_8–F2_8	1.315(10)
C1_4–C4_4	1.559(9)	C2_8–F3_8	1.322(11)
C1_4–C2_4	1.583(9)	C2_8–F1_8	1.348(11)
C2_4–F1_4	1.320(9)	C3_8–F6_8	1.321(9)
C2_4–F3_4	1.328(10)	C3_8–F4_8	1.343(9)
C2_4–F2_4	1.329(10)	C3_8–F5_8	1.435(11)
C3_4–F4_4	1.308(9)	C4_8–F9_8	1.305(11)
C3_4–F5_4	1.333(10)	C4_8–F8_8	1.332(10)
C3_4–F6_4	1.336(10)	C4_8–F7_8	1.347(11)
C4_4–F7_4	1.284(10)	O1_9–C1_9	1.365(8)
C4_4–F9_4	1.302(9)	C1_9–C4_9	1.548(9)
C4_4–F8_4	1.330(8)	C1_9–C2_9	1.553(9)
O1_5–C1_5	1.348(5)	C1_9–C3_9	1.561(9)
C1_5–C2_5	1.540(8)	C2_9–F3_9	1.318(9)
C1_5–C3_5	1.544(6)	C2_9–F1_9	1.331(10)
C1_5–C4_5	1.561(7)	C2_9–F2_9	1.335(8)
C2_5–F1_5	1.299(7)	C3_9–F6_9	1.320(9)
C2_5–F3_5	1.317(7)	C3_9–F4_9	1.331(10)
C2_5–F2_5	1.330(8)	C3_9–F5_9	1.342(10)
C3_5–F6_5	1.310(6)	C4_9–F9_9	1.326(11)
C3_5–F4_5	1.318(7)	C4_9–F7_9	1.327(10)
C3_5–F5_5	1.336(7)	C4_9–F8_9	1.368(10)
C4_5–F9_5	1.314(7)	O1_10–C1_10	1.353(4)
C4_5–F8_5	1.316(6)	C1_10–C4_10	1.539(6)
C4_5–F7_5	1.317(7)	C1_10–C3_10	1.552(5)
O1_6–C1_6	1.354(7)	C1_10–C2_10	1.564(6)
C1_6–C4_6	1.537(9)	C2_10–F2_10	1.328(5)
C1_6–C3_6	1.542(8)	C2_10–F3_10	1.332(6)
C1_6–C2_6	1.555(9)	C2_10–F1_10	1.339(5)
C2_6–F1_6	1.326(10)	C3_10–F5_10	1.328(6)
C2_6–F2_6	1.330(9)	C3_10–F6_10	1.335(5)
C2_6–F3_6	1.334(10)	C3_10–F4_10	1.343(6)
C3_6–F5_6	1.323(8)	C4_10–F9_10	1.306(5)
C3_6–F4_6	1.326(8)	C4_10–F8_10	1.345(5)
C3_6–F6_6	1.342(8)	C4_10–F7_10	1.350(6)
C4_6–F9_6	1.331(9)	O1_11–C1_11	1.356(5)
C4_6–F8_6	1.336(8)	C1_11–C3_11	1.531(6)
C4_6–F7_6	1.341(9)	C1_11–C2_11	1.547(7)
O1_7–C1_7	1.348(9)	C1_11–C4_11	1.560(7)
C1_7–C3_7	1.548(9)	C2_11–F3_11	1.317(7)
C1_7–C2_7	1.551(9)	C2_11–F2_11	1.335(7)
C1_7–C4_7	1.564(9)	C2_11–F1_11	1.352(8)
C2_7–F1_7	1.313(11)	C3_11–F4_11	1.315(7)
C2_7–F3_7	1.328(9)	C3_11–F6_11	1.343(7)
C2_7–F2_7	1.342(8)	C3_11–F5_11	1.351(8)
C3_7–F5_7	1.330(9)	C4_11–F9_11	1.284(7)
C3_7–F4_7	1.330(11)	C4_11–F7_11	1.333(7)
C3_7–F6_7	1.341(10)	C4_11–F8_11	1.347(7)
C4_7–F8_7	1.298(8)	O1_12–C1_12	1.354(9)
C4_7–F9_7	1.324(10)	C1_12–C3_12	1.540(9)
C4_7–F7_7	1.327(8)	C1_12–C4_12	1.546(9)

C1_12–C2_12	1.546(9)	C2_16–F1_16	1.348(9)
C2_12–F3_12	1.315(9)	C3_16–F4_16	1.320(9)
C2_12–F1_12	1.332(9)	C3_16–F6_16	1.337(9)
C2_12–F2_12	1.348(9)	C3_16–F5_16	1.372(9)
C3_12–F4_12	1.329(8)	C4_16–F9_16	1.319(9)
C3_12–F6_12	1.329(9)	C4_16–F8_16	1.321(8)
C3_12–F5_12	1.341(8)	C4_16–F7_16	1.363(9)
C4_12–F7_12	1.321(9)	O1_17–C1_17	1.317(7)
C4_12–F9_12	1.340(8)	C1_17–C2_17	1.540(8)
C4_12–F8_12	1.344(10)	C1_17–C4_17	1.566(8)
O1_13–C1_13	1.344(7)	C1_17–C3_17	1.572(9)
C1_13–C4_13	1.541(7)	C2_17–F3_17	1.319(8)
C1_13–C2_13	1.547(7)	C2_17–F1_17	1.334(8)
C1_13–C3_13	1.565(7)	C2_17–F2_17	1.339(7)
C2_13–F3_13	1.319(7)	C3_17–F5_17	1.295(9)
C2_13–F1_13	1.330(7)	C3_17–F6_17	1.329(8)
C2_13–F2_13	1.351(7)	C3_17–F4_17	1.380(9)
C3_13–F5_13	1.321(7)	C4_17–F8_17	1.289(8)
C3_13–F6_13	1.334(6)	C4_17–F7_17	1.334(8)
C3_13–F4_13	1.337(7)	C4_17–F9_17	1.378(8)
C4_13–F9_13	1.328(6)	C1_18–F1_18	1.346(6)
C4_13–F7_13	1.336(7)	C1_18–C6_18	1.363(7)
C4_13–F8_13	1.358(6)	C1_18–C2_18	1.375(6)
O1_14–C1_14	1.368(8)	C2_18–F2_18	1.345(6)
C1_14–C4_14	1.531(9)	C2_18–C3_18	1.367(7)
C1_14–C2_14	1.544(9)	C3_18–C4_18	1.382(7)
C1_14–C3_14	1.549(9)	C3_18–H3_18	0.9500
C2_14–F3_14	1.289(9)	C4_18–C5_18	1.372(7)
C2_14–F2_14	1.299(8)	C4_18–H4_18	0.9500
C2_14–F1_14	1.388(10)	C5_18–C6_18	1.373(7)
C3_14–F4_14	1.297(10)	C5_18–H5_18	0.9500
C3_14–F6_14	1.321(9)	C6_18–H6_18	0.9500
C3_14–F5_14	1.370(10)	O1_20–C1_20	1.345(7)
C4_14–F9_14	1.234(10)	C1_20–C4_20	1.519(9)
C4_14–F8_14	1.333(11)	C1_20–C3_20	1.548(9)
C4_14–F7_14	1.383(10)	C1_20–C2_20	1.578(9)
O1_15–C1_15	1.346(7)	C2_20–F3_20	1.287(9)
C1_15–C4_15	1.547(8)	C2_20–F2_20	1.342(8)
C1_15–C3_15	1.558(7)	C2_20–F1_20	1.387(9)
C1_15–C2_15	1.561(7)	C3_20–F4_20	1.321(8)
C2_15–F2_15	1.326(7)	C3_20–F6_20	1.353(8)
C2_15–F3_15	1.327(7)	C3_20–F5_20	1.379(9)
C2_15–F1_15	1.327(6)	C4_20–F9_20	1.277(8)
C3_15–F4_15	1.314(7)	C4_20–F8_20	1.330(7)
C3_15–F5_15	1.332(7)	C4_20–F7_20	1.388(10)
C3_15–F6_15	1.334(7)	O1_23–C1_23	1.358(10)
C4_15–F9_15	1.323(7)	C1_23–C3_23	1.543(11)
C4_15–F8_15	1.332(7)	C1_23–C2_23	1.545(11)
C4_15–F7_15	1.333(8)	C1_23–C4_23	1.551(11)
O1_16–C1_16	1.347(9)	C2_23–F1_23	1.312(11)
C1_16–C3_16	1.537(9)	C2_23–F3_23	1.313(11)
C1_16–C4_16	1.558(9)	C2_23–F2_23	1.328(11)
C1_16–C2_16	1.562(9)	C3_23–F5_23	1.330(12)
C2_16–F3_16	1.315(8)	C3_23–F6_23	1.336(12)
C2_16–F2_16	1.340(8)	C3_23–F4_23	1.336(11)

C4_23–F9_23	1.313(11)	O1_30–C1_30	1.353(10)
C4_23–F8_23	1.319(11)	C1_30–C2_30	1.535(11)
C4_23–F7_23	1.324(11)	C1_30–C4_30	1.545(11)
O1_24–C1_24	1.362(10)	C1_30–C3_30	1.550(11)
C1_24–C4_24	1.546(11)	C2_30–F3_30	1.270(12)
C1_24–C2_24	1.552(10)	C2_30–F1_30	1.276(11)
C1_24–C3_24	1.559(11)	C2_30–F2_30	1.355(11)
C2_24–F3_24	1.320(10)	C3_30–F6_30	1.308(10)
C2_24–F2_24	1.330(9)	C3_30–F5_30	1.315(11)
C2_24–F1_24	1.332(11)	C3_30–F4_30	1.327(11)
C3_24–F5_24	1.332(11)	C4_30–F9_30	1.301(12)
C3_24–F4_24	1.334(10)	C4_30–F7_30	1.333(11)
C3_24–F6_24	1.341(9)	C4_30–F8_30	1.341(11)
C4_24–F7_24	1.316(10)	O1_31–C1_31	1.349(11)
C4_24–F9_24	1.319(10)	C1_31–C3_31	1.539(10)
C4_24–F8_24	1.351(9)	C1_31–C2_31	1.547(11)
O1_25–C1_25	1.356(10)	C1_31–C4_31	1.549(11)
C1_25–C3_25	1.538(10)	C2_31–F3_31	1.310(11)
C1_25–C4_25	1.551(11)	C2_31–F2_31	1.325(11)
C1_25–C2_25	1.554(11)	C2_31–F1_31	1.337(12)
C2_25–F3_25	1.313(11)	C3_31–F4_31	1.294(11)
C2_25–F1_25	1.323(10)	C3_31–F6_31	1.321(11)
C2_25–F2_25	1.342(10)	C3_31–F5_31	1.343(11)
C3_25–F6_25	1.258(10)	C4_31–F9_31	1.318(11)
C3_25–F5_25	1.278(12)	C4_31–F7_31	1.324(12)
C3_25–F4_25	1.325(10)	C4_31–F8_31	1.326(11)
C4_25–F8_25	1.286(10)	O1_33–C1_33	1.344(12)
C4_25–F9_25	1.292(11)	C1_33–C2_33	1.545(11)
C4_25–F7_25	1.385(11)	C1_33–C3_33	1.551(11)
O1_26–C1_26	1.345(10)	C1_33–C4_33	1.555(11)
C1_26–C2_26	1.538(10)	C2_33–F2_33	1.287(11)
C1_26–C3_26	1.561(10)	C2_33–F3_33	1.340(11)
C1_26–C4_26	1.563(10)	C2_33–F1_33	1.395(12)
C2_26–F3_26	1.336(11)	C3_33–F4_33	1.325(11)
C2_26–F2_26	1.336(10)	C3_33–F6_33	1.327(11)
C2_26–F1_26	1.345(11)	C3_33–F5_33	1.358(12)
C3_26–F4_26	1.308(10)	C4_33–F7_33	1.340(12)
C3_26–F5_26	1.328(9)	C4_33–F8_33	1.343(11)
C3_26–F6_26	1.340(11)	C4_33–F9_33	1.347(12)
C4_26–F8_26	1.308(9)	O1_34–C1_34	1.303(11)
C4_26–F7_26	1.330(11)	C1_34–C4_34	1.531(11)
C4_26–F9_26	1.349(11)	C1_34–C3_34	1.560(11)
O1_29–C1_29	1.375(10)	C1_34–C2_34	1.564(11)
C1_29–C3_29	1.547(10)	C2_34–F3_34	1.308(11)
C1_29–C4_29	1.553(10)	C2_34–F2_34	1.312(12)
C1_29–C2_29	1.564(10)	C2_34–F1_34	1.360(11)
C2_29–F1_29	1.303(11)	C3_34–F6_34	1.295(11)
C2_29–F3_29	1.327(11)	C3_34–F5_34	1.328(11)
C2_29–F2_29	1.328(11)	C3_34–F4_34	1.337(12)
C3_29–F4_29	1.317(9)	C4_34–F9_34	1.318(12)
C3_29–F5_29	1.339(9)	C4_34–F8_34	1.327(11)
C3_29–F6_29	1.342(11)	C4_34–F7_34	1.339(11)
C4_29–F7_29	1.299(10)	O1_35–C1_35	1.361(13)
C4_29–F8_29	1.328(10)	C1_35–C3_35	1.542(12)
C4_29–F9_29	1.354(9)	C1_35–C4_35	1.546(12)

C1_35–C2_35	1.551(12)	C2_41–F1_41	1.334(12)
C2_35–F3_35	1.320(12)	C3_41–F5_41	1.328(12)
C2_35–F1_35	1.325(13)	C3_41–F4_41	1.340(12)
C2_35–F2_35	1.329(13)	C3_41–F6_41	1.341(12)
C3_35–F5_35	1.323(13)	C4_41–F7_41	1.282(13)
C3_35–F4_35	1.323(13)	C4_41–F8_41	1.307(12)
C3_35–F6_35	1.335(12)	C4_41–F9_41	1.322(12)
C4_35–F9_35	1.323(13)	O1_42–C1_42	1.337(13)
C4_35–F8_35	1.337(12)	C1_42–C4_42	1.540(12)
C4_35–F7_35	1.344(13)	C1_42–C3_42	1.544(12)
O1_27–C1_27	1.325(9)	C1_42–C2_42	1.560(12)
C1_27–C2_27	1.531(10)	C2_42–F1_42	1.311(13)
C1_27–C4_27	1.546(10)	C2_42–F2_42	1.320(13)
C1_27–C3_27	1.559(10)	C2_42–F3_42	1.321(13)
C2_27–F3_27	1.313(11)	C3_42–F4_42	1.327(13)
C2_27–F2_27	1.314(10)	C3_42–F6_42	1.340(13)
C2_27–F1_27	1.323(10)	C3_42–F5_42	1.354(13)
C3_27–F6_27	1.280(10)	C4_42–F9_42	1.333(13)
C3_27–F4_27	1.312(11)	C4_42–F8_42	1.335(13)
C3_27–F5_27	1.336(11)	C4_42–F7_42	1.340(13)
C4_27–F9_27	1.298(11)	O1_43–C1_43	1.347(9)
C4_27–F8_27	1.326(10)	C1_43–C4_43	1.534(10)
C4_27–F7_27	1.344(11)	C1_43–C2_43	1.545(10)
O1_36–C1_36	1.351(10)	C1_43–C3_43	1.583(10)
C1_36–C3_36	1.546(11)	C2_43–F3_43	1.325(10)
C1_36–C2_36	1.547(10)	C2_43–F2_43	1.331(9)
C1_36–C4_36	1.548(10)	C2_43–F1_43	1.339(10)
C2_36–F2_36	1.318(11)	C3_43–F6_43	1.324(9)
C2_36–F3_36	1.329(10)	C3_43–F4_43	1.334(10)
C2_36–F1_36	1.338(10)	C3_43–F5_43	1.359(10)
C3_36–F5_36	1.305(11)	C4_43–F9_43	1.334(10)
C3_36–F4_36	1.326(11)	C4_43–F8_43	1.358(9)
C3_36–F6_36	1.339(11)	C4_43–F7_43	1.356(10)
C4_36–F7_36	1.312(10)	O1_44–C1_44	1.349(9)
C4_36–F8_36	1.330(11)	C1_44–C2_44	1.534(10)
C4_36–F9_36	1.332(11)	C1_44–C3_44	1.534(10)
O1_37–C1_37	1.348(12)	C1_44–C4_44	1.558(10)
C1_37–C2_37	1.549(12)	C2_44–F2_44	1.312(10)
C1_37–C4_37	1.550(12)	C2_44–F3_44	1.317(10)
C1_37–C3_37	1.550(12)	C2_44–F1_44	1.320(9)
C2_37–F1_37	1.324(12)	C3_44–F4_44	1.310(10)
C2_37–F3_37	1.327(12)	C3_44–F6_44	1.330(9)
C2_37–F2_37	1.346(12)	C3_44–F5_44	1.341(11)
C3_37–F5_37	1.319(13)	C4_44–F8_44	1.315(11)
C3_37–F4_37	1.329(12)	C4_44–F9_44	1.328(11)
C3_37–F6_37	1.348(13)	C4_44–F7_44	1.343(11)
C4_37–F8_37	1.338(12)	O1_46–C1_46	1.363(10)
C4_37–F9_37	1.342(12)	C1_46–C2_46	1.541(11)
C4_37–F7_37	1.345(12)	C1_46–C4_46	1.551(11)
O1_41–C1_41	1.354(12)	C1_46–C3_46	1.557(11)
C1_41–C2_41	1.536(12)	C2_46–F2_46	1.337(11)
C1_41–C3_41	1.540(12)	C2_46–F1_46	1.338(12)
C1_41–C4_41	1.551(12)	C2_46–F3_46	1.338(11)
C2_41–F2_41	1.322(12)	C3_46–F5_46	1.323(10)
C2_41–F3_41	1.326(12)	C3_46–F4_46	1.328(10)

C3_46–F6_46	1.342(11)	C4_64–F9_64	1.350(12)
C4_46–F7_46	1.324(12)	O1_65–C1_65	1.345(13)
C4_46–F8_46	1.336(11)	C1_65–C3_65	1.546(12)
C4_46–F9_46	1.343(11)	C1_65–C2_65	1.550(12)
O1_61–C1_61	1.356(12)	C1_65–C4_65	1.565(12)
C1_61–C4_61	1.546(12)	C2_65–F2_65	1.329(13)
C1_61–C3_61	1.552(12)	C2_65–F3_65	1.331(13)
C1_61–C2_61	1.554(12)	C2_65–F1_65	1.340(13)
C2_61–F3_61	1.324(13)	C3_65–F5_65	1.326(13)
C2_61–F2_61	1.332(12)	C3_65–F6_65	1.331(13)
C2_61–F1_61	1.333(12)	C3_65–F4_65	1.336(12)
C3_61–F6_61	1.325(12)	C4_65–F7_65	1.314(12)
C3_61–F5_61	1.325(13)	C4_65–F8_65	1.327(12)
C3_61–F4_61	1.334(12)	C4_65–F9_65	1.329(13)
C4_61–F9_61	1.336(12)	C1_19–C6_19	1.328(9)
C4_61–F8_61	1.337(12)	C1_19–F1_19	1.341(9)
C4_61–F7_61	1.338(13)	C1_19–C2_19	1.396(10)
O1_62–C1_62	1.335(13)	C2_19–F2_19	1.330(9)
C1_62–C4_62	1.547(12)	C2_19–C3_19	1.370(10)
C1_62–C2_62	1.551(12)	C3_19–C4_19	1.363(10)
C1_62–C3_62	1.559(12)	C3_19–H3_19	0.9500
C2_62–F3_62	1.314(12)	C4_19–C5_19	1.367(9)
C2_62–F1_62	1.317(13)	C4_19–H4_19	0.9500
C2_62–F2_62	1.392(14)	C5_19–C6_19	1.365(9)
C3_62–F6_62	1.310(12)	C5_19–H5_19	0.9500
C3_62–F5_62	1.316(13)	C6_19–H6_19	0.9500
C3_62–F4_62	1.332(13)	O1_67–C1_67	1.343(13)
C4_62–F7_62	1.307(13)	C1_67–C2_67	1.541(12)
C4_62–F8_62	1.330(12)	C1_67–C4_67	1.542(12)
C4_62–F9_62	1.344(13)	C1_67–C3_67	1.558(13)
O1_63–C1_63	1.326(13)	C2_67–F3_67	1.322(13)
C1_63–C4_63	1.541(12)	C2_67–F1_67	1.330(13)
C1_63–C3_63	1.549(12)	C2_67–F2_67	1.347(13)
C1_63–C2_63	1.567(12)	C3_67–F6_67	1.313(13)
C2_63–F2_63	1.301(13)	C3_67–F5_67	1.320(13)
C2_63–F3_63	1.323(13)	C3_67–F4_67	1.324(13)
C2_63–F1_63	1.344(13)	C4_67–F9_67	1.319(13)
C3_63–F4_63	1.301(12)	C4_67–F7_67	1.329(13)
C3_63–F5_63	1.343(13)	C4_67–F8_67	1.340(13)
C3_63–F6_63	1.364(13)	O1_38–C1_38	1.367(12)
C4_63–F8_63	1.302(13)	C1_38–C2_38	1.549(11)
C4_63–F9_63	1.345(13)	C1_38–C4_38	1.555(12)
C4_63–F7_63	1.345(13)	C1_38–C3_38	1.566(11)
O1_64–C1_64	1.335(12)	C2_38–F2_38	1.331(12)
C1_64–C2_64	1.538(12)	C2_38–F1_38	1.331(13)
C1_64–C3_64	1.541(12)	C2_38–F3_38	1.338(12)
C1_64–C4_64	1.584(12)	C3_38–F6_38	1.319(12)
C2_64–F3_64	1.320(12)	C3_38–F5_38	1.342(13)
C2_64–F2_64	1.344(13)	C3_38–F4_38	1.392(12)
C2_64–F1_64	1.352(12)	C4_38–F8_38	1.281(12)
C3_64–F4_64	1.325(12)	C4_38–F7_38	1.329(12)
C3_64–F5_64	1.338(13)	C4_38–F9_38	1.354(12)
C3_64–F6_64	1.394(13)	O1_21–C1_21	1.377(10)
C4_64–F8_64	1.256(12)	C1_21–C3_21	1.530(9)
C4_64–F7_64	1.332(12)	C1_21–C4_21	1.549(9)

C1_21–C2_21	1.561(9)	C9A_45–H9AB_45	0.9800
C2_21–F2_21	1.319(9)	C9A_45–H9AC_45	0.9800
C2_21–F3_21	1.332(10)	C8A_45–H8AA_45	0.9800
C2_21–F1_21	1.357(10)	C8A_45–H8AB_45	0.9800
C3_21–F5_21	1.327(9)	C8A_45–H8AC_45	0.9800
C3_21–F4_21	1.337(8)	C7A_45–H7AA_45	0.9800
C3_21–F6_21	1.345(8)	C7A_45–H7AB_45	0.9800
C4_21–F9_21	1.304(10)	C7A_45–H7AC_45	0.9800
C4_21–F7_21	1.322(9)	C6A_45–H6AA_45	0.9800
C4_21–F8_21	1.355(9)	C6A_45–H6AB_45	0.9800
O1_28–C1_28	1.340(12)	C6A_45–H6AC_45	0.9800
C1_28–C4_28	1.535(11)	C1B_45–C5B_45	1.419(5)
C1_28–C2_28	1.558(11)	C1B_45–C2B_45	1.419(5)
C1_28–C3_28	1.562(11)	C1B_45–C6B_45	1.505(5)
C2_28–F1_28	1.315(12)	C2B_45–C3B_45	1.417(5)
C2_28–F3_28	1.323(12)	C2B_45–C7B_45	1.513(5)
C2_28–F2_28	1.333(12)	C3B_45–C4B_45	1.422(4)
C3_28–F5_28	1.318(12)	C3B_45–C8B_45	1.499(5)
C3_28–F6_28	1.344(12)	C4B_45–C5B_45	1.420(4)
C3_28–F4_28	1.347(12)	C4B_45–C9B_45	1.501(4)
C4_28–F7_28	1.332(12)	C5B_45–C10B_45	1.508(5)
C4_28–F9_28	1.333(11)	C10B_45–H10D_45	0.9800
C4_28–F8_28	1.337(11)	C10B_45–H10E_45	0.9800
In1_45–Al3_45	2.7396(15)	C10B_45–H10F_45	0.9800
In1_45–Al1_45	2.7575(13)	C9B_45–H9BA_45	0.9800
In1_45–Al2_45	2.7635(13)	C9B_45–H9BB_45	0.9800
Al2_45–C1B_45	2.221(4)	C9B_45–H9BC_45	0.9800
Al2_45–C5B_45	2.227(3)	C8B_45–H8BA_45	0.9800
Al2_45–C4B_45	2.243(3)	C8B_45–H8BB_45	0.9800
Al2_45–C2B_45	2.244(4)	C8B_45–H8BC_45	0.9800
Al2_45–C3B_45	2.255(3)	C7B_45–H7BA_45	0.9800
Al3_45–C1C_45	2.226(3)	C7B_45–H7BB_45	0.9800
Al3_45–C5C_45	2.228(3)	C7B_45–H7BC_45	0.9800
Al3_45–C2C_45	2.229(3)	C6B_45–H6BA_45	0.9800
Al3_45–C4C_45	2.241(3)	C6B_45–H6BB_45	0.9800
Al3_45–C3C_45	2.251(4)	C6B_45–H6BC_45	0.9800
Al1_45–C3A_45	2.204(3)	C1C_45–C2C_45	1.420(4)
Al1_45–C2A_45	2.221(3)	C1C_45–C5C_45	1.431(4)
Al1_45–C4A_45	2.221(3)	C1C_45–C6C_45	1.495(5)
Al1_45–C5A_45	2.240(3)	C2C_45–C3C_45	1.403(5)
Al1_45–C1A_45	2.243(3)	C2C_45–C7C_45	1.514(5)
C1A_45–C2A_45	1.424(4)	C3C_45–C4C_45	1.409(5)
C1A_45–C5A_45	1.428(4)	C3C_45–C8C_45	1.508(5)
C1A_45–C6A_45	1.504(5)	C4C_45–C5C_45	1.430(5)
C2A_45–C3A_45	1.429(5)	C4C_45–C9C_45	1.507(5)
C2A_45–C7A_45	1.505(4)	C5C_45–C10C_45	1.496(5)
C3A_45–C4A_45	1.437(4)	C10C_45–H10G_45	0.9800
C3A_45–C8A_45	1.493(5)	C10C_45–H10H_45	0.9800
C4A_45–C5A_45	1.418(4)	C10C_45–H10I_45	0.9800
C4A_45–C9A_45	1.502(4)	C9C_45–H9CA_45	0.9800
C5A_45–C10A_45	1.504(4)	C9C_45–H9CB_45	0.9800
C10A_45–H10A_45	0.9800	C9C_45–H9CC_45	0.9800
C10A_45–H10B_45	0.9800	C8C_45–H8CA_45	0.9800
C10A_45–H10C_45	0.9800	C8C_45–H8CB_45	0.9800
C9A_45–H9AA_45	0.9800	C8C_45–H8CC_45	0.9800

C7C_45–H7CA_45	0.9800	C3B_66–C8B_66	1.498(5)
C7C_45–H7CB_45	0.9800	C4B_66–C5B_66	1.424(5)
C7C_45–H7CC_45	0.9800	C4B_66–C9B_66	1.502(5)
C6C_45–H6CA_45	0.9800	C5B_66–C10B_66	1.503(5)
C6C_45–H6CB_45	0.9800	C10B_66–H10D_66	0.9800
C6C_45–H6CC_45	0.9800	C10B_66–H10E_66	0.9800
In1_66–Al1_66	2.7322(19)	C10B_66–H10F_66	0.9800
In1_66–Al3_66	2.7411(19)	C9B_66–H9BA_66	0.9800
In1_66–Al2_66	2.7500(14)	C9B_66–H9BB_66	0.9800
Al2_66–C5B_66	2.214(3)	C9B_66–H9BC_66	0.9800
Al2_66–C1B_66	2.220(3)	C8B_66–H8BA_66	0.9800
Al2_66–C2B_66	2.232(3)	C8B_66–H8BB_66	0.9800
Al2_66–C4B_66	2.238(3)	C8B_66–H8BC_66	0.9800
Al2_66–C3B_66	2.246(3)	C7B_66–H7BA_66	0.9800
Al3_66–C1C_66	2.199(3)	C7B_66–H7BB_66	0.9800
Al3_66–C2C_66	2.203(4)	C7B_66–H7BC_66	0.9800
Al3_66–C5C_66	2.224(3)	C6B_66–H6BA_66	0.9800
Al3_66–C3C_66	2.237(3)	C6B_66–H6BB_66	0.9800
Al3_66–C4C_66	2.242(3)	C6B_66–H6BC_66	0.9800
Al1_66–C2A_66	2.218(4)	C1C_66–C5C_66	1.424(4)
Al1_66–C1A_66	2.224(4)	C1C_66–C2C_66	1.436(4)
Al1_66–C3A_66	2.231(3)	C1C_66–C6C_66	1.501(5)
Al1_66–C5A_66	2.247(4)	C2C_66–C3C_66	1.424(5)
Al1_66–C4A_66	2.248(4)	C2C_66–C7C_66	1.507(5)
C1A_66–C5A_66	1.426(6)	C3C_66–C4C_66	1.422(5)
C1A_66–C2A_66	1.436(5)	C3C_66–C8C_66	1.506(5)
C1A_66–C6A_66	1.502(6)	C4C_66–C5C_66	1.426(4)
C2A_66–C3A_66	1.414(5)	C4C_66–C9C_66	1.504(5)
C2A_66–C7A_66	1.503(5)	C5C_66–C10C_66	1.503(4)
C3A_66–C4A_66	1.421(5)	C10C_66–H10G_66	0.9800
C3A_66–C8A_66	1.506(5)	C10C_66–H10H_66	0.9800
C4A_66–C5A_66	1.405(5)	C10C_66–H10I_66	0.9800
C4A_66–C9A_66	1.500(6)	C9C_66–H9CA_66	0.9800
C5A_66–C10A_66	1.511(5)	C9C_66–H9CB_66	0.9800
C10A_66–H10A_66	0.9800	C9C_66–H9CC_66	0.9800
C10A_66–H10B_66	0.9800	C8C_66–H8CA_66	0.9800
C10A_66–H10C_66	0.9800	C8C_66–H8CB_66	0.9800
C9A_66–H9AA_66	0.9800	C8C_66–H8CC_66	0.9800
C9A_66–H9AB_66	0.9800	C7C_66–H7CA_66	0.9800
C9A_66–H9AC_66	0.9800	C7C_66–H7CB_66	0.9800
C8A_66–H8AA_66	0.9800	C7C_66–H7CC_66	0.9800
C8A_66–H8AB_66	0.9800	C6C_66–H6CA_66	0.9800
C8A_66–H8AC_66	0.9800	C6C_66–H6CB_66	0.9800
C7A_66–H7AA_66	0.9800	C6C_66–H6CC_66	0.9800
C7A_66–H7AB_66	0.9800	In1_68–Al3_68	2.7318(12)
C7A_66–H7AC_66	0.9800	In1_68–Al2_68	2.7351(15)
C6A_66–H6AA_66	0.9800	In1_68–Al1_68	2.7396(13)
C6A_66–H6AB_66	0.9800	Al2_68–C5B_68	2.199(5)
C6A_66–H6AC_66	0.9800	Al2_68–C4B_68	2.207(5)
C1B_66–C2B_66	1.415(5)	Al2_68–C3B_68	2.209(5)
C1B_66–C5B_66	1.427(5)	Al2_68–C1B_68	2.210(5)
C1B_66–C6B_66	1.506(5)	Al2_68–C2B_68	2.225(5)
C2B_66–C3B_66	1.413(5)	Al3_68–C1C_68	2.207(4)
C2B_66–C7B_66	1.507(5)	Al3_68–C2C_68	2.212(4)
C3B_66–C4B_66	1.425(5)	Al3_68–C5C_68	2.232(4)

Al3_68–C3C_68	2.233(4)	C6B_68–H6BB_68	0.9800
Al3_68–C4C_68	2.240(3)	C6B_68–H6BC_68	0.9800
Al1_68–C1A_68	2.220(4)	C1C_68–C2C_68	1.422(6)
Al1_68–C2A_68	2.222(4)	C1C_68–C5C_68	1.439(6)
Al1_68–C4A_68	2.233(4)	C1C_68–C6C_68	1.490(6)
Al1_68–C5A_68	2.233(4)	C2C_68–C3C_68	1.410(5)
Al1_68–C3A_68	2.239(4)	C2C_68–C7C_68	1.519(6)
C1A_68–C2A_68	1.425(7)	C3C_68–C4C_68	1.416(5)
C1A_68–C5A_68	1.430(6)	C3C_68–C8C_68	1.508(5)
C1A_68–C6A_68	1.499(6)	C4C_68–C5C_68	1.410(5)
C2A_68–C3A_68	1.425(6)	C4C_68–C9C_68	1.495(5)
C2A_68–C7A_68	1.506(7)	C5C_68–C10C_68	1.501(6)
C3A_68–C4A_68	1.421(7)	C10C_68–H10G_68	0.9800
C3A_68–C8A_68	1.502(7)	C10C_68–H10H_68	0.9800
C4A_68–C5A_68	1.423(7)	C10C_68–H10I_68	0.9800
C4A_68–C9A_68	1.504(6)	C9C_68–H9CA_68	0.9800
C5A_68–C10A_68	1.502(7)	C9C_68–H9CB_68	0.9800
C10A_68–H10A_68	0.9800	C9C_68–H9CC_68	0.9800
C10A_68–H10B_68	0.9800	C8C_68–H8CA_68	0.9800
C10A_68–H10C_68	0.9800	C8C_68–H8CB_68	0.9800
C9A_68–H9AA_68	0.9800	C8C_68–H8CC_68	0.9800
C9A_68–H9AB_68	0.9800	C7C_68–H7CA_68	0.9800
C9A_68–H9AC_68	0.9800	C7C_68–H7CB_68	0.9800
C8A_68–H8AA_68	0.9800	C7C_68–H7CC_68	0.9800
C8A_68–H8AB_68	0.9800	C6C_68–H6CA_68	0.9800
C8A_68–H8AC_68	0.9800	C6C_68–H6CB_68	0.9800
C7A_68–H7AA_68	0.9800	C6C_68–H6CC_68	0.9800
C7A_68–H7AB_68	0.9800	In1_69–Al1_69	2.7317(11)
C7A_68–H7AC_68	0.9800	In1_69–Al2_69	2.7553(13)
C6A_68–H6AA_68	0.9800	In1_69–Al3_69	2.7616(13)
C6A_68–H6AB_68	0.9800	Al2_69–C5B_69	2.193(4)
C6A_68–H6AC_68	0.9800	Al2_69–C4B_69	2.220(4)
C1B_68–C2B_68	1.401(6)	Al2_69–C1B_69	2.220(4)
C1B_68–C5B_68	1.411(7)	Al2_69–C2B_69	2.233(4)
C1B_68–C6B_68	1.518(7)	Al2_69–C3B_69	2.243(4)
C2B_68–C3B_68	1.409(7)	Al3_69–C2C_69	2.222(4)
C2B_68–C7B_68	1.509(7)	Al3_69–C1C_69	2.224(4)
C3B_68–C4B_68	1.438(8)	Al3_69–C5C_69	2.233(4)
C3B_68–C8B_68	1.504(7)	Al3_69–C3C_69	2.236(4)
C4B_68–C5B_68	1.432(7)	Al3_69–C4C_69	2.239(4)
C4B_68–C9B_68	1.506(8)	Al1_69–C1A_69	2.223(3)
C5B_68–C10B_68	1.505(7)	Al1_69–C2A_69	2.224(3)
C10B_68–H10D_68	0.9800	Al1_69–C3A_69	2.235(3)
C10B_68–H10E_68	0.9800	Al1_69–C5A_69	2.235(4)
C10B_68–H10F_68	0.9800	Al1_69–C4A_69	2.249(3)
C9B_68–H9BA_68	0.9800	C1A_69–C2A_69	1.418(5)
C9B_68–H9BB_68	0.9800	C1A_69–C5A_69	1.436(6)
C9B_68–H9BC_68	0.9800	C1A_69–C6A_69	1.502(6)
C8B_68–H8BA_68	0.9800	C2A_69–C3A_69	1.407(5)
C8B_68–H8BB_68	0.9800	C2A_69–C7A_69	1.509(5)
C8B_68–H8BC_68	0.9800	C3A_69–C4A_69	1.402(5)
C7B_68–H7BA_68	0.9800	C3A_69–C8A_69	1.510(5)
C7B_68–H7BB_68	0.9800	C4A_69–C5A_69	1.408(6)
C7B_68–H7BC_68	0.9800	C4A_69–C9A_69	1.507(6)
C6B_68–H6BA_68	0.9800	C5A_69–C10A_69	1.513(6)

C10A_69–H10A_69	0.9800	C9C_69–H9CC_69	0.9800
C10A_69–H10B_69	0.9800	C8C_69–H8CA_69	0.9800
C10A_69–H10C_69	0.9800	C8C_69–H8CB_69	0.9800
C9A_69–H9AA_69	0.9800	C8C_69–H8CC_69	0.9800
C9A_69–H9AB_69	0.9800	C7C_69–H7CA_69	0.9800
C9A_69–H9AC_69	0.9800	C7C_69–H7CB_69	0.9800
C8A_69–H8AA_69	0.9800	C7C_69–H7CC_69	0.9800
C8A_69–H8AB_69	0.9800	C6C_69–H6CA_69	0.9800
C8A_69–H8AC_69	0.9800	C6C_69–H6CB_69	0.9800
C7A_69–H7AA_69	0.9800	C6C_69–H6CC_69	0.9800
C7A_69–H7AB_69	0.9800	In1_47–Al3_47	2.734(13)
C7A_69–H7AC_69	0.9800	In1_47–Al2_47	2.734(13)
C6A_69–H6AA_69	0.9800	In1_47–Al1_47	2.746(12)
C6A_69–H6AB_69	0.9800	Al2_47–C5B_47	2.207(15)
C6A_69–H6AC_69	0.9800	Al2_47–C1B_47	2.219(15)
C1B_69–C5B_69	1.408(6)	Al2_47–C4B_47	2.220(15)
C1B_69–C2B_69	1.423(5)	Al2_47–C3B_47	2.229(15)
C1B_69–C6B_69	1.518(6)	Al2_47–C2B_47	2.230(15)
C2B_69–C3B_69	1.407(6)	Al3_47–C1C_47	2.217(15)
C2B_69–C7B_69	1.504(6)	Al3_47–C2C_47	2.221(15)
C3B_69–C4B_69	1.416(6)	Al3_47–C5C_47	2.229(15)
C3B_69–C8B_69	1.512(6)	Al3_47–C4C_47	2.240(15)
C4B_69–C5B_69	1.437(6)	Al3_47–C3C_47	2.242(15)
C4B_69–C9B_69	1.492(7)	Al1_47–C2A_47	2.226(15)
C5B_69–C10B_69	1.502(5)	Al1_47–C1A_47	2.228(15)
C10B_69–H10D_69	0.9800	Al1_47–C3A_47	2.232(15)
C10B_69–H10E_69	0.9800	Al1_47–C4A_47	2.239(15)
C10B_69–H10F_69	0.9800	Al1_47–C5A_47	2.246(15)
C9B_69–H9BA_69	0.9800	C1A_47–C2A_47	1.426(15)
C9B_69–H9BB_69	0.9800	C1A_47–C5A_47	1.426(14)
C9B_69–H9BC_69	0.9800	C1A_47–C6A_47	1.503(15)
C8B_69–H8BA_69	0.9800	C2A_47–C3A_47	1.422(14)
C8B_69–H8BB_69	0.9800	C2A_47–C7A_47	1.512(15)
C8B_69–H8BC_69	0.9800	C3A_47–C4A_47	1.417(14)
C7B_69–H7BA_69	0.9800	C3A_47–C8A_47	1.504(15)
C7B_69–H7BB_69	0.9800	C4A_47–C5A_47	1.421(15)
C7B_69–H7BC_69	0.9800	C4A_47–C9A_47	1.510(15)
C6B_69–H6BA_69	0.9800	C5A_47–C10A_47	1.513(15)
C6B_69–H6BB_69	0.9800	C10A_47–H10A_47	0.9800
C6B_69–H6BC_69	0.9800	C10A_47–H10B_47	0.9800
C1C_69–C5C_69	1.419(6)	C10A_47–H10C_47	0.9800
C1C_69–C2C_69	1.423(6)	C9A_47–H9AA_47	0.9800
C1C_69–C6C_69	1.496(6)	C9A_47–H9AB_47	0.9800
C2C_69–C3C_69	1.428(6)	C9A_47–H9AC_47	0.9800
C2C_69–C7C_69	1.504(6)	C8A_47–H8AA_47	0.9800
C3C_69–C4C_69	1.430(6)	C8A_47–H8AB_47	0.9800
C3C_69–C8C_69	1.494(6)	C8A_47–H8AC_47	0.9800
C4C_69–C5C_69	1.433(5)	C7A_47–H7AA_47	0.9800
C4C_69–C9C_69	1.487(6)	C7A_47–H7AB_47	0.9800
C5C_69–C10C_69	1.497(6)	C7A_47–H7AC_47	0.9800
C10C_69–H10G_69	0.9800	C6A_47–H6AA_47	0.9800
C10C_69–H10H_69	0.9800	C6A_47–H6AB_47	0.9800
C10C_69–H10I_69	0.9800	C6A_47–H6AC_47	0.9800
C9C_69–H9CA_69	0.9800	C1B_47–C5B_47	1.415(15)
C9C_69–H9CB_69	0.9800	C1B_47–C2B_47	1.418(14)

C1B_47–C6B_47	1.520(15)	Al2_48–C4B_48	2.227(15)
C2B_47–C3B_47	1.417(15)	Al3_48–C1C_48	2.225(15)
C2B_47–C7B_47	1.511(15)	Al3_48–C2C_48	2.240(15)
C3B_47–C4B_47	1.421(15)	Al3_48–C5C_48	2.250(15)
C3B_47–C8B_47	1.506(15)	Al3_48–C3C_48	2.266(15)
C4B_47–C5B_47	1.434(15)	Al3_48–C4C_48	2.274(15)
C4B_47–C9B_47	1.504(15)	Al1_48–C3A_48	2.220(15)
C5B_47–C10B_47	1.509(15)	Al1_48–C4A_48	2.225(15)
C10B_47–H10D_47	0.9800	Al1_48–C1A_48	2.224(15)
C10B_47–H10E_47	0.9800	Al1_48–C2A_48	2.228(15)
C10B_47–H10F_47	0.9800	Al1_48–C5A_48	2.251(15)
C9B_47–H9BA_47	0.9800	C1A_48–C5A_48	1.424(14)
C9B_47–H9BB_47	0.9800	C1A_48–C2A_48	1.426(14)
C9B_47–H9BC_47	0.9800	C1A_48–C6A_48	1.505(15)
C8B_47–H8BA_47	0.9800	C2A_48–C3A_48	1.422(14)
C8B_47–H8BB_47	0.9800	C2A_48–C7A_48	1.511(15)
C8B_47–H8BC_47	0.9800	C3A_48–C4A_48	1.417(14)
C7B_47–H7BA_47	0.9800	C3A_48–C8A_48	1.498(14)
C7B_47–H7BB_47	0.9800	C4A_48–C5A_48	1.418(15)
C7B_47–H7BC_47	0.9800	C4A_48–C9A_48	1.506(15)
C6B_47–H6BA_47	0.9800	C5A_48–C10A_48	1.505(15)
C6B_47–H6BB_47	0.9800	C10A_48–H10A_48	0.9800
C6B_47–H6BC_47	0.9800	C10A_48–H10B_48	0.9800
C1C_47–C2C_47	1.426(15)	C10A_48–H10C_48	0.9800
C1C_47–C5C_47	1.431(15)	C9A_48–H9AA_48	0.9800
C1C_47–C6C_47	1.497(15)	C9A_48–H9AB_48	0.9800
C2C_47–C3C_47	1.415(15)	C9A_48–H9AC_48	0.9800
C2C_47–C7C_47	1.514(15)	C8A_48–H8AA_48	0.9800
C3C_47–C4C_47	1.422(15)	C8A_48–H8AB_48	0.9800
C3C_47–C8C_47	1.513(15)	C8A_48–H8AC_48	0.9800
C4C_47–C5C_47	1.424(15)	C7A_48–H7AA_48	0.9800
C4C_47–C9C_47	1.490(15)	C7A_48–H7AB_48	0.9800
C5C_47–C10C_47	1.503(15)	C7A_48–H7AC_48	0.9800
C10C_47–H10G_47	0.9800	C6A_48–H6AA_48	0.9800
C10C_47–H10H_47	0.9800	C6A_48–H6AB_48	0.9800
C10C_47–H10I_47	0.9800	C6A_48–H6AC_48	0.9800
C9C_47–H9CA_47	0.9800	C1B_48–C5B_48	1.415(14)
C9C_47–H9CB_47	0.9800	C1B_48–C2B_48	1.418(14)
C9C_47–H9CC_47	0.9800	C1B_48–C6B_48	1.519(15)
C8C_47–H8CA_47	0.9800	C2B_48–C3B_48	1.411(15)
C8C_47–H8CB_47	0.9800	C2B_48–C7B_48	1.509(15)
C8C_47–H8CC_47	0.9800	C3B_48–C4B_48	1.431(15)
C7C_47–H7CA_47	0.9800	C3B_48–C8B_48	1.501(15)
C7C_47–H7CB_47	0.9800	C4B_48–C5B_48	1.435(14)
C7C_47–H7CC_47	0.9800	C4B_48–C9B_48	1.505(15)
C6C_47–H6CA_47	0.9800	C5B_48–C10B_48	1.514(15)
C6C_47–H6CB_47	0.9800	C10B_48–H10D_48	0.9800
C6C_47–H6CC_47	0.9800	C10B_48–H10E_48	0.9800
In1_48–Al3_48	2.716(10)	C10B_48–H10F_48	0.9800
In1_48–Al2_48	2.742(13)	C9B_48–H9BA_48	0.9800
In1_48–Al1_48	2.752(11)	C9B_48–H9BB_48	0.9800
Al2_48–C5B_48	2.211(15)	C9B_48–H9BC_48	0.9800
Al2_48–C1B_48	2.213(15)	C8B_48–H8BA_48	0.9800
Al2_48–C2B_48	2.217(15)	C8B_48–H8BB_48	0.9800
Al2_48–C3B_48	2.221(15)	C8B_48–H8BC_48	0.9800

C7B_48–H7BA_48	0.9800	C10_49–H10C_49	0.9800
C7B_48–H7BB_48	0.9800	O1_50–C1_50	1.350(12)
C7B_48–H7BC_48	0.9800	C1_50–C2_50	1.548(12)
C6B_48–H6BA_48	0.9800	C1_50–C4_50	1.548(12)
C6B_48–H6BB_48	0.9800	C1_50–C3_50	1.549(12)
C6B_48–H6BC_48	0.9800	C2_50–F3_50	1.310(13)
C1C_48–C2C_48	1.424(14)	C2_50–F2_50	1.338(12)
C1C_48–C5C_48	1.426(14)	C2_50–F1_50	1.346(13)
C1C_48–C6C_48	1.498(15)	C3_50–F4_50	1.317(13)
C2C_48–C3C_48	1.404(14)	C3_50–F5_50	1.345(13)
C2C_48–C7C_48	1.510(14)	C3_50–F6_50	1.346(12)
C3C_48–C4C_48	1.420(14)	C4_50–F9_50	1.320(13)
C3C_48–C8C_48	1.514(14)	C4_50–F8_50	1.331(13)
C4C_48–C5C_48	1.417(14)	C4_50–F7_50	1.346(13)
C4C_48–C9C_48	1.498(14)	O1_22–C1_22	1.348(8)
C5C_48–C10C_48	1.496(14)	C1_22–C3_22	1.545(9)
C10C_48–H10G_48	0.9800	C1_22–C2_22	1.550(9)
C10C_48–H10H_48	0.9800	C1_22–C4_22	1.559(9)
C10C_48–H10I_48	0.9800	C2_22–F2_22	1.285(8)
C9C_48–H9CA_48	0.9800	C2_22–F3_22	1.338(8)
C9C_48–H9CB_48	0.9800	C2_22–F1_22	1.371(11)
C9C_48–H9CC_48	0.9800	C3_22–F6_22	1.321(8)
C8C_48–H8CA_48	0.9800	C3_22–F4_22	1.334(9)
C8C_48–H8CB_48	0.9800	C3_22–F5_22	1.341(10)
C8C_48–H8CC_48	0.9800	C4_22–F9_22	1.324(10)
C7C_48–H7CA_48	0.9800	C4_22–F8_22	1.327(10)
C7C_48–H7CB_48	0.9800	C4_22–F7_22	1.331(10)
C7C_48–H7CC_48	0.9800	O1_51–C1_51	1.347(12)
C6C_48–H6CA_48	0.9800	C1_51–C4_51	1.539(12)
C6C_48–H6CB_48	0.9800	C1_51–C3_51	1.550(12)
C6C_48–H6CC_48	0.9800	C1_51–C2_51	1.567(12)
C1_49–C2_49	1.412(11)	C2_51–F2_51	1.313(13)
C1_49–C5_49	1.413(10)	C2_51–F3_51	1.323(13)
C1_49–C10_49	1.495(11)	C2_51–F1_51	1.341(13)
C2_49–C3_49	1.401(12)	C3_51–F6_51	1.315(13)
C2_49–C9_49	1.521(12)	C3_51–F4_51	1.329(13)
C3_49–C4_49	1.420(12)	C3_51–F5_51	1.343(13)
C3_49–C8_49	1.496(12)	C4_51–F9_51	1.324(13)
C4_49–C5_49	1.426(12)	C4_51–F7_51	1.333(13)
C4_49–C7_49	1.490(12)	C4_51–F8_51	1.352(13)
C5_49–C6_49	1.509(11)	O1_32–C1_32	1.339(12)
C6_49–H6A_49	0.9800	C1_32–C2_32	1.532(11)
C6_49–H6B_49	0.9800	C1_32–C4_32	1.546(12)
C6_49–H6C_49	0.9800	C1_32–C3_32	1.564(12)
C7_49–H7A_49	0.9800	C2_32–F1_32	1.310(12)
C7_49–H7B_49	0.9800	C2_32–F2_32	1.327(12)
C7_49–H7C_49	0.9800	C2_32–F3_32	1.335(12)
C8_49–H8A_49	0.9800	C3_32–F6_32	1.324(12)
C8_49–H8B_49	0.9800	C3_32–F4_32	1.326(12)
C8_49–H8C_49	0.9800	C3_32–F5_32	1.336(13)
C9_49–H9A_49	0.9800	C4_32–F9_32	1.323(12)
C9_49–H9B_49	0.9800	C4_32–F7_32	1.328(12)
C9_49–H9C_49	0.9800	C4_32–F8_32	1.354(12)
C10_49–H10A_49	0.9800	C1_40–C5_40	1.424(6)
C10_49–H10B_49	0.9800	C1_40–C2_40	1.432(5)

C1_40–C10_40	1.502(6)
C2_40–C3_40	1.416(5)
C2_40–C9_40	1.497(5)
C3_40–C4_40	1.394(6)
C3_40–C8_40	1.499(6)
C4_40–C5_40	1.409(6)
C4_40–C7_40	1.510(6)
C5_40–C6_40	1.496(6)
C6_40–H6A_40	0.9800
C6_40–H6B_40	0.9800
C6_40–H6C_40	0.9800
C7_40–H7A_40	0.9800
C7_40–H7B_40	0.9800
C7_40–H7C_40	0.9800
C8_40–H8A_40	0.9800
C8_40–H8B_40	0.9800
C8_40–H8C_40	0.9800
C9_40–H9A_40	0.9800
C9_40–H9B_40	0.9800
C9_40–H9C_40	0.9800
C10_40–H10A_40	0.9800
C10_40–H10B_40	0.9800
C10_40–H10C_40	0.9800
C1_52–C2_52	1.413(5)
C1_52–C5_52	1.427(4)
C1_52–C10_52	1.502(5)
C2_52–C3_52	1.432(6)
C2_52–C9_52	1.511(5)
C3_52–C4_52	1.422(5)
C3_52–C8_52	1.501(5)
C4_52–C5_52	1.420(4)
C4_52–C7_52	1.499(5)
C5_52–C6_52	1.502(4)
C6_52–H6A_52	0.9800
C6_52–H6B_52	0.9800
C6_52–H6C_52	0.9800
C7_52–H7A_52	0.9800
C7_52–H7B_52	0.9800
C7_52–H7C_52	0.9800
C8_52–H8A_52	0.9800
C8_52–H8B_52	0.9800
C8_52–H8C_52	0.9800
C9_52–H9A_52	0.9800
C9_52–H9B_52	0.9800
C9_52–H9C_52	0.9800
C10_52–H10A_52	0.9800
C10_52–H10B_52	0.9800
C10_52–H10C_52	0.9800
C1_53–C5_53	1.409(8)
C1_53–C2_53	1.408(7)
C1_53–C10_53	1.520(7)
C2_53–C3_53	1.413(7)
C2_53–C9_53	1.529(8)
C3_53–C4_53	1.432(8)
C3_53–C8_53	1.493(7)
C4_53–C5_53	1.431(8)
C4_53–C7_53	1.493(8)
C5_53–C6_53	1.513(8)
C6_53–H6A_53	0.9800
C6_53–H6B_53	0.9800
C6_53–H6C_53	0.9800
C7_53–H7A_53	0.9800
C7_53–H7B_53	0.9800
C7_53–H7C_53	0.9800
C8_53–H8A_53	0.9800
C8_53–H8B_53	0.9800
C8_53–H8C_53	0.9800
C9_53–H9A_53	0.9800
C9_53–H9B_53	0.9800
C9_53–H9C_53	0.9800
C10_53–H10A_53	0.9800
C10_53–H10B_53	0.9800
C10_53–H10C_53	0.9800

Atom–Atom–Atom	**Angle [°]**
O1_44–Al16–O1_67	106.7(10)
O1_12–Al16–O1_10	108.8(4)
O1_44–Al16–O1_29	122.0(5)
O1_67–Al16–O1_29	111.6(12)
O1_44–Al16–O1_23	116.0(5)
O1_67–Al16–O1_23	113.4(11)
O1_29–Al16–O1_23	86.4(4)
O1_12–Al16–O1_11	124.1(4)
O1_10–Al16–O1_11	110.06(17)
O1_12–Al16–O1_9	96.0(3)
O1_10–Al16–O1_9	109.3(2)
O1_11–Al16–O1_9	107.05(17)
O1_15–Al17–O1_13	110.2(3)
O1_15–Al17–O1_20	109.3(2)
O1_13–Al17–O1_20	113.3(4)
O1_30–Al17–O1_31	114.1(6)
O1_30–Al17–O1_24	115.9(4)
O1_31–Al17–O1_24	104.0(6)
O1_30–Al17–O1_25	110.0(4)
O1_31–Al17–O1_25	109.3(8)
O1_24–Al17–O1_25	102.7(3)
O1_15–Al17–O1_14	109.9(2)
O1_13–Al17–O1_14	106.8(4)
O1_20–Al17–O1_14	107.4(2)
O1_38–Al18–O1_32	103.1(11)
O1_22–Al18–O1_16	121.8(7)
O1_63–Al18–O1_33	99.7(15)
O1_51–Al18–O1_65	109.7(12)
O1_63–Al18–O1_28	108.3(16)
O1_33–Al18–O1_28	107.0(12)
O1_22–Al18–O1_17	106.4(5)
O1_16–Al18–O1_17	108.9(7)
O1_63–Al18–O1_27	106.5(15)
O1_33–Al18–O1_27	106.4(8)
O1_28–Al18–O1_27	125.9(9)

O1_22–Al18–O1_21	108.2(5)	C5_40–Al3–C3_40	61.47(16)
O1_16–Al18–O1_21	103.4(7)	C2_40–Al3–C3_40	36.90(13)
O1_17–Al18–O1_21	107.5(6)	C4_40–Al3–C3_40	36.13(15)
O1_26–Al19–O1_42	108.6(10)	C1_40–Al3–In1	170.09(12)
O1_8–Al19–O1_5	118.5(4)	C5_40–Al3–In1	141.64(12)
O1_8–Al19–O1_6	84.3(3)	C2_40–Al3–In1	150.46(11)
O1_5–Al19–O1_6	112.7(2)	C4_40–Al3–In1	123.82(11)
O1_8–Al19–O1_7	116.1(4)	C3_40–Al3–In1	127.40(11)
O1_5–Al19–O1_7	106.7(4)	C4_53–Al1–C3_53	38.3(2)
O1_6–Al19–O1_7	117.7(5)	C4_53–Al1–C5_53	38.2(2)
O1_26–Al19–O1_46	106.9(5)	C3_53–Al1–C5_53	63.8(2)
O1_42–Al19–O1_46	119.8(8)	C4_53–Al1–C2_53	62.6(2)
O1_26–Al19–O1_43	89.8(5)	C3_53–Al1–C2_53	37.3(2)
O1_42–Al19–O1_43	93.3(9)	C5_53–Al1–C2_53	62.3(2)
O1_46–Al19–O1_43	133.7(4)	C3_49–Al1–C4_49	37.1(4)
O1_37–Al20–O1_36	114.6(6)	C4_53–Al1–C1_53	62.5(2)
O1_37–Al20–O1_35	108.6(10)	C3_53–Al1–C1_53	62.52(19)
O1_36–Al20–O1_35	111.1(10)	C5_53–Al1–C1_53	37.0(2)
O1_4–Al20–O1_1	109.6(3)	C2_53–Al1–C1_53	36.80(17)
O1_4–Al20–O1_2	106.2(3)	C3_49–Al1–C2_49	35.8(3)
O1_1–Al20–O1_2	119.0(3)	C4_49–Al1–C2_49	59.7(5)
O1_50–Al20–O1_62	115.9(9)	C3_49–Al1–C5_49	59.8(4)
O1_37–Al20–O1_34	107.0(6)	C4_49–Al1–C5_49	35.6(4)
O1_36–Al20–O1_34	108.2(5)	C2_49–Al1–C5_49	58.0(4)
O1_35–Al20–O1_34	106.8(9)	C3_49–Al1–C1_49	58.8(4)
O1_4–Al20–O1_3	111.4(4)	C4_49–Al1–C1_49	58.3(5)
O1_1–Al20–O1_3	104.9(3)	C2_49–Al1–C1_49	34.5(3)
O1_2–Al20–O1_3	105.7(4)	C5_49–Al1–C1_49	34.0(3)
O1_50–Al20–O1_61	104.3(6)	C4_53–Al1–In1	125.44(19)
O1_62–Al20–O1_61	114.1(10)	C3_53–Al1–In1	111.01(15)
Al3–In1–Al2	70.07(4)	C5_53–Al1–In1	160.1(2)
Al3–In1–Al1	70.96(4)	C2_53–Al1–In1	126.45(14)
Al2–In1–Al1	70.53(4)	C3_49–Al1–In1	145.0(4)
C5_52–Al2–C1_52	37.31(11)	C4_49–Al1–In1	166.5(4)
C5_52–Al2–C2_52	61.75(12)	C1_53–Al1–In1	160.10(17)
C1_52–Al2–C2_52	36.76(13)	C2_49–Al1–In1	114.9(3)
C5_52–Al2–C4_52	36.94(11)	C5_49–Al1–In1	130.9(3)
C1_52–Al2–C4_52	61.85(12)	C1_49–Al1–In1	109.7(2)
C2_52–Al2–C4_52	61.61(14)	C1_1–O1_1–Al20	151.7(4)
C5_52–Al2–C3_52	61.50(12)	O1_1–C1_1–C2_1	109.5(4)
C1_52–Al2–C3_52	61.58(13)	O1_1–C1_1–C4_1	110.5(4)
C2_52–Al2–C3_52	36.98(14)	C2_1–C1_1–C4_1	112.0(5)
C4_52–Al2–C3_52	36.66(13)	O1_1–C1_1–C3_1	111.0(5)
C5_52–Al2–In1	166.58(9)	C2_1–C1_1–C3_1	107.9(4)
C1_52–Al2–In1	155.76(10)	C4_1–C1_1–C3_1	106.0(5)
C2_52–Al2–In1	126.64(10)	F3_1–C2_1–F2_1	107.7(6)
C4_52–Al2–In1	133.81(9)	F3_1–C2_1–F1_1	106.9(6)
C3_52–Al2–In1	117.55(10)	F2_1–C2_1–F1_1	108.4(5)
C1_40–Al3–C5_40	37.77(15)	F3_1–C2_1–C1_1	111.1(5)
C1_40–Al3–C2_40	37.95(14)	F2_1–C2_1–C1_1	112.8(5)
C5_40–Al3–C2_40	62.48(14)	F1_1–C2_1–C1_1	109.7(5)
C1_40–Al3–C4_40	62.27(15)	F4_1–C3_1–F5_1	107.2(6)
C5_40–Al3–C4_40	36.89(16)	F4_1–C3_1–F6_1	107.6(5)
C2_40–Al3–C4_40	61.41(13)	F5_1–C3_1–F6_1	107.6(5)
C1_40–Al3–C3_40	62.38(14)	F4_1–C3_1–C1_1	111.0(5)

F5_1–C3_1–C1_1	111.2(5)	F9_3–C4_3–C1_3	111.0(7)
F6_1–C3_1–C1_1	112.1(5)	F8_3–C4_3–C1_3	112.2(8)
F7_1–C4_1–F8_1	109.4(6)	F7_3–C4_3–C1_3	111.3(7)
F7_1–C4_1–F9_1	109.7(7)	C1_4–O1_4–Al20	149.1(6)
F8_1–C4_1–F9_1	105.0(7)	O1_4–C1_4–C3_4	110.8(7)
F7_1–C4_1–C1_1	113.0(6)	O1_4–C1_4–C4_4	109.5(7)
F8_1–C4_1–C1_1	111.8(5)	C3_4–C1_4–C4_4	117.3(7)
F9_1–C4_1–C1_1	107.6(5)	O1_4–C1_4–C2_4	104.8(7)
C1_2–O1_2–Al20	147.0(7)	C3_4–C1_4–C2_4	105.3(7)
O1_2–C1_2–C3_2	108.3(6)	C4_4–C1_4–C2_4	108.2(7)
O1_2–C1_2–C2_2	110.3(6)	F1_4–C2_4–F3_4	115.3(9)
C3_2–C1_2–C2_2	109.3(6)	F1_4–C2_4–F2_4	105.6(9)
O1_2–C1_2–C4_2	110.9(6)	F3_4–C2_4–F2_4	109.2(8)
C3_2–C1_2–C4_2	109.9(6)	F1_4–C2_4–C1_4	107.9(8)
C2_2–C1_2–C4_2	108.2(6)	F3_4–C2_4–C1_4	109.6(7)
F3_2–C2_2–F1_2	108.5(8)	F2_4–C2_4–C1_4	109.2(8)
F3_2–C2_2–F2_2	106.7(7)	F4_4–C3_4–F5_4	107.1(9)
F1_2–C2_2–F2_2	106.7(7)	F4_4–C3_4–F6_4	107.3(9)
F3_2–C2_2–C1_2	110.9(7)	F5_4–C3_4–F6_4	100.4(8)
F1_2–C2_2–C1_2	111.4(6)	F4_4–C3_4–C1_4	110.9(8)
F2_2–C2_2–C1_2	112.4(7)	F5_4–C3_4–C1_4	112.0(8)
F4_2–C3_2–F5_2	107.8(7)	F6_4–C3_4–C1_4	118.3(8)
F4_2–C3_2–F6_2	108.2(7)	F7_4–C4_4–F9_4	103.3(8)
F5_2–C3_2–F6_2	107.8(6)	F7_4–C4_4–F8_4	101.5(8)
F4_2–C3_2–C1_2	110.8(6)	F9_4–C4_4–F8_4	112.1(8)
F5_2–C3_2–C1_2	110.5(6)	F7_4–C4_4–C1_4	109.3(7)
F6_2–C3_2–C1_2	111.6(6)	F9_4–C4_4–C1_4	114.9(7)
F9_2–C4_2–F7_2	107.8(7)	F8_4–C4_4–C1_4	114.1(7)
F9_2–C4_2–F8_2	107.6(7)	C1_5–O1_5–Al19	152.7(4)
F7_2–C4_2–F8_2	107.8(7)	O1_5–C1_5–C2_5	112.2(5)
F9_2–C4_2–C1_2	111.3(6)	O1_5–C1_5–C3_5	111.7(4)
F7_2–C4_2–C1_2	109.4(6)	C2_5–C1_5–C3_5	108.7(5)
F8_2–C4_2–C1_2	112.8(6)	O1_5–C1_5–C4_5	104.8(4)
C1_3–O1_3–Al20	145.3(7)	C2_5–C1_5–C4_5	109.3(4)
O1_3–C1_3–C4_3	114.3(7)	C3_5–C1_5–C4_5	110.0(4)
O1_3–C1_3–C2_3	107.8(8)	F1_5–C2_5–F3_5	107.4(6)
C4_3–C1_3–C2_3	107.7(7)	F1_5–C2_5–F2_5	104.2(6)
O1_3–C1_3–C3_3	108.9(7)	F3_5–C2_5–F2_5	112.6(7)
C4_3–C1_3–C3_3	108.1(7)	F1_5–C2_5–C1_5	113.0(6)
C2_3–C1_3–C3_3	110.1(7)	F3_5–C2_5–C1_5	108.2(5)
F3_3–C2_3–F1_3	106.1(8)	F2_5–C2_5–C1_5	111.4(5)
F3_3–C2_3–F2_3	107.9(10)	F6_5–C3_5–F4_5	107.3(5)
F1_3–C2_3–F2_3	107.8(11)	F6_5–C3_5–F5_5	109.5(5)
F3_3–C2_3–C1_3	111.2(7)	F4_5–C3_5–F5_5	108.1(5)
F1_3–C2_3–C1_3	110.9(7)	F6_5–C3_5–C1_5	111.5(4)
F2_3–C2_3–C1_3	112.7(10)	F4_5–C3_5–C1_5	109.8(5)
F6_3–C3_3–F4_3	110.6(8)	F5_5–C3_5–C1_5	110.5(5)
F6_3–C3_3–F5_3	108.5(8)	F9_5–C4_5–F8_5	104.4(5)
F4_3–C3_3–F5_3	104.7(7)	F9_5–C4_5–F7_5	110.7(6)
F6_3–C3_3–C1_3	113.4(8)	F8_5–C4_5–F7_5	110.6(5)
F4_3–C3_3–C1_3	110.2(7)	F9_5–C4_5–C1_5	109.8(5)
F5_3–C3_3–C1_3	109.1(7)	F8_5–C4_5–C1_5	112.0(5)
F9_3–C4_3–F8_3	108.7(8)	F7_5–C4_5–C1_5	109.3(5)
F9_3–C4_3–F7_3	105.3(8)	C1_6–O1_6–Al19	149.6(5)
F8_3–C4_3–F7_3	108.0(8)	O1_6–C1_6–C4_6	110.0(6)

O1_6–C1_6–C3_6	112.6(6)	F2_8–C2_8–F3_8	111.0(10)
C4_6–C1_6–C3_6	108.1(6)	F2_8–C2_8–F1_8	107.4(10)
O1_6–C1_6–C2_6	109.5(6)	F3_8–C2_8–F1_8	108.9(11)
C4_6–C1_6–C2_6	109.1(7)	F2_8–C2_8–C1_8	111.1(10)
C3_6–C1_6–C2_6	107.5(6)	F3_8–C2_8–C1_8	109.0(9)
F1_6–C2_6–F2_6	109.4(9)	F1_8–C2_8–C1_8	109.4(9)
F1_6–C2_6–F3_6	106.2(8)	F6_8–C3_8–F4_8	108.1(9)
F2_6–C2_6–F3_6	109.1(9)	F6_8–C3_8–F5_8	92.5(8)
F1_6–C2_6–C1_6	110.1(7)	F4_8–C3_8–F5_8	121.6(9)
F2_6–C2_6–C1_6	111.1(8)	F6_8–C3_8–C1_8	109.3(8)
F3_6–C2_6–C1_6	110.9(8)	F4_8–C3_8–C1_8	110.0(8)
F5_6–C3_6–F4_6	106.7(7)	F5_8–C3_8–C1_8	113.4(8)
F5_6–C3_6–F6_6	107.1(6)	F9_8–C4_8–F8_8	110.2(11)
F4_6–C3_6–F6_6	107.6(6)	F9_8–C4_8–F7_8	100.7(10)
F5_6–C3_6–C1_6	111.5(6)	F8_8–C4_8–F7_8	107.9(11)
F4_6–C3_6–C1_6	109.8(5)	F9_8–C4_8–C1_8	107.5(8)
F6_6–C3_6–C1_6	113.9(7)	F8_8–C4_8–C1_8	115.7(11)
F9_6–C4_6–F8_6	107.9(7)	F7_8–C4_8–C1_8	113.8(9)
F9_6–C4_6–F7_6	106.9(9)	C1_9–O1_9–Al16	147.9(4)
F8_6–C4_6–F7_6	109.3(9)	O1_9–C1_9–C4_9	110.1(6)
F9_6–C4_6–C1_6	109.8(7)	O1_9–C1_9–C2_9	108.0(6)
F8_6–C4_6–C1_6	113.5(8)	C4_9–C1_9–C2_9	108.4(7)
F7_6–C4_6–C1_6	109.2(8)	O1_9–C1_9–C3_9	111.1(6)
C1_7–O1_7–Al19	146.6(8)	C4_9–C1_9–C3_9	110.1(7)
O1_7–C1_7–C3_7	115.4(7)	C2_9–C1_9–C3_9	109.1(7)
O1_7–C1_7–C2_7	112.0(8)	F3_9–C2_9–F1_9	106.7(9)
C3_7–C1_7–C2_7	109.9(7)	F3_9–C2_9–F2_9	108.2(7)
O1_7–C1_7–C4_7	101.6(7)	F1_9–C2_9–F2_9	107.7(9)
C3_7–C1_7–C4_7	108.7(6)	F3_9–C2_9–C1_9	110.0(7)
C2_7–C1_7–C4_7	108.7(7)	F1_9–C2_9–C1_9	110.0(8)
F1_7–C2_7–F3_7	106.1(9)	F2_9–C2_9–C1_9	113.9(8)
F1_7–C2_7–F2_7	110.5(10)	F6_9–C3_9–F4_9	108.2(9)
F3_7–C2_7–F2_7	105.9(7)	F6_9–C3_9–F5_9	107.0(9)
F1_7–C2_7–C1_7	110.9(8)	F4_9–C3_9–F5_9	109.8(9)
F3_7–C2_7–C1_7	112.0(7)	F6_9–C3_9–C1_9	112.4(8)
F2_7–C2_7–C1_7	111.3(7)	F4_9–C3_9–C1_9	110.2(7)
F5_7–C3_7–F4_7	107.4(10)	F5_9–C3_9–C1_9	109.2(7)
F5_7–C3_7–F6_7	106.8(10)	F9_9–C4_9–F7_9	104.9(10)
F4_7–C3_7–F6_7	104.1(11)	F9_9–C4_9–F8_9	111.6(9)
F5_7–C3_7–C1_7	109.8(7)	F7_9–C4_9–F8_9	105.1(9)
F4_7–C3_7–C1_7	113.9(9)	F9_9–C4_9–C1_9	111.0(8)
F6_7–C3_7–C1_7	114.3(11)	F7_9–C4_9–C1_9	111.7(9)
F8_7–C4_7–F9_7	112.4(8)	F8_9–C4_9–C1_9	112.2(8)
F8_7–C4_7–F7_7	109.7(6)	C1_10–O1_10–Al16	146.1(3)
F9_7–C4_7–F7_7	104.8(8)	O1_10–C1_10–C4_10	109.8(4)
F8_7–C4_7–C1_7	113.2(7)	O1_10–C1_10–C3_10	107.3(3)
F9_7–C4_7–C1_7	106.8(7)	C4_10–C1_10–C3_10	110.4(3)
F7_7–C4_7–C1_7	109.6(6)	O1_10–C1_10–C2_10	112.7(3)
C1_8–O1_8–Al19	152.9(8)	C4_10–C1_10–C2_10	108.7(4)
O1_8–C1_8–C3_8	113.6(8)	C3_10–C1_10–C2_10	108.1(4)
O1_8–C1_8–C2_8	105.6(8)	F2_10–C2_10–F3_10	108.9(5)
C3_8–C1_8–C2_8	113.3(8)	F2_10–C2_10–F1_10	106.5(4)
O1_8–C1_8–C4_8	106.3(8)	F3_10–C2_10–F1_10	107.7(4)
C3_8–C1_8–C4_8	108.1(8)	F2_10–C2_10–C1_10	112.4(4)
C2_8–C1_8–C4_8	109.7(8)	F3_10–C2_10–C1_10	110.2(4)

F1_10–C2_10–C1_10	111.0(4)	F6_12–C3_12–C1_12	113.7(8)
F5_10–C3_10–F6_10	107.2(4)	F5_12–C3_12–C1_12	110.6(6)
F5_10–C3_10–F4_10	106.5(4)	F7_12–C4_12–F9_12	107.2(7)
F6_10–C3_10–F4_10	108.0(4)	F7_12–C4_12–F8_12	110.0(10)
F5_10–C3_10–C1_10	110.6(4)	F9_12–C4_12–F8_12	108.0(10)
F6_10–C3_10–C1_10	113.1(4)	F7_12–C4_12–C1_12	110.3(7)
F4_10–C3_10–C1_10	111.2(4)	F9_12–C4_12–C1_12	110.2(6)
F9_10–C4_10–F8_10	108.4(4)	F8_12–C4_12–C1_12	111.0(10)
F9_10–C4_10–F7_10	108.2(4)	C1_13–O1_13–Al17	150.9(5)
F8_10–C4_10–F7_10	106.7(4)	O1_13–C1_13–C4_13	109.9(6)
F9_10–C4_10–C1_10	111.3(4)	O1_13–C1_13–C2_13	108.5(5)
F8_10–C4_10–C1_10	111.9(4)	C4_13–C1_13–C2_13	110.5(5)
F7_10–C4_10–C1_10	110.2(4)	O1_13–C1_13–C3_13	110.7(6)
C1_11–O1_11–Al16	146.6(3)	C4_13–C1_13–C3_13	109.1(4)
O1_11–C1_11–C3_11	111.2(4)	C2_13–C1_13–C3_13	108.2(4)
O1_11–C1_11–C2_11	110.2(4)	F3_13–C2_13–F1_13	108.6(6)
C3_11–C1_11–C2_11	110.5(5)	F3_13–C2_13–F2_13	108.4(5)
O1_11–C1_11–C4_11	107.3(4)	F1_13–C2_13–F2_13	107.6(5)
C3_11–C1_11–C4_11	109.1(4)	F3_13–C2_13–C1_13	111.0(5)
C2_11–C1_11–C4_11	108.5(4)	F1_13–C2_13–C1_13	109.8(5)
F3_11–C2_11–F2_11	108.2(6)	F2_13–C2_13–C1_13	111.3(5)
F3_11–C2_11–F1_11	107.3(5)	F5_13–C3_13–F6_13	108.3(5)
F2_11–C2_11–F1_11	108.5(6)	F5_13–C3_13–F4_13	107.6(5)
F3_11–C2_11–C1_11	110.0(5)	F6_13–C3_13–F4_13	107.0(5)
F2_11–C2_11–C1_11	112.0(5)	F5_13–C3_13–C1_13	111.8(5)
F1_11–C2_11–C1_11	110.7(5)	F6_13–C3_13–C1_13	112.5(4)
F4_11–C3_11–F6_11	107.1(6)	F4_13–C3_13–C1_13	109.4(4)
F4_11–C3_11–F5_11	107.1(5)	F9_13–C4_13–F7_13	107.4(5)
F6_11–C3_11–F5_11	107.9(6)	F9_13–C4_13–F8_13	107.3(5)
F4_11–C3_11–C1_11	111.8(5)	F7_13–C4_13–F8_13	106.2(5)
F6_11–C3_11–C1_11	112.1(6)	F9_13–C4_13–C1_13	111.7(5)
F5_11–C3_11–C1_11	110.6(5)	F7_13–C4_13–C1_13	111.8(5)
F9_11–C4_11–F7_11	107.6(6)	F8_13–C4_13–C1_13	112.1(5)
F9_11–C4_11–F8_11	108.7(5)	C1_14–O1_14–Al17	148.3(6)
F7_11–C4_11–F8_11	106.6(5)	O1_14–C1_14–C4_14	112.1(7)
F9_11–C4_11–C1_11	112.3(5)	O1_14–C1_14–C2_14	110.1(6)
F7_11–C4_11–C1_11	110.2(5)	C4_14–C1_14–C2_14	110.3(7)
F8_11–C4_11–C1_11	111.2(5)	O1_14–C1_14–C3_14	107.0(6)
C1_12–O1_12–Al16	145.7(10)	C4_14–C1_14–C3_14	110.3(7)
O1_12–C1_12–C3_12	113.8(8)	C2_14–C1_14–C3_14	106.8(7)
O1_12–C1_12–C4_12	99.9(7)	F3_14–C2_14–F2_14	111.8(7)
C3_12–C1_12–C4_12	109.0(6)	F3_14–C2_14–F1_14	103.6(8)
O1_12–C1_12–C2_12	113.0(8)	F2_14–C2_14–F1_14	99.6(8)
C3_12–C1_12–C2_12	110.1(6)	F3_14–C2_14–C1_14	116.8(7)
C4_12–C1_12–C2_12	110.5(7)	F2_14–C2_14–C1_14	116.0(6)
F3_12–C2_12–F1_12	108.3(7)	F1_14–C2_14–C1_14	106.4(7)
F3_12–C2_12–F2_12	105.7(7)	F4_14–C3_14–F6_14	110.7(9)
F1_12–C2_12–F2_12	107.1(7)	F4_14–C3_14–F5_14	101.5(9)
F3_12–C2_12–C1_12	112.4(7)	F6_14–C3_14–F5_14	107.5(9)
F1_12–C2_12–C1_12	112.0(7)	F4_14–C3_14–C1_14	114.0(7)
F2_12–C2_12–C1_12	111.0(7)	F6_14–C3_14–C1_14	113.8(9)
F4_12–C3_12–F6_12	108.6(7)	F5_14–C3_14–C1_14	108.4(7)
F4_12–C3_12–F5_12	105.3(7)	F9_14–C4_14–F8_14	110.8(10)
F6_12–C3_12–F5_12	106.9(7)	F9_14–C4_14–F7_14	101.8(9)
F4_12–C3_12–C1_12	111.3(6)	F8_14–C4_14–F7_14	104.6(9)

F9_14–C4_14–C1_14	116.4(8)	O1_17–C1_17–C4_17	110.8(7)
F8_14–C4_14–C1_14	115.0(9)	C2_17–C1_17–C4_17	110.2(5)
F7_14–C4_14–C1_14	106.5(7)	O1_17–C1_17–C3_17	107.4(7)
C1_15–O1_15–Al17	150.5(4)	C2_17–C1_17–C3_17	105.7(5)
O1_15–C1_15–C4_15	110.3(5)	C4_17–C1_17–C3_17	108.2(6)
O1_15–C1_15–C3_15	107.8(5)	F3_17–C2_17–F1_17	109.4(6)
C4_15–C1_15–C3_15	109.2(5)	F3_17–C2_17–F2_17	105.0(6)
O1_15–C1_15–C2_15	111.1(5)	F1_17–C2_17–F2_17	109.4(6)
C4_15–C1_15–C2_15	109.3(5)	F3_17–C2_17–C1_17	111.6(5)
C3_15–C1_15–C2_15	108.9(5)	F1_17–C2_17–C1_17	109.4(5)
F2_15–C2_15–F3_15	107.2(6)	F2_17–C2_17–C1_17	111.9(6)
F2_15–C2_15–F1_15	108.1(6)	F5_17–C3_17–F6_17	108.8(6)
F3_15–C2_15–F1_15	107.7(4)	F5_17–C3_17–F4_17	106.7(7)
F2_15–C2_15–C1_15	112.5(5)	F6_17–C3_17–F4_17	105.1(7)
F3_15–C2_15–C1_15	110.9(5)	F5_17–C3_17–C1_17	113.1(6)
F1_15–C2_15–C1_15	110.3(5)	F6_17–C3_17–C1_17	112.7(7)
F4_15–C3_15–F5_15	107.4(5)	F4_17–C3_17–C1_17	109.9(6)
F4_15–C3_15–F6_15	107.4(5)	F8_17–C4_17–F7_17	108.6(7)
F5_15–C3_15–F6_15	107.5(5)	F8_17–C4_17–F9_17	105.6(6)
F4_15–C3_15–C1_15	111.1(5)	F7_17–C4_17–F9_17	106.8(6)
F5_15–C3_15–C1_15	111.1(5)	F8_17–C4_17–C1_17	116.2(6)
F6_15–C3_15–C1_15	112.1(5)	F7_17–C4_17–C1_17	111.0(6)
F9_15–C4_15–F8_15	108.0(5)	F9_17–C4_17–C1_17	108.2(6)
F9_15–C4_15–F7_15	107.1(6)	F1_18–C1_18–C6_18	120.9(5)
F8_15–C4_15–F7_15	106.1(5)	F1_18–C1_18–C2_18	118.3(5)
F9_15–C4_15–C1_15	111.2(5)	C6_18–C1_18–C2_18	120.8(5)
F8_15–C4_15–C1_15	112.6(5)	F2_18–C2_18–C3_18	120.5(5)
F7_15–C4_15–C1_15	111.6(5)	F2_18–C2_18–C1_18	118.7(5)
C1_16–O1_16–Al18	145.8(12)	C3_18–C2_18–C1_18	120.7(5)
O1_16–C1_16–C3_16	108.4(9)	C2_18–C3_18–C4_18	118.8(5)
O1_16–C1_16–C4_16	110.3(9)	C2_18–C3_18–H3_18	120.6
C3_16–C1_16–C4_16	108.4(6)	C4_18–C3_18–H3_18	120.6
O1_16–C1_16–C2_16	112.4(9)	C5_18–C4_18–C3_18	119.8(5)
C3_16–C1_16–C2_16	110.7(6)	C5_18–C4_18–H4_18	120.1
C4_16–C1_16–C2_16	106.6(6)	C3_18–C4_18–H4_18	120.1
F3_16–C2_16–F2_16	106.8(7)	C4_18–C5_18–C6_18	121.2(5)
F3_16–C2_16–F1_16	108.1(7)	C4_18–C5_18–H5_18	119.4
F2_16–C2_16–F1_16	111.7(7)	C6_18–C5_18–H5_18	119.4
F3_16–C2_16–C1_16	110.6(6)	C1_18–C6_18–C5_18	118.6(5)
F2_16–C2_16–C1_16	111.7(6)	C1_18–C6_18–H6_18	120.7
F1_16–C2_16–C1_16	108.0(7)	C5_18–C6_18–H6_18	120.7
F4_16–C3_16–F6_16	106.7(7)	C1_20–O1_20–Al17	147.0(4)
F4_16–C3_16–F5_16	107.9(7)	O1_20–C1_20–C4_20	112.0(5)
F6_16–C3_16–F5_16	106.8(8)	O1_20–C1_20–C3_20	107.2(5)
F4_16–C3_16–C1_16	112.3(6)	C4_20–C1_20–C3_20	113.1(6)
F6_16–C3_16–C1_16	113.4(7)	O1_20–C1_20–C2_20	111.2(6)
F5_16–C3_16–C1_16	109.4(7)	C4_20–C1_20–C2_20	105.7(6)
F9_16–C4_16–F8_16	107.8(7)	C3_20–C1_20–C2_20	107.6(6)
F9_16–C4_16–F7_16	105.6(7)	F3_20–C2_20–F2_20	109.7(7)
F8_16–C4_16–F7_16	108.4(7)	F3_20–C2_20–F1_20	108.8(8)
F9_16–C4_16–C1_16	112.2(6)	F2_20–C2_20–F1_20	112.3(7)
F8_16–C4_16–C1_16	113.9(7)	F3_20–C2_20–C1_20	111.5(6)
F7_16–C4_16–C1_16	108.6(7)	F2_20–C2_20–C1_20	109.3(6)
C1_17–O1_17–Al18	153.3(9)	F1_20–C2_20–C1_20	105.2(6)
O1_17–C1_17–C2_17	114.3(7)	F4_20–C3_20–F6_20	107.0(7)

F4_20–C3_20–F5_20	109.8(7)	F7_24–C4_24–F9_24	106.3(8)
F6_20–C3_20–F5_20	109.7(6)	F7_24–C4_24–F8_24	106.9(8)
F4_20–C3_20–C1_20	112.0(6)	F9_24–C4_24–F8_24	107.5(9)
F6_20–C3_20–C1_20	111.9(6)	F7_24–C4_24–C1_24	112.7(8)
F5_20–C3_20–C1_20	106.5(6)	F9_24–C4_24–C1_24	111.3(8)
F9_20–C4_20–F8_20	111.1(6)	F8_24–C4_24–C1_24	111.9(8)
F9_20–C4_20–F7_20	102.0(7)	C1_25–O1_25–Al17	145.5(7)
F8_20–C4_20–F7_20	103.4(7)	O1_25–C1_25–C3_25	113.2(8)
F9_20–C4_20–C1_20	115.5(6)	O1_25–C1_25–C4_25	110.7(8)
F8_20–C4_20–C1_20	115.5(6)	C3_25–C1_25–C4_25	109.0(8)
F7_20–C4_20–C1_20	107.6(7)	O1_25–C1_25–C2_25	106.9(8)
C1_23–O1_23–Al16	146.7(7)	C3_25–C1_25–C2_25	111.9(8)
O1_23–C1_23–C3_23	110.6(8)	C4_25–C1_25–C2_25	104.8(8)
O1_23–C1_23–C2_23	110.2(8)	F3_25–C2_25–F1_25	107.0(9)
C3_23–C1_23–C2_23	108.2(8)	F3_25–C2_25–F2_25	106.8(10)
O1_23–C1_23–C4_23	106.4(8)	F1_25–C2_25–F2_25	106.5(9)
C3_23–C1_23–C4_23	110.8(8)	F3_25–C2_25–C1_25	112.6(8)
C2_23–C1_23–C4_23	110.6(8)	F1_25–C2_25–C1_25	112.2(8)
F1_23–C2_23–F3_23	103.8(10)	F2_25–C2_25–C1_25	111.4(8)
F1_23–C2_23–F2_23	105.1(11)	F6_25–C3_25–F5_25	97.2(11)
F3_23–C2_23–F2_23	112.8(12)	F6_25–C3_25–F4_25	114.3(9)
F1_23–C2_23–C1_23	110.7(9)	F5_25–C3_25–F4_25	99.3(11)
F3_23–C2_23–C1_23	113.0(9)	F6_25–C3_25–C1_25	117.3(9)
F2_23–C2_23–C1_23	111.1(10)	F5_25–C3_25–C1_25	117.7(10)
F5_23–C3_23–F6_23	110.8(13)	F4_25–C3_25–C1_25	109.5(8)
F5_23–C3_23–F4_23	107.1(11)	F8_25–C4_25–F9_25	109.9(11)
F6_23–C3_23–F4_23	103.3(13)	F8_25–C4_25–F7_25	105.7(10)
F5_23–C3_23–C1_23	110.9(9)	F9_25–C4_25–F7_25	107.5(11)
F6_23–C3_23–C1_23	111.8(11)	F8_25–C4_25–C1_25	113.7(9)
F4_23–C3_23–C1_23	112.6(10)	F9_25–C4_25–C1_25	113.7(9)
F9_23–C4_23–F8_23	106.2(12)	F7_25–C4_25–C1_25	105.8(8)
F9_23–C4_23–F7_23	106.6(10)	C1_26–O1_26–Al19	153.7(10)
F8_23–C4_23–F7_23	107.5(12)	O1_26–C1_26–C2_26	116.8(9)
F9_23–C4_23–C1_23	112.9(8)	O1_26–C1_26–C3_26	110.8(8)
F8_23–C4_23–C1_23	112.3(10)	C2_26–C1_26–C3_26	108.4(7)
F7_23–C4_23–C1_23	111.0(9)	O1_26–C1_26–C4_26	101.2(8)
C1_24–O1_24–Al17	148.3(7)	C2_26–C1_26–C4_26	110.7(7)
O1_24–C1_24–C4_24	112.3(8)	C3_26–C1_26–C4_26	108.6(7)
O1_24–C1_24–C2_24	107.3(8)	F3_26–C2_26–F2_26	106.4(9)
C4_24–C1_24–C2_24	108.9(8)	F3_26–C2_26–F1_26	105.5(11)
O1_24–C1_24–C3_24	110.2(8)	F2_26–C2_26–F1_26	106.3(11)
C4_24–C1_24–C3_24	108.1(8)	F3_26–C2_26–C1_26	116.0(8)
C2_24–C1_24–C3_24	110.0(8)	F2_26–C2_26–C1_26	112.6(8)
F3_24–C2_24–F2_24	107.3(8)	F1_26–C2_26–C1_26	109.4(8)
F3_24–C2_24–F1_24	108.6(10)	F4_26–C3_26–F5_26	107.2(9)
F2_24–C2_24–F1_24	107.5(9)	F4_26–C3_26–F6_26	109.1(11)
F3_24–C2_24–C1_24	109.5(8)	F5_26–C3_26–F6_26	110.0(9)
F2_24–C2_24–C1_24	112.7(8)	F4_26–C3_26–C1_26	108.7(8)
F1_24–C2_24–C1_24	111.1(9)	F5_26–C3_26–C1_26	110.6(7)
F5_24–C3_24–F4_24	107.9(10)	F6_26–C3_26–C1_26	111.0(10)
F5_24–C3_24–F6_24	109.4(9)	F8_26–C4_26–F7_26	105.9(10)
F4_24–C3_24–F6_24	107.1(8)	F8_26–C4_26–F9_26	113.2(8)
F5_24–C3_24–C1_24	108.7(9)	F7_26–C4_26–F9_26	107.7(9)
F4_24–C3_24–C1_24	110.9(8)	F8_26–C4_26–C1_26	112.2(8)
F6_24–C3_24–C1_24	112.8(8)	F7_26–C4_26–C1_26	111.1(9)

F9_26–C4_26–C1_26	106.8(9)	O1_31–C1_31–C4_31	111.7(10)
C1_29–O1_29–Al16	146.6(8)	C3_31–C1_31–C4_31	109.2(8)
O1_29–C1_29–C3_29	119.1(8)	C2_31–C1_31–C4_31	108.2(8)
O1_29–C1_29–C4_29	111.5(9)	F3_31–C2_31–F2_31	106.9(11)
C3_29–C1_29–C4_29	107.7(7)	F3_31–C2_31–F1_31	105.7(13)
O1_29–C1_29–C2_29	100.7(8)	F2_31–C2_31–F1_31	109.1(12)
C3_29–C1_29–C2_29	107.8(8)	F3_31–C2_31–C1_31	113.0(9)
C4_29–C1_29–C2_29	109.4(8)	F2_31–C2_31–C1_31	113.2(9)
F1_29–C2_29–F3_29	107.7(9)	F1_31–C2_31–C1_31	108.6(11)
F1_29–C2_29–F2_29	108.2(9)	F4_31–C3_31–F6_31	107.6(10)
F3_29–C2_29–F2_29	107.5(9)	F4_31–C3_31–F5_31	111.1(12)
F1_29–C2_29–C1_29	109.5(8)	F6_31–C3_31–F5_31	102.7(10)
F3_29–C2_29–C1_29	110.4(8)	F4_31–C3_31–C1_31	111.0(9)
F2_29–C2_29–C1_29	113.4(9)	F6_31–C3_31–C1_31	115.3(9)
F4_29–C3_29–F5_29	107.9(8)	F5_31–C3_31–C1_31	108.8(9)
F4_29–C3_29–F6_29	108.9(11)	F9_31–C4_31–F7_31	103.5(11)
F5_29–C3_29–F6_29	106.7(11)	F9_31–C4_31–F8_31	111.2(11)
F4_29–C3_29–C1_29	109.1(8)	F7_31–C4_31–F8_31	106.3(10)
F5_29–C3_29–C1_29	112.5(7)	F9_31–C4_31–C1_31	111.6(9)
F6_29–C3_29–C1_29	111.7(11)	F7_31–C4_31–C1_31	110.5(10)
F7_29–C4_29–F8_29	108.5(10)	F8_31–C4_31–C1_31	113.1(9)
F7_29–C4_29–F9_29	107.0(9)	C1_33–O1_33–Al18	152.8(18)
F8_29–C4_29–F9_29	107.2(10)	O1_33–C1_33–C2_33	109.8(13)
F7_29–C4_29–C1_29	112.6(7)	O1_33–C1_33–C3_33	108.8(12)
F8_29–C4_29–C1_29	113.6(9)	C2_33–C1_33–C3_33	107.0(9)
F9_29–C4_29–C1_29	107.7(8)	O1_33–C1_33–C4_33	110.9(13)
C1_30–O1_30–Al17	150.6(8)	C2_33–C1_33–C4_33	110.0(9)
O1_30–C1_30–C2_30	109.3(8)	C3_33–C1_33–C4_33	110.3(9)
O1_30–C1_30–C4_30	108.5(8)	F2_33–C2_33–F3_33	107.8(11)
C2_30–C1_30–C4_30	108.9(8)	F2_33–C2_33–F1_33	105.0(11)
O1_30–C1_30–C3_30	109.3(8)	F3_33–C2_33–F1_33	113.6(12)
C2_30–C1_30–C3_30	110.2(8)	F2_33–C2_33–C1_33	115.9(10)
C4_30–C1_30–C3_30	110.6(9)	F3_33–C2_33–C1_33	109.9(9)
F3_30–C2_30–F1_30	107.1(10)	F1_33–C2_33–C1_33	104.7(10)
F3_30–C2_30–F2_30	97.0(10)	F4_33–C3_33–F6_33	106.2(11)
F1_30–C2_30–F2_30	111.0(10)	F4_33–C3_33–F5_33	112.8(12)
F3_30–C2_30–C1_30	110.6(9)	F6_33–C3_33–F5_33	107.5(12)
F1_30–C2_30–C1_30	116.7(10)	F4_33–C3_33–C1_33	111.1(9)
F2_30–C2_30–C1_30	112.5(9)	F6_33–C3_33–C1_33	111.8(10)
F6_30–C3_30–F5_30	101.6(10)	F5_33–C3_33–C1_33	107.3(10)
F6_30–C3_30–F4_30	112.8(11)	F7_33–C4_33–F8_33	106.7(11)
F5_30–C3_30–F4_30	106.9(10)	F7_33–C4_33–F9_33	110.0(12)
F6_30–C3_30–C1_30	111.4(9)	F8_33–C4_33–F9_33	114.1(12)
F5_30–C3_30–C1_30	113.7(9)	F7_33–C4_33–C1_33	106.3(10)
F4_30–C3_30–C1_30	110.1(8)	F8_33–C4_33–C1_33	109.0(10)
F9_30–C4_30–F7_30	106.1(11)	F9_33–C4_33–C1_33	110.3(9)
F9_30–C4_30–F8_30	106.0(11)	C1_34–O1_34–Al20	156.9(9)
F7_30–C4_30–F8_30	112.2(11)	O1_34–C1_34–C4_34	115.8(10)
F9_30–C4_30–C1_30	111.1(10)	O1_34–C1_34–C3_34	109.7(9)
F7_30–C4_30–C1_30	113.1(9)	C4_34–C1_34–C3_34	107.5(9)
F8_30–C4_30–C1_30	108.1(9)	O1_34–C1_34–C2_34	105.1(9)
C1_31–O1_31–Al17	154.2(12)	C4_34–C1_34–C2_34	100.8(8)
O1_31–C1_31–C3_31	110.6(12)	C3_34–C1_34–C2_34	117.9(9)
O1_31–C1_31–C2_31	107.4(10)	F3_34–C2_34–F2_34	110.5(12)
C3_31–C1_31–C2_31	109.7(8)	F3_34–C2_34–F1_34	114.9(11)

F2_34–C2_34–F1_34	103.2(10)	F6_27–C3_27–F5_27	107.7(10)
F3_34–C2_34–C1_34	114.1(10)	F4_27–C3_27–F5_27	103.2(10)
F2_34–C2_34–C1_34	105.0(10)	F6_27–C3_27–C1_27	118.1(9)
F1_34–C2_34–C1_34	108.2(10)	F4_27–C3_27–C1_27	113.7(9)
F6_34–C3_34–F5_34	107.9(11)	F5_27–C3_27–C1_27	108.6(8)
F6_34–C3_34–F4_34	104.1(12)	F9_27–C4_27–F8_27	109.3(11)
F5_34–C3_34–F4_34	102.0(11)	F9_27–C4_27–F7_27	108.2(11)
F6_34–C3_34–C1_34	115.8(10)	F8_27–C4_27–F7_27	103.0(9)
F5_34–C3_34–C1_34	111.3(9)	F9_27–C4_27–C1_27	112.9(9)
F4_34–C3_34–C1_34	114.7(11)	F8_27–C4_27–C1_27	110.6(9)
F9_34–C4_34–F8_34	106.3(11)	F7_27–C4_27–C1_27	112.4(9)
F9_34–C4_34–F7_34	101.8(11)	C1_36–O1_36–Al20	149.4(10)
F8_34–C4_34–F7_34	107.9(10)	O1_36–C1_36–C3_36	108.5(9)
F9_34–C4_34–C1_34	119.3(11)	O1_36–C1_36–C2_36	114.2(9)
F8_34–C4_34–C1_34	112.8(9)	C3_36–C1_36–C2_36	109.2(8)
F7_34–C4_34–C1_34	107.8(9)	O1_36–C1_36–C4_36	108.2(8)
C1_35–O1_35–Al20	150(2)	C3_36–C1_36–C4_36	108.8(8)
O1_35–C1_35–C3_35	110.2(14)	C2_36–C1_36–C4_36	107.8(8)
O1_35–C1_35–C4_35	108.1(15)	F2_36–C2_36–F3_36	107.9(9)
C3_35–C1_35–C4_35	108.7(11)	F2_36–C2_36–F1_36	109.4(10)
O1_35–C1_35–C2_35	109.3(13)	F3_36–C2_36–F1_36	106.3(9)
C3_35–C1_35–C2_35	110.1(11)	F2_36–C2_36–C1_36	112.8(10)
C4_35–C1_35–C2_35	110.3(11)	F3_36–C2_36–C1_36	109.0(9)
F3_35–C2_35–F1_35	105.9(17)	F1_36–C2_36–C1_36	111.2(8)
F3_35–C2_35–F2_35	108.7(17)	F5_36–C3_36–F4_36	105.1(11)
F1_35–C2_35–F2_35	107.2(18)	F5_36–C3_36–F6_36	110.6(13)
F3_35–C2_35–C1_35	110.1(12)	F4_36–C3_36–F6_36	106.8(14)
F1_35–C2_35–C1_35	111.6(13)	F5_36–C3_36–C1_36	110.0(9)
F2_35–C2_35–C1_35	113.0(16)	F4_36–C3_36–C1_36	111.8(10)
F5_35–C3_35–F4_35	107.3(15)	F6_36–C3_36–C1_36	112.2(13)
F5_35–C3_35–F6_35	107.1(15)	F7_36–C4_36–F8_36	107.1(9)
F4_35–C3_35–F6_35	106.6(15)	F7_36–C4_36–F9_36	104.6(9)
F5_35–C3_35–C1_35	111.1(12)	F8_36–C4_36–F9_36	107.5(9)
F4_35–C3_35–C1_35	111.8(13)	F7_36–C4_36–C1_36	112.3(9)
F6_35–C3_35–C1_35	112.6(13)	F8_36–C4_36–C1_36	113.7(9)
F9_35–C4_35–F8_35	107.2(14)	F9_36–C4_36–C1_36	111.1(8)
F9_35–C4_35–F7_35	108.1(15)	C1_37–O1_37–Al20	152.2(10)
F8_35–C4_35–F7_35	107.6(14)	O1_37–C1_37–C2_37	108.7(10)
F9_35–C4_35–C1_35	111.2(12)	O1_37–C1_37–C4_37	111.1(11)
F8_35–C4_35–C1_35	111.9(12)	C2_37–C1_37–C4_37	108.2(10)
F7_35–C4_35–C1_35	110.7(13)	O1_37–C1_37–C3_37	108.6(11)
C1_27–O1_27–Al18	154.6(8)	C2_37–C1_37–C3_37	109.9(10)
O1_27–C1_27–C2_27	108.7(8)	C4_37–C1_37–C3_37	110.2(10)
O1_27–C1_27–C4_27	114.3(8)	F1_37–C2_37–F3_37	112.9(13)
C2_27–C1_27–C4_27	107.5(7)	F1_37–C2_37–F2_37	109.7(12)
O1_27–C1_27–C3_27	107.0(8)	F3_37–C2_37–F2_37	105.6(13)
C2_27–C1_27–C3_27	112.4(8)	F1_37–C2_37–C1_37	109.5(10)
C4_27–C1_27–C3_27	107.1(7)	F3_37–C2_37–C1_37	110.2(11)
F3_27–C2_27–F2_27	98.4(10)	F2_37–C2_37–C1_37	108.7(11)
F3_27–C2_27–F1_27	105.4(9)	F5_37–C3_37–F4_37	115.0(14)
F2_27–C2_27–F1_27	106.1(10)	F5_37–C3_37–F6_37	109.1(15)
F3_27–C2_27–C1_27	114.5(9)	F4_37–C3_37–F6_37	103.4(13)
F2_27–C2_27–C1_27	114.4(9)	F5_37–C3_37–C1_37	109.7(12)
F1_27–C2_27–C1_27	116.2(8)	F4_37–C3_37–C1_37	109.6(11)
F6_27–C3_27–F4_27	104.3(9)	F6_37–C3_37–C1_37	109.8(12)

F8_37–C4_37–F9_37	109.5(12)	F7_42–C4_42–C1_42	106.9(13)
F8_37–C4_37–F7_37	110.6(13)	C1_43–O1_43–Al19	144.0(7)
F9_37–C4_37–F7_37	107.1(13)	O1_43–C1_43–C4_43	119.9(9)
F8_37–C4_37–C1_37	111.2(11)	O1_43–C1_43–C2_43	105.3(7)
F9_37–C4_37–C1_37	108.1(11)	C4_43–C1_43–C2_43	108.7(8)
F7_37–C4_37–C1_37	110.1(10)	O1_43–C1_43–C3_43	101.4(7)
C1_41–O1_41–Al18	153.6(13)	C4_43–C1_43–C3_43	110.1(7)
O1_41–C1_41–C2_41	113.8(11)	C2_43–C1_43–C3_43	111.1(8)
O1_41–C1_41–C3_41	111.4(11)	F3_43–C2_43–F2_43	109.7(9)
C2_41–C1_41–C3_41	112.4(10)	F3_43–C2_43–F1_43	104.4(9)
O1_41–C1_41–C4_41	103.3(10)	F2_43–C2_43–F1_43	107.2(8)
C2_41–C1_41–C4_41	106.2(9)	F3_43–C2_43–C1_43	112.1(8)
C3_41–C1_41–C4_41	109.1(10)	F2_43–C2_43–C1_43	111.2(9)
F2_41–C2_41–F3_41	111.0(12)	F1_43–C2_43–C1_43	111.9(9)
F2_41–C2_41–F1_41	107.2(12)	F6_43–C3_43–F4_43	110.4(8)
F3_41–C2_41–F1_41	106.0(12)	F6_43–C3_43–F5_43	127.0(10)
F2_41–C2_41–C1_41	112.3(11)	F4_43–C3_43–F5_43	97.5(7)
F3_41–C2_41–C1_41	109.4(10)	F6_43–C3_43–C1_43	111.9(7)
F1_41–C2_41–C1_41	110.7(11)	F4_43–C3_43–C1_43	110.8(8)
F5_41–C3_41–F4_41	105.3(12)	F5_43–C3_43–C1_43	97.8(7)
F5_41–C3_41–F6_41	107.8(14)	F9_43–C4_43–F8_43	102.1(10)
F4_41–C3_41–F6_41	111.7(14)	F9_43–C4_43–F7_43	108.2(10)
F5_41–C3_41–C1_41	114.2(12)	F8_43–C4_43–F7_43	104.4(9)
F4_41–C3_41–C1_41	109.6(11)	F9_43–C4_43–C1_43	118.5(9)
F6_41–C3_41–C1_41	108.2(12)	F8_43–C4_43–C1_43	111.1(10)
F7_41–C4_41–F8_41	112.8(13)	F7_43–C4_43–C1_43	111.3(8)
F7_41–C4_41–F9_41	103.8(12)	C1_44–O1_44–Al16	154.8(7)
F8_41–C4_41–F9_41	107.9(11)	O1_44–C1_44–C2_44	106.2(8)
F7_41–C4_41–C1_41	107.8(11)	O1_44–C1_44–C3_44	113.1(8)
F8_41–C4_41–C1_41	113.9(11)	C2_44–C1_44–C3_44	111.0(7)
F9_41–C4_41–C1_41	110.2(11)	O1_44–C1_44–C4_44	110.7(8)
C1_42–O1_42–Al19	154(2)	C2_44–C1_44–C4_44	106.2(8)
O1_42–C1_42–C4_42	109.8(14)	C3_44–C1_44–C4_44	109.3(8)
O1_42–C1_42–C3_42	112.0(14)	F2_44–C2_44–F3_44	101.0(10)
C4_42–C1_42–C3_42	116.1(11)	F2_44–C2_44–F1_44	112.0(10)
O1_42–C1_42–C2_42	101.7(13)	F3_44–C2_44–F1_44	109.9(10)
C4_42–C1_42–C2_42	107.4(11)	F2_44–C2_44–C1_44	113.1(10)
C3_42–C1_42–C2_42	108.7(11)	F3_44–C2_44–C1_44	108.8(8)
F1_42–C2_42–F2_42	112.6(16)	F1_44–C2_44–C1_44	111.6(8)
F1_42–C2_42–F3_42	104.8(15)	F4_44–C3_44–F6_44	112.8(10)
F2_42–C2_42–F3_42	108.8(15)	F4_44–C3_44–F5_44	106.6(10)
F1_42–C2_42–C1_42	114.4(14)	F6_44–C3_44–F5_44	107.2(10)
F2_42–C2_42–C1_42	111.2(14)	F4_44–C3_44–C1_44	109.9(8)
F3_42–C2_42–C1_42	104.3(13)	F6_44–C3_44–C1_44	110.1(9)
F4_42–C3_42–F6_42	107.7(15)	F5_44–C3_44–C1_44	110.1(10)
F4_42–C3_42–F5_42	105.3(15)	F8_44–C4_44–F9_44	107.9(12)
F6_42–C3_42–F5_42	108.4(16)	F8_44–C4_44–F7_44	109.4(12)
F4_42–C3_42–C1_42	117.2(15)	F9_44–C4_44–F7_44	105.7(11)
F6_42–C3_42–C1_42	109.0(13)	F8_44–C4_44–C1_44	111.4(10)
F5_42–C3_42–C1_42	108.9(14)	F9_44–C4_44–C1_44	111.2(10)
F9_42–C4_42–F8_42	110.8(16)	F7_44–C4_44–C1_44	111.2(10)
F9_42–C4_42–F7_42	110.0(16)	C1_46–O1_46–Al19	150.7(7)
F8_42–C4_42–F7_42	104.9(16)	O1_46–C1_46–C2_46	112.3(9)
F9_42–C4_42–C1_42	116.2(14)	O1_46–C1_46–C4_46	107.9(8)
F8_42–C4_42–C1_42	107.3(14)	C2_46–C1_46–C4_46	109.2(9)

O1_46–C1_46–C3_46	108.2(8)	F1_62–C2_62–F2_62	90.8(14)
C2_46–C1_46–C3_46	109.3(8)	F3_62–C2_62–C1_62	117.1(12)
C4_46–C1_46–C3_46	109.9(8)	F1_62–C2_62–C1_62	115.4(14)
F2_46–C2_46–F1_46	107.8(12)	F2_62–C2_62–C1_62	99.0(13)
F2_46–C2_46–F3_46	106.4(12)	F6_62–C3_62–F5_62	122.5(17)
F1_46–C2_46–F3_46	106.4(11)	F6_62–C3_62–F4_62	108.8(15)
F2_46–C2_46–C1_46	115.0(12)	F5_62–C3_62–F4_62	90.8(13)
F1_46–C2_46–C1_46	110.5(10)	F6_62–C3_62–C1_62	109.3(12)
F3_46–C2_46–C1_46	110.4(10)	F5_62–C3_62–C1_62	108.6(12)
F5_46–C3_46–F4_46	107.7(9)	F4_62–C3_62–C1_62	116.2(14)
F5_46–C3_46–F6_46	108.4(9)	F7_62–C4_62–F8_62	110.7(14)
F4_46–C3_46–F6_46	106.5(9)	F7_62–C4_62–F9_62	106.7(15)
F5_46–C3_46–C1_46	111.8(9)	F8_62–C4_62–F9_62	110.0(14)
F4_46–C3_46–C1_46	111.8(8)	F7_62–C4_62–C1_62	108.4(13)
F6_46–C3_46–C1_46	110.4(9)	F8_62–C4_62–C1_62	114.4(13)
F7_46–C4_46–F8_46	105.9(11)	F9_62–C4_62–C1_62	106.3(12)
F7_46–C4_46–F9_46	108.4(12)	C1_63–O1_63–Al18	148(3)
F8_46–C4_46–F9_46	109.2(10)	O1_63–C1_63–C4_63	111.9(17)
F7_46–C4_46–C1_46	109.4(10)	O1_63–C1_63–C3_63	113.8(19)
F8_46–C4_46–C1_46	112.6(9)	C4_63–C1_63–C3_63	108.4(11)
F9_46–C4_46–C1_46	111.2(9)	O1_63–C1_63–C2_63	109.5(17)
C1_61–O1_61–Al20	147.2(11)	C4_63–C1_63–C2_63	114.6(11)
O1_61–C1_61–C4_61	112.2(11)	C3_63–C1_63–C2_63	98.0(10)
O1_61–C1_61–C3_61	107.1(10)	F2_63–C2_63–F3_63	109.1(15)
C4_61–C1_61–C3_61	109.8(10)	F2_63–C2_63–F1_63	111.5(15)
O1_61–C1_61–C2_61	109.7(10)	F3_63–C2_63–F1_63	106.4(15)
C4_61–C1_61–C2_61	108.4(10)	F2_63–C2_63–C1_63	110.6(13)
C3_61–C1_61–C2_61	109.6(10)	F3_63–C2_63–C1_63	110.5(13)
F3_61–C2_61–F2_61	106.4(13)	F1_63–C2_63–C1_63	108.7(12)
F3_61–C2_61–F1_61	106.5(13)	F4_63–C3_63–F5_63	106.4(15)
F2_61–C2_61–F1_61	108.5(12)	F4_63–C3_63–F6_63	125.6(16)
F3_61–C2_61–C1_61	111.0(11)	F5_63–C3_63–F6_63	96.6(14)
F2_61–C2_61–C1_61	112.2(11)	F4_63–C3_63–C1_63	106.0(11)
F1_61–C2_61–C1_61	112.0(11)	F5_63–C3_63–C1_63	116.5(14)
F6_61–C3_61–F5_61	107.8(13)	F6_63–C3_63–C1_63	106.3(12)
F6_61–C3_61–F4_61	108.4(13)	F8_63–C4_63–F9_63	98.5(13)
F5_61–C3_61–F4_61	106.3(13)	F8_63–C4_63–F7_63	111.7(17)
F6_61–C3_61–C1_61	111.3(11)	F9_63–C4_63–F7_63	104.3(14)
F5_61–C3_61–C1_61	111.0(12)	F8_63–C4_63–C1_63	110.9(15)
F4_61–C3_61–C1_61	111.8(11)	F9_63–C4_63–C1_63	118.7(14)
F9_61–C4_61–F8_61	109.6(13)	F7_63–C4_63–C1_63	112.0(13)
F9_61–C4_61–F7_61	105.1(15)	C1_64–O1_64–Al17	147.8(18)
F8_61–C4_61–F7_61	104.8(14)	O1_64–C1_64–C2_64	112.1(13)
F9_61–C4_61–C1_61	112.2(12)	O1_64–C1_64–C3_64	125.8(14)
F8_61–C4_61–C1_61	113.2(12)	C2_64–C1_64–C3_64	110.0(10)
F7_61–C4_61–C1_61	111.3(12)	O1_64–C1_64–C4_64	94.0(12)
C1_62–O1_62–Al20	143(2)	C2_64–C1_64–C4_64	114.2(11)
O1_62–C1_62–C4_62	111.5(15)	C3_64–C1_64–C4_64	98.5(10)
O1_62–C1_62–C2_62	119.4(15)	F3_64–C2_64–F2_64	108.2(16)
C4_62–C1_62–C2_62	106.9(11)	F3_64–C2_64–F1_64	111.6(13)
O1_62–C1_62–C3_62	109.1(14)	F2_64–C2_64–F1_64	104.8(16)
C4_62–C1_62–C3_62	107.0(11)	F3_64–C2_64–C1_64	113.9(11)
C2_62–C1_62–C3_62	102.0(11)	F2_64–C2_64–C1_64	111.1(15)
F3_62–C2_62–F1_62	126.6(15)	F1_64–C2_64–C1_64	106.7(10)
F3_62–C2_62–F2_62	90.3(14)	F4_64–C3_64–F5_64	106.9(16)

F4_64–C3_64–F6_64	119.3(15)	O1_67–C1_67–C2_67	113.9(16)
F5_64–C3_64–F6_64	104.1(16)	O1_67–C1_67–C4_67	112.3(14)
F4_64–C3_64–C1_64	111.8(11)	C2_67–C1_67–C4_67	110.4(12)
F5_64–C3_64–C1_64	112.8(16)	O1_67–C1_67–C3_67	102.7(15)
F6_64–C3_64–C1_64	101.9(12)	C2_67–C1_67–C3_67	108.2(12)
F8_64–C4_64–F7_64	115.3(14)	C4_67–C1_67–C3_67	108.9(13)
F8_64–C4_64–F9_64	110.4(15)	F3_67–C2_67–F1_67	111.8(18)
F7_64–C4_64–F9_64	102.4(14)	F3_67–C2_67–F2_67	108.1(17)
F8_64–C4_64–C1_64	113.8(13)	F1_67–C2_67–F2_67	105.3(17)
F7_64–C4_64–C1_64	106.1(11)	F3_67–C2_67–C1_67	111.2(14)
F9_64–C4_64–C1_64	108.0(13)	F1_67–C2_67–C1_67	110.6(15)
C1_65–O1_65–Al18	146(2)	F2_67–C2_67–C1_67	109.6(15)
O1_65–C1_65–C3_65	110.8(14)	F6_67–C3_67–F5_67	108.2(17)
O1_65–C1_65–C2_65	111.7(16)	F6_67–C3_67–F4_67	114.2(19)
C3_65–C1_65–C2_65	112.9(11)	F5_67–C3_67–F4_67	106.4(17)
O1_65–C1_65–C4_65	107.7(14)	F6_67–C3_67–C1_67	112.1(17)
C3_65–C1_65–C4_65	108.1(11)	F5_67–C3_67–C1_67	111.2(15)
C2_65–C1_65–C4_65	105.3(10)	F4_67–C3_67–C1_67	104.5(14)
F2_65–C2_65–F3_65	115.9(17)	F9_67–C4_67–F7_67	107.7(18)
F2_65–C2_65–F1_65	99.3(15)	F9_67–C4_67–F8_67	107.7(18)
F3_65–C2_65–F1_65	106.7(17)	F7_67–C4_67–F8_67	105.7(17)
F2_65–C2_65–C1_65	109.1(14)	F9_67–C4_67–C1_67	110.9(15)
F3_65–C2_65–C1_65	113.0(16)	F7_67–C4_67–C1_67	114.4(15)
F1_65–C2_65–C1_65	112.0(15)	F8_67–C4_67–C1_67	110.1(15)
F5_65–C3_65–F6_65	104.8(16)	C1_38–O1_38–Al18	160.7(15)
F5_65–C3_65–F4_65	114.7(16)	O1_38–C1_38–C2_38	106.7(11)
F6_65–C3_65–F4_65	108.3(17)	O1_38–C1_38–C4_38	103.0(11)
F5_65–C3_65–C1_65	108.9(13)	C2_38–C1_38–C4_38	107.2(9)
F6_65–C3_65–C1_65	112.9(15)	O1_38–C1_38–C3_38	100.5(11)
F4_65–C3_65–C1_65	107.3(12)	C2_38–C1_38–C3_38	127.1(11)
F7_65–C4_65–F8_65	115.9(16)	C4_38–C1_38–C3_38	109.6(10)
F7_65–C4_65–F9_65	106.6(14)	F2_38–C2_38–F1_38	97.5(12)
F8_65–C4_65–F9_65	104.0(15)	F2_38–C2_38–F3_38	112.9(13)
F7_65–C4_65–C1_65	111.4(13)	F1_38–C2_38–F3_38	96.4(12)
F8_65–C4_65–C1_65	111.1(13)	F2_38–C2_38–C1_38	118.1(12)
F9_65–C4_65–C1_65	107.2(11)	F1_38–C2_38–C1_38	112.3(11)
C6_19–C1_19–F1_19	121.7(9)	F3_38–C2_38–C1_38	115.7(11)
C6_19–C1_19–C2_19	118.5(9)	F6_38–C3_38–F5_38	105.4(14)
F1_19–C1_19–C2_19	119.8(8)	F6_38–C3_38–F4_38	99.2(12)
F2_19–C2_19–C3_19	122.8(9)	F5_38–C3_38–F4_38	102.3(13)
F2_19–C2_19–C1_19	116.8(9)	F6_38–C3_38–C1_38	118.0(12)
C3_19–C2_19–C1_19	120.4(9)	F5_38–C3_38–C1_38	104.9(12)
C4_19–C3_19–C2_19	120.0(9)	F4_38–C3_38–C1_38	124.7(12)
C4_19–C3_19–H3_19	120.0	F8_38–C4_38–F7_38	107.5(13)
C2_19–C3_19–H3_19	120.0	F8_38–C4_38–F9_38	102.2(12)
C3_19–C4_19–C5_19	118.8(9)	F7_38–C4_38–F9_38	110.1(14)
C3_19–C4_19–H4_19	120.6	F8_38–C4_38–C1_38	114.8(12)
C5_19–C4_19–H4_19	120.6	F7_38–C4_38–C1_38	108.9(11)
C6_19–C5_19–C4_19	120.9(9)	F9_38–C4_38–C1_38	113.1(11)
C6_19–C5_19–H5_19	119.6	C1_21–O1_21–Al18	146.5(11)
C4_19–C5_19–H5_19	119.6	O1_21–C1_21–C3_21	111.6(7)
C1_19–C6_19–C5_19	121.4(9)	O1_21–C1_21–C4_21	110.6(8)
C1_19–C6_19–H6_19	119.3	C3_21–C1_21–C4_21	109.4(6)
C5_19–C6_19–H6_19	119.3	O1_21–C1_21–C2_21	105.2(8)
C1_67–O1_67–Al16	156(2)	C3_21–C1_21–C2_21	110.1(6)

C4_21–C1_21–C2_21	109.8(6)	C5B_45–Al2_45–C4B_45	37.05(11)
F2_21–C2_21–F3_21	109.5(9)	C1B_45–Al2_45–C2B_45	37.05(14)
F2_21–C2_21–F1_21	107.0(8)	C5B_45–Al2_45–C2B_45	61.76(13)
F3_21–C2_21–F1_21	106.6(9)	C4B_45–Al2_45–C2B_45	61.40(12)
F2_21–C2_21–C1_21	111.6(7)	C1B_45–Al2_45–C3B_45	61.85(13)
F3_21–C2_21–C1_21	111.4(8)	C5B_45–Al2_45–C3B_45	61.83(12)
F1_21–C2_21–C1_21	110.4(7)	C4B_45–Al2_45–C3B_45	36.85(11)
F5_21–C3_21–F4_21	106.9(7)	C2B_45–Al2_45–C3B_45	36.73(13)
F5_21–C3_21–F6_21	108.0(7)	C1B_45–Al2_45–In1_45	149.94(12)
F4_21–C3_21–F6_21	106.5(7)	C5B_45–Al2_45–In1_45	171.83(11)
F5_21–C3_21–C1_21	111.1(7)	C4B_45–Al2_45–In1_45	136.19(10)
F4_21–C3_21–C1_21	111.4(6)	C2B_45–Al2_45–In1_45	121.56(11)
F6_21–C3_21–C1_21	112.7(6)	C3B_45–Al2_45–In1_45	115.65(10)
F9_21–C4_21–F7_21	108.5(8)	C1C_45–Al3_45–C5C_45	37.47(12)
F9_21–C4_21–F8_21	106.9(8)	C1C_45–Al3_45–C2C_45	37.17(11)
F7_21–C4_21–F8_21	107.4(7)	C5C_45–Al3_45–C2C_45	61.78(12)
F9_21–C4_21–C1_21	111.6(7)	C1C_45–Al3_45–C4C_45	62.24(13)
F7_21–C4_21–C1_21	111.8(7)	C5C_45–Al3_45–C4C_45	37.33(14)
F8_21–C4_21–C1_21	110.4(7)	C2C_45–Al3_45–C4C_45	61.14(13)
C1_28–O1_28–Al18	149(2)	C1C_45–Al3_45–C3C_45	61.97(12)
O1_28–C1_28–C4_28	115.7(13)	C5C_45–Al3_45–C3C_45	61.82(14)
O1_28–C1_28–C2_28	107.4(14)	C2C_45–Al3_45–C3C_45	36.50(13)
C4_28–C1_28–C2_28	110.1(9)	C4C_45–Al3_45–C3C_45	36.56(14)
O1_28–C1_28–C3_28	106.5(14)	C1C_45–Al3_45–In1_45	160.81(10)
C4_28–C1_28–C3_28	108.6(9)	C5C_45–Al3_45–In1_45	127.38(10)
C2_28–C1_28–C3_28	108.1(9)	C2C_45–Al3_45–In1_45	159.98(10)
F1_28–C2_28–F3_28	107.7(12)	C4C_45–Al3_45–In1_45	113.65(10)
F1_28–C2_28–F2_28	108.5(12)		
F3_28–C2_28–F2_28	109.5(11)		
F1_28–C2_28–C1_28	108.7(11)		
F3_28–C2_28–C1_28	111.4(10)		
F2_28–C2_28–C1_28	111.1(10)		
F5_28–C3_28–F6_28	109.5(12)		
F5_28–C3_28–F4_28	105.3(14)		
F6_28–C3_28–F4_28	109.8(13)		
F5_28–C3_28–C1_28	111.4(10)		
F6_28–C3_28–C1_28	112.5(11)		
F4_28–C3_28–C1_28	108.1(13)		
F7_28–C4_28–F9_28	109.7(11)		
F7_28–C4_28–F8_28	105.6(11)		
F9_28–C4_28–F8_28	107.2(11)		
F7_28–C4_28–C1_28	111.8(10)		
F9_28–C4_28–C1_28	109.4(9)		
F8_28–C4_28–C1_28	112.9(10)		
Al3_45–In1_45–Al1_45	66.24(4)		
Al3_45–In1_45–Al2_45	68.22(4)		
Al1_45–In1_45–Al2_45	68.96(4)		
C1B_45–Al2_45–C5B_45	37.20(13)		
C1B_45–Al2_45–C4B_45	61.86(12)		

C3C_45–Al3_45–In1_45	127.28(10)	C7A_45–C2A_45–Al1_45	126.1(2)
C3A_45–Al1_45–C2A_45	37.68(12)	C2A_45–C3A_45–C4A_45	107.6(3)
C3A_45–Al1_45–C4A_45	37.89(12)	C2A_45–C3A_45–C8A_45	126.2(3)
C2A_45–Al1_45–C4A_45	62.76(12)	C4A_45–C3A_45–C8A_45	126.1(3)
C3A_45–Al1_45–C5A_45	62.64(12)	C2A_45–C3A_45–Al1_45	71.80(18)
C2A_45–Al1_45–C5A_45	62.35(12)	C4A_45–C3A_45–Al1_45	71.71(17)
C4A_45–Al1_45–C5A_45	37.06(12)	C8A_45–C3A_45–Al1_45	125.2(2)
C3A_45–Al1_45–C1A_45	62.56(12)	C5A_45–C4A_45–C3A_45	108.0(3)
C2A_45–Al1_45–C1A_45	37.21(12)	C5A_45–C4A_45–C9A_45	126.9(3)
C4A_45–Al1_45–C1A_45	62.20(12)	C3A_45–C4A_45–C9A_45	125.0(3)
C5A_45–Al1_45–C1A_45	37.17(11)	C5A_45–C4A_45–Al1_45	72.17(17)
C3A_45–Al1_45–In1_45	148.44(10)	C3A_45–C4A_45–Al1_45	70.41(17)
C2A_45–Al1_45–In1_45	173.86(10)	C9A_45–C4A_45–Al1_45	121.4(2)
C4A_45–Al1_45–In1_45	121.73(10)	C4A_45–C5A_45–C1A_45	108.2(3)
C5A_45–Al1_45–In1_45	118.14(9)	C4A_45–C5A_45–C10A_45	127.4(3)
C1A_45–Al1_45–In1_45	139.34(10)	C1A_45–C5A_45–C10A_45	124.4(3)
C2A_45–C1A_45–C5A_45	108.1(3)	C4A_45–C5A_45–Al1_45	70.77(17)
C2A_45–C1A_45–C6A_45	127.2(3)	C1A_45–C5A_45–Al1_45	71.53(17)
C5A_45–C1A_45–C6A_45	124.6(3)	C10A_45–C5A_45–Al1_45	123.8(2)
C2A_45–C1A_45–Al1_45	70.56(18)	C5A_45–C10A_45–H10A_45	109.5
C5A_45–C1A_45–Al1_45	71.30(17)	C5A_45–C10A_45–H10B_45	109.5
C6A_45–C1A_45–Al1_45	126.7(2)	H10A_45–C10A_45–H10B_45	109.5
C1A_45–C2A_45–C3A_45	108.0(3)	C5A_45–C10A_45–H10C_45	109.5
C1A_45–C2A_45–C7A_45	127.0(3)	H10A_45–C10A_45–H10C_45	109.5
C3A_45–C2A_45–C7A_45	124.8(3)	H10B_45–C10A_45–H10C_45	109.5
C1A_45–C2A_45–Al1_45	72.22(17)	C4A_45–C9A_45–H9AA_45	109.5
C3A_45–C2A_45–Al1_45	70.52(17)	C4A_45–C9A_45–H9AB_45	109.5

H9AA_45–C9A_45–H9AB_45	109.5	C6B_45–C1B_45–Al2_45	126.5(3)
C4A_45–C9A_45–H9AC_45	109.5	C3B_45–C2B_45–C1B_45	108.4(3)
H9AA_45–C9A_45–H9AC_45	109.5	C3B_45–C2B_45–C7B_45	126.4(4)
H9AB_45–C9A_45–H9AC_45	109.5	C1B_45–C2B_45–C7B_45	125.2(4)
C3A_45–C8A_45–H8AA_45	109.5	C3B_45–C2B_45–Al2_45	72.05(19)
C3A_45–C8A_45–H8AB_45	109.5	C1B_45–C2B_45–Al2_45	70.6(2)
H8AA_45–C8A_45–H8AB_45	109.5	C7B_45–C2B_45–Al2_45	123.6(3)
C3A_45–C8A_45–H8AC_45	109.5	C2B_45–C3B_45–C4B_45	107.6(3)
H8AA_45–C8A_45–H8AC_45	109.5	C2B_45–C3B_45–C8B_45	127.4(4)
H8AB_45–C8A_45–H8AC_45	109.5	C4B_45–C3B_45–C8B_45	125.0(4)
C2A_45–C7A_45–H7AA_45	109.5	C2B_45–C3B_45–Al2_45	71.22(19)
C2A_45–C7A_45–H7AB_45	109.5	C4B_45–C3B_45–Al2_45	71.13(18)
H7AA_45–C7A_45–H7AB_45	109.5	C8B_45–C3B_45–Al2_45	124.0(3)
C2A_45–C7A_45–H7AC_45	109.5	C5B_45–C4B_45–C3B_45	108.3(3)
H7AA_45–C7A_45–H7AC_45	109.5	C5B_45–C4B_45–C9B_45	127.3(3)
H7AB_45–C7A_45–H7AC_45	109.5	C3B_45–C4B_45–C9B_45	124.3(3)
C1A_45–C6A_45–H6AA_45	109.5	C5B_45–C4B_45–Al2_45	70.88(18)
C1A_45–C6A_45–H6AB_45	109.5	C3B_45–C4B_45–Al2_45	72.02(18)
H6AA_45–C6A_45–H6AB_45	109.5	C9B_45–C4B_45–Al2_45	126.2(2)
C1A_45–C6A_45–H6AC_45	109.5	C1B_45–C5B_45–C4B_45	107.8(3)
H6AA_45–C6A_45–H6AC_45	109.5	C1B_45–C5B_45–C10B_45	125.4(3)
H6AB_45–C6A_45–H6AC_45	109.5	C4B_45–C5B_45–C10B_45	126.6(3)
C5B_45–C1B_45–C2B_45	107.9(3)	C1B_45–C5B_45–Al2_45	71.1(2)
C5B_45–C1B_45–C6B_45	125.3(4)	C4B_45–C5B_45–Al2_45	72.08(18)
C2B_45–C1B_45–C6B_45	126.5(4)	C10B_45–C5B_45–Al2_45	125.7(2)
C5B_45–C1B_45–Al2_45	71.65(19)	C5B_45–C10B_45–H10D_45	109.5
C2B_45–C1B_45–Al2_45	72.4(2)	C5B_45–C10B_45–H10E_45	109.5

H10D_45–C10B_45–H10E_45	109.5	H6BB_45–C6B_45–H6BC_45	109.5
C5B_45–C10B_45–H10F_45	109.5	C2C_45–C1C_45–C5C_45	106.8(3)
H10D_45–C10B_45–H10F_45	109.5	C2C_45–C1C_45–C6C_45	124.9(3)
H10E_45–C10B_45–H10F_45	109.5	C5C_45–C1C_45–C6C_45	128.0(3)
C4B_45–C9B_45–H9BA_45	109.5	C2C_45–C1C_45–Al3_45	71.54(18)
C4B_45–C9B_45–H9BB_45	109.5	C5C_45–C1C_45–Al3_45	71.32(17)
H9BA_45–C9B_45–H9BB_45	109.5	C6C_45–C1C_45–Al3_45	126.7(2)
C4B_45–C9B_45–H9BC_45	109.5	C3C_45–C2C_45–C1C_45	109.4(3)
H9BA_45–C9B_45–H9BC_45	109.5	C3C_45–C2C_45–C7C_45	125.7(3)
H9BB_45–C9B_45–H9BC_45	109.5	C1C_45–C2C_45–C7C_45	124.7(3)
C3B_45–C8B_45–H8BA_45	109.5	C3C_45–C2C_45–Al3_45	72.58(19)
C3B_45–C8B_45–H8BB_45	109.5	C1C_45–C2C_45–Al3_45	71.29(17)
H8BA_45–C8B_45–H8BB_45	109.5	C7C_45–C2C_45–Al3_45	126.3(2)
C3B_45–C8B_45–H8BC_45	109.5	C2C_45–C3C_45–C4C_45	107.9(3)
H8BA_45–C8B_45–H8BC_45	109.5	C2C_45–C3C_45–C8C_45	126.8(4)
H8BB_45–C8B_45–H8BC_45	109.5	C4C_45–C3C_45–C8C_45	125.3(4)
C2B_45–C7B_45–H7BA_45	109.5	C2C_45–C3C_45–Al3_45	70.92(18)
C2B_45–C7B_45–H7BB_45	109.5	C4C_45–C3C_45–Al3_45	71.4(2)
H7BA_45–C7B_45–H7BB_45	109.5	C8C_45–C3C_45–Al3_45	124.4(3)
C2B_45–C7B_45–H7BC_45	109.5	C3C_45–C4C_45–C5C_45	108.2(3)
H7BA_45–C7B_45–H7BC_45	109.5	C3C_45–C4C_45–C9C_45	125.5(4)
H7BB_45–C7B_45–H7BC_45	109.5	C5C_45–C4C_45–C9C_45	126.3(4)
C1B_45–C6B_45–H6BA_45	109.5	C3C_45–C4C_45–Al3_45	72.08(19)
C1B_45–C6B_45–H6BB_45	109.5	C5C_45–C4C_45–Al3_45	70.81(19)
H6BA_45–C6B_45–H6BB_45	109.5	C9C_45–C4C_45–Al3_45	123.7(3)
C1B_45–C6B_45–H6BC_45	109.5	C1C_45–C5C_45–C4C_45	107.6(3)
H6BA_45–C6B_45–H6BC_45	109.5	C1C_45–C5C_45–C10C_45	125.5(4)

C4C_45–C5C_45–C10C_45	126.8(4)	H7CB_45–C7C_45–H7CC_45	109.5
C1C_45–C5C_45–Al3_45	71.20(17)	C1C_45–C6C_45–H6CA_45	109.5
C4C_45–C5C_45–Al3_45	71.86(19)	C1C_45–C6C_45–H6CB_45	109.5
C10C_45–C5C_45–Al3_45	122.3(3)	H6CA_45–C6C_45–H6CB_45	109.5
C5C_45–C10C_45–H10G_45	109.5	C1C_45–C6C_45–H6CC_45	109.5
C5C_45–C10C_45–H10H_45	109.5	H6CA_45–C6C_45–H6CC_45	109.5
H10G_45–C10C_45–H10H_45	109.5	H6CB_45–C6C_45–H6CC_45	109.5
C5C_45–C10C_45–H10I_45	109.5	Al1_66–In1_66–Al3_66	68.01(6)
H10G_45–C10C_45–H10I_45	109.5	Al1_66–In1_66–Al2_66	67.87(6)
H10H_45–C10C_45–H10I_45	109.5	Al3_66–In1_66–Al2_66	69.98(5)
C4C_45–C9C_45–H9CA_45	109.5	C5B_66–Al2_66–C1B_66	37.54(12)
C4C_45–C9C_45–H9CB_45	109.5	C5B_66–Al2_66–C2B_66	62.22(13)
H9CA_45–C9C_45–H9CB_45	109.5	C1B_66–Al2_66–C2B_66	37.06(13)
C4C_45–C9C_45–H9CC_45	109.5	C5B_66–Al2_66–C4B_66	37.30(13)
H9CA_45–C9C_45–H9CC_45	109.5	C1B_66–Al2_66–C4B_66	62.30(13)
H9CB_45–C9C_45–H9CC_45	109.5	C2B_66–Al2_66–C4B_66	61.97(13)
C3C_45–C8C_45–H8CA_45	109.5	C5B_66–Al2_66–C3B_66	61.98(13)
C3C_45–C8C_45–H8CB_45	109.5	C1B_66–Al2_66–C3B_66	61.76(13)
H8CA_45–C8C_45–H8CB_45	109.5	C2B_66–Al2_66–C3B_66	36.79(13)
C3C_45–C8C_45–H8CC_45	109.5	C4B_66–Al2_66–C3B_66	37.05(13)
H8CA_45–C8C_45–H8CC_45	109.5	C5B_66–Al2_66–In1_66	152.52(11)
H8CB_45–C8C_45–H8CC_45	109.5	C1B_66–Al2_66–In1_66	164.70(11)
C2C_45–C7C_45–H7CA_45	109.5	C2B_66–Al2_66–In1_66	128.52(11)
C2C_45–C7C_45–H7CB_45	109.5	C4B_66–Al2_66–In1_66	119.75(11)
H7CA_45–C7C_45–H7CB_45	109.5	C3B_66–Al2_66–In1_66	109.82(10)
C2C_45–C7C_45–H7CC_45	109.5	C1C_66–Al3_66–C2C_66	38.08(12)
H7CA_45–C7C_45–H7CC_45	109.5	C1C_66–Al3_66–C5C_66	37.56(12)

C2C_66–Al3_66–C5C_66	62.82(13)	C4A_66–Al1_66–In1_66	114.57(14)
C1C_66–Al3_66–C3C_66	63.04(13)	C5A_66–C1A_66–C2A_66	107.9(3)
C2C_66–Al3_66–C3C_66	37.42(12)	C5A_66–C1A_66–C6A_66	126.0(4)
C5C_66–Al3_66–C3C_66	62.49(13)	C2A_66–C1A_66–C6A_66	125.9(4)
C1C_66–Al3_66–C4C_66	62.53(13)	C5A_66–C1A_66–Al1_66	72.3(2)
C2C_66–Al3_66–C4C_66	62.21(13)	C2A_66–C1A_66–Al1_66	70.92(19)
C5C_66–Al3_66–C4C_66	37.25(12)	C6A_66–C1A_66–Al1_66	125.9(3)
C3C_66–Al3_66–C4C_66	37.03(12)	C3A_66–C2A_66–C1A_66	107.1(3)
C1C_66–Al3_66–In1_66	155.28(13)	C3A_66–C2A_66–C7A_66	126.1(3)
C2C_66–Al3_66–In1_66	166.11(13)	C1A_66–C2A_66–C7A_66	126.8(3)
C5C_66–Al3_66–In1_66	125.31(12)	C3A_66–C2A_66–Al1_66	72.0(2)
C3C_66–Al3_66–In1_66	132.57(13)	C1A_66–C2A_66–Al1_66	71.4(2)
C4C_66–Al3_66–In1_66	116.16(12)	C7A_66–C2A_66–Al1_66	124.2(3)
C2A_66–Al1_66–C1A_66	37.72(13)	C2A_66–C3A_66–C4A_66	108.7(3)
C2A_66–Al1_66–C3A_66	37.06(12)	C2A_66–C3A_66–C8A_66	125.9(3)
C1A_66–Al1_66–C3A_66	61.92(13)	C4A_66–C3A_66–C8A_66	125.4(3)
C2A_66–Al1_66–C5A_66	62.44(14)	C2A_66–C3A_66–Al1_66	70.96(19)
C1A_66–Al1_66–C5A_66	37.20(16)	C4A_66–C3A_66–Al1_66	72.15(19)
C3A_66–Al1_66–C5A_66	61.50(13)	C8A_66–C3A_66–Al1_66	124.0(2)
C2A_66–Al1_66–C4A_66	62.11(14)	C5A_66–C4A_66–C3A_66	108.2(3)
C1A_66–Al1_66–C4A_66	61.65(15)	C5A_66–C4A_66–C9A_66	126.7(4)
C3A_66–Al1_66–C4A_66	36.99(12)	C3A_66–C4A_66–C9A_66	125.1(4)
C5A_66–Al1_66–C4A_66	36.44(14)	C5A_66–C4A_66–Al1_66	71.7(2)
C2A_66–Al1_66–In1_66	168.27(14)	C3A_66–C4A_66–Al1_66	70.86(19)
C1A_66–Al1_66–In1_66	152.55(14)	C9A_66–C4A_66–Al1_66	122.3(3)
C3A_66–Al1_66–In1_66	133.37(14)	C4A_66–C5A_66–C1A_66	108.1(3)
C5A_66–Al1_66–In1_66	122.48(14)	C4A_66–C5A_66–C10A_66	125.9(5)

C1A_66–C5A_66–C10A_66	126.0(4)	H7AB_66–C7A_66–H7AC_66	109.5
C4A_66–C5A_66–Al1_66	71.8(2)	C1A_66–C6A_66–H6AA_66	109.5
C1A_66–C5A_66–Al1_66	70.5(2)	C1A_66–C6A_66–H6AB_66	109.5
C10A_66–C5A_66–Al1_66	122.6(3)	H6AA_66–C6A_66–H6AB_66	109.5
C5A_66–C10A_66–H10A_66	109.5	C1A_66–C6A_66–H6AC_66	109.5
C5A_66–C10A_66–H10B_66	109.5	H6AA_66–C6A_66–H6AC_66	109.5
H10A_66–C10A_66–H10B_66	109.5	H6AB_66–C6A_66–H6AC_66	109.5
C5A_66–C10A_66–H10C_66	109.5	C2B_66–C1B_66–C5B_66	107.9(3)
H10A_66–C10A_66–H10C_66	109.5	C2B_66–C1B_66–C6B_66	127.4(3)
H10B_66–C10A_66–H10C_66	109.5	C5B_66–C1B_66–C6B_66	124.5(3)
C4A_66–C9A_66–H9AA_66	109.5	C2B_66–C1B_66–Al2_66	71.93(19)
C4A_66–C9A_66–H9AB_66	109.5	C5B_66–C1B_66–Al2_66	70.98(19)
H9AA_66–C9A_66–H9AB_66	109.5	C6B_66–C1B_66–Al2_66	126.2(3)
C4A_66–C9A_66–H9AC_66	109.5	C3B_66–C2B_66–C1B_66	108.3(3)
H9AA_66–C9A_66–H9AC_66	109.5	C3B_66–C2B_66–C7B_66	125.1(4)
H9AB_66–C9A_66–H9AC_66	109.5	C1B_66–C2B_66–C7B_66	126.6(4)
C3A_66–C8A_66–H8AA_66	109.5	C3B_66–C2B_66–Al2_66	72.13(19)
C3A_66–C8A_66–H8AB_66	109.5	C1B_66–C2B_66–Al2_66	71.01(19)
H8AA_66–C8A_66–H8AB_66	109.5	C7B_66–C2B_66–Al2_66	123.7(3)
C3A_66–C8A_66–H8AC_66	109.5	C2B_66–C3B_66–C4B_66	108.4(3)
H8AA_66–C8A_66–H8AC_66	109.5	C2B_66–C3B_66–C8B_66	124.5(4)
H8AB_66–C8A_66–H8AC_66	109.5	C4B_66–C3B_66–C8B_66	127.1(4)
C2A_66–C7A_66–H7AA_66	109.5	C2B_66–C3B_66–Al2_66	71.08(19)
C2A_66–C7A_66–H7AB_66	109.5	C4B_66–C3B_66–Al2_66	71.15(19)
H7AA_66–C7A_66–H7AB_66	109.5	C8B_66–C3B_66–Al2_66	123.0(3)
C2A_66–C7A_66–H7AC_66	109.5	C5B_66–C4B_66–C3B_66	107.5(3)
H7AA_66–C7A_66–H7AC_66	109.5	C5B_66–C4B_66–C9B_66	126.1(4)

C3B_66–C4B_66–C9B_66	126.4(4)	H8BB_66–C8B_66–H8BC_66	109.5
C5B_66–C4B_66–Al2_66	70.43(19)	C2B_66–C7B_66–H7BA_66	109.5
C3B_66–C4B_66–Al2_66	71.80(19)	C2B_66–C7B_66–H7BB_66	109.5
C9B_66–C4B_66–Al2_66	123.5(3)	H7BA_66–C7B_66–H7BB_66	109.5
C4B_66–C5B_66–C1B_66	108.0(3)	C2B_66–C7B_66–H7BC_66	109.5
C4B_66–C5B_66–C10B_66	125.9(3)	H7BA_66–C7B_66–H7BC_66	109.5
C1B_66–C5B_66–C10B_66	125.8(4)	H7BB_66–C7B_66–H7BC_66	109.5
C4B_66–C5B_66–Al2_66	72.26(19)	C1B_66–C6B_66–H6BA_66	109.5
C1B_66–C5B_66–Al2_66	71.48(19)	C1B_66–C6B_66–H6BB_66	109.5
C10B_66–C5B_66–Al2_66	126.7(2)	H6BA_66–C6B_66–H6BB_66	109.5
C5B_66–C10B_66–H10D_66	109.5	C1B_66–C6B_66–H6BC_66	109.5
C5B_66–C10B_66–H10E_66	109.5	H6BA_66–C6B_66–H6BC_66	109.5
H10D_66–C10B_66–H10E_66	109.5	H6BB_66–C6B_66–H6BC_66	109.5
C5B_66–C10B_66–H10F_66	109.5	C5C_66–C1C_66–C2C_66	107.6(3)
H10D_66–C10B_66–H10F_66	109.5	C5C_66–C1C_66–C6C_66	126.9(3)
H10E_66–C10B_66–H10F_66	109.5	C2C_66–C1C_66–C6C_66	125.5(3)
C4B_66–C9B_66–H9BA_66	109.5	C5C_66–C1C_66–Al3_66	72.18(19)
C4B_66–C9B_66–H9BB_66	109.5	C2C_66–C1C_66–Al3_66	71.13(19)
H9BA_66–C9B_66–H9BB_66	109.5	C6C_66–C1C_66–Al3_66	124.2(3)
C4B_66–C9B_66–H9BC_66	109.5	C3C_66–C2C_66–C1C_66	108.3(3)
H9BA_66–C9B_66–H9BC_66	109.5	C3C_66–C2C_66–C7C_66	127.2(3)
H9BB_66–C9B_66–H9BC_66	109.5	C1C_66–C2C_66–C7C_66	124.2(3)
C3B_66–C8B_66–H8BA_66	109.5	C3C_66–C2C_66–Al3_66	72.6(2)
C3B_66–C8B_66–H8BB_66	109.5	C1C_66–C2C_66–Al3_66	70.79(19)
H8BA_66–C8B_66–H8BB_66	109.5	C7C_66–C2C_66–Al3_66	126.9(3)
C3B_66–C8B_66–H8BC_66	109.5	C4C_66–C3C_66–C2C_66	107.6(3)
H8BA_66–C8B_66–H8BC_66	109.5	C4C_66–C3C_66–C8C_66	125.8(3)

C2C_66–C3C_66–C8C_66	126.7(3)	H9CB_66–C9C_66–H9CC_66	109.5
C4C_66–C3C_66–Al3_66	71.67(19)	C3C_66–C8C_66–H8CA_66	109.5
C2C_66–C3C_66–Al3_66	70.03(19)	C3C_66–C8C_66–H8CB_66	109.5
C8C_66–C3C_66–Al3_66	124.3(3)	H8CA_66–C8C_66–H8CB_66	109.5
C3C_66–C4C_66–C5C_66	108.6(3)	C3C_66–C8C_66–H8CC_66	109.5
C3C_66–C4C_66–C9C_66	126.1(3)	H8CA_66–C8C_66–H8CC_66	109.5
C5C_66–C4C_66–C9C_66	125.3(3)	H8CB_66–C8C_66–H8CC_66	109.5
C3C_66–C4C_66–Al3_66	71.29(18)	C2C_66–C7C_66–H7CA_66	109.5
C5C_66–C4C_66–Al3_66	70.70(18)	C2C_66–C7C_66–H7CB_66	109.5
C9C_66–C4C_66–Al3_66	124.3(3)	H7CA_66–C7C_66–H7CB_66	109.5
C1C_66–C5C_66–C4C_66	107.9(3)	C2C_66–C7C_66–H7CC_66	109.5
C1C_66–C5C_66–C10C_66	126.6(3)	H7CA_66–C7C_66–H7CC_66	109.5
C4C_66–C5C_66–C10C_66	125.5(3)	H7CB_66–C7C_66–H7CC_66	109.5
C1C_66–C5C_66–Al3_66	70.27(18)	C1C_66–C6C_66–H6CA_66	109.5
C4C_66–C5C_66–Al3_66	72.05(18)	C1C_66–C6C_66–H6CB_66	109.5
C10C_66–C5C_66–Al3_66	123.7(3)	H6CA_66–C6C_66–H6CB_66	109.5
C5C_66–C10C_66–H10G_66	109.5	C1C_66–C6C_66–H6CC_66	109.5
C5C_66–C10C_66–H10H_66	109.5	H6CA_66–C6C_66–H6CC_66	109.5
H10G_66–C10C_66–H10H_66	109.5	H6CB_66–C6C_66–H6CC_66	109.5
C5C_66–C10C_66–H10I_66	109.5	Al3_68–In1_68–Al2_68	68.25(4)
H10G_66–C10C_66–H10I_66	109.5	Al3_68–In1_68–Al1_68	67.73(4)
H10H_66–C10C_66–H10I_66	109.5	Al2_68–In1_68–Al1_68	68.04(4)
C4C_66–C9C_66–H9CA_66	109.5	C5B_68–Al2_68–C4B_68	37.92(19)
C4C_66–C9C_66–H9CB_66	109.5	C5B_68–Al2_68–C3B_68	63.09(19)
H9CA_66–C9C_66–H9CB_66	109.5	C4B_68–Al2_68–C3B_68	38.0(2)
C4C_66–C9C_66–H9CC_66	109.5	C5B_68–Al2_68–C1B_68	37.32(19)
H9CA_66–C9C_66–H9CC_66	109.5	C4B_68–Al2_68–C1B_68	62.48(19)

C3B_68–Al2_68–C1B_68	61.94(17)	C2A_68–Al1_68–C4A_68	61.80(16)
C5B_68–Al2_68–C2B_68	62.49(19)	C1A_68–Al1_68–C5A_68	37.45(16)
C4B_68–Al2_68–C2B_68	62.7(2)	C2A_68–Al1_68–C5A_68	62.26(18)
C3B_68–Al2_68–C2B_68	37.04(19)	C4A_68–Al1_68–C5A_68	37.15(17)
C1B_68–Al2_68–C2B_68	36.84(16)	C1A_68–Al1_68–C3A_68	62.62(17)
C5B_68–Al2_68–In1_68	153.57(17)	C2A_68–Al1_68–C3A_68	37.24(15)
C4B_68–Al2_68–In1_68	126.12(16)	C4A_68–Al1_68–C3A_68	37.05(18)
C3B_68–Al2_68–In1_68	119.56(14)	C5A_68–Al1_68–C3A_68	62.38(19)
C1B_68–Al2_68–In1_68	169.10(14)	C1A_68–Al1_68–In1_68	155.66(15)
C2B_68–Al2_68–In1_68	137.37(12)	C2A_68–Al1_68–In1_68	163.93(14)
C1C_68–Al3_68–C2C_68	37.54(16)	C4A_68–Al1_68–In1_68	112.10(12)
C1C_68–Al3_68–C5C_68	37.82(15)	C5A_68–Al1_68–In1_68	123.07(13)
C2C_68–Al3_68–C5C_68	62.90(15)	C3A_68–Al1_68–In1_68	128.73(12)
C1C_68–Al3_68–C3C_68	61.99(14)	C2A_68–C1A_68–C5A_68	107.6(4)
C2C_68–Al3_68–C3C_68	37.00(14)	C2A_68–C1A_68–C6A_68	125.0(4)
C5C_68–Al3_68–C3C_68	62.08(13)	C5A_68–C1A_68–C6A_68	127.2(5)
C1C_68–Al3_68–C4C_68	61.83(14)	C2A_68–C1A_68–Al1_68	71.4(2)
C2C_68–Al3_68–C4C_68	61.91(14)	C5A_68–C1A_68–Al1_68	71.8(2)
C5C_68–Al3_68–C4C_68	36.74(13)	C6A_68–C1A_68–Al1_68	126.9(3)
C3C_68–Al3_68–C4C_68	36.92(12)	C3A_68–C2A_68–C1A_68	108.8(4)
C1C_68–Al3_68–In1_68	158.30(13)	C3A_68–C2A_68–C7A_68	126.8(5)
C2C_68–Al3_68–In1_68	163.09(12)	C1A_68–C2A_68–C7A_68	124.2(4)
C5C_68–Al3_68–In1_68	126.11(12)	C3A_68–C2A_68–Al1_68	72.1(2)
C3C_68–Al3_68–In1_68	130.25(11)	C1A_68–C2A_68–Al1_68	71.2(2)
C4C_68–Al3_68–In1_68	115.26(10)	C7A_68–C2A_68–Al1_68	126.3(3)
C1A_68–Al1_68–C2A_68	37.42(18)	C4A_68–C3A_68–C2A_68	107.0(4)
C1A_68–Al1_68–C4A_68	62.21(16)	C4A_68–C3A_68–C8A_68	126.0(4)

C2A_68–C3A_68–C8A_68	127.0(5)	H9AB_68–C9A_68–H9AC_68	109.5
C4A_68–C3A_68–Al1_68	71.2(2)	C3A_68–C8A_68–H8AA_68	109.5
C2A_68–C3A_68–Al1_68	70.7(2)	C3A_68–C8A_68–H8AB_68	109.5
C8A_68–C3A_68–Al1_68	124.0(3)	H8AA_68–C8A_68–H8AB_68	109.5
C3A_68–C4A_68–C5A_68	109.1(4)	C3A_68–C8A_68–H8AC_68	109.5
C3A_68–C4A_68–C9A_68	124.9(5)	H8AA_68–C8A_68–H8AC_68	109.5
C5A_68–C4A_68–C9A_68	126.0(5)	H8AB_68–C8A_68–H8AC_68	109.5
C3A_68–C4A_68–Al1_68	71.7(2)	C2A_68–C7A_68–H7AA_68	109.5
C5A_68–C4A_68–Al1_68	71.4(2)	C2A_68–C7A_68–H7AB_68	109.5
C9A_68–C4A_68–Al1_68	122.5(3)	H7AA_68–C7A_68–H7AB_68	109.5
C4A_68–C5A_68–C1A_68	107.5(4)	C2A_68–C7A_68–H7AC_68	109.5
C4A_68–C5A_68–C10A_68	125.9(5)	H7AA_68–C7A_68–H7AC_68	109.5
C1A_68–C5A_68–C10A_68	126.6(5)	H7AB_68–C7A_68–H7AC_68	109.5
C4A_68–C5A_68–Al1_68	71.4(2)	C1A_68–C6A_68–H6AA_68	109.5
C1A_68–C5A_68–Al1_68	70.8(2)	C1A_68–C6A_68–H6AB_68	109.5
C10A_68–C5A_68–Al1_68	122.8(3)	H6AA_68–C6A_68–H6AB_68	109.5
C5A_68–C10A_68–H10A_68	109.5	C1A_68–C6A_68–H6AC_68	109.5
C5A_68–C10A_68–H10B_68	109.5	H6AA_68–C6A_68–H6AC_68	109.5
H10A_68–C10A_68–H10B_68	109.5	H6AB_68–C6A_68–H6AC_68	109.5
C5A_68–C10A_68–H10C_68	109.5	C2B_68–C1B_68–C5B_68	109.4(4)
H10A_68–C10A_68–H10C_68	109.5	C2B_68–C1B_68–C6B_68	126.5(5)
H10B_68–C10A_68–H10C_68	109.5	C5B_68–C1B_68–C6B_68	124.0(5)
C4A_68–C9A_68–H9AA_68	109.5	C2B_68–C1B_68–Al2_68	72.2(3)
C4A_68–C9A_68–H9AB_68	109.5	C5B_68–C1B_68–Al2_68	70.9(3)
H9AA_68–C9A_68–H9AB_68	109.5	C6B_68–C1B_68–Al2_68	125.6(3)
C4A_68–C9A_68–H9AC_68	109.5	C1B_68–C2B_68–C3B_68	108.1(5)
H9AA_68–C9A_68–H9AC_68	109.5	C1B_68–C2B_68–C7B_68	126.2(6)

C3B_68–C2B_68–C7B_68	125.8(5)	H10E_68–C10B_68–H10F_68	109.5
C1B_68–C2B_68–Al2_68	71.0(3)	C4B_68–C9B_68–H9BA_68	109.5
C3B_68–C2B_68–Al2_68	70.9(3)	C4B_68–C9B_68–H9BB_68	109.5
C7B_68–C2B_68–Al2_68	123.9(4)	H9BA_68–C9B_68–H9BB_68	109.5
C2B_68–C3B_68–C4B_68	108.1(4)	C4B_68–C9B_68–H9BC_68	109.5
C2B_68–C3B_68–C8B_68	126.3(7)	H9BA_68–C9B_68–H9BC_68	109.5
C4B_68–C3B_68–C8B_68	125.5(7)	H9BB_68–C9B_68–H9BC_68	109.5
C2B_68–C3B_68–Al2_68	72.1(3)	C3B_68–C8B_68–H8BA_68	109.5
C4B_68–C3B_68–Al2_68	70.9(3)	C3B_68–C8B_68–H8BB_68	109.5
C8B_68–C3B_68–Al2_68	123.4(4)	H8BA_68–C8B_68–H8BB_68	109.5
C5B_68–C4B_68–C3B_68	107.0(5)	C3B_68–C8B_68–H8BC_68	109.5
C5B_68–C4B_68–C9B_68	125.3(7)	H8BA_68–C8B_68–H8BC_68	109.5
C3B_68–C4B_68–C9B_68	127.7(6)	H8BB_68–C8B_68–H8BC_68	109.5
C5B_68–C4B_68–Al2_68	70.7(3)	C2B_68–C7B_68–H7BA_68	109.5
C3B_68–C4B_68–Al2_68	71.1(3)	C2B_68–C7B_68–H7BB_68	109.5
C9B_68–C4B_68–Al2_68	124.0(5)	H7BA_68–C7B_68–H7BB_68	109.5
C1B_68–C5B_68–C4B_68	107.4(4)	C2B_68–C7B_68–H7BC_68	109.5
C1B_68–C5B_68–C10B_68	124.8(6)	H7BA_68–C7B_68–H7BC_68	109.5
C4B_68–C5B_68–C10B_68	127.5(6)	H7BB_68–C7B_68–H7BC_68	109.5
C1B_68–C5B_68–Al2_68	71.8(2)	C1B_68–C6B_68–H6BA_68	109.5
C4B_68–C5B_68–Al2_68	71.4(3)	C1B_68–C6B_68–H6BB_68	109.5
C10B_68–C5B_68–Al2_68	126.4(5)	H6BA_68–C6B_68–H6BB_68	109.5
C5B_68–C10B_68–H10D_68	109.5	C1B_68–C6B_68–H6BC_68	109.5
C5B_68–C10B_68–H10E_68	109.5	H6BA_68–C6B_68–H6BC_68	109.5
H10D_68–C10B_68–H10E_68	109.5	H6BB_68–C6B_68–H6BC_68	109.5
C5B_68–C10B_68–H10F_68	109.5	C2C_68–C1C_68–C5C_68	108.3(3)
H10D_68–C10B_68–H10F_68	109.5	C2C_68–C1C_68–C6C_68	125.0(5)

C5C_68–C1C_68–C6C_68	126.5(5)	C10C_68–C5C_68–Al3_68	123.0(3)
C2C_68–C1C_68–Al3_68	71.4(2)	C5C_68–C10C_68–H10G_68	109.5
C5C_68–C1C_68–Al3_68	72.0(2)	C5C_68–C10C_68–H10H_68	109.5
C6C_68–C1C_68–Al3_68	126.0(3)	H10G_68–C10C_68–H10H_68	109.5
C3C_68–C2C_68–C1C_68	107.7(3)	C5C_68–C10C_68–H10I_68	109.5
C3C_68–C2C_68–C7C_68	126.9(4)	H10G_68–C10C_68–H10I_68	109.5
C1C_68–C2C_68–C7C_68	125.2(4)	H10H_68–C10C_68–H10I_68	109.5
C3C_68–C2C_68–Al3_68	72.3(2)	C4C_68–C9C_68–H9CA_68	109.5
C1C_68–C2C_68–Al3_68	71.0(2)	C4C_68–C9C_68–H9CB_68	109.5
C7C_68–C2C_68–Al3_68	125.9(3)	H9CA_68–C9C_68–H9CB_68	109.5
C2C_68–C3C_68–C4C_68	108.2(3)	C4C_68–C9C_68–H9CC_68	109.5
C2C_68–C3C_68–C8C_68	126.3(4)	H9CA_68–C9C_68–H9CC_68	109.5
C4C_68–C3C_68–C8C_68	125.5(4)	H9CB_68–C9C_68–H9CC_68	109.5
C2C_68–C3C_68–Al3_68	70.7(2)	C3C_68–C8C_68–H8CA_68	109.5
C4C_68–C3C_68–Al3_68	71.82(19)	C3C_68–C8C_68–H8CB_68	109.5
C8C_68–C3C_68–Al3_68	123.6(3)	H8CA_68–C8C_68–H8CB_68	109.5
C5C_68–C4C_68–C3C_68	109.1(3)	C3C_68–C8C_68–H8CC_68	109.5
C5C_68–C4C_68–C9C_68	125.5(4)	H8CA_68–C8C_68–H8CC_68	109.5
C3C_68–C4C_68–C9C_68	125.4(4)	H8CB_68–C8C_68–H8CC_68	109.5
C5C_68–C4C_68–Al3_68	71.3(2)	C2C_68–C7C_68–H7CA_68	109.5
C3C_68–C4C_68–Al3_68	71.26(19)	C2C_68–C7C_68–H7CB_68	109.5
C9C_68–C4C_68–Al3_68	121.8(3)	H7CA_68–C7C_68–H7CB_68	109.5
C4C_68–C5C_68–C1C_68	106.7(3)	C2C_68–C7C_68–H7CC_68	109.5
C4C_68–C5C_68–C10C_68	125.6(4)	H7CA_68–C7C_68–H7CC_68	109.5
C1C_68–C5C_68–C10C_68	127.7(4)	H7CB_68–C7C_68–H7CC_68	109.5
C4C_68–C5C_68–Al3_68	71.93(19)	C1C_68–C6C_68–H6CA_68	109.5
C1C_68–C5C_68–Al3_68	70.1(2)	C1C_68–C6C_68–H6CB_68	109.5

H6CA_68–C6C_68–H6CB_68	109.5	C5C_69–Al3_69–C3C_69	62.30(15)
C1C_68–C6C_68–H6CC_68	109.5	C2C_69–Al3_69–C4C_69	62.48(17)
H6CA_68–C6C_68–H6CC_68	109.5	C1C_69–Al3_69–C4C_69	62.16(16)
H6CB_68–C6C_68–H6CC_68	109.5	C5C_69–Al3_69–C4C_69	37.37(14)
Al1_69–In1_69–Al2_69	70.18(4)	C3C_69–Al3_69–C4C_69	37.27(16)
Al1_69–In1_69–Al3_69	68.97(4)	C2C_69–Al3_69–In1_69	171.76(12)
Al2_69–In1_69–Al3_69	69.41(4)	C1C_69–Al3_69–In1_69	150.71(12)
C5B_69–Al2_69–C4B_69	38.01(17)	C5C_69–Al3_69–In1_69	122.82(12)
C5B_69–Al2_69–C1B_69	37.21(17)	C3C_69–Al3_69–In1_69	137.14(13)
C4B_69–Al2_69–C1B_69	62.78(17)	C4C_69–Al3_69–In1_69	117.10(13)
C5B_69–Al2_69–C2B_69	61.84(15)	C1A_69–Al1_69–C2A_69	37.19(14)
C4B_69–Al2_69–C2B_69	61.69(17)	C1A_69–Al1_69–C3A_69	61.60(13)
C1B_69–Al2_69–C2B_69	37.27(13)	C2A_69–Al1_69–C3A_69	36.77(12)
C5B_69–Al2_69–C3B_69	62.33(14)	C1A_69–Al1_69–C5A_69	37.56(15)
C4B_69–Al2_69–C3B_69	36.99(15)	C2A_69–Al1_69–C5A_69	61.95(14)
C1B_69–Al2_69–C3B_69	62.27(15)	C3A_69–Al1_69–C5A_69	61.07(13)
C2B_69–Al2_69–C3B_69	36.64(16)	C1A_69–Al1_69–C4A_69	61.93(14)
C5B_69–Al2_69–In1_69	154.99(15)	C2A_69–Al1_69–C4A_69	61.55(13)
C4B_69–Al2_69–In1_69	126.46(14)	C3A_69–Al1_69–C4A_69	36.45(13)
C1B_69–Al2_69–In1_69	167.80(13)	C5A_69–Al1_69–C4A_69	36.59(15)
C2B_69–Al2_69–In1_69	136.09(10)	C1A_69–Al1_69–In1_69	153.13(12)
C3B_69–Al2_69–In1_69	119.10(11)	C2A_69–Al1_69–In1_69	169.29(11)
C2C_69–Al3_69–C1C_69	37.33(15)	C3A_69–Al1_69–In1_69	135.68(10)
C2C_69–Al3_69–C5C_69	62.45(16)	C5A_69–Al1_69–In1_69	124.29(11)
C1C_69–Al3_69–C5C_69	37.13(16)	C4A_69–Al1_69–In1_69	117.26(10)
C2C_69–Al3_69–C3C_69	37.36(16)	C2A_69–C1A_69–C5A_69	107.1(3)
C1C_69–Al3_69–C3C_69	62.13(15)	C2A_69–C1A_69–C6A_69	126.4(5)

C5A_69–C1A_69–C6A_69	126.4(5)	C10A_69–C5A_69–Al1_69	122.5(3)
C2A_69–C1A_69–Al1_69	71.44(19)	C5A_69–C10A_69–H10A_69	109.5
C5A_69–C1A_69–Al1_69	71.7(2)	C5A_69–C10A_69–H10B_69	109.5
C6A_69–C1A_69–Al1_69	126.1(3)	H10A_69–C10A_69–H10B_69	109.5
C3A_69–C2A_69–C1A_69	107.8(3)	C5A_69–C10A_69–H10C_69	109.5
C3A_69–C2A_69–C7A_69	125.5(4)	H10A_69–C10A_69–H10C_69	109.5
C1A_69–C2A_69–C7A_69	126.5(4)	H10B_69–C10A_69–H10C_69	109.5
C3A_69–C2A_69–Al1_69	72.04(19)	C4A_69–C9A_69–H9AA_69	109.5
C1A_69–C2A_69–Al1_69	71.4(2)	C4A_69–C9A_69–H9AB_69	109.5
C7A_69–C2A_69–Al1_69	125.5(3)	H9AA_69–C9A_69–H9AB_69	109.5
C4A_69–C3A_69–C2A_69	109.1(3)	C4A_69–C9A_69–H9AC_69	109.5
C4A_69–C3A_69–C8A_69	125.6(4)	H9AA_69–C9A_69–H9AC_69	109.5
C2A_69–C3A_69–C8A_69	125.3(4)	H9AB_69–C9A_69–H9AC_69	109.5
C4A_69–C3A_69–Al1_69	72.30(19)	C3A_69–C8A_69–H8AA_69	109.5
C2A_69–C3A_69–Al1_69	71.19(19)	C3A_69–C8A_69–H8AB_69	109.5
C8A_69–C3A_69–Al1_69	123.3(3)	H8AA_69–C8A_69–H8AB_69	109.5
C3A_69–C4A_69–C5A_69	107.9(3)	C3A_69–C8A_69–H8AC_69	109.5
C3A_69–C4A_69–C9A_69	125.4(4)	H8AA_69–C8A_69–H8AC_69	109.5
C5A_69–C4A_69–C9A_69	126.7(4)	H8AB_69–C8A_69–H8AC_69	109.5
C3A_69–C4A_69–Al1_69	71.25(19)	C2A_69–C7A_69–H7AA_69	109.5
C5A_69–C4A_69–Al1_69	71.2(2)	C2A_69–C7A_69–H7AB_69	109.5
C9A_69–C4A_69–Al1_69	123.7(3)	H7AA_69–C7A_69–H7AB_69	109.5
C4A_69–C5A_69–C1A_69	108.1(3)	C2A_69–C7A_69–H7AC_69	109.5
C4A_69–C5A_69–C10A_69	125.0(5)	H7AA_69–C7A_69–H7AC_69	109.5
C1A_69–C5A_69–C10A_69	126.9(5)	H7AB_69–C7A_69–H7AC_69	109.5
C4A_69–C5A_69–Al1_69	72.2(2)	C1A_69–C6A_69–H6AA_69	109.5
C1A_69–C5A_69–Al1_69	70.8(2)	C1A_69–C6A_69–H6AB_69	109.5

H6AA_69–C6A_69–H6AB_69	109.5	C9B_69–C4B_69–Al2_69	125.0(3)
C1A_69–C6A_69–H6AC_69	109.5	C1B_69–C5B_69–C4B_69	108.7(3)
H6AA_69–C6A_69–H6AC_69	109.5	C1B_69–C5B_69–C10B_69	124.6(5)
H6AB_69–C6A_69–H6AC_69	109.5	C4B_69–C5B_69–C10B_69	126.4(5)
C5B_69–C1B_69–C2B_69	106.9(4)	C1B_69–C5B_69–Al2_69	72.4(2)
C5B_69–C1B_69–C6B_69	126.2(4)	C4B_69–C5B_69–Al2_69	72.0(2)
C2B_69–C1B_69–C6B_69	126.7(4)	C10B_69–C5B_69–Al2_69	126.1(3)
C5B_69–C1B_69–Al2_69	70.4(2)	C5B_69–C10B_69–H10D_69	109.5
C2B_69–C1B_69–Al2_69	71.9(2)	C5B_69–C10B_69–H10E_69	109.5
C6B_69–C1B_69–Al2_69	126.8(3)	H10D_69–C10B_69–H10E_69	109.5
C3B_69–C2B_69–C1B_69	109.2(4)	C5B_69–C10B_69–H10F_69	109.5
C3B_69–C2B_69–C7B_69	124.5(4)	H10D_69–C10B_69–H10F_69	109.5
C1B_69–C2B_69–C7B_69	126.2(4)	H10E_69–C10B_69–H10F_69	109.5
C3B_69–C2B_69–Al2_69	72.1(2)	C4B_69–C9B_69–H9BA_69	109.5
C1B_69–C2B_69–Al2_69	70.9(2)	C4B_69–C9B_69–H9BB_69	109.5
C7B_69–C2B_69–Al2_69	125.9(3)	H9BA_69–C9B_69–H9BB_69	109.5
C2B_69–C3B_69–C4B_69	107.9(4)	C4B_69–C9B_69–H9BC_69	109.5
C2B_69–C3B_69–C8B_69	125.3(4)	H9BA_69–C9B_69–H9BC_69	109.5
C4B_69–C3B_69–C8B_69	126.7(5)	H9BB_69–C9B_69–H9BC_69	109.5
C2B_69–C3B_69–Al2_69	71.3(2)	C3B_69–C8B_69–H8BA_69	109.5
C4B_69–C3B_69–Al2_69	70.6(2)	C3B_69–C8B_69–H8BB_69	109.5
C8B_69–C3B_69–Al2_69	124.3(3)	H8BA_69–C8B_69–H8BB_69	109.5
C3B_69–C4B_69–C5B_69	107.2(4)	C3B_69–C8B_69–H8BC_69	109.5
C3B_69–C4B_69–C9B_69	126.5(5)	H8BA_69–C8B_69–H8BC_69	109.5
C5B_69–C4B_69–C9B_69	126.3(5)	H8BB_69–C8B_69–H8BC_69	109.5
C3B_69–C4B_69–Al2_69	72.4(2)	C2B_69–C7B_69–H7BA_69	109.5
C5B_69–C4B_69–Al2_69	70.0(2)	C2B_69–C7B_69–H7BB_69	109.5

H7BA_69–C7B_69–H7BB_69	109.5	C8C_69–C3C_69–Al3_69	126.5(3)
C2B_69–C7B_69–H7BC_69	109.5	C3C_69–C4C_69–C5C_69	107.7(4)
H7BA_69–C7B_69–H7BC_69	109.5	C3C_69–C4C_69–C9C_69	125.5(4)
H7BB_69–C7B_69–H7BC_69	109.5	C5C_69–C4C_69–C9C_69	126.8(4)
C1B_69–C6B_69–H6BA_69	109.5	C3C_69–C4C_69–Al3_69	71.2(2)
C1B_69–C6B_69–H6BB_69	109.5	C5C_69–C4C_69–Al3_69	71.1(2)
H6BA_69–C6B_69–H6BB_69	109.5	C9C_69–C4C_69–Al3_69	123.9(3)
C1B_69–C6B_69–H6BC_69	109.5	C1C_69–C5C_69–C4C_69	107.8(4)
H6BA_69–C6B_69–H6BC_69	109.5	C1C_69–C5C_69–C10C_69	126.2(4)
H6BB_69–C6B_69–H6BC_69	109.5	C4C_69–C5C_69–C10C_69	126.0(4)
C5C_69–C1C_69–C2C_69	108.7(4)	C1C_69–C5C_69–Al3_69	71.1(2)
C5C_69–C1C_69–C6C_69	125.7(4)	C4C_69–C5C_69–Al3_69	71.6(2)
C2C_69–C1C_69–C6C_69	125.5(4)	C10C_69–C5C_69–Al3_69	122.5(3)
C5C_69–C1C_69–Al3_69	71.8(2)	C5C_69–C10C_69–H10G_69	109.5
C2C_69–C1C_69–Al3_69	71.3(2)	C5C_69–C10C_69–H10H_69	109.5
C6C_69–C1C_69–Al3_69	126.3(3)	H10G_69–C10C_69–H10H_69	109.5
C1C_69–C2C_69–C3C_69	107.7(4)	C5C_69–C10C_69–H10I_69	109.5
C1C_69–C2C_69–C7C_69	126.0(4)	H10G_69–C10C_69–H10I_69	109.5
C3C_69–C2C_69–C7C_69	126.1(4)	H10H_69–C10C_69–H10I_69	109.5
C1C_69–C2C_69–Al3_69	71.4(2)	C4C_69–C9C_69–H9CA_69	109.5
C3C_69–C2C_69–Al3_69	71.8(2)	C4C_69–C9C_69–H9CB_69	109.5
C7C_69–C2C_69–Al3_69	126.0(3)	H9CA_69–C9C_69–H9CB_69	109.5
C2C_69–C3C_69–C4C_69	108.1(4)	C4C_69–C9C_69–H9CC_69	109.5
C2C_69–C3C_69–C8C_69	125.4(5)	H9CA_69–C9C_69–H9CC_69	109.5
C4C_69–C3C_69–C8C_69	126.4(5)	H9CB_69–C9C_69–H9CC_69	109.5
C2C_69–C3C_69–Al3_69	70.8(2)	C3C_69–C8C_69–H8CA_69	109.5
C4C_69–C3C_69–Al3_69	71.5(2)	C3C_69–C8C_69–H8CB_69	109.5

H8CA_69–C8C_69–H8CB_69	109.5	C4B_47–Al2_47–C2B_47	62.0(7)
C3C_69–C8C_69–H8CC_69	109.5	C3B_47–Al2_47–C2B_47	37.1(4)
H8CA_69–C8C_69–H8CC_69	109.5	C5B_47–Al2_47–In1_47	159.4(13)
H8CB_69–C8C_69–H8CC_69	109.5	C1B_47–Al2_47–In1_47	163.1(13)
C2C_69–C7C_69–H7CA_69	109.5	C4B_47–Al2_47–In1_47	128.7(12)
C2C_69–C7C_69–H7CB_69	109.5	C3B_47–Al2_47–In1_47	117.4(11)
H7CA_69–C7C_69–H7CB_69	109.5	C2B_47–Al2_47–In1_47	131.8(12)
C2C_69–C7C_69–H7CC_69	109.5	C1C_47–Al3_47–C2C_47	37.5(4)
H7CA_69–C7C_69–H7CC_69	109.5	C1C_47–Al3_47–C5C_47	37.5(4)
H7CB_69–C7C_69–H7CC_69	109.5	C2C_47–Al3_47–C5C_47	62.6(7)
C1C_69–C6C_69–H6CA_69	109.5	C1C_47–Al3_47–C4C_47	61.7(7)
C1C_69–C6C_69–H6CB_69	109.5	C2C_47–Al3_47–C4C_47	61.4(7)
H6CA_69–C6C_69–H6CB_69	109.5	C5C_47–Al3_47–C4C_47	37.2(4)
C1C_69–C6C_69–H6CC_69	109.5	C1C_47–Al3_47–C3C_47	62.4(7)
H6CA_69–C6C_69–H6CC_69	109.5	C2C_47–Al3_47–C3C_47	37.0(4)
H6CB_69–C6C_69–H6CC_69	109.5	C5C_47–Al3_47–C3C_47	62.7(7)
Al3_47–In1_47–Al2_47	67.3(7)	C4C_47–Al3_47–C3C_47	37.0(4)
Al3_47–In1_47–Al1_47	67.7(7)	C1C_47–Al3_47–In1_47	156.9(13)
Al2_47–In1_47–Al1_47	67.3(7)	C2C_47–Al3_47–In1_47	165.2(13)
C5B_47–Al2_47–C1B_47	37.3(4)	C5C_47–Al3_47–In1_47	126.4(12)
C5B_47–Al2_47–C4B_47	37.8(4)	C4C_47–Al3_47–In1_47	117.3(11)
C1B_47–Al2_47–C4B_47	62.6(7)	C3C_47–Al3_47–In1_47	132.6(12)
C5B_47–Al2_47–C3B_47	62.6(7)	C2A_47–Al1_47–C1A_47	37.3(4)
C1B_47–Al2_47–C3B_47	62.4(7)	C2A_47–Al1_47–C3A_47	37.2(4)
C4B_47–Al2_47–C3B_47	37.3(4)	C1A_47–Al1_47–C3A_47	62.0(7)
C5B_47–Al2_47–C2B_47	62.1(7)	C2A_47–Al1_47–C4A_47	62.1(7)
C1B_47–Al2_47–C2B_47	37.2(4)	C1A_47–Al1_47–C4A_47	61.9(7)

C3A_47–Al1_47–C4A_47	36.9(4)	C8A_47–C3A_47–Al1_47	124(2)
C2A_47–Al1_47–C5A_47	62.2(7)	C3A_47–C4A_47–C5A_47	108.2(13)
C1A_47–Al1_47–C5A_47	37.2(4)	C3A_47–C4A_47–C9A_47	127(2)
C3A_47–Al1_47–C5A_47	61.8(7)	C5A_47–C4A_47–C9A_47	125(2)
C4A_47–Al1_47–C5A_47	36.9(4)	C3A_47–C4A_47–Al1_47	71.2(8)
C2A_47–Al1_47–In1_47	171.7(12)	C5A_47–C4A_47–Al1_47	71.8(8)
C1A_47–Al1_47–In1_47	150.4(11)	C9A_47–C4A_47–Al1_47	121(2)
C3A_47–Al1_47–In1_47	136.5(11)	C4A_47–C5A_47–C1A_47	107.6(13)
C4A_47–Al1_47–In1_47	116.4(10)	C4A_47–C5A_47–C10A_47	124(2)
C5A_47–Al1_47–In1_47	122.1(10)	C1A_47–C5A_47–C10A_47	129(2)
C2A_47–C1A_47–C5A_47	108.2(13)	C4A_47–C5A_47–Al1_47	71.3(8)
C2A_47–C1A_47–C6A_47	125(2)	C1A_47–C5A_47–Al1_47	70.7(8)
C5A_47–C1A_47–C6A_47	127(2)	C10A_47–C5A_47–Al1_47	120(2)
C2A_47–C1A_47–Al1_47	71.2(8)	C5A_47–C10A_47–H10A_47	109.5
C5A_47–C1A_47–Al1_47	72.1(8)	C5A_47–C10A_47–H10B_47	109.5
C6A_47–C1A_47–Al1_47	127(2)	H10A_47–C10A_47–H10B_47	109.5
C3A_47–C2A_47–C1A_47	107.5(13)	C5A_47–C10A_47–H10C_47	109.5
C3A_47–C2A_47–C7A_47	126(2)	H10A_47–C10A_47–H10C_47	109.5
C1A_47–C2A_47–C7A_47	126(2)	H10B_47–C10A_47–H10C_47	109.5
C3A_47–C2A_47–Al1_47	71.6(8)	C4A_47–C9A_47–H9AA_47	109.5
C1A_47–C2A_47–Al1_47	71.4(8)	C4A_47–C9A_47–H9AB_47	109.5
C7A_47–C2A_47–Al1_47	123(2)	H9AA_47–C9A_47–H9AB_47	109.5
C4A_47–C3A_47–C2A_47	108.4(13)	C4A_47–C9A_47–H9AC_47	109.5
C4A_47–C3A_47–C8A_47	128(2)	H9AA_47–C9A_47–H9AC_47	109.5
C2A_47–C3A_47–C8A_47	124(2)	H9AB_47–C9A_47–H9AC_47	109.5
C4A_47–C3A_47–Al1_47	71.8(8)	C3A_47–C8A_47–H8AA_47	109.5
C2A_47–C3A_47–Al1_47	71.2(8)	C3A_47–C8A_47–H8AB_47	109.5

H8AA_47–C8A_47–H8AB_47	109.5	C7B_47–C2B_47–Al2_47	122(2)
C3A_47–C8A_47–H8AC_47	109.5	C2B_47–C3B_47–C4B_47	107.8(13)
H8AA_47–C8A_47–H8AC_47	109.5	C2B_47–C3B_47–C8B_47	125(2)
H8AB_47–C8A_47–H8AC_47	109.5	C4B_47–C3B_47–C8B_47	127(2)
C2A_47–C7A_47–H7AA_47	109.5	C2B_47–C3B_47–Al2_47	71.5(8)
C2A_47–C7A_47–H7AB_47	109.5	C4B_47–C3B_47–Al2_47	71.1(8)
H7AA_47–C7A_47–H7AB_47	109.5	C8B_47–C3B_47–Al2_47	122(2)
C2A_47–C7A_47–H7AC_47	109.5	C3B_47–C4B_47–C5B_47	107.6(13)
H7AA_47–C7A_47–H7AC_47	109.5	C3B_47–C4B_47–C9B_47	127(2)
H7AB_47–C7A_47–H7AC_47	109.5	C5B_47–C4B_47–C9B_47	125(2)
C1A_47–C6A_47–H6AA_47	109.5	C3B_47–C4B_47–Al2_47	71.7(8)
C1A_47–C6A_47–H6AB_47	109.5	C5B_47–C4B_47–Al2_47	70.6(8)
H6AA_47–C6A_47–H6AB_47	109.5	C9B_47–C4B_47–Al2_47	124(2)
C1A_47–C6A_47–H6AC_47	109.5	C1B_47–C5B_47–C4B_47	108.2(13)
H6AA_47–C6A_47–H6AC_47	109.5	C1B_47–C5B_47–C10B_47	127(2)
H6AB_47–C6A_47–H6AC_47	109.5	C4B_47–C5B_47–C10B_47	124(2)
C5B_47–C1B_47–C2B_47	107.7(13)	C1B_47–C5B_47–Al2_47	71.8(8)
C5B_47–C1B_47–C6B_47	126(2)	C4B_47–C5B_47–Al2_47	71.6(8)
C2B_47–C1B_47–C6B_47	127(2)	C10B_47–C5B_47–Al2_47	124(2)
C5B_47–C1B_47–Al2_47	70.9(8)	C5B_47–C10B_47–H10D_47	109.5
C2B_47–C1B_47–Al2_47	71.8(8)	C5B_47–C10B_47–H10E_47	109.5
C6B_47–C1B_47–Al2_47	123(2)	H10D_47–C10B_47–H10E_47	109.5
C3B_47–C2B_47–C1B_47	108.8(13)	C5B_47–C10B_47–H10F_47	109.5
C3B_47–C2B_47–C7B_47	126(2)	H10D_47–C10B_47–H10F_47	109.5
C1B_47–C2B_47–C7B_47	125(2)	H10E_47–C10B_47–H10F_47	109.5
C3B_47–C2B_47–Al2_47	71.4(8)	C4B_47–C9B_47–H9BA_47	109.5
C1B_47–C2B_47–Al2_47	71.0(8)	C4B_47–C9B_47–H9BB_47	109.5

H9BA_47–C9B_47–H9BB_47	109.5	C6C_47–C1C_47–Al3_47	126(2)
C4B_47–C9B_47–H9BC_47	109.5	C3C_47–C2C_47–C1C_47	108.7(14)
H9BA_47–C9B_47–H9BC_47	109.5	C3C_47–C2C_47–C7C_47	126(2)
H9BB_47–C9B_47–H9BC_47	109.5	C1C_47–C2C_47–C7C_47	125(2)
C3B_47–C8B_47–H8BA_47	109.5	C3C_47–C2C_47–Al3_47	72.3(8)
C3B_47–C8B_47–H8BB_47	109.5	C1C_47–C2C_47–Al3_47	71.1(8)
H8BA_47–C8B_47–H8BB_47	109.5	C7C_47–C2C_47–Al3_47	126(2)
C3B_47–C8B_47–H8BC_47	109.5	C2C_47–C3C_47–C4C_47	106.9(13)
H8BA_47–C8B_47–H8BC_47	109.5	C2C_47–C3C_47–C8C_47	128(2)
H8BB_47–C8B_47–H8BC_47	109.5	C4C_47–C3C_47–C8C_47	125(2)
C2B_47–C7B_47–H7BA_47	109.5	C2C_47–C3C_47–Al3_47	70.7(8)
C2B_47–C7B_47–H7BB_47	109.5	C4C_47–C3C_47–Al3_47	71.4(8)
H7BA_47–C7B_47–H7BB_47	109.5	C8C_47–C3C_47–Al3_47	122(2)
C2B_47–C7B_47–H7BC_47	109.5	C5C_47–C4C_47–C3C_47	109.7(13)
H7BA_47–C7B_47–H7BC_47	109.5	C5C_47–C4C_47–C9C_47	125(2)
H7BB_47–C7B_47–H7BC_47	109.5	C3C_47–C4C_47–C9C_47	125(2)
C1B_47–C6B_47–H6BA_47	109.5	C5C_47–C4C_47–Al3_47	71.0(8)
C1B_47–C6B_47–H6BB_47	109.5	C3C_47–C4C_47–Al3_47	71.6(8)
H6BA_47–C6B_47–H6BB_47	109.5	C9C_47–C4C_47–Al3_47	129(2)
C1B_47–C6B_47–H6BC_47	109.5	C4C_47–C5C_47–C1C_47	106.4(13)
H6BA_47–C6B_47–H6BC_47	109.5	C4C_47–C5C_47–C10C_47	126(2)
H6BB_47–C6B_47–H6BC_47	109.5	C1C_47–C5C_47–C10C_47	127(2)
C2C_47–C1C_47–C5C_47	108.2(14)	C4C_47–C5C_47–Al3_47	71.8(8)
C2C_47–C1C_47–C6C_47	127(2)	C1C_47–C5C_47–Al3_47	70.8(8)
C5C_47–C1C_47–C6C_47	125(2)	C10C_47–C5C_47–Al3_47	122(2)
C2C_47–C1C_47–Al3_47	71.4(8)	C5C_47–C10C_47–H10G_47	109.5
C5C_47–C1C_47–Al3_47	71.7(8)	C5C_47–C10C_47–H10H_47	109.5

H10G_47–C10C_47–H10H_47	109.5	H6CB_47–C6C_47–H6CC_47	109.5
C5C_47–C10C_47–H10I_47	109.5	Al3_48–In1_48–Al2_48	67.4(6)
H10G_47–C10C_47–H10I_47	109.5	Al3_48–In1_48–Al1_48	68.5(5)
H10H_47–C10C_47–H10I_47	109.5	Al2_48–In1_48–Al1_48	67.1(6)
C4C_47–C9C_47–H9CA_47	109.5	C5B_48–Al2_48–C1B_48	37.3(4)
C4C_47–C9C_47–H9CB_47	109.5	C5B_48–Al2_48–C2B_48	62.6(7)
H9CA_47–C9C_47–H9CB_47	109.5	C1B_48–Al2_48–C2B_48	37.3(4)
C4C_47–C9C_47–H9CC_47	109.5	C5B_48–Al2_48–C3B_48	63.1(7)
H9CA_47–C9C_47–H9CC_47	109.5	C1B_48–Al2_48–C3B_48	62.4(7)
H9CB_47–C9C_47–H9CC_47	109.5	C2B_48–Al2_48–C3B_48	37.1(4)
C3C_47–C8C_47–H8CA_47	109.5	C5B_48–Al2_48–C4B_48	37.7(4)
C3C_47–C8C_47–H8CB_47	109.5	C1B_48–Al2_48–C4B_48	62.2(7)
H8CA_47–C8C_47–H8CB_47	109.5	C2B_48–Al2_48–C4B_48	62.1(7)
C3C_47–C8C_47–H8CC_47	109.5	C3B_48–Al2_48–C4B_48	37.5(4)
H8CA_47–C8C_47–H8CC_47	109.5	C5B_48–Al2_48–In1_48	155.3(12)
H8CB_47–C8C_47–H8CC_47	109.5	C1B_48–Al2_48–In1_48	167.4(12)
C2C_47–C7C_47–H7CA_47	109.5	C2B_48–Al2_48–In1_48	135.7(12)
C2C_47–C7C_47–H7CB_47	109.5	C3B_48–Al2_48–In1_48	119.0(12)
H7CA_47–C7C_47–H7CB_47	109.5	C4B_48–Al2_48–In1_48	127.4(11)
C2C_47–C7C_47–H7CC_47	109.5	C1C_48–Al3_48–C2C_48	37.2(4)
H7CA_47–C7C_47–H7CC_47	109.5	C1C_48–Al3_48–C5C_48	37.2(4)
H7CB_47–C7C_47–H7CC_47	109.5	C2C_48–Al3_48–C5C_48	61.4(7)
C1C_47–C6C_47–H6CA_47	109.5	C1C_48–Al3_48–C3C_48	61.8(7)
C1C_47–C6C_47–H6CB_47	109.5	C2C_48–Al3_48–C3C_48	36.3(4)
H6CA_47–C6C_47–H6CB_47	109.5	C5C_48–Al3_48–C3C_48	61.6(6)
C1C_47–C6C_47–H6CC_47	109.5	C1C_48–Al3_48–C4C_48	61.2(7)
H6CA_47–C6C_47–H6CC_47	109.5	C2C_48–Al3_48–C4C_48	60.4(6)

C5C_48–Al3_48–C4C_48	36.5(4)	C6A_48–C1A_48–Al1_48	125(2)
C3C_48–Al3_48–C4C_48	36.4(4)	C3A_48–C2A_48–C1A_48	107.5(13)
C1C_48–Al3_48–In1_48	158.2(8)	C3A_48–C2A_48–C7A_48	126(2)
C2C_48–Al3_48–In1_48	160.6(8)	C1A_48–C2A_48–C7A_48	127(2)
C5C_48–Al3_48–In1_48	124.5(8)	C3A_48–C2A_48–Al1_48	71.0(8)
C3C_48–Al3_48–In1_48	126.5(7)	C1A_48–C2A_48–Al1_48	71.2(8)
C4C_48–Al3_48–In1_48	112.0(7)	C7A_48–C2A_48–Al1_48	123(2)
C3A_48–Al1_48–C4A_48	37.2(4)	C4A_48–C3A_48–C2A_48	108.8(13)
C3A_48–Al1_48–C1A_48	62.3(7)	C4A_48–C3A_48–C8A_48	129(2)
C4A_48–Al1_48–C1A_48	62.5(7)	C2A_48–C3A_48–C8A_48	122(2)
C3A_48–Al1_48–C2A_48	37.3(4)	C4A_48–C3A_48–Al1_48	71.6(8)
C4A_48–Al1_48–C2A_48	62.4(7)	C2A_48–C3A_48–Al1_48	71.7(8)
C1A_48–Al1_48–C2A_48	37.4(4)	C8A_48–C3A_48–Al1_48	127(2)
C3A_48–Al1_48–C5A_48	61.5(7)	C5A_48–C4A_48–C3A_48	107.5(13)
C4A_48–Al1_48–C5A_48	36.9(4)	C5A_48–C4A_48–C9A_48	126(2)
C1A_48–Al1_48–C5A_48	37.1(4)	C3A_48–C4A_48–C9A_48	127(2)
C2A_48–Al1_48–C5A_48	61.8(7)	C5A_48–C4A_48–Al1_48	72.5(8)
C3A_48–Al1_48–In1_48	140.4(10)	C3A_48–C4A_48–Al1_48	71.2(8)
C4A_48–Al1_48–In1_48	120.0(9)	C9A_48–C4A_48–Al1_48	122(2)
C1A_48–Al1_48–In1_48	149.4(9)	C4A_48–C5A_48–C1A_48	108.5(13)
C2A_48–Al1_48–In1_48	173.1(9)	C4A_48–C5A_48–C10A_48	124(2)
C5A_48–Al1_48–In1_48	124.4(9)	C1A_48–C5A_48–C10A_48	128(2)
C5A_48–C1A_48–C2A_48	107.6(13)	C4A_48–C5A_48–Al1_48	70.5(8)
C5A_48–C1A_48–C6A_48	127(2)	C1A_48–C5A_48–Al1_48	70.4(8)
C2A_48–C1A_48–C6A_48	125(2)	C10A_48–C5A_48–Al1_48	123(2)
C5A_48–C1A_48–Al1_48	72.5(8)	C5A_48–C10A_48–H10A_48	109.5
C2A_48–C1A_48–Al1_48	71.5(8)	C5A_48–C10A_48–H10B_48	109.5

H10A_48–C10A_48–H10B_48	109.5	H6AB_48–C6A_48–H6AC_48	109.5
C5A_48–C10A_48–H10C_48	109.5	C5B_48–C1B_48–C2B_48	108.6(13)
H10A_48–C10A_48–H10C_48	109.5	C5B_48–C1B_48–C6B_48	126.9(19)
H10B_48–C10A_48–H10C_48	109.5	C2B_48–C1B_48–C6B_48	124.4(19)
C4A_48–C9A_48–H9AA_48	109.5	C5B_48–C1B_48–Al2_48	71.2(8)
C4A_48–C9A_48–H9AB_48	109.5	C2B_48–C1B_48–Al2_48	71.5(8)
H9AA_48–C9A_48–H9AB_48	109.5	C6B_48–C1B_48–Al2_48	127(2)
C4A_48–C9A_48–H9AC_48	109.5	C3B_48–C2B_48–C1B_48	108.6(13)
H9AA_48–C9A_48–H9AC_48	109.5	C3B_48–C2B_48–C7B_48	126(2)
H9AB_48–C9A_48–H9AC_48	109.5	C1B_48–C2B_48–C7B_48	125(2)
C3A_48–C8A_48–H8AA_48	109.5	C3B_48–C2B_48–Al2_48	71.6(8)
C3A_48–C8A_48–H8AB_48	109.5	C1B_48–C2B_48–Al2_48	71.2(8)
H8AA_48–C8A_48–H8AB_48	109.5	C7B_48–C2B_48–Al2_48	125(2)
C3A_48–C8A_48–H8AC_48	109.5	C2B_48–C3B_48–C4B_48	107.6(13)
H8AA_48–C8A_48–H8AC_48	109.5	C2B_48–C3B_48–C8B_48	126(2)
H8AB_48–C8A_48–H8AC_48	109.5	C4B_48–C3B_48–C8B_48	126(2)
C2A_48–C7A_48–H7AA_48	109.5	C2B_48–C3B_48–Al2_48	71.3(8)
C2A_48–C7A_48–H7AB_48	109.5	C4B_48–C3B_48–Al2_48	71.4(8)
H7AA_48–C7A_48–H7AB_48	109.5	C8B_48–C3B_48–Al2_48	126(2)
C2A_48–C7A_48–H7AC_48	109.5	C3B_48–C4B_48–C5B_48	108.0(13)
H7AA_48–C7A_48–H7AC_48	109.5	C3B_48–C4B_48–C9B_48	124(2)
H7AB_48–C7A_48–H7AC_48	109.5	C5B_48–C4B_48–C9B_48	128(2)
C1A_48–C6A_48–H6AA_48	109.5	C3B_48–C4B_48–Al2_48	71.0(8)
C1A_48–C6A_48–H6AB_48	109.5	C5B_48–C4B_48–Al2_48	70.5(8)
H6AA_48–C6A_48–H6AB_48	109.5	C9B_48–C4B_48–Al2_48	122(2)
C1A_48–C6A_48–H6AC_48	109.5	C1B_48–C5B_48–C4B_48	107.3(13)
H6AA_48–C6A_48–H6AC_48	109.5	C1B_48–C5B_48–C10B_48	128(2)

C4B_48–C5B_48–C10B_48	125(2)	H7BB_48–C7B_48–H7BC_48	109.5
C1B_48–C5B_48–Al2_48	71.4(8)	C1B_48–C6B_48–H6BA_48	109.5
C4B_48–C5B_48–Al2_48	71.7(8)	C1B_48–C6B_48–H6BB_48	109.5
C10B_48–C5B_48–Al2_48	123(2)	H6BA_48–C6B_48–H6BB_48	109.5
C5B_48–C10B_48–H10D_48	109.5	C1B_48–C6B_48–H6BC_48	109.5
C5B_48–C10B_48–H10E_48	109.5	H6BA_48–C6B_48–H6BC_48	109.5
H10D_48–C10B_48–H10E_48	109.5	H6BB_48–C6B_48–H6BC_48	109.5
C5B_48–C10B_48–H10F_48	109.5	C2C_48–C1C_48–C5C_48	107.2(13)
H10D_48–C10B_48–H10F_48	109.5	C2C_48–C1C_48–C6C_48	126(2)
H10E_48–C10B_48–H10F_48	109.5	C5C_48–C1C_48–C6C_48	126(2)
C4B_48–C9B_48–H9BA_48	109.5	C2C_48–C1C_48–Al3_48	72.0(8)
C4B_48–C9B_48–H9BB_48	109.5	C5C_48–C1C_48–Al3_48	72.4(8)
H9BA_48–C9B_48–H9BB_48	109.5	C6C_48–C1C_48–Al3_48	125(2)
C4B_48–C9B_48–H9BC_48	109.5	C3C_48–C2C_48–C1C_48	109.4(13)
H9BA_48–C9B_48–H9BC_48	109.5	C3C_48–C2C_48–C7C_48	126.0(19)
H9BB_48–C9B_48–H9BC_48	109.5	C1C_48–C2C_48–C7C_48	124.4(19)
C3B_48–C8B_48–H8BA_48	109.5	C3C_48–C2C_48–Al3_48	72.8(8)
C3B_48–C8B_48–H8BB_48	109.5	C1C_48–C2C_48–Al3_48	70.8(8)
H8BA_48–C8B_48–H8BB_48	109.5	C7C_48–C2C_48–Al3_48	127(2)
C3B_48–C8B_48–H8BC_48	109.5	C2C_48–C3C_48–C4C_48	107.0(13)
H8BA_48–C8B_48–H8BC_48	109.5	C2C_48–C3C_48–C8C_48	129(2)
H8BB_48–C8B_48–H8BC_48	109.5	C4C_48–C3C_48–C8C_48	123.6(19)
C2B_48–C7B_48–H7BA_48	109.5	C2C_48–C3C_48–Al3_48	70.8(8)
C2B_48–C7B_48–H7BB_48	109.5	C4C_48–C3C_48–Al3_48	72.1(8)
H7BA_48–C7B_48–H7BB_48	109.5	C8C_48–C3C_48–Al3_48	120.2(18)
C2B_48–C7B_48–H7BC_48	109.5	C5C_48–C4C_48–C3C_48	109.1(12)
H7BA_48–C7B_48–H7BC_48	109.5	C5C_48–C4C_48–C9C_48	128.0(19)

C3C_48–C4C_48–C9C_48	122.8(18)
C5C_48–C4C_48–Al3_48	70.8(8)
C3C_48–C4C_48–Al3_48	71.5(8)
C9C_48–C4C_48–Al3_48	124.4(18)
C4C_48–C5C_48–C1C_48	107.4(13)
C4C_48–C5C_48–C10C_48	126.2(19)
C1C_48–C5C_48–C10C_48	126.2(19)
C4C_48–C5C_48–Al3_48	72.7(8)
C1C_48–C5C_48–Al3_48	70.4(8)
C10C_48–C5C_48–Al3_48	126(2)
C5C_48–C10C_48–H10G_48	109.5
C5C_48–C10C_48–H10H_48	109.5
H10G_48–C10C_48–H10H_48	109.5
C5C_48–C10C_48–H10I_48	109.5
H10G_48–C10C_48–H10I_48	109.5
H10H_48–C10C_48–H10I_48	109.5
C4C_48–C9C_48–H9CA_48	109.5
C4C_48–C9C_48–H9CB_48	109.5
H9CA_48–C9C_48–H9CB_48	109.5
C4C_48–C9C_48–H9CC_48	109.5
H9CA_48–C9C_48–H9CC_48	109.5
H9CB_48–C9C_48–H9CC_48	109.5
C3C_48–C8C_48–H8CA_48	109.5
C3C_48–C8C_48–H8CB_48	109.5
H8CA_48–C8C_48–H8CB_48	109.5
C3C_48–C8C_48–H8CC_48	109.5
H8CA_48–C8C_48–H8CC_48	109.5
H8CB_48–C8C_48–H8CC_48	109.5
C2C_48–C7C_48–H7CA_48	109.5
C2C_48–C7C_48–H7CB_48	109.5
H7CA_48–C7C_48–H7CB_48	109.5
C2C_48–C7C_48–H7CC_48	109.5
H7CA_48–C7C_48–H7CC_48	109.5
H7CB_48–C7C_48–H7CC_48	109.5
C1C_48–C6C_48–H6CA_48	109.5
C1C_48–C6C_48–H6CB_48	109.5
H6CA_48–C6C_48–H6CB_48	109.5
C1C_48–C6C_48–H6CC_48	109.5
H6CA_48–C6C_48–H6CC_48	109.5
H6CB_48–C6C_48–H6CC_48	109.5
C2_49–C1_49–C5_49	108.1(9)
C2_49–C1_49–C10_49	125.3(12)
C5_49–C1_49–C10_49	126.6(12)
C2_49–C1_49–Al1	68.3(5)
C5_49–C1_49–Al1	71.7(7)
C10_49–C1_49–Al1	126.8(8)
C3_49–C2_49–C1_49	109.2(9)
C3_49–C2_49–C9_49	127.2(13)
C1_49–C2_49–C9_49	123.6(13)
C3_49–C2_49–Al1	68.6(5)
C1_49–C2_49–Al1	77.2(5)
C9_49–C2_49–Al1	121.9(9)
C2_49–C3_49–C4_49	107.0(9)
C2_49–C3_49–C8_49	126.9(14)
C4_49–C3_49–C8_49	126.0(14)
C2_49–C3_49–Al1	75.6(6)
C4_49–C3_49–Al1	71.7(11)
C8_49–C3_49–Al1	121.0(9)
C3_49–C4_49–C5_49	108.6(9)
C3_49–C4_49–C7_49	127.7(13)
C5_49–C4_49–C7_49	123.3(13)
C3_49–C4_49–Al1	71.2(9)
C5_49–C4_49–Al1	78.4(11)
C7_49–C4_49–Al1	122.3(15)
C1_49–C5_49–C4_49	107.0(9)
C1_49–C5_49–C6_49	123.7(12)
C4_49–C5_49–C6_49	129.2(12)
C1_49–C5_49–Al1	74.3(7)
C4_49–C5_49–Al1	66.0(11)

C6_49–C5_49–Al1	128.3(11)	C4_50–C1_50–C3_50	107.4(11)
C5_49–C6_49–H6A_49	109.5	F3_50–C2_50–F2_50	109.0(14)
C5_49–C6_49–H6B_49	109.5	F3_50–C2_50–F1_50	109.0(17)
H6A_49–C6_49–H6B_49	109.5	F2_50–C2_50–F1_50	109.0(15)
C5_49–C6_49–H6C_49	109.5	F3_50–C2_50–C1_50	109.6(12)
H6A_49–C6_49–H6C_49	109.5	F2_50–C2_50–C1_50	112.0(12)
H6B_49–C6_49–H6C_49	109.5	F1_50–C2_50–C1_50	108.2(14)
C4_49–C7_49–H7A_49	109.5	F4_50–C3_50–F5_50	108.2(16)
C4_49–C7_49–H7B_49	109.5	F4_50–C3_50–F6_50	108.8(14)
H7A_49–C7_49–H7B_49	109.5	F5_50–C3_50–F6_50	109.0(15)
C4_49–C7_49–H7C_49	109.5	F4_50–C3_50–C1_50	112.5(12)
H7A_49–C7_49–H7C_49	109.5	F5_50–C3_50–C1_50	108.0(13)
H7B_49–C7_49–H7C_49	109.5	F6_50–C3_50–C1_50	110.2(12)
C3_49–C8_49–H8A_49	109.5	F9_50–C4_50–F8_50	108.3(16)
C3_49–C8_49–H8B_49	109.5	F9_50–C4_50–F7_50	111.0(19)
H8A_49–C8_49–H8B_49	109.5	F8_50–C4_50–F7_50	109.2(18)
C3_49–C8_49–H8C_49	109.5	F9_50–C4_50–C1_50	111.6(15)
H8A_49–C8_49–H8C_49	109.5	F8_50–C4_50–C1_50	111.3(15)
H8B_49–C8_49–H8C_49	109.5	F7_50–C4_50–C1_50	105.4(13)
C2_49–C9_49–H9A_49	109.5	C1_22–O1_22–Al18	146.6(7)
C2_49–C9_49–H9B_49	109.5	O1_22–C1_22–C3_22	111.8(6)
H9A_49–C9_49–H9B_49	109.5	O1_22–C1_22–C2_22	112.1(6)
C2_49–C9_49–H9C_49	109.5	C3_22–C1_22–C2_22	107.7(6)
H9A_49–C9_49–H9C_49	109.5	O1_22–C1_22–C4_22	107.4(7)
H9B_49–C9_49–H9C_49	109.5	C3_22–C1_22–C4_22	108.2(6)
C1_49–C10_49–H10A_49	109.5	C2_22–C1_22–C4_22	109.6(6)
C1_49–C10_49–H10B_49	109.5	F2_22–C2_22–F3_22	110.7(7)
H10A_49–C10_49–H10B_49	109.5	F2_22–C2_22–F1_22	107.3(8)
C1_49–C10_49–H10C_49	109.5	F3_22–C2_22–F1_22	102.3(8)
H10A_49–C10_49–H10C_49	109.5	F2_22–C2_22–C1_22	115.9(7)
H10B_49–C10_49–H10C_49	109.5	F3_22–C2_22–C1_22	110.4(6)
C1_50–O1_50–Al20	148.5(11)	F1_22–C2_22–C1_22	109.3(7)
O1_50–C1_50–C2_50	112.3(11)	F6_22–C3_22–F4_22	108.1(7)
O1_50–C1_50–C4_50	110.7(11)	F6_22–C3_22–F5_22	106.8(7)
C2_50–C1_50–C4_50	108.3(12)	F4_22–C3_22–F5_22	105.7(7)
O1_50–C1_50–C3_50	110.8(11)	F6_22–C3_22–C1_22	113.4(7)
C2_50–C1_50–C3_50	107.2(11)	F4_22–C3_22–C1_22	110.5(6)
		F5_22–C3_22–C1_22	112.0(7)
		F9_22–C4_22–F8_22	111.2(9)
		F9_22–C4_22–F7_22	103.9(9)
		F8_22–C4_22–F7_22	105.1(9)
		F9_22–C4_22–C1_22	110.3(7)
		F8_22–C4_22–C1_22	112.6(8)
		F7_22–C4_22–C1_22	113.3(8)
		C1_51–O1_51–Al18	139.5(13)
		O1_51–C1_51–C4_51	118.9(13)
		O1_51–C1_51–C3_51	106.0(11)
		C4_51–C1_51–C3_51	110.2(11)
		O1_51–C1_51–C2_51	105.7(12)
		C4_51–C1_51–C2_51	105.4(10)
		C3_51–C1_51–C2_51	110.6(11)
		F2_51–C2_51–F3_51	106.5(15)
		F2_51–C2_51–F1_51	105.5(16)
		F3_51–C2_51–F1_51	113.8(16)
		F2_51–C2_51–C1_51	112.7(15)

F3_51–C2_51–C1_51	112.4(13)	C2_40–C3_40–Al3	70.1(2)
F1_51–C2_51–C1_51	105.8(13)	C8_40–C3_40–Al3	126.4(3)
F6_51–C3_51–F4_51	107.1(14)	C3_40–C4_40–C5_40	109.0(3)
F6_51–C3_51–F5_51	108.2(14)	C3_40–C4_40–C7_40	125.7(5)
F4_51–C3_51–F5_51	108.3(15)	C5_40–C4_40–C7_40	125.3(5)
F6_51–C3_51–C1_51	114.1(13)	C3_40–C4_40–Al3	72.5(2)
F4_51–C3_51–C1_51	110.0(13)	C5_40–C4_40–Al3	70.4(2)
F5_51–C3_51–C1_51	109.0(12)	C7_40–C4_40–Al3	124.7(3)
F9_51–C4_51–F7_51	107.2(16)	C4_40–C5_40–C1_40	107.9(3)
F9_51–C4_51–F8_51	106.9(15)	C4_40–C5_40–C6_40	127.2(5)
F7_51–C4_51–F8_51	105.5(15)	C1_40–C5_40–C6_40	124.9(5)
F9_51–C4_51–C1_51	114.4(14)	C4_40–C5_40–Al3	72.8(2)
F7_51–C4_51–C1_51	114.9(14)	C1_40–C5_40–Al3	70.2(2)
F8_51–C4_51–C1_51	107.3(13)	C6_40–C5_40–Al3	124.1(3)
C1_32–O1_32–Al18	164.5(19)	C5_40–C6_40–H6A_40	109.5
O1_32–C1_32–C2_32	109.8(13)	C5_40–C6_40–H6B_40	109.5
O1_32–C1_32–C4_32	110.7(12)	H6A_40–C6_40–H6B_40	109.5
C2_32–C1_32–C4_32	111.1(10)		
O1_32–C1_32–C3_32	106.1(13)	C5_40–C6_40–H6C_40	109.5
C2_32–C1_32–C3_32	110.7(10)	H6A_40–C6_40–H6C_40	109.5
C4_32–C1_32–C3_32	108.2(10)		
F1_32–C2_32–F2_32	106.5(13)	H6B_40–C6_40–H6C_40	109.5
F1_32–C2_32–F3_32	103.6(12)		
F2_32–C2_32–F3_32	107.8(12)	C4_40–C7_40–H7A_40	109.5
F1_32–C2_32–C1_32	112.7(11)	C4_40–C7_40–H7B_40	109.5
F2_32–C2_32–C1_32	113.2(11)	H7A_40–C7_40–H7B_40	109.5
F3_32–C2_32–C1_32	112.4(10)		
F6_32–C3_32–F4_32	111.3(12)	C4_40–C7_40–H7C_40	109.5
F6_32–C3_32–F5_32	107.1(13)	H7A_40–C7_40–H7C_40	109.5
F4_32–C3_32–F5_32	108.5(13)		
F6_32–C3_32–C1_32	112.0(11)	H7B_40–C7_40–H7C_40	109.5
F4_32–C3_32–C1_32	110.6(11)		
F5_32–C3_32–C1_32	107.2(13)	C3_40–C8_40–H8A_40	109.5
F9_32–C4_32–F7_32	107.0(13)	C3_40–C8_40–H8B_40	109.5
F9_32–C4_32–F8_32	104.7(13)	H8A_40–C8_40–H8B_40	109.5
F7_32–C4_32–F8_32	107.4(14)		
F9_32–C4_32–C1_32	113.0(12)	C3_40–C8_40–H8C_40	109.5
F7_32–C4_32–C1_32	112.1(12)	H8A_40–C8_40–H8C_40	109.5
F8_32–C4_32–C1_32	112.2(13)		
C5_40–C1_40–C2_40	107.0(3)	H8B_40–C8_40–H8C_40	109.5
C5_40–C1_40–C10_40	127.1(4)		
C2_40–C1_40–C10_40	125.8(4)	C2_40–C9_40–H9A_40	109.5
C5_40–C1_40–Al3	72.0(2)	C2_40–C9_40–H9B_40	109.5
C2_40–C1_40–Al3	72.17(19)	H9A_40–C9_40–H9B_40	109.5
C10_40–C1_40–Al3	122.9(3)		
C3_40–C2_40–C1_40	107.8(3)	C2_40–C9_40–H9C_40	109.5
C3_40–C2_40–C9_40	126.9(4)	H9A_40–C9_40–H9C_40	109.5
C1_40–C2_40–C9_40	125.1(4)		
C3_40–C2_40–Al3	73.0(2)	H9B_40–C9_40–H9C_40	109.5
C1_40–C2_40–Al3	69.88(19)		
C9_40–C2_40–Al3	125.7(3)	C1_40–C10_40–H10A_40	109.5
C4_40–C3_40–C2_40	108.2(4)		
C4_40–C3_40–C8_40	126.3(4)	C1_40–C10_40–H10B_40	109.5
C2_40–C3_40–C8_40	125.4(4)		
C4_40–C3_40–Al3	71.4(2)		

H10A_40–C10_40–H10B_40	109.5
C1_40–C10_40–H10C_40	109.5
H10A_40–C10_40–H10C_40	109.5
H10B_40–C10_40–H10C_40	109.5
C2_52–C1_52–C5_52	108.0(3)
C2_52–C1_52–C10_52	126.7(3)
C5_52–C1_52–C10_52	125.2(3)
C2_52–C1_52–Al2	72.28(18)
C5_52–C1_52–Al2	71.21(18)
C10_52–C1_52–Al2	124.5(3)
C1_52–C2_52–C3_52	108.1(3)
C1_52–C2_52–C9_52	125.4(4)
C3_52–C2_52–C9_52	126.5(4)
C1_52–C2_52–Al2	70.97(18)
C3_52–C2_52–Al2	72.14(19)
C9_52–C2_52–Al2	123.4(3)
C4_52–C3_52–C2_52	107.9(3)
C4_52–C3_52–C8_52	126.6(4)
C2_52–C3_52–C8_52	125.5(4)
C4_52–C3_52–Al2	71.25(19)
C2_52–C3_52–Al2	70.9(2)
C8_52–C3_52–Al2	123.9(3)
C5_52–C4_52–C3_52	107.9(3)
C5_52–C4_52–C7_52	126.8(3)
C3_52–C4_52–C7_52	125.3(3)
C5_52–C4_52–Al2	70.53(19)
C3_52–C4_52–Al2	72.1(2)
C7_52–C4_52–Al2	124.3(3)
C4_52–C5_52–C1_52	108.2(3)
C4_52–C5_52–C6_52	126.2(3)
C1_52–C5_52–C6_52	125.5(3)
C4_52–C5_52–Al2	72.52(19)
C1_52–C5_52–Al2	71.48(18)
C6_52–C5_52–Al2	125.5(3)
C5_52–C6_52–H6A_52	109.5
C5_52–C6_52–H6B_52	109.5
H6A_52–C6_52–H6B_52	109.5
C5_52–C6_52–H6C_52	109.5
H6A_52–C6_52–H6C_52	109.5
H6B_52–C6_52–H6C_52	109.5
C4_52–C7_52–H7A_52	109.5
C4_52–C7_52–H7B_52	109.5
H7A_52–C7_52–H7B_52	109.5
C4_52–C7_52–H7C_52	109.5
H7A_52–C7_52–H7C_52	109.5
H7B_52–C7_52–H7C_52	109.5
C3_52–C8_52–H8A_52	109.5
C3_52–C8_52–H8B_52	109.5
H8A_52–C8_52–H8B_52	109.5
C3_52–C8_52–H8C_52	109.5
H8A_52–C8_52–H8C_52	109.5
H8B_52–C8_52–H8C_52	109.5
C2_52–C9_52–H9A_52	109.5
C2_52–C9_52–H9B_52	109.5
H9A_52–C9_52–H9B_52	109.5
C2_52–C9_52–H9C_52	109.5
H9A_52–C9_52–H9C_52	109.5
H9B_52–C9_52–H9C_52	109.5
C1_52–C10_52–H10A_52	109.5
C1_52–C10_52–H10B_52	109.5
H10A_52–C10_52–H10B_52	109.5
C1_52–C10_52–H10C_52	109.5
H10A_52–C10_52–H10C_52	109.5
H10B_52–C10_52–H10C_52	109.5
C5_53–C1_53–C2_53	108.5(5)
C5_53–C1_53–C10_53	127.1(6)
C2_53–C1_53–C10_53	124.3(6)
C5_53–C1_53–Al1	70.0(4)
C2_53–C1_53–Al1	71.0(3)
C10_53–C1_53–Al1	128.2(4)
C1_53–C2_53–C3_53	109.2(5)
C1_53–C2_53–C9_53	126.1(6)
C3_53–C2_53–C9_53	124.6(6)
C1_53–C2_53–Al1	72.2(3)
C3_53–C2_53–Al1	70.2(3)
C9_53–C2_53–Al1	125.9(4)
C2_53–C3_53–C4_53	106.7(5)
C2_53–C3_53–C8_53	125.2(7)
C4_53–C3_53–C8_53	128.2(7)
C2_53–C3_53–Al1	72.5(3)
C4_53–C3_53–Al1	69.8(3)
C8_53–C3_53–Al1	123.2(4)
C5_53–C4_53–C3_53	108.3(5)
C5_53–C4_53–C7_53	124.0(7)
C3_53–C4_53–C7_53	127.7(7)
C5_53–C4_53–Al1	72.1(5)
C3_53–C4_53–Al1	71.8(3)

C7_53–C4_53–Al1	122.5(5)
C1_53–C5_53–C4_53	107.3(5)
C1_53–C5_53–C6_53	123.5(7)
C4_53–C5_53–C6_53	128.9(8)
C1_53–C5_53–Al1	72.9(4)
C4_53–C5_53–Al1	69.6(4)
C6_53–C5_53–Al1	127.4(6)
C5_53–C6_53–H6A_53	109.5
C5_53–C6_53–H6B_53	109.5
H6A_53–C6_53–H6B_53	109.5
C5_53–C6_53–H6C_53	109.5
H6A_53–C6_53–H6C_53	109.5
H6B_53–C6_53–H6C_53	109.5
C4_53–C7_53–H7A_53	109.5
C4_53–C7_53–H7B_53	109.5
H7A_53–C7_53–H7B_53	109.5
C4_53–C7_53–H7C_53	109.5
H7A_53–C7_53–H7C_53	109.5
H7B_53–C7_53–H7C_53	109.5
C3_53–C8_53–H8A_53	109.5
C3_53–C8_53–H8B_53	109.5
H8A_53–C8_53–H8B_53	109.5
C3_53–C8_53–H8C_53	109.5
H8A_53–C8_53–H8C_53	109.5
H8B_53–C8_53–H8C_53	109.5
C2_53–C9_53–H9A_53	109.5
C2_53–C9_53–H9B_53	109.5
H9A_53–C9_53–H9B_53	109.5
C2_53–C9_53–H9C_53	109.5
H9A_53–C9_53–H9C_53	109.5
H9B_53–C9_53–H9C_53	109.5
C1_53–C10_53–H10A_53	109.5
C1_53–C10_53–H10B_53	109.5
H10A_53–C10_53–H10B_53	109.5
C1_53–C10_53–H10C_53	109.5
H10A_53–C10_53–H10C_53	109.5
H10B_53–C10_53–H10C_53	109.5

S-Table 10: Bond lengths and angles for **3**

Atom–Atom	**Length [Å]**
Tl1–Al2	2.725(3)
Tl1–Al3	2.771(3)
Tl1–Al1	2.799(3)
Tl2–Al4	2.742(3)
Tl2–Al6	2.785(3)
Tl2–Al5	2.790(3)
Tl3–Al8	2.760(3)
Tl3–Al7	2.760(3)
Tl3–Al9	2.766(3)
Al1–C2_9	2.170(9)
Al1–C1_9	2.195(9)
Al1–C3_9	2.203(10)
Al1–C5_57	2.22(3)
Al1–C5_9	2.233(9)
Al1–C4_9	2.243(9)
Al1–C1_57	2.28(3)
Al1–C4_57	2.32(3)
Al1–C2_57	2.40(2)
Al1–C3_57	2.44(2)
Al8–C5_11	2.201(7)
Al8–C4_11	2.205(8)
Al8–C2_11	2.230(6)
Al8–C3_11	2.233(7)
Al8–C1_11	2.234(7)
Al9–C4_12	2.217(7)
Al9–C5_12	2.231(7)
Al9–C3_12	2.236(8)
Al9–C2_12	2.238(7)
Al9–C1_12	2.249(7)
Al10–O1_46	1.614(12)
Al10–O1_29	1.676(7)
Al10–O1_28	1.703(9)
Al10–O1_40	1.716(8)
Al10–O1_43	1.715(15)
Al10–O1_59	1.75(2)
Al10–O1_45	1.756(10)
Al10–O1_35	1.771(11)
Al10–O1_30	1.799(19)
Al11–O1_54	1.66(3)
Al11–O1_26	1.694(14)
Al11–O1_24	1.712(6)
Al11–O1_25	1.714(5)
Al11–O1_34	1.730(12)
Al11–O1_33	1.740(16)
Al11–O1_27	1.749(6)
Al12–O1_56	1.49(3)
Al12–O1_22	1.619(12)
Al12–O1_2	1.65(3)
Al12–O1_36	1.682(18)
Al12–O1_20	1.705(8)
Al12–O1_21	1.713(9)
Al12–O1_23	1.727(16)
Al12–O1_62	1.756(11)
Al12–O1_55	1.796(11)
Al13–O1_38	1.581(13)
Al13–O1_49	1.605(15)
Al13–O1_58	1.654(16)
Al13–O1_44	1.677(16)
Al13–O1_50	1.70(2)
Al13–O1_60	1.71(3)
Al13–O1_32	1.732(15)
Al13–O1_31	1.767(9)
Al13–O1_51	1.767(17)
Al13–O1_39	1.809(14)
Al13–O1_37	1.818(11)
Al14–O1_48	1.641(14)
Al14–O1_15	1.653(18)
Al14–O1_53	1.67(3)
Al14–O1_19	1.684(14)
Al14–O1_16	1.699(10)
Al14–O1_17	1.706(6)
Al14–O1_61	1.72(3)
Al14–O1_47	1.769(15)
Al14–O1_18	1.775(10)
Al14–O1_3	1.83(2)
Al2–C4_7	2.282(7)
Al2–C3_7	2.283(6)
Al2–C5_7	2.295(7)
Al2–C2_7	2.299(6)
Al2–C1_7	2.311(6)
Al3–C4_8	2.187(7)
Al3–C5_8	2.220(7)
Al3–C3_8	2.228(7)
Al3–C1_8	2.253(7)
Al3–C2_8	2.263(7)
Al4–C3_4	2.241(6)
Al4–C2_4	2.245(6)
Al4–C1_4	2.254(6)
Al4–C4_4	2.258(7)
Al4–C5_4	2.263(7)
Al5–C2_5	2.222(7)
Al5–C3_5	2.229(7)
Al5–C5_5	2.235(8)
Al5–C4_5	2.236(8)
Al5–C1_5	2.244(7)
Al6–C3_6	2.203(7)
Al6–C4_6	2.216(9)
Al6–C2_6	2.223(7)
Al6–C1_6	2.242(7)
Al6–C5_6	2.247(7)
Al7–C4_10	2.207(9)
Al7–C2_10	2.211(7)
Al7–C3_10	2.211(8)
Al7–C1_10	2.222(8)
Al7–C5_10	2.225(9)
C1_4–C5_4	1.403(8)
C1_4–C2_4	1.404(8)

C1_4–C10_4	1.513(8)	C4_6–C5_6	1.412(9)
C2_4–C3_4	1.402(8)	C4_6–C7_6	1.508(10)
C2_4–C9_4	1.514(8)	C5_6–C6_6	1.510(9)
C3_4–C4_4	1.424(9)	C6_6–H6A_6	0.9800
C3_4–C8_4	1.519(9)	C6_6–H6B_6	0.9800
C4_4–C5_4	1.408(9)	C6_6–H6C_6	0.9800
C4_4–C7_4	1.513(9)	C7_6–H7A_6	0.9800
C5_4–C6_4	1.510(9)	C7_6–H7B_6	0.9800
C6_4–H6A_4	0.9800	C7_6–H7C_6	0.9800
C6_4–H6B_4	0.9800	C8_6–H8A_6	0.9800
C6_4–H6C_4	0.9800	C8_6–H8B_6	0.9800
C7_4–H7A_4	0.9800	C8_6–H8C_6	0.9800
C7_4–H7B_4	0.9800	C9_6–H9A_6	0.9800
C7_4–H7C_4	0.9800	C9_6–H9B_6	0.9800
C8_4–H8A_4	0.9800	C9_6–H9C_6	0.9800
C8_4–H8B_4	0.9800	C10_6–H10A_6	0.9800
C8_4–H8C_4	0.9800	C10_6–H10B_6	0.9800
C9_4–H9A_4	0.9800	C10_6–H10C_6	0.9800
C9_4–H9B_4	0.9800	C1_7–C2_7	1.420(8)
C9_4–H9C_4	0.9800	C1_7–C5_7	1.420(8)
C10_4–H10A_4	0.9800	C1_7–C10_7	1.505(8)
C10_4–H10B_4	0.9800	C2_7–C3_7	1.417(7)
C10_4–H10C_4	0.9800	C2_7–C9_7	1.509(8)
C1_5–C2_5	1.413(9)	C3_7–C4_7	1.424(7)
C1_5–C5_5	1.425(9)	C3_7–C8_7	1.511(8)
C1_5–C10_5	1.502(9)	C4_7–C5_7	1.417(8)
C2_5–C3_5	1.421(9)	C4_7–C7_7	1.509(8)
C2_5–C9_5	1.505(9)	C5_7–C6_7	1.519(8)
C3_5–C4_5	1.423(9)	C6_7–H6A_7	0.9800
C3_5–C8_5	1.509(9)	C6_7–H6B_7	0.9800
C4_5–C5_5	1.424(9)	C6_7–H6C_7	0.9800
C4_5–C7_5	1.507(9)	C7_7–H7A_7	0.9800
C5_5–C6_5	1.510(9)	C7_7–H7B_7	0.9800
C6_5–H6A_5	0.9800	C7_7–H7C_7	0.9800
C6_5–H6B_5	0.9800	C8_7–H8A_7	0.9800
C6_5–H6C_5	0.9800	C8_7–H8B_7	0.9800
C7_5–H7A_5	0.9800	C8_7–H8C_7	0.9800
C7_5–H7B_5	0.9800	C9_7–H9A_7	0.9800
C7_5–H7C_5	0.9800	C9_7–H9B_7	0.9800
C8_5–H8A_5	0.9800	C9_7–H9C_7	0.9800
C8_5–H8B_5	0.9800	C10_7–H10A_7	0.9800
C8_5–H8C_5	0.9800	C10_7–H10B_7	0.9800
C9_5–H9A_5	0.9800	C10_7–H10C_7	0.9800
C9_5–H9B_5	0.9800	C1_8–C2_8	1.394(9)
C9_5–H9C_5	0.9800	C1_8–C5_8	1.419(9)
C10_5–H10A_5	0.9800	C1_8–C10_8	1.513(9)
C10_5–H10B_5	0.9800	C2_8–C3_8	1.411(8)
C10_5–H10C_5	0.9800	C2_8–C9_8	1.495(9)
C1_6–C2_6	1.413(8)	C3_8–C4_8	1.437(8)
C1_6–C5_6	1.429(9)	C3_8–C8_8	1.495(8)
C1_6–C10_6	1.497(9)	C4_8–C5_8	1.415(8)
C2_6–C3_6	1.411(9)	C4_8–C7_8	1.498(9)
C2_6–C9_6	1.513(10)	C5_8–C6_8	1.503(9)
C3_6–C4_6	1.427(9)	C6_8–H6A_8	0.9800
C3_6–C8_6	1.511(9)	C6_8–H6B_8	0.9800

C6_8–H6C_8	0.9800	C8_10–H8B_10	0.9800
C7_8–H7A_8	0.9800	C8_10–H8C_10	0.9800
C7_8–H7B_8	0.9800	C9_10–H9A_10	0.9800
C7_8–H7C_8	0.9800	C9_10–H9B_10	0.9800
C8_8–H8A_8	0.9800	C9_10–H9C_10	0.9800
C8_8–H8B_8	0.9800	C10_10–H10A_10	0.9800
C8_8–H8C_8	0.9800	C10_10–H10B_10	0.9800
C9_8–H9A_8	0.9800	C10_10–H10C_10	0.9800
C9_8–H9B_8	0.9800	C1_11–C2_11	1.403(8)
C9_8–H9C_8	0.9800	C1_11–C5_11	1.435(9)
C10_8–H10A_8	0.9800	C1_11–C10_11	1.504(9)
C10_8–H10B_8	0.9800	C2_11–C3_11	1.413(8)
C10_8–H10C_8	0.9800	C2_11–C9_11	1.503(8)
C1_9–C5_9	1.416(10)	C3_11–C4_11	1.405(8)
C1_9–C2_9	1.420(10)	C3_11–C8_11	1.511(9)
C1_9–C10_9	1.509(10)	C4_11–C5_11	1.421(9)
C2_9–C3_9	1.423(10)	C4_11–C7_11	1.517(9)
C2_9–C9_9	1.508(11)	C5_11–C6_11	1.507(9)
C3_9–C4_9	1.401(10)	C6_11–H6A_11	0.9800
C3_9–C8_9	1.514(10)	C6_11–H6B_11	0.9800
C4_9–C5_9	1.414(9)	C6_11–H6C_11	0.9800
C4_9–C7_9	1.518(10)	C7_11–H7A_11	0.9800
C5_9–C6_9	1.499(10)	C7_11–H7B_11	0.9800
C6_9–H6A_9	0.9800	C7_11–H7C_11	0.9800
C6_9–H6B_9	0.9800	C8_11–H8A_11	0.9800
C6_9–H6C_9	0.9800	C8_11–H8B_11	0.9800
C7_9–H7A_9	0.9800	C8_11–H8C_11	0.9800
C7_9–H7B_9	0.9800	C9_11–H9A_11	0.9800
C7_9–H7C_9	0.9800	C9_11–H9B_11	0.9800
C8_9–H8A_9	0.9800	C9_11–H9C_11	0.9800
C8_9–H8B_9	0.9800	C10_11–H10A_11	0.9800
C8_9–H8C_9	0.9800	C10_11–H10B_11	0.9800
C9_9–H9A_9	0.9800	C10_11–H10C_11	0.9800
C9_9–H9B_9	0.9800	C1_12–C2_12	1.413(9)
C9_9–H9C_9	0.9800	C1_12–C5_12	1.416(8)
C10_9–H10A_9	0.9800	C1_12–C10_12	1.506(10)
C10_9–H10B_9	0.9800	C2_12–C3_12	1.414(9)
C10_9–H10C_9	0.9800	C2_12–C9_12	1.508(9)
C1_10–C5_10	1.402(9)	C3_12–C4_12	1.429(9)
C1_10–C2_10	1.406(9)	C3_12–C8_12	1.512(10)
C1_10–C10_10	1.505(10)	C4_12–C5_12	1.429(9)
C2_10–C3_10	1.421(9)	C4_12–C7_12	1.503(9)
C2_10–C9_10	1.511(9)	C5_12–C6_12	1.510(9)
C3_10–C4_10	1.427(10)	C6_12–H6A_12	0.9800
C3_10–C8_10	1.490(10)	C6_12–H6B_12	0.9800
C4_10–C5_10	1.416(10)	C6_12–H6C_12	0.9800
C4_10–C7_10	1.506(10)	C7_12–H7A_12	0.9800
C5_10–C6_10	1.513(10)	C7_12–H7B_12	0.9800
C6_10–H6A_10	0.9800	C7_12–H7C_12	0.9800
C6_10–H6B_10	0.9800	C8_12–H8A_12	0.9800
C6_10–H6C_10	0.9800	C8_12–H8B_12	0.9800
C7_10–H7A_10	0.9800	C8_12–H8C_12	0.9800
C7_10–H7B_10	0.9800	C9_12–H9A_12	0.9800
C7_10–H7C_10	0.9800	C9_12–H9B_12	0.9800
C8_10–H8A_10	0.9800	C9_12–H9C_12	0.9800

C10_12–H10A_12	0.9800	O1_20–C1_20	1.346(9)
C10_12–H10B_12	0.9800	C1_20–C3_20	1.543(10)
C10_12–H10C_12	0.9800	C1_20–C4_20	1.550(10)
O1_16–C1_16	1.348(10)	C1_20–C2_20	1.552(10)
C1_16–C2_16	1.543(11)	C2_20–F3_20	1.317(10)
C1_16–C4_16	1.548(11)	C2_20–F1_20	1.324(10)
C1_16–C3_16	1.562(11)	C2_20–F2_20	1.326(9)
C2_16–F3_16	1.326(10)	C3_20–F6_20	1.299(11)
C2_16–F1_16	1.344(11)	C3_20–F5_20	1.301(10)
C2_16–F2_16	1.354(11)	C3_20–F4_20	1.322(10)
C3_16–F4_16	1.320(11)	C4_20–F9_20	1.314(10)
C3_16–F6_16	1.327(10)	C4_20–F8_20	1.318(9)
C3_16–F5_16	1.344(11)	C4_20–F7_20	1.332(10)
C4_16–F9_16	1.275(11)	O1_21–C1_21	1.363(11)
C4_16–F8_16	1.343(10)	C1_21–C3_21	1.542(11)
C4_16–F7_16	1.377(11)	C1_21–C4_21	1.542(11)
O1_17–C1_17	1.351(8)	C1_21–C2_21	1.569(11)
C1_17–C4_17	1.533(10)	C2_21–F1_21	1.321(12)
C1_17–C2_17	1.541(9)	C2_21–F2_21	1.329(11)
C1_17–C3_17	1.569(10)	C2_21–F3_21	1.343(12)
C2_17–F3_17	1.304(10)	C3_21–F4_21	1.313(11)
C2_17–F2_17	1.320(10)	C3_21–F5_21	1.314(11)
C2_17–F1_17	1.349(10)	C3_21–F6_21	1.336(11)
C3_17–F4_17	1.307(10)	C4_21–F9_21	1.324(11)
C3_17–F5_17	1.332(10)	C4_21–F7_21	1.330(11)
C3_17–F6_17	1.339(10)	C4_21–F8_21	1.344(11)
C4_17–F7_17	1.325(11)	O1_22–C1_22	1.348(12)
C4_17–F9_17	1.337(10)	C1_22–C3_22	1.543(12)
C4_17–F8_17	1.341(10)	C1_22–C2_22	1.547(11)
O1_18–C1_18	1.349(10)	C1_22–C4_22	1.555(12)
C1_18–C4_18	1.542(11)	C2_22–F2_22	1.320(11)
C1_18–C2_18	1.549(11)	C2_22–F1_22	1.325(12)
C1_18–C3_18	1.595(11)	C2_22–F3_22	1.328(11)
C2_18–F1_18	1.325(11)	C3_22–F4_22	1.326(12)
C2_18–F2_18	1.327(11)	C3_22–F6_22	1.335(12)
C2_18–F3_18	1.331(11)	C3_22–F5_22	1.343(12)
C3_18–F5_18	1.313(11)	C4_22–F8_22	1.309(12)
C3_18–F4_18	1.324(11)	C4_22–F9_22	1.330(12)
C3_18–F6_18	1.338(11)	C4_22–F7_22	1.338(12)
C4_18–F7_18	1.314(11)	O1_23–C1_23	1.349(11)
C4_18–F8_18	1.331(11)	C1_23–C2_23	1.553(11)
C4_18–F9_18	1.338(11)	C1_23–C4_23	1.554(11)
O1_19–C1_19	1.361(11)	C1_23–C3_23	1.558(11)
C1_19–C2_19	1.550(11)	C2_23–F3_23	1.325(12)
C1_19–C3_19	1.557(11)	C2_23–F2_23	1.326(11)
C1_19–C4_19	1.568(12)	C2_23–F1_23	1.334(11)
C2_19–F2_19	1.328(12)	C3_23–F6_23	1.317(10)
C2_19–F1_19	1.331(12)	C3_23–F5_23	1.321(11)
C2_19–F3_19	1.345(12)	C3_23–F4_23	1.335(11)
C3_19–F5_19	1.307(12)	C4_23–F9_23	1.309(11)
C3_19–F4_19	1.308(12)	C4_23–F7_23	1.322(12)
C3_19–F6_19	1.319(11)	C4_23–F8_23	1.328(11)
C4_19–F7_19	1.322(12)	O1_24–C1_24	1.348(8)
C4_19–F8_19	1.325(12)	C1_24–C3_24	1.548(9)
C4_19–F9_19	1.338(12)	C1_24–C4_24	1.553(9)

C1_24–C2_24	1.557(9)	C2_28–F3_28	1.330(10)
C2_24–F1_24	1.317(8)	C3_28–F4_28	1.336(10)
C2_24–F3_24	1.323(9)	C3_28–F5_28	1.335(11)
C2_24–F2_24	1.344(8)	C3_28–F6_28	1.337(10)
C3_24–F6_24	1.313(9)	C4_28–F9_28	1.317(11)
C3_24–F4_24	1.314(9)	C4_28–F7_28	1.327(10)
C3_24–F5_24	1.356(9)	C4_28–F8_28	1.341(10)
C4_24–F9_24	1.302(9)	O1_29–C1_29	1.361(10)
C4_24–F8_24	1.336(9)	C1_29–C4_29	1.537(10)
C4_24–F7_24	1.353(9)	C1_29–C2_29	1.551(10)
O1_25–C1_25	1.366(7)	C1_29–C3_29	1.553(10)
C1_25–C4_25	1.543(8)	C2_29–F3_29	1.324(10)
C1_25–C2_25	1.547(9)	C2_29–F2_29	1.334(11)
C1_25–C3_25	1.549(9)	C2_29–F1_29	1.335(10)
C2_25–F3_25	1.304(8)	C3_29–F4_29	1.311(10)
C2_25–F1_25	1.330(8)	C3_29–F5_29	1.322(10)
C2_25–F2_25	1.358(8)	C3_29–F6_29	1.331(10)
C3_25–F4_25	1.320(8)	C4_29–F9_29	1.326(10)
C3_25–F6_25	1.324(8)	C4_29–F8_29	1.328(10)
C3_25–F5_25	1.353(8)	C4_29–F7_29	1.329(11)
C4_25–F9_25	1.314(8)	O1_30–C1_30	1.356(12)
C4_25–F7_25	1.327(9)	C1_30–C4_30	1.548(12)
C4_25–F8_25	1.333(8)	C1_30–C2_30	1.549(12)
O1_26–C1_26	1.359(11)	C1_30–C3_30	1.551(12)
C1_26–C4_26	1.542(11)	C2_30–F1_30	1.329(13)
C1_26–C3_26	1.556(11)	C2_30–F2_30	1.328(13)
C1_26–C2_26	1.556(11)	C2_30–F3_30	1.329(13)
C2_26–F3_26	1.320(11)	C3_30–F5_30	1.324(12)
C2_26–F1_26	1.328(11)	C3_30–F4_30	1.335(13)
C2_26–F2_26	1.331(11)	C3_30–F6_30	1.338(13)
C3_26–F6_26	1.317(11)	C4_30–F9_30	1.329(12)
C3_26–F5_26	1.328(11)	C4_30–F8_30	1.332(12)
C3_26–F4_26	1.341(11)	C4_30–F7_30	1.341(12)
C4_26–F7_26	1.325(11)	O1_31–C1_31	1.337(10)
C4_26–F9_26	1.333(11)	C1_31–C2_31	1.533(11)
C4_26–F8_26	1.346(11)	C1_31–C4_31	1.552(11)
O1_27–C1_27	1.364(9)	C1_31–C3_31	1.577(11)
C1_27–C2_27	1.535(10)	C2_31–F1_31	1.288(11)
C1_27–C3_27	1.552(10)	C2_31–F3_31	1.324(11)
C1_27–C4_27	1.553(10)	C2_31–F2_31	1.360(10)
C2_27–F3_27	1.325(10)	C3_31–F5_31	1.291(11)
C2_27–F2_27	1.330(10)	C3_31–F6_31	1.328(11)
C2_27–F1_27	1.338(10)	C3_31–F4_31	1.340(11)
C3_27–F4_27	1.304(10)	C4_31–F9_31	1.297(11)
C3_27–F6_27	1.331(10)	C4_31–F7_31	1.317(11)
C3_27–F5_27	1.335(10)	C4_31–F8_31	1.330(10)
C4_27–F9_27	1.322(10)	O1_32–C1_32	1.348(12)
C4_27–F8_27	1.330(10)	C1_32–C3_32	1.543(11)
C4_27–F7_27	1.343(11)	C1_32–C2_32	1.559(11)
O1_28–C1_28	1.340(10)	C1_32–C4_32	1.563(11)
C1_28–C4_28	1.548(10)	C2_32–F3_32	1.328(12)
C1_28–C3_28	1.552(10)	C2_32–F1_32	1.336(12)
C1_28–C2_28	1.570(10)	C2_32–F2_32	1.341(11)
C2_28–F1_28	1.316(11)	C3_32–F6_32	1.330(12)
C2_28–F2_28	1.318(10)	C3_32–F4_32	1.337(11)

C3_32–F5_32	1.351(12)	C4_36–F7_36	1.325(12)
C4_32–F8_32	1.309(12)	C4_36–F8_36	1.327(12)
C4_32–F9_32	1.320(12)	O1_37–C1_37	1.373(11)
C4_32–F7_32	1.364(12)	C1_37–C2_37	1.534(11)
O1_33–C1_33	1.355(11)	C1_37–C3_37	1.543(11)
C1_33–C4_33	1.540(11)	C1_37–C4_37	1.547(11)
C1_33–C2_33	1.551(11)	C2_37–F3_37	1.340(12)
C1_33–C3_33	1.555(11)	C2_37–F1_37	1.345(12)
C2_33–F2_33	1.318(12)	C2_37–F2_37	1.352(12)
C2_33–F3_33	1.324(12)	C3_37–F5_37	1.319(12)
C2_33–F1_33	1.327(12)	C3_37–F4_37	1.324(12)
C3_33–F5_33	1.306(12)	C3_37–F6_37	1.344(11)
C3_33–F6_33	1.314(12)	C4_37–F8_37	1.317(12)
C3_33–F4_33	1.349(12)	C4_37–F9_37	1.343(12)
F5_33–F4_54	1.42(3)	C4_37–F7_37	1.350(12)
C4_33–F7_33	1.319(12)	O1_38–C1_38	1.348(12)
C4_33–F9_33	1.325(12)	C1_38–C2_38	1.550(12)
C4_33–F8_33	1.346(12)	C1_38–C4_38	1.551(12)
O1_34–C1_34	1.352(12)	C1_38–C3_38	1.553(12)
C1_34–C4_34	1.547(12)	C2_38–F2_38	1.326(12)
C1_34–C3_34	1.553(12)	C2_38–F3_38	1.333(12)
C1_34–C2_34	1.553(12)	C2_38–F1_38	1.338(12)
C2_34–F2_34	1.320(13)	C3_38–F6_38	1.330(12)
C2_34–F3_34	1.323(13)	C3_38–F4_38	1.333(12)
C2_34–F1_34	1.327(13)	C3_38–F5_38	1.343(12)
C3_34–F5_34	1.322(13)	C4_38–F8_38	1.314(12)
C3_34–F6_34	1.323(13)	C4_38–F9_38	1.331(12)
C3_34–F4_34	1.324(13)	C4_38–F7_38	1.343(13)
C4_34–F8_34	1.331(13)	O1_39–C1_39	1.352(12)
C4_34–F9_34	1.335(13)	C1_39–C2_39	1.535(12)
C4_34–F7_34	1.338(13)	C1_39–C3_39	1.549(12)
O1_35–C1_35	1.368(12)	C1_39–C4_39	1.550(12)
C1_35–C2_35	1.551(12)	C2_39–F3_39	1.312(13)
C1_35–C4_35	1.552(12)	C2_39–F1_39	1.324(13)
C1_35–C3_35	1.555(12)	C2_39–F2_39	1.326(12)
C2_35–F1_35	1.327(13)	C3_39–F4_39	1.313(13)
C2_35–F2_35	1.328(12)	C3_39–F6_39	1.326(12)
C2_35–F3_35	1.334(12)	C3_39–F5_39	1.327(13)
C3_35–F4_35	1.327(12)	C4_39–F8_39	1.296(13)
C3_35–F5_35	1.330(13)	C4_39–F9_39	1.321(13)
C3_35–F6_35	1.341(12)	C4_39–F7_39	1.328(13)
C4_35–F7_35	1.322(12)	O1_40–C1_40	1.353(10)
C4_35–F9_35	1.334(12)	C1_40–C2_40	1.540(11)
C4_35–F8_35	1.338(12)	C1_40–C4_40	1.548(11)
O1_36–C1_36	1.351(12)	C1_40–C3_40	1.572(11)
C1_36–C3_36	1.544(12)	C2_40–F3_40	1.298(11)
C1_36–C2_36	1.553(12)	C2_40–F2_40	1.327(10)
C1_36–C4_36	1.564(11)	C2_40–F1_40	1.351(12)
C2_36–F2_36	1.322(11)	C3_40–F4_40	1.291(12)
C2_36–F1_36	1.329(12)	C3_40–F6_40	1.339(11)
C2_36–F3_36	1.339(12)	C3_40–F5_40	1.364(12)
C3_36–F4_36	1.323(12)	C4_40–F9_40	1.321(11)
C3_36–F6_36	1.327(11)	C4_40–F8_40	1.335(11)
C3_36–F5_36	1.341(12)	C4_40–F7_40	1.351(12)
C4_36–F9_36	1.320(12)	C1_41–F1_41	1.334(10)

C1_41–C6_41	1.369(10)	C2_45–F3_45	1.326(12)
C1_41–C2_41	1.379(10)	C3_45–F4_45	1.303(12)
C2_41–F2_41	1.333(10)	C3_45–F6_45	1.306(12)
C2_41–C3_41	1.369(10)	C3_45–F5_45	1.349(12)
C3_41–C4_41	1.381(10)	C4_45–F9_45	1.306(12)
C3_41–H3_41	0.9500	C4_45–F7_45	1.334(12)
C4_41–C5_41	1.378(10)	C4_45–F8_45	1.343(12)
C4_41–H4_41	0.9500	O1_46–C1_46	1.366(12)
C5_41–C6_41	1.384(10)	C1_46–C4_46	1.547(12)
C5_41–H5_41	0.9500	C1_46–C3_46	1.550(12)
C6_41–H6_41	0.9500	C1_46–C2_46	1.556(12)
C1_42–F1_42	1.324(12)	C2_46–F1_46	1.319(13)
C1_42–C6_42	1.371(12)	C2_46–F3_46	1.322(13)
C1_42–C2_42	1.398(12)	C2_46–F2_46	1.338(12)
C2_42–F2_42	1.343(12)	C3_46–F6_46	1.325(13)
C2_42–C3_42	1.344(12)	C3_46–F5_46	1.336(13)
C3_42–C4_42	1.380(12)	C3_46–F4_46	1.345(13)
C3_42–H3_42	0.9500	C4_46–F9_46	1.326(13)
C4_42–C5_42	1.395(12)	C4_46–F8_46	1.329(13)
C4_42–H4_42	0.9500	C4_46–F7_46	1.331(13)
C5_42–C6_42	1.368(12)	O1_47–C1_47	1.333(12)
C5_42–H5_42	0.9500	C1_47–C4_47	1.552(12)
C6_42–H6_42	0.9500	C1_47–C3_47	1.555(12)
O1_43–C1_43	1.343(13)	C1_47–C2_47	1.565(12)
C1_43–C4_43	1.544(12)	C2_47–F2_47	1.310(13)
C1_43–C3_43	1.552(12)	C2_47–F1_47	1.320(13)
C1_43–C2_43	1.553(12)	C2_47–F3_47	1.336(13)
C2_43–F3_43	1.310(13)	C3_47–F4_47	1.320(13)
C2_43–F1_43	1.317(13)	C3_47–F6_47	1.321(13)
C2_43–F2_43	1.325(13)	C3_47–F5_47	1.332(13)
C3_43–F6_43	1.323(12)	C4_47–F8_47	1.327(13)
C3_43–F4_43	1.327(13)	C4_47–F7_47	1.338(13)
C3_43–F5_43	1.334(13)	C4_47–F9_47	1.338(13)
C4_43–F9_43	1.307(12)	O1_48–C1_48	1.345(12)
C4_43–F8_43	1.315(13)	C1_48–C2_48	1.542(11)
C4_43–F7_43	1.327(13)	C1_48–C3_48	1.543(12)
O1_44–C1_44	1.341(13)	C1_48–C4_48	1.559(12)
C1_44–C2_44	1.536(12)	C2_48–F3_48	1.308(12)
C1_44–C4_44	1.547(12)	C2_48–F1_48	1.331(12)
C1_44–C3_44	1.578(12)	C2_48–F2_48	1.342(12)
C2_44–F1_44	1.312(13)	C3_48–F4_48	1.312(12)
C2_44–F3_44	1.338(13)	C3_48–F6_48	1.327(12)
C2_44–F2_44	1.345(12)	C3_48–F5_48	1.342(12)
C3_44–F6_44	1.306(13)	C4_48–F8_48	1.315(12)
C3_44–F5_44	1.315(13)	C4_48–F9_48	1.332(12)
C3_44–F4_44	1.354(13)	C4_48–F7_48	1.345(12)
C4_44–F9_44	1.304(12)	O1_49–C1_49	1.332(12)
C4_44–F8_44	1.332(12)	C1_49–C3_49	1.547(12)
C4_44–F7_44	1.341(13)	C1_49–C2_49	1.551(12)
O1_45–C1_45	1.349(11)	C1_49–C4_49	1.553(12)
C1_45–C2_45	1.538(11)	C2_49–F1_49	1.314(13)
C1_45–C3_45	1.550(12)	C2_49–F2_49	1.314(13)
C1_45–C4_45	1.552(12)	C2_49–F3_49	1.356(13)
C2_45–F2_45	1.283(12)	C3_49–F6_49	1.304(13)
C2_45–F1_45	1.313(13)	C3_49–F4_49	1.324(13)

C3_49–F5_49	1.331(13)	C7A_52–H7AB_52	0.9800
C4_49–F7_49	1.295(13)	C7A_52–H7AC_52	0.9800
C4_49–F8_49	1.297(13)	C6A_52–H6AA_52	0.9800
C4_49–F9_49	1.337(13)	C6A_52–H6AB_52	0.9800
O1_50–C1_50	1.343(13)	C6A_52–H6AC_52	0.9800
C1_50–C3_50	1.552(12)	C1B_52–C2B_52	1.425(8)
C1_50–C4_50	1.553(12)	C1B_52–C5B_52	1.430(8)
C1_50–C2_50	1.558(12)	C1B_52–C6B_52	1.504(8)
C2_50–F2_50	1.323(13)	C2B_52–C3B_52	1.424(7)
C2_50–F3_50	1.325(13)	C2B_52–C7B_52	1.499(8)
C2_50–F1_50	1.344(13)	C3B_52–C4B_52	1.416(8)
C3_50–F6_50	1.332(13)	C3B_52–C8B_52	1.513(8)
C3_50–F4_50	1.333(13)	C4B_52–C5B_52	1.430(8)
C3_50–F5_50	1.349(13)	C4B_52–C9B_52	1.503(8)
C4_50–F8_50	1.298(13)	C5B_52–C10B_52	1.499(8)
C4_50–F9_50	1.327(13)	C10B_52–H10D_52	0.9800
C4_50–F7_50	1.363(13)	C10B_52–H10E_52	0.9800
Tl1_52–Al3_52	2.769(3)	C10B_52–H10F_52	0.9800
Tl1_52–Al2_52	2.788(3)	C9B_52–H9BA_52	0.9800
Tl1_52–Al1_52	2.789(3)	C9B_52–H9BB_52	0.9800
Al2_52–C5B_52	2.209(6)	C9B_52–H9BC_52	0.9800
Al2_52–C1B_52	2.224(6)	C8B_52–H8BA_52	0.9800
Al2_52–C4B_52	2.224(6)	C8B_52–H8BB_52	0.9800
Al2_52–C2B_52	2.240(6)	C8B_52–H8BC_52	0.9800
Al2_52–C3B_52	2.239(6)	C7B_52–H7BA_52	0.9800
Al3_52–C5C_52	2.225(6)	C7B_52–H7BB_52	0.9800
Al3_52–C4C_52	2.229(6)	C7B_52–H7BC_52	0.9800
Al3_52–C2C_52	2.232(6)	C6B_52–H6BA_52	0.9800
Al3_52–C1C_52	2.235(6)	C6B_52–H6BB_52	0.9800
Al3_52–C3C_52	2.244(7)	C6B_52–H6BC_52	0.9800
Al1_52–C1A_52	2.236(6)	C1C_52–C5C_52	1.427(8)
Al1_52–C2A_52	2.240(7)	C1C_52–C2C_52	1.431(8)
Al1_52–C3A_52	2.249(7)	C1C_52–C6C_52	1.496(8)
Al1_52–C5A_52	2.251(6)	C2C_52–C3C_52	1.406(8)
Al1_52–C4A_52	2.265(6)	C2C_52–C7C_52	1.498(8)
C1A_52–C5A_52	1.418(8)	C3C_52–C4C_52	1.411(8)
C1A_52–C2A_52	1.424(8)	C3C_52–C8C_52	1.502(9)
C1A_52–C6A_52	1.508(8)	C4C_52–C5C_52	1.413(8)
C2A_52–C3A_52	1.413(8)	C4C_52–C9C_52	1.505(8)
C2A_52–C7A_52	1.509(8)	C5C_52–C10C_52	1.498(8)
C3A_52–C4A_52	1.419(8)	C10C_52–H10G_52	0.9800
C3A_52–C8A_52	1.512(8)	C10C_52–H10H_52	0.9800
C4A_52–C5A_52	1.420(8)	C10C_52–H10I_52	0.9800
C4A_52–C9A_52	1.499(8)	C9C_52–H9CA_52	0.9800
C5A_52–C10A_52	1.504(8)	C9C_52–H9CB_52	0.9800
C10A_52–H10A_52	0.9800	C9C_52–H9CC_52	0.9800
C10A_52–H10B_52	0.9800	C8C_52–H8CA_52	0.9800
C10A_52–H10C_52	0.9800	C8C_52–H8CB_52	0.9800
C9A_52–H9AA_52	0.9800	C8C_52–H8CC_52	0.9800
C9A_52–H9AB_52	0.9800	C7C_52–H7CA_52	0.9800
C9A_52–H9AC_52	0.9800	C7C_52–H7CB_52	0.9800
C8A_52–H8AA_52	0.9800	C7C_52–H7CC_52	0.9800
C8A_52–H8AB_52	0.9800	C6C_52–H6CA_52	0.9800
C8A_52–H8AC_52	0.9800	C6C_52–H6CB_52	0.9800
C7A_52–H7AA_52	0.9800	C6C_52–H6CC_52	0.9800

Tl1_13–Al3_13	2.745(12)	C10B_13–H10D_13	0.9800
Tl1_13–Al1_13	2.742(12)	C10B_13–H10E_13	0.9800
Tl1_13–Al2_13	2.797(12)	C10B_13–H10F_13	0.9800
Al2_13–C3B_13	2.225(14)	C9B_13–H9BA_13	0.9800
Al2_13–C2B_13	2.204(14)	C9B_13–H9BB_13	0.9800
Al2_13–C4B_13	2.256(14)	C9B_13–H9BC_13	0.9800
Al2_13–C1B_13	2.219(14)	C8B_13–H8BA_13	0.9800
Al2_13–C5B_13	2.246(14)	C8B_13–H8BB_13	0.9800
Al2_13–Al1_13	3.053(13)	C8B_13–H8BC_13	0.9800
Al3_13–C4C_13	2.242(14)	C7B_13–H7BA_13	0.9800
Al3_13–C5C_13	2.234(14)	C7B_13–H7BB_13	0.9800
Al3_13–C3C_13	2.244(14)	C7B_13–H7BC_13	0.9800
Al3_13–C2C_13	2.233(14)	C6B_13–H6BA_13	0.9800
Al3_13–C1C_13	2.232(14)	C6B_13–H6BB_13	0.9800
Al3_13–Al1_13	3.020(13)	C6B_13–H6BC_13	0.9800
Al1_13–C3A_13	2.244(14)	C1C_13–C5C_13	1.418(14)
Al1_13–C4A_13	2.245(14)	C1C_13–C2C_13	1.422(14)
Al1_13–C2A_13	2.256(14)	C1C_13–C6C_13	1.506(14)
Al1_13–C5A_13	2.254(14)	C2C_13–C3C_13	1.422(14)
Al1_13–C1A_13	2.260(14)	C2C_13–C7C_13	1.500(14)
C1A_13–C2A_13	1.415(14)	C3C_13–C4C_13	1.415(16)
C1A_13–C5A_13	1.418(14)	C3C_13–C8C_13	1.504(14)
C1A_13–C6A_13	1.510(14)	C4C_13–C5C_13	1.425(14)
C2A_13–C3A_13	1.422(14)	C4C_13–C9C_13	1.504(14)
C2A_13–C7A_13	1.511(14)	C5C_13–C10C_13	1.505(14)
C3A_13–C4A_13	1.415(16)	C10C_13–H10G_13	0.9800
C3A_13–C8A_13	1.505(14)	C10C_13–H10H_13	0.9800
C4A_13–C5A_13	1.416(14)	C10C_13–H10I_13	0.9800
C4A_13–C9A_13	1.509(14)	C9C_13–H9CA_13	0.9800
C5A_13–C10A_13	1.508(14)	C9C_13–H9CB_13	0.9800
C10A_13–H10A_13	0.9800	C9C_13–H9CC_13	0.9800
C10A_13–H10B_13	0.9800	C8C_13–H8CA_13	0.9800
C10A_13–H10C_13	0.9800	C8C_13–H8CB_13	0.9800
C9A_13–H9AA_13	0.9800	C8C_13–H8CC_13	0.9800
C9A_13–H9AB_13	0.9800	C7C_13–H7CA_13	0.9800
C9A_13–H9AC_13	0.9800	C7C_13–H7CB_13	0.9800
C8A_13–H8AA_13	0.9800	C7C_13–H7CC_13	0.9800
C8A_13–H8AB_13	0.9800	C6C_13–H6CA_13	0.9800
C8A_13–H8AC_13	0.9800	C6C_13–H6CB_13	0.9800
C7A_13–H7AA_13	0.9800	C6C_13–H6CC_13	0.9800
C7A_13–H7AB_13	0.9800	Tl1_14–Al1_14	2.759(5)
C7A_13–H7AC_13	0.9800	Tl1_14–Al3_14	2.771(4)
C6A_13–H6AA_13	0.9800	Tl1_14–Al2_14	2.785(3)
C6A_13–H6AB_13	0.9800	Al2_14–C5B_14	2.221(7)
C6A_13–H6AC_13	0.9800	Al2_14–C4B_14	2.223(7)
C1B_13–C5B_13	1.410(14)	Al2_14–C3B_14	2.233(7)
C1B_13–C2B_13	1.432(14)	Al2_14–C1B_14	2.242(7)
C1B_13–C6B_13	1.511(14)	Al2_14–C2B_14	2.247(6)
C2B_13–C3B_13	1.411(14)	Al3_14–C4C_14	2.207(7)
C2B_13–C7B_13	1.504(14)	Al3_14–C5C_14	2.224(7)
C3B_13–C4B_13	1.415(16)	Al3_14–C2C_14	2.230(6)
C3B_13–C8B_13	1.511(14)	Al3_14–C1C_14	2.234(7)
C4B_13–C5B_13	1.421(14)	Al3_14–C3C_14	2.232(6)
C4B_13–C9B_13	1.516(14)	Al1_14–C1A_14	2.219(7)
C5B_13–C10B_13	1.508(14)	Al1_14–C5A_14	2.231(7)

Al1_14–C2A_14	2.227(7)	C1C_14–C6C_14	1.508(8)
Al1_14–C3A_14	2.256(8)	C2C_14–C3C_14	1.434(8)
Al1_14–C4A_14	2.263(8)	C2C_14–C7C_14	1.501(8)
C1A_14–C5A_14	1.417(8)	C3C_14–C4C_14	1.420(8)
C1A_14–C2A_14	1.421(8)	C3C_14–C8C_14	1.501(8)
C1A_14–C6A_14	1.511(9)	C4C_14–C5C_14	1.433(8)
C2A_14–C3A_14	1.417(9)	C4C_14–C9C_14	1.502(8)
C2A_14–C7A_14	1.500(9)	C5C_14–C10C_14	1.502(8)
C3A_14–C4A_14	1.411(9)	C10C_14–H10G_14	0.9800
C3A_14–C8A_14	1.512(9)	C10C_14–H10H_14	0.9800
C4A_14–C5A_14	1.418(8)	C10C_14–H10I_14	0.9800
C4A_14–C9A_14	1.501(9)	C9C_14–H9CA_14	0.9800
C5A_14–C10A_14	1.503(8)	C9C_14–H9CB_14	0.9800
C10A_14–H10A_14	0.9800	C9C_14–H9CC_14	0.9800
C10A_14–H10B_14	0.9800	C8C_14–H8CA_14	0.9800
C10A_14–H10C_14	0.9800	C8C_14–H8CB_14	0.9800
C9A_14–H9AA_14	0.9800	C8C_14–H8CC_14	0.9800
C9A_14–H9AB_14	0.9800	C7C_14–H7CA_14	0.9800
C9A_14–H9AC_14	0.9800	C7C_14–H7CB_14	0.9800
C8A_14–H8AA_14	0.9800	C7C_14–H7CC_14	0.9800
C8A_14–H8AB_14	0.9800	C6C_14–H6CA_14	0.9800
C8A_14–H8AC_14	0.9800	C6C_14–H6CB_14	0.9800
C7A_14–H7AA_14	0.9800	C6C_14–H6CC_14	0.9800
C7A_14–H7AB_14	0.9800	Tl1_1–Al1_1	2.695(11)
C7A_14–H7AC_14	0.9800	Tl1_1–Al2_1	2.747(12)
C6A_14–H6AA_14	0.9800	Tl1_1–Al3_1	2.771(11)
C6A_14–H6AB_14	0.9800	Al2_1–C1B_1	2.216(14)
C6A_14–H6AC_14	0.9800	Al2_1–C5B_1	2.217(14)
C1B_14–C5B_14	1.417(8)	Al2_1–C2B_1	2.233(14)
C1B_14–C2B_14	1.427(8)	Al2_1–C4B_1	2.231(14)
C1B_14–C6B_14	1.505(9)	Al2_1–C3B_1	2.246(14)
C2B_14–C3B_14	1.415(8)	Al3_1–C3C_1	2.221(14)
C2B_14–C7B_14	1.493(9)	Al3_1–C2C_1	2.224(14)
C3B_14–C4B_14	1.403(9)	Al3_1–C4C_1	2.239(14)
C3B_14–C8B_14	1.502(8)	Al3_1–C5C_1	2.259(14)
C4B_14–C5B_14	1.420(8)	Al3_1–C1C_1	2.264(14)
C4B_14–C9B_14	1.511(9)	Al1_1–C2A_1	2.250(13)
C5B_14–C10B_14	1.501(8)	Al1_1–C3A_1	2.257(13)
C10B_14–H10D_14	0.9800	Al1_1–C1A_1	2.262(13)
C10B_14–H10E_14	0.9800	Al1_1–C4A_1	2.275(13)
C10B_14–H10F_14	0.9800	Al1_1–C5A_1	2.275(13)
C9B_14–H9BA_14	0.9800	C1A_1–C5A_1	1.407(13)
C9B_14–H9BB_14	0.9800	C1A_1–C2A_1	1.421(14)
C9B_14–H9BC_14	0.9800	C1A_1–C6A_1	1.514(14)
C8B_14–H8BA_14	0.9800	C2A_1–C3A_1	1.410(14)
C8B_14–H8BB_14	0.9800	C2A_1–C7A_1	1.502(14)
C8B_14–H8BC_14	0.9800	C3A_1–C4A_1	1.415(16)
C7B_14–H7BA_14	0.9800	C3A_1–C8A_1	1.510(14)
C7B_14–H7BB_14	0.9800	C4A_1–C5A_1	1.419(14)
C7B_14–H7BC_14	0.9800	C4A_1–C9A_1	1.506(14)
C6B_14–H6BA_14	0.9800	C5A_1–C10A_1	1.509(14)
C6B_14–H6BB_14	0.9800	C10A_1–H10A_1	0.9800
C6B_14–H6BC_14	0.9800	C10A_1–H10B_1	0.9800
C1C_14–C5C_14	1.426(8)	C10A_1–H10C_1	0.9800
C1C_14–C2C_14	1.425(8)	C9A_1–H9AA_1	0.9800

C9A_1–H9AB_1	0.9800	C7C_1–H7CA_1	0.9800
C9A_1–H9AC_1	0.9800	C7C_1–H7CB_1	0.9800
C8A_1–H8AA_1	0.9800	C7C_1–H7CC_1	0.9800
C8A_1–H8AB_1	0.9800	C6C_1–H6CA_1	0.9800
C8A_1–H8AC_1	0.9800	C6C_1–H6CB_1	0.9800
C7A_1–H7AA_1	0.9800	C6C_1–H6CC_1	0.9800
C7A_1–H7AB_1	0.9800	O1_2–C1_2	1.348(13)
C7A_1–H7AC_1	0.9800	C1_2–C4_2	1.543(13)
C6A_1–H6AA_1	0.9800	C1_2–C3_2	1.548(13)
C6A_1–H6AB_1	0.9800	C1_2–C2_2	1.561(13)
C6A_1–H6AC_1	0.9800	C2_2–F1_2	1.311(13)
C1B_1–C2B_1	1.412(14)	C2_2–F3_2	1.319(14)
C1B_1–C5B_1	1.432(14)	C2_2–F2_2	1.321(13)
C1B_1–C6B_1	1.509(14)	C3_2–F6_2	1.325(14)
C2B_1–C3B_1	1.424(14)	C3_2–F4_2	1.327(13)
C2B_1–C7B_1	1.504(14)	C3_2–F5_2	1.349(14)
C3B_1–C4B_1	1.414(15)	C4_2–F9_2	1.331(14)
C3B_1–C8B_1	1.512(14)	C4_2–F7_2	1.332(14)
C4B_1–C5B_1	1.419(14)	C4_2–F8_2	1.333(14)
C4B_1–C9B_1	1.510(14)	O1_3–C1_3	1.351(13)
C5B_1–C10B_1	1.511(14)	C1_3–C4_3	1.543(13)
C10B_1–H10D_1	0.9800	C1_3–C3_3	1.556(13)
C10B_1–H10E_1	0.9800	C1_3–C2_3	1.570(13)
C10B_1–H10F_1	0.9800	C2_3–F2_3	1.322(14)
C9B_1–H9BA_1	0.9800	C2_3–F3_3	1.331(14)
C9B_1–H9BB_1	0.9800	C2_3–F1_3	1.338(14)
C9B_1–H9BC_1	0.9800	C3_3–F6_3	1.323(14)
C8B_1–H8BA_1	0.9800	C3_3–F5_3	1.328(14)
C8B_1–H8BB_1	0.9800	C3_3–F4_3	1.332(14)
C8B_1–H8BC_1	0.9800	C4_3–F9_3	1.328(14)
C7B_1–H7BA_1	0.9800	C4_3–F7_3	1.333(14)
C7B_1–H7BB_1	0.9800	C4_3–F8_3	1.364(14)
C7B_1–H7BC_1	0.9800	O1_15–C1_15	1.355(13)
C6B_1–H6BA_1	0.9800	C1_15–C3_15	1.546(13)
C6B_1–H6BB_1	0.9800	C1_15–C2_15	1.555(12)
C6B_1–H6BC_1	0.9800	C1_15–C4_15	1.557(13)
C1C_1–C5C_1	1.412(14)	C2_15–F1_15	1.327(13)
C1C_1–C2C_1	1.423(14)	C2_15–F3_15	1.330(13)
C1C_1–C6C_1	1.502(14)	C2_15–F2_15	1.332(13)
C2C_1–C3C_1	1.416(14)	C3_15–F4_15	1.324(13)
C2C_1–C7C_1	1.504(14)	C3_15–F5_15	1.326(13)
C3C_1–C4C_1	1.417(16)	C3_15–F6_15	1.339(14)
C3C_1–C8C_1	1.498(14)	C4_15–F9_15	1.326(13)
C4C_1–C5C_1	1.422(14)	C4_15–F7_15	1.334(13)
C4C_1–C9C_1	1.506(14)	C4_15–F8_15	1.336(13)
C5C_1–C10C_1	1.508(14)	O1_51–C1_51	1.351(13)
C10C_1–H10G_1	0.9800	C1_51–C4_51	1.543(12)
C10C_1–H10H_1	0.9800	C1_51–C2_51	1.543(12)
C10C_1–H10I_1	0.9800	C1_51–C3_51	1.560(13)
C9C_1–H9CA_1	0.9800	C2_51–F3_51	1.329(13)
C9C_1–H9CB_1	0.9800	C2_51–F1_51	1.332(13)
C9C_1–H9CC_1	0.9800	C2_51–F2_51	1.341(13)
C8C_1–H8CA_1	0.9800	C3_51–F5_51	1.299(13)
C8C_1–H8CB_1	0.9800	C3_51–F6_51	1.317(13)
C8C_1–H8CC_1	0.9800	C3_51–F4_51	1.328(13)

C4_51–F8_51	1.318(13)	C1_57–C5_57	1.414(13)
C4_51–F9_51	1.321(13)	C1_57–C2_57	1.417(13)
C4_51–F7_51	1.339(13)	C1_57–C10_57	1.505(13)
O1_53–C1_53	1.352(13)	C2_57–C3_57	1.410(13)
C1_53–C3_53	1.546(13)	C2_57–C9_57	1.511(13)
C1_53–C2_53	1.551(13)	C3_57–C4_57	1.418(13)
C1_53–C4_53	1.555(13)	C3_57–C8_57	1.510(13)
C2_53–F3_53	1.325(13)	C4_57–C5_57	1.413(13)
C2_53–F2_53	1.334(13)	C4_57–C7_57	1.507(13)
C2_53–F1_53	1.351(13)	C5_57–C6_57	1.506(13)
C3_53–F4_53	1.325(13)	C6_57–H6A_57	0.9800
C3_53–F6_53	1.328(13)	C6_57–H6B_57	0.9800
C3_53–F5_53	1.336(13)	C6_57–H6C_57	0.9800
C4_53–F7_53	1.323(13)	C7_57–H7A_57	0.9800
C4_53–F8_53	1.328(13)	C7_57–H7B_57	0.9800
C4_53–F9_53	1.336(13)	C7_57–H7C_57	0.9800
O1_54–C1_54	1.347(14)	C8_57–H8A_57	0.9800
C1_54–C2_54	1.545(13)	C8_57–H8B_57	0.9800
C1_54–C3_54	1.551(13)	C8_57–H8C_57	0.9800
C1_54–C4_54	1.566(13)	C9_57–H9A_57	0.9800
C2_54–F3_54	1.321(14)	C9_57–H9B_57	0.9800
C2_54–F1_54	1.328(14)	C9_57–H9C_57	0.9800
C2_54–F2_54	1.344(14)	C10_57–H10A_57	0.9800
C3_54–F5_54	1.322(14)	C10_57–H10B_57	0.9800
C3_54–F6_54	1.323(14)	C10_57–H10C_57	0.9800
C3_54–F4_54	1.323(14)	O1_58–C1_58	1.352(13)
C4_54–F8_54	1.306(14)	C1_58–C4_58	1.535(12)
C4_54–F7_54	1.322(14)	C1_58–C2_58	1.565(12)
C4_54–F9_54	1.323(14)	C1_58–C3_58	1.568(13)
O1_55–C1_55	1.352(11)	C2_58–F2_58	1.316(13)
C1_55–C3_55	1.551(11)	C2_58–F3_58	1.335(13)
C1_55–C4_55	1.554(12)	C2_58–F1_58	1.335(13)
C1_55–C2_55	1.555(11)	C3_58–F4_58	1.317(13)
C2_55–F2_55	1.326(12)	C3_58–F5_58	1.320(13)
C2_55–F3_55	1.329(12)	C3_58–F6_58	1.326(13)
C2_55–F1_55	1.344(12)	C4_58–F7_58	1.333(13)
C3_55–F4_55	1.340(12)	C4_58–F9_58	1.335(13)
C3_55–F5_55	1.340(12)	C4_58–F8_58	1.353(14)
C3_55–F6_55	1.342(12)	O1_59–C1_59	1.356(13)
C4_55–F8_55	1.313(11)	C1_59–C2_59	1.546(12)
C4_55–F9_55	1.325(12)	C1_59–C3_59	1.550(12)
C4_55–F7_55	1.342(12)	C1_59–C4_59	1.552(12)
O1_56–C1_56	1.361(14)	C2_59–F1_59	1.328(13)
C1_56–C2_56	1.544(13)	C2_59–F3_59	1.329(13)
C1_56–C3_56	1.549(13)	C2_59–F2_59	1.336(13)
C1_56–C4_56	1.552(13)	C3_59–F5_59	1.330(13)
C2_56–F1_56	1.325(14)	C3_59–F6_59	1.333(13)
C2_56–F2_56	1.327(14)	C3_59–F4_59	1.339(13)
C2_56–F3_56	1.335(14)	C4_59–F7_59	1.320(13)
C3_56–F5_56	1.328(14)	C4_59–F9_59	1.334(13)
C3_56–F6_56	1.329(14)	C4_59–F8_59	1.335(13)
C3_56–F4_56	1.331(14)	O1_60–C1_60	1.343(13)
C4_56–F8_56	1.318(14)	C1_60–C4_60	1.553(13)
C4_56–F7_56	1.328(14)	C1_60–C2_60	1.555(13)
C4_56–F9_56	1.334(14)	C1_60–C3_60	1.566(13)

C2_60–F1_60	1.325(13)
C2_60–F3_60	1.330(13)
C2_60–F2_60	1.333(14)
C3_60–F6_60	1.315(13)
C3_60–F5_60	1.321(13)
C3_60–F4_60	1.324(13)
C4_60–F7_60	1.331(13)
C4_60–F8_60	1.335(13)
C4_60–F9_60	1.338(13)
O1_61–C1_61	1.358(13)
C1_61–C2_61	1.550(13)
C1_61–C3_61	1.555(13)
C1_61–C4_61	1.557(13)
C2_61–F1_61	1.310(13)
C2_61–F2_61	1.314(13)
C2_61–F3_61	1.343(14)
C3_61–F5_61	1.323(13)
C3_61–F6_61	1.333(13)
C3_61–F4_61	1.339(13)
C4_61–F8_61	1.325(14)
C4_61–F9_61	1.340(13)
C4_61–F7_61	1.341(13)
O1_62–C1_62	1.360(11)
C1_62–C3_62	1.549(12)
C1_62–C4_62	1.549(12)
C1_62–C2_62	1.552(12)
C2_62–F3_62	1.320(12)
C2_62–F1_62	1.325(12)
C2_62–F2_62	1.346(12)
C3_62–F6_62	1.331(12)
C3_62–F5_62	1.344(12)
C3_62–F4_62	1.347(12)
C4_62–F9_62	1.318(12)
C4_62–F7_62	1.325(12)
C4_62–F8_62	1.350(12)

Atom–Atom–Atom	**Angle [°]**
Al2–Tl1–Al3	69.53(9)
Al2–Tl1–Al1	70.52(8)
Al3–Tl1–Al1	71.21(9)
Al4–Tl2–Al6	69.58(9)
Al4–Tl2–Al5	68.72(8)
Al6–Tl2–Al5	69.17(10)
Al8–Tl3–Al7	67.74(8)
Al8–Tl3–Al9	67.45(8)
Al7–Tl3–Al9	67.60(9)
C2_9–Al1–C1_9	38.0(3)
C2_9–Al1–C3_9	38.0(3)
C1_9–Al1–C3_9	62.9(3)
C2_9–Al1–C5_9	62.6(3)
C1_9–Al1–C5_9	37.3(3)
C3_9–Al1–C5_9	61.8(3)
C2_9–Al1–C4_9	62.5(3)
C1_9–Al1–C4_9	62.2(3)
C3_9–Al1–C4_9	36.7(3)
C5_9–Al1–C4_9	36.8(3)
C5_57–Al1–C1_57	36.6(5)
C5_57–Al1–C4_57	36.2(5)
C1_57–Al1–C4_57	59.7(7)
C5_57–Al1–C2_57	59.2(7)
C1_57–Al1–C2_57	35.2(5)
C4_57–Al1–C2_57	57.8(6)
C5_57–Al1–C3_57	58.8(6)
C1_57–Al1–C3_57	58.1(6)
C4_57–Al1–C3_57	34.6(4)
C2_57–Al1–C3_57	33.9(4)
C2_9–Al1–Tl1	124.2(3)
C1_9–Al1–Tl1	109.2(2)
C3_9–Al1–Tl1	159.9(3)
C5_57–Al1–Tl1	144.9(6)
C5_9–Al1–Tl1	124.4(2)
C4_9–Al1–Tl1	158.7(3)
C1_57–Al1–Tl1	165.7(6)
C4_57–Al1–Tl1	114.0(6)
C2_57–Al1–Tl1	130.6(5)
C3_57–Al1–Tl1	108.9(5)
C5_11–Al8–C4_11	37.6(2)
C5_11–Al8–C2_11	61.8(2)
C4_11–Al8–C2_11	61.7(2)
C5_11–Al8–C3_11	62.2(3)
C4_11–Al8–C3_11	36.9(2)
C2_11–Al8–C3_11	36.9(2)
C5_11–Al8–C1_11	37.8(2)
C4_11–Al8–C1_11	62.7(3)
C2_11–Al8–C1_11	36.6(2)
C3_11–Al8–C1_11	62.0(2)
C5_11–Al8–Tl3	158.3(2)
C4_11–Al8–Tl3	162.7(2)
C2_11–Al8–Tl3	114.76(19)
C3_11–Al8–Tl3	129.59(19)
C1_11–Al8–Tl3	125.9(2)
C4_12–Al9–C5_12	37.5(2)
C4_12–Al9–C3_12	37.4(2)
C5_12–Al9–C3_12	62.1(3)
C4_12–Al9–C2_12	62.1(3)
C5_12–Al9–C2_12	61.6(3)
C3_12–Al9–C2_12	36.8(2)
C4_12–Al9–C1_12	62.1(3)
C5_12–Al9–C1_12	36.8(2)
C3_12–Al9–C1_12	61.6(3)
C2_12–Al9–C1_12	36.7(2)
C4_12–Al9–Tl3	155.6(2)
C5_12–Al9–Tl3	163.2(2)
C3_12–Al9–Tl3	122.7(2)
C2_12–Al9–Tl3	111.4(2)
C1_12–Al9–Tl3	128.3(2)
O1_29–Al10–O1_28	110.3(5)
O1_29–Al10–O1_40	111.1(4)
O1_28–Al10–O1_40	112.7(6)
O1_46–Al10–O1_43	114.1(9)

O1_46–Al10–O1_45	106.5(7)	O1_47–Al14–O1_3	108.5(13)
O1_43–Al10–O1_45	110.9(10)	C4_7–Al2–C3_7	36.37(19)
O1_46–Al10–O1_35	115.4(8)	C4_7–Al2–C5_7	36.1(2)
O1_43–Al10–O1_35	104.2(9)	C3_7–Al2–C5_7	60.2(2)
O1_45–Al10–O1_35	105.5(6)	C4_7–Al2–C2_7	60.2(2)
O1_29–Al10–O1_30	110.7(9)	C3_7–Al2–C2_7	36.02(19)
O1_28–Al10–O1_30	106.2(9)	C5_7–Al2–C2_7	60.0(2)
O1_40–Al10–O1_30	105.6(8)	C4_7–Al2–C1_7	60.0(2)
O1_26–Al11–O1_24	109.6(5)	C3_7–Al2–C1_7	60.0(2)
O1_26–Al11–O1_25	107.9(7)	C5_7–Al2–C1_7	35.9(2)
O1_24–Al11–O1_25	110.5(3)	C2_7–Al2–C1_7	35.9(2)
O1_54–Al11–O1_34	106.5(14)	C4_7–Al2–Tl1	153.99(17)
O1_54–Al11–O1_33	121.0(13)	C3_7–Al2–Tl1	168.70(17)
O1_34–Al11–O1_33	99.7(8)	C5_7–Al2–Tl1	125.33(18)
O1_26–Al11–O1_27	115.1(6)	C2_7–Al2–Tl1	135.19(17)
O1_24–Al11–O1_27	102.9(4)	C1_7–Al2–Tl1	117.60(17)
O1_25–Al11–O1_27	110.8(3)	C4_8–Al3–C5_8	37.5(2)
O1_56–Al12–O1_2	113(2)	C4_8–Al3–C3_8	38.0(2)
O1_56–Al12–O1_36	120(2)	C5_8–Al3–C3_8	62.1(2)
O1_2–Al12–O1_36	109.1(16)	C4_8–Al3–C1_8	62.2(2)
O1_22–Al12–O1_20	117.1(7)	C5_8–Al3–C1_8	37.0(2)
O1_22–Al12–O1_21	84.7(7)	C3_8–Al3–C1_8	61.1(2)
O1_20–Al12–O1_21	113.2(5)	C4_8–Al3–C2_8	62.2(2)
O1_22–Al12–O1_23	110.8(9)	C5_8–Al3–C2_8	61.2(3)
O1_20–Al12–O1_23	108.7(8)	C3_8–Al3–C2_8	36.6(2)
O1_21–Al12–O1_23	121.0(8)	C1_8–Al3–C2_8	36.0(2)
O1_56–Al12–O1_55	112(2)	C4_8–Al3–Tl1	167.5(2)
O1_2–Al12–O1_55	98.4(14)	C5_8–Al3–Tl1	141.7(2)
O1_36–Al12–O1_55	102.3(9)	C3_8–Al3–Tl1	152.4(2)
O1_49–Al13–O1_44	104.6(13)	C1_8–Al3–Tl1	125.5(2)
O1_49–Al13–O1_50	113.1(12)	C2_8–Al3–Tl1	130.14(19)
O1_44–Al13–O1_50	108.7(14)	C3_4–Al4–C2_4	36.4(2)
O1_58–Al13–O1_60	108.7(15)	C3_4–Al4–C1_4	60.5(2)
O1_38–Al13–O1_32	121.5(10)	C2_4–Al4–C1_4	36.4(2)
O1_38–Al13–O1_31	110.2(7)	C3_4–Al4–C4_4	36.9(2)
O1_32–Al13–O1_31	105.5(8)	C2_4–Al4–C4_4	61.2(2)
O1_58–Al13–O1_51	78.2(11)	C1_4–Al4–C4_4	60.6(2)
O1_60–Al13–O1_51	102.6(13)	C3_4–Al4–C5_4	60.8(2)
O1_49–Al13–O1_39	100.2(10)	C2_4–Al4–C5_4	60.8(2)
O1_44–Al13–O1_39	124.9(10)	C1_4–Al4–C5_4	36.2(2)
O1_50–Al13–O1_39	105.2(11)	C4_4–Al4–C5_4	36.3(2)
O1_38–Al13–O1_37	109.3(8)	C3_4–Al4–Tl2	152.2(2)
O1_32–Al13–O1_37	103.9(9)	C2_4–Al4–Tl2	170.88(19)
O1_31–Al13–O1_37	104.9(6)	C1_4–Al4–Tl2	137.02(18)
O1_48–Al14–O1_15	109.5(12)	C4_4–Al4–Tl2	123.9(2)
O1_19–Al14–O1_16	105.6(8)	C5_4–Al4–Tl2	117.91(18)
O1_19–Al14–O1_17	108.8(6)	C2_5–Al5–C3_5	37.2(2)
O1_16–Al14–O1_17	118.3(6)	C2_5–Al5–C5_5	61.8(3)
O1_48–Al14–O1_47	118.6(10)	C3_5–Al5–C5_5	62.3(3)
O1_15–Al14–O1_47	109.3(10)	C2_5–Al5–C4_5	61.7(3)
O1_19–Al14–O1_18	106.8(8)	C3_5–Al5–C4_5	37.2(2)
O1_16–Al14–O1_18	108.9(6)	C5_5–Al5–C4_5	37.1(2)
O1_17–Al14–O1_18	107.9(5)	C2_5–Al5–C1_5	36.9(2)
O1_48–Al14–O1_3	120.7(13)	C3_5–Al5–C1_5	62.2(3)
O1_15–Al14–O1_3	84.9(14)	C5_5–Al5–C1_5	37.1(2)

C4_5–Al5–C1_5	61.9(3)	C5_4–C4_4–C7_4	125.0(8)
C2_5–Al5–Tl2	151.0(2)	C3_4–C4_4–C7_4	127.8(8)
C3_5–Al5–Tl2	171.0(2)	C5_4–C4_4–Al4	72.0(4)
C5_5–Al5–Tl2	115.8(2)	C3_4–C4_4–Al4	70.9(4)
C4_5–Al5–Tl2	135.9(2)	C7_4–C4_4–Al4	122.7(5)
C1_5–Al5–Tl2	122.2(2)	C1_4–C5_4–C4_4	108.1(5)
C3_6–Al6–C4_6	37.7(2)	C1_4–C5_4–C6_4	125.4(7)
C3_6–Al6–C2_6	37.2(3)	C4_4–C5_4–C6_4	126.4(7)
C4_6–Al6–C2_6	62.5(3)	C1_4–C5_4–Al4	71.5(3)
C3_6–Al6–C1_6	61.7(3)	C4_4–C5_4–Al4	71.7(4)
C4_6–Al6–C1_6	62.0(3)	C6_4–C5_4–Al4	123.5(5)
C2_6–Al6–C1_6	36.9(2)	C5_4–C6_4–H6A_4	109.5
C3_6–Al6–C5_6	62.0(2)	C5_4–C6_4–H6B_4	109.5
C4_6–Al6–C5_6	36.9(2)	H6A_4–C6_4–H6B_4	109.5
C2_6–Al6–C5_6	62.0(3)	C5_4–C6_4–H6C_4	109.5
C1_6–Al6–C5_6	37.1(2)	H6A_4–C6_4–H6C_4	109.5
C3_6–Al6–Tl2	155.6(3)	H6B_4–C6_4–H6C_4	109.5
C4_6–Al6–Tl2	127.6(3)	C4_4–C7_4–H7A_4	109.5
C2_6–Al6–Tl2	167.2(3)	C4_4–C7_4–H7B_4	109.5
C1_6–Al6–Tl2	136.44(19)	H7A_4–C7_4–H7B_4	109.5
C5_6–Al6–Tl2	120.0(2)	C4_4–C7_4–H7C_4	109.5
C4_10–Al7–C2_10	62.5(3)	H7A_4–C7_4–H7C_4	109.5
C4_10–Al7–C3_10	37.7(3)	H7B_4–C7_4–H7C_4	109.5
C2_10–Al7–C3_10	37.5(3)	C3_4–C8_4–H8A_4	109.5
C4_10–Al7–C1_10	61.9(3)	C3_4–C8_4–H8B_4	109.5
C2_10–Al7–C1_10	37.0(3)	H8A_4–C8_4–H8B_4	109.5
C3_10–Al7–C1_10	62.2(3)	C3_4–C8_4–H8C_4	109.5
C4_10–Al7–C5_10	37.3(3)	H8A_4–C8_4–H8C_4	109.5
C2_10–Al7–C5_10	62.0(3)	H8B_4–C8_4–H8C_4	109.5
C3_10–Al7–C5_10	62.5(3)	C2_4–C9_4–H9A_4	109.5
C1_10–Al7–C5_10	36.8(2)	C2_4–C9_4–H9B_4	109.5
C4_10–Al7–Tl3	119.8(2)	H9A_4–C9_4–H9B_4	109.5
C2_10–Al7–Tl3	154.1(3)	C2_4–C9_4–H9C_4	109.5
C3_10–Al7–Tl3	126.7(3)	H9A_4–C9_4–H9C_4	109.5
C1_10–Al7–Tl3	168.9(2)	H9B_4–C9_4–H9C_4	109.5
C5_10–Al7–Tl3	137.4(2)	C1_4–C10_4–H10A_4	109.5
C5_4–C1_4–C2_4	108.7(5)	C1_4–C10_4–H10B_4	109.5
C5_4–C1_4–C10_4	125.9(7)	H10A_4–C10_4–H10B_4	109.5
C2_4–C1_4–C10_4	125.4(6)		
C5_4–C1_4–Al4	72.3(4)	C1_4–C10_4–H10C_4	109.5
C2_4–C1_4–Al4	71.5(3)	H10A_4–C10_4–H10C_4	109.5
C10_4–C1_4–Al4	122.6(5)		
C3_4–C2_4–C1_4	107.6(5)	H10B_4–C10_4–H10C_4	109.5
C3_4–C2_4–C9_4	126.5(7)		
C1_4–C2_4–C9_4	125.7(7)	C2_5–C1_5–C5_5	107.4(6)
C3_4–C2_4–Al4	71.6(3)	C2_5–C1_5–C10_5	126.5(7)
C1_4–C2_4–Al4	72.2(3)	C5_5–C1_5–C10_5	126.0(7)
C9_4–C2_4–Al4	125.5(5)	C2_5–C1_5–Al5	70.7(4)
C2_4–C3_4–C4_4	108.4(5)	C5_5–C1_5–Al5	71.1(4)
C2_4–C3_4–C8_4	125.8(8)	C10_5–C1_5–Al5	121.8(5)
C4_4–C3_4–C8_4	125.6(8)	C1_5–C2_5–C3_5	109.3(6)
C2_4–C3_4–Al4	72.0(3)	C1_5–C2_5–C9_5	125.2(7)
C4_4–C3_4–Al4	72.2(4)	C3_5–C2_5–C9_5	125.4(7)
C8_4–C3_4–Al4	125.6(5)	C1_5–C2_5–Al5	72.4(4)
C5_4–C4_4–C3_4	107.2(5)	C3_5–C2_5–Al5	71.6(4)

C9_5–C2_5–Al5	125.7(5)	C2_6–C1_6–Al6	70.8(4)
C2_5–C3_5–C4_5	107.0(6)	C5_6–C1_6–Al6	71.6(4)
C2_5–C3_5–C8_5	125.4(7)	C10_6–C1_6–Al6	125.5(5)
C4_5–C3_5–C8_5	127.5(7)	C3_6–C2_6–C1_6	107.8(7)
C2_5–C3_5–Al5	71.1(4)	C3_6–C2_6–C9_6	125.6(7)
C4_5–C3_5–Al5	71.7(4)	C1_6–C2_6–C9_6	126.5(8)
C8_5–C3_5–Al5	125.6(5)	C3_6–C2_6–Al6	70.7(4)
C3_5–C4_5–C5_5	108.4(6)	C1_6–C2_6–Al6	72.3(4)
C3_5–C4_5–C7_5	125.5(8)	C9_6–C2_6–Al6	126.1(5)
C5_5–C4_5–C7_5	126.0(8)	C2_6–C3_6–C4_6	108.5(6)
C3_5–C4_5–Al5	71.1(4)	C2_6–C3_6–C8_6	123.8(9)
C5_5–C4_5–Al5	71.4(5)	C4_6–C3_6–C8_6	127.6(9)
C7_5–C4_5–Al5	126.7(6)	C2_6–C3_6–Al6	72.2(4)
C4_5–C5_5–C1_5	107.9(6)	C4_6–C3_6–Al6	71.6(4)
C4_5–C5_5–C6_5	125.2(7)	C8_6–C3_6–Al6	125.1(5)
C1_5–C5_5–C6_5	126.8(7)	C5_6–C4_6–C3_6	107.6(7)
C4_5–C5_5–Al5	71.5(4)	C5_6–C4_6–C7_6	125.0(8)
C1_5–C5_5–Al5	71.8(4)	C3_6–C4_6–C7_6	127.3(8)
C6_5–C5_5–Al5	124.1(6)	C5_6–C4_6–Al6	72.7(4)
C5_5–C6_5–H6A_5	109.5	C3_6–C4_6–Al6	70.7(4)
C5_5–C6_5–H6B_5	109.5	C7_6–C4_6–Al6	125.1(6)
H6A_5–C6_5–H6B_5	109.5	C4_6–C5_6–C1_6	107.8(6)
C5_5–C6_5–H6C_5	109.5	C4_6–C5_6–C6_6	127.7(8)
H6A_5–C6_5–H6C_5	109.5	C1_6–C5_6–C6_6	124.5(7)
H6B_5–C6_5–H6C_5	109.5	C4_6–C5_6–Al6	70.4(4)
C4_5–C7_5–H7A_5	109.5	C1_6–C5_6–Al6	71.3(4)
C4_5–C7_5–H7B_5	109.5	C6_6–C5_6–Al6	124.7(5)
H7A_5–C7_5–H7B_5	109.5	C5_6–C6_6–H6A_6	109.5
C4_5–C7_5–H7C_5	109.5	C5_6–C6_6–H6B_6	109.5
H7A_5–C7_5–H7C_5	109.5	H6A_6–C6_6–H6B_6	109.5
H7B_5–C7_5–H7C_5	109.5	C5_6–C6_6–H6C_6	109.5
C3_5–C8_5–H8A_5	109.5	H6A_6–C6_6–H6C_6	109.5
C3_5–C8_5–H8B_5	109.5	H6B_6–C6_6–H6C_6	109.5
H8A_5–C8_5–H8B_5	109.5	C4_6–C7_6–H7A_6	109.5
C3_5–C8_5–H8C_5	109.5	C4_6–C7_6–H7B_6	109.5
H8A_5–C8_5–H8C_5	109.5	H7A_6–C7_6–H7B_6	109.5
H8B_5–C8_5–H8C_5	109.5	C4_6–C7_6–H7C_6	109.5
C2_5–C9_5–H9A_5	109.5	H7A_6–C7_6–H7C_6	109.5
C2_5–C9_5–H9B_5	109.5	H7B_6–C7_6–H7C_6	109.5
H9A_5–C9_5–H9B_5	109.5	C3_6–C8_6–H8A_6	109.5
C2_5–C9_5–H9C_5	109.5	C3_6–C8_6–H8B_6	109.5
H9A_5–C9_5–H9C_5	109.5	H8A_6–C8_6–H8B_6	109.5
H9B_5–C9_5–H9C_5	109.5	C3_6–C8_6–H8C_6	109.5
C1_5–C10_5–H10A_5	109.5	H8A_6–C8_6–H8C_6	109.5
C1_5–C10_5–H10B_5	109.5	H8B_6–C8_6–H8C_6	109.5
H10A_5–C10_5–H10B_5	109.5	C2_6–C9_6–H9A_6	109.5
		C2_6–C9_6–H9B_6	109.5
C1_5–C10_5–H10C_5	109.5	H9A_6–C9_6–H9B_6	109.5
H10A_5–C10_5–H10C_5	109.5	C2_6–C9_6–H9C_6	109.5
		H9A_6–C9_6–H9C_6	109.5
H10B_5–C10_5–H10C_5	109.5	H9B_6–C9_6–H9C_6	109.5
		C1_6–C10_6–H10A_6	109.5
C2_6–C1_6–C5_6	108.3(6)	C1_6–C10_6–H10B_6	109.5
C2_6–C1_6–C10_6	127.0(8)	H10A_6–C10_6–H10B_6	109.5
C5_6–C1_6–C10_6	124.6(7)		

C1_6–C10_6–H10C_6	109.5
H10A_6–C10_6–H10C_6	109.5
H10B_6–C10_6–H10C_6	109.5
C2_7–C1_7–C5_7	107.9(5)
C2_7–C1_7–C10_7	126.1(7)
C5_7–C1_7–C10_7	125.9(7)
C2_7–C1_7–Al2	71.6(3)
C5_7–C1_7–Al2	71.4(4)
C10_7–C1_7–Al2	123.3(5)
C3_7–C2_7–C1_7	108.0(5)
C3_7–C2_7–C9_7	126.3(6)
C1_7–C2_7–C9_7	125.6(6)
C3_7–C2_7–Al2	71.3(3)
C1_7–C2_7–Al2	72.5(3)
C9_7–C2_7–Al2	123.3(4)
C2_7–C3_7–C4_7	108.0(5)
C2_7–C3_7–C8_7	125.7(5)
C4_7–C3_7–C8_7	126.2(5)
C2_7–C3_7–Al2	72.6(3)
C4_7–C3_7–Al2	71.8(3)
C8_7–C3_7–Al2	124.1(4)
C5_7–C4_7–C3_7	107.8(5)
C5_7–C4_7–C7_7	126.9(6)
C3_7–C4_7–C7_7	125.2(6)
C5_7–C4_7–Al2	72.5(4)
C3_7–C4_7–Al2	71.8(3)
C7_7–C4_7–Al2	123.9(5)
C4_7–C5_7–C1_7	108.2(5)
C4_7–C5_7–C6_7	125.4(7)
C1_7–C5_7–C6_7	126.4(7)
C4_7–C5_7–Al2	71.5(4)
C1_7–C5_7–Al2	72.7(4)
C6_7–C5_7–Al2	122.9(5)
C5_7–C6_7–H6A_7	109.5
C5_7–C6_7–H6B_7	109.5
H6A_7–C6_7–H6B_7	109.5
C5_7–C6_7–H6C_7	109.5
H6A_7–C6_7–H6C_7	109.5
H6B_7–C6_7–H6C_7	109.5
C4_7–C7_7–H7A_7	109.5
C4_7–C7_7–H7B_7	109.5
H7A_7–C7_7–H7B_7	109.5
C4_7–C7_7–H7C_7	109.5
H7A_7–C7_7–H7C_7	109.5
H7B_7–C7_7–H7C_7	109.5
C3_7–C8_7–H8A_7	109.5
C3_7–C8_7–H8B_7	109.5
H8A_7–C8_7–H8B_7	109.5
C3_7–C8_7–H8C_7	109.5
H8A_7–C8_7–H8C_7	109.5
H8B_7–C8_7–H8C_7	109.5
C2_7–C9_7–H9A_7	109.5
C2_7–C9_7–H9B_7	109.5
H9A_7–C9_7–H9B_7	109.5
C2_7–C9_7–H9C_7	109.5
H9A_7–C9_7–H9C_7	109.5
H9B_7–C9_7–H9C_7	109.5
C1_7–C10_7–H10A_7	109.5
C1_7–C10_7–H10B_7	109.5
H10A_7–C10_7–H10B_7	109.5
C1_7–C10_7–H10C_7	109.5
H10A_7–C10_7–H10C_7	109.5
H10B_7–C10_7–H10C_7	109.5
C2_8–C1_8–C5_8	108.4(6)
C2_8–C1_8–C10_8	126.0(8)
C5_8–C1_8–C10_8	125.5(8)
C2_8–C1_8–Al3	72.4(4)
C5_8–C1_8–Al3	70.2(4)
C10_8–C1_8–Al3	124.5(5)
C1_8–C2_8–C3_8	108.7(6)
C1_8–C2_8–C9_8	125.9(7)
C3_8–C2_8–C9_8	125.4(7)
C1_8–C2_8–Al3	71.6(4)
C3_8–C2_8–Al3	70.3(3)
C9_8–C2_8–Al3	125.7(5)
C2_8–C3_8–C4_8	107.7(5)
C2_8–C3_8–C8_8	126.3(7)
C4_8–C3_8–C8_8	125.9(6)
C2_8–C3_8–Al3	73.0(3)
C4_8–C3_8–Al3	69.5(4)
C8_8–C3_8–Al3	125.3(5)
C5_8–C4_8–C3_8	107.0(6)
C5_8–C4_8–C7_8	127.8(7)
C3_8–C4_8–C7_8	125.1(7)
C5_8–C4_8–Al3	72.5(4)
C3_8–C4_8–Al3	72.6(4)
C7_8–C4_8–Al3	123.2(5)
C4_8–C5_8–C1_8	108.2(6)
C4_8–C5_8–C6_8	125.6(8)
C1_8–C5_8–C6_8	126.3(8)
C4_8–C5_8–Al3	70.0(4)
C1_8–C5_8–Al3	72.8(4)
C6_8–C5_8–Al3	123.6(6)
C5_8–C6_8–H6A_8	109.5
C5_8–C6_8–H6B_8	109.5
H6A_8–C6_8–H6B_8	109.5
C5_8–C6_8–H6C_8	109.5
H6A_8–C6_8–H6C_8	109.5
H6B_8–C6_8–H6C_8	109.5
C4_8–C7_8–H7A_8	109.5
C4_8–C7_8–H7B_8	109.5
H7A_8–C7_8–H7B_8	109.5
C4_8–C7_8–H7C_8	109.5
H7A_8–C7_8–H7C_8	109.5
H7B_8–C7_8–H7C_8	109.5

C3_8–C8_8–H8A_8	109.5
C3_8–C8_8–H8B_8	109.5
H8A_8–C8_8–H8B_8	109.5
C3_8–C8_8–H8C_8	109.5
H8A_8–C8_8–H8C_8	109.5
H8B_8–C8_8–H8C_8	109.5
C2_8–C9_8–H9A_8	109.5
C2_8–C9_8–H9B_8	109.5
H9A_8–C9_8–H9B_8	109.5
C2_8–C9_8–H9C_8	109.5
H9A_8–C9_8–H9C_8	109.5
H9B_8–C9_8–H9C_8	109.5
C1_8–C10_8–H10A_8	109.5
C1_8–C10_8–H10B_8	109.5
H10A_8–C10_8–H10B_8	109.5
C1_8–C10_8–H10C_8	109.5
H10A_8–C10_8–H10C_8	109.5
H10B_8–C10_8–H10C_8	109.5
C5_9–C1_9–C2_9	107.5(7)
C5_9–C1_9–C10_9	124.1(9)
C2_9–C1_9–C10_9	128.4(9)
C5_9–C1_9–Al1	72.8(5)
C2_9–C1_9–Al1	70.0(4)
C10_9–C1_9–Al1	122.8(6)
C1_9–C2_9–C3_9	107.7(7)
C1_9–C2_9–C9_9	126.1(10)
C3_9–C2_9–C9_9	126.2(10)
C1_9–C2_9–Al1	72.0(5)
C3_9–C2_9–Al1	72.3(5)
C9_9–C2_9–Al1	123.2(7)
C4_9–C3_9–C2_9	108.3(7)
C4_9–C3_9–C8_9	124.2(9)
C2_9–C3_9–C8_9	127.3(10)
C4_9–C3_9–Al1	73.2(5)
C2_9–C3_9–Al1	69.7(4)
C8_9–C3_9–Al1	126.6(7)
C3_9–C4_9–C5_9	108.1(7)
C3_9–C4_9–C7_9	126.8(9)
C5_9–C4_9–C7_9	125.0(9)
C3_9–C4_9–Al1	70.1(5)
C5_9–C4_9–Al1	71.2(5)
C7_9–C4_9–Al1	127.2(7)
C4_9–C5_9–C1_9	108.4(7)
C4_9–C5_9–C6_9	125.4(9)
C1_9–C5_9–C6_9	126.2(9)
C4_9–C5_9–Al1	72.0(5)
C1_9–C5_9–Al1	69.9(5)
C6_9–C5_9–Al1	125.5(7)
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
C5_10–C1_10–C2_10	108.9(7)
C5_10–C1_10–C10_10	125.6(8)
C2_10–C1_10–C10_10	125.5(7)
C5_10–C1_10–Al7	71.7(5)
C2_10–C1_10–Al7	71.1(4)
C10_10–C1_10–Al7	125.5(6)
C1_10–C2_10–C3_10	108.1(6)
C1_10–C2_10–C9_10	123.9(8)
C3_10–C2_10–C9_10	127.9(9)
C1_10–C2_10–Al7	71.9(4)
C3_10–C2_10–Al7	71.3(4)
C9_10–C2_10–Al7	125.4(7)
C2_10–C3_10–C4_10	107.1(7)
C2_10–C3_10–C8_10	125.4(10)
C4_10–C3_10–C8_10	127.5(10)
C2_10–C3_10–Al7	71.2(4)
C4_10–C3_10–Al7	71.0(5)
C8_10–C3_10–Al7	124.2(7)
C5_10–C4_10–C3_10	108.1(7)
C5_10–C4_10–C7_10	126.0(10)
C3_10–C4_10–C7_10	125.9(10)
C5_10–C4_10–Al7	72.1(5)
C3_10–C4_10–Al7	71.3(5)
C7_10–C4_10–Al7	123.1(7)
C1_10–C5_10–C4_10	107.8(7)
C1_10–C5_10–C6_10	126.8(9)

C4_10–C5_10–C6_10	125.3(8)	C2_11–C1_11–Al8	71.5(3)
C1_10–C5_10–Al7	71.5(5)	C5_11–C1_11–Al8	69.9(4)
C4_10–C5_10–Al7	70.7(5)	C10_11–C1_11–Al8	123.2(5)
C6_10–C5_10–Al7	124.0(7)	C1_11–C2_11–C3_11	109.7(6)
C5_10–C6_10–H6A_10	109.5	C1_11–C2_11–C9_11	125.1(6)
C5_10–C6_10–H6B_10	109.5	C3_11–C2_11–C9_11	125.2(6)
H6A_10–C6_10–H6B_10	109.5	C1_11–C2_11–Al8	71.8(3)
		C3_11–C2_11–Al8	71.7(3)
C5_10–C6_10–H6C_10	109.5	C9_11–C2_11–Al8	122.7(4)
H6A_10–C6_10–H6C_10	109.5	C4_11–C3_11–C2_11	107.5(6)
		C4_11–C3_11–C8_11	127.1(7)
H6B_10–C6_10–H6C_10	109.5	C2_11–C3_11–C8_11	125.4(6)
		C4_11–C3_11–Al8	70.5(4)
C4_10–C7_10–H7A_10	109.5	C2_11–C3_11–Al8	71.4(3)
C4_10–C7_10–H7B_10	109.5	C8_11–C3_11–Al8	123.6(5)
H7A_10–C7_10–H7B_10	109.5	C3_11–C4_11–C5_11	108.3(6)
		C3_11–C4_11–C7_11	126.6(8)
C4_10–C7_10–H7C_10	109.5	C5_11–C4_11–C7_11	125.0(7)
H7A_10–C7_10–H7C_10	109.5	C3_11–C4_11–Al8	72.6(4)
		C5_11–C4_11–Al8	71.0(4)
H7B_10–C7_10–H7C_10	109.5	C7_11–C4_11–Al8	125.5(5)
		C4_11–C5_11–C1_11	107.8(6)
C3_10–C8_10–H8A_10	109.5	C4_11–C5_11–C6_11	126.8(8)
C3_10–C8_10–H8B_10	109.5	C1_11–C5_11–C6_11	125.2(8)
H8A_10–C8_10–H8B_10	109.5	C4_11–C5_11–Al8	71.3(4)
		C1_11–C5_11–Al8	72.3(4)
C3_10–C8_10–H8C_10	109.5	C6_11–C5_11–Al8	125.9(6)
H8A_10–C8_10–H8C_10	109.5	C5_11–C6_11–H6A_11	109.5
		C5_11–C6_11–H6B_11	109.5
H8B_10–C8_10–H8C_10	109.5	H6A_11–C6_11–H6B_11	109.5
C2_10–C9_10–H9A_10	109.5	C5_11–C6_11–H6C_11	109.5
C2_10–C9_10–H9B_10	109.5	H6A_11–C6_11–H6C_11	109.5
H9A_10–C9_10–H9B_10	109.5	H6B_11–C6_11–H6C_11	109.5
C2_10–C9_10–H9C_10	109.5	C4_11–C7_11–H7A_11	109.5
H9A_10–C9_10–H9C_10	109.5	C4_11–C7_11–H7B_11	109.5
H9B_10–C9_10–H9C_10	109.5	H7A_11–C7_11–H7B_11	109.5
C1_10–C10_10–H10A_10	109.5	C4_11–C7_11–H7C_11	109.5
C1_10–C10_10–H10B_10	109.5	H7A_11–C7_11–H7C_11	109.5
H10A_10–C10_10–H10B_10	109.5	H7B_11–C7_11–H7C_11	109.5
C1_10–C10_10–H10C_10	109.5	C3_11–C8_11–H8A_11	109.5
H10A_10–C10_10–H10C_10	109.5	C3_11–C8_11–H8B_11	109.5
H10B_10–C10_10–H10C_10	109.5	H8A_11–C8_11–H8B_11	109.5
C2_11–C1_11–C5_11	106.7(6)	C3_11–C8_11–H8C_11	109.5
C2_11–C1_11–C10_11	125.6(7)	H8A_11–C8_11–H8C_11	109.5
C5_11–C1_11–C10_11	127.8(7)	H8B_11–C8_11–H8C_11	109.5
		C2_11–C9_11–H9A_11	109.5

C2_11–C9_11–H9B_11	109.5	H6A_12–C6_12–H6C_12	109.5
H9A_11–C9_11–H9B_11	109.5	H6B_12–C6_12–H6C_12	109.5
C2_11–C9_11–H9C_11	109.5	C4_12–C7_12–H7A_12	109.5
H9A_11–C9_11–H9C_11	109.5	C4_12–C7_12–H7B_12	109.5
H9B_11–C9_11–H9C_11	109.5	H7A_12–C7_12–H7B_12	109.5
C1_11–C10_11–H10A_11	109.5	C4_12–C7_12–H7C_12	109.5
C1_11–C10_11–H10B_11	109.5	H7A_12–C7_12–H7C_12	109.5
H10A_11–C10_11–H10B_11	109.5	H7B_12–C7_12–H7C_12	109.5
C1_11–C10_11–H10C_11	109.5	C3_12–C8_12–H8A_12	109.5
H10A_11–C10_11–H10C_11	109.5	C3_12–C8_12–H8B_12	109.5
H10B_11–C10_11–H10C_11	109.5	H8A_12–C8_12–H8B_12	109.5
C2_12–C1_12–C5_12	108.0(6)	C3_12–C8_12–H8C_12	109.5
C2_12–C1_12–C10_12	125.1(7)	H8A_12–C8_12–H8C_12	109.5
C5_12–C1_12–C10_12	126.9(7)	H8B_12–C8_12–H8C_12	109.5
C2_12–C1_12–Al9	71.2(4)	C2_12–C9_12–H9A_12	109.5
C5_12–C1_12–Al9	70.9(4)	C2_12–C9_12–H9B_12	109.5
C10_12–C1_12–Al9	123.0(5)	H9A_12–C9_12–H9B_12	109.5
C1_12–C2_12–C3_12	108.6(6)	C2_12–C9_12–H9C_12	109.5
C1_12–C2_12–C9_12	124.9(8)	H9A_12–C9_12–H9C_12	109.5
C3_12–C2_12–C9_12	126.5(8)	H9B_12–C9_12–H9C_12	109.5
C1_12–C2_12–Al9	72.1(4)	C1_12–C10_12–H10A_12	109.5
C3_12–C2_12–Al9	71.5(4)	C1_12–C10_12–H10B_12	109.5
C9_12–C2_12–Al9	122.0(5)	H10A_12–C10_12–H10B_12	109.5
C2_12–C3_12–C4_12	107.8(6)	C1_12–C10_12–H10C_12	109.5
C2_12–C3_12–C8_12	126.7(7)	H10A_12–C10_12–H10C_12	109.5
C4_12–C3_12–C8_12	125.5(7)	H10B_12–C10_12–H10C_12	109.5
C2_12–C3_12–Al9	71.6(4)	C1_16–O1_16–Al14	150.0(10)
C4_12–C3_12–Al9	70.6(4)	O1_16–C1_16–C2_16	112.2(9)
C8_12–C3_12–Al9	122.8(5)	O1_16–C1_16–C4_16	109.3(9)
C3_12–C4_12–C5_12	107.4(6)	C2_16–C1_16–C4_16	109.6(8)
C3_12–C4_12–C7_12	126.8(8)	O1_16–C1_16–C3_16	108.9(9)
C5_12–C4_12–C7_12	125.5(7)	C2_16–C1_16–C3_16	109.8(8)
C3_12–C4_12–Al9	72.0(4)	C4_16–C1_16–C3_16	106.9(8)
C5_12–C4_12–Al9	71.8(4)	F3_16–C2_16–F1_16	106.9(9)
C7_12–C4_12–Al9	126.8(5)	F3_16–C2_16–F2_16	107.6(9)
C1_12–C5_12–C4_12	108.1(6)	F1_16–C2_16–F2_16	109.6(10)
C1_12–C5_12–C6_12	127.6(7)	F3_16–C2_16–C1_16	111.2(8)
C4_12–C5_12–C6_12	124.1(7)	F1_16–C2_16–C1_16	109.6(9)
C1_12–C5_12–Al9	72.3(4)		
C4_12–C5_12–Al9	70.7(4)		
C6_12–C5_12–Al9	125.7(6)		
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		

F2_16–C2_16–C1_16	111.7(8)	F4_18–C3_18–C1_18	107.6(9)
F4_16–C3_16–F6_16	107.9(9)	F6_18–C3_18–C1_18	108.9(11)
F4_16–C3_16–F5_16	107.6(10)	F7_18–C4_18–F8_18	109.0(10)
F6_16–C3_16–F5_16	111.2(10)	F7_18–C4_18–F9_18	105.6(11)
F4_16–C3_16–C1_16	110.0(9)	F8_18–C4_18–F9_18	104.2(10)
F6_16–C3_16–C1_16	110.6(9)	F7_18–C4_18–C1_18	112.2(9)
F5_16–C3_16–C1_16	109.5(9)	F8_18–C4_18–C1_18	113.7(10)
F9_16–C4_16–F8_16	111.0(10)	F9_18–C4_18–C1_18	111.6(9)
F9_16–C4_16–F7_16	107.9(10)	C1_19–O1_19–Al14	150.5(14)
F8_16–C4_16–F7_16	107.0(9)	O1_19–C1_19–C2_19	109.6(11)
F9_16–C4_16–C1_16	110.6(9)	O1_19–C1_19–C3_19	110.4(10)
F8_16–C4_16–C1_16	110.7(9)	C2_19–C1_19–C3_19	110.2(9)
F7_16–C4_16–C1_16	109.5(9)	O1_19–C1_19–C4_19	105.8(11)
C1_17–O1_17–Al14	151.8(6)	C2_19–C1_19–C4_19	110.6(9)
O1_17–C1_17–C4_17	110.4(7)	C3_19–C1_19–C4_19	110.1(9)
O1_17–C1_17–C2_17	109.6(7)	F2_19–C2_19–F1_19	100.6(11)
C4_17–C1_17–C2_17	111.7(7)	F2_19–C2_19–F3_19	109.6(12)
O1_17–C1_17–C3_17	110.2(7)	F1_19–C2_19–F3_19	110.7(12)
C4_17–C1_17–C3_17	107.2(7)	F2_19–C2_19–C1_19	115.6(11)
C2_17–C1_17–C3_17	107.7(7)	F1_19–C2_19–C1_19	110.4(10)
F3_17–C2_17–F2_17	108.8(8)	F3_19–C2_19–C1_19	109.6(10)
F3_17–C2_17–F1_17	105.9(9)	F5_19–C3_19–F4_19	104.5(12)
F2_17–C2_17–F1_17	109.3(9)	F5_19–C3_19–F6_19	98.7(11)
F3_17–C2_17–C1_17	111.0(8)	F4_19–C3_19–F6_19	112.3(11)
F2_17–C2_17–C1_17	112.8(8)	F5_19–C3_19–C1_19	108.9(10)
F1_17–C2_17–C1_17	108.7(8)	F4_19–C3_19–C1_19	113.5(10)
F4_17–C3_17–F5_17	108.5(9)	F6_19–C3_19–C1_19	117.0(11)
F4_17–C3_17–F6_17	107.8(9)	F7_19–C4_19–F8_19	106.1(12)
F5_17–C3_17–F6_17	108.5(8)	F7_19–C4_19–F9_19	112.9(12)
F4_17–C3_17–C1_17	110.7(8)	F8_19–C4_19–F9_19	107.7(11)
F5_17–C3_17–C1_17	110.1(8)	F7_19–C4_19–C1_19	108.3(11)
F6_17–C3_17–C1_17	111.3(8)	F8_19–C4_19–C1_19	110.8(11)
F7_17–C4_17–F9_17	109.2(10)	F9_19–C4_19–C1_19	110.9(10)
F7_17–C4_17–F8_17	107.7(9)	C1_20–O1_20–Al12	153.8(8)
F9_17–C4_17–F8_17	106.9(9)	O1_20–C1_20–C3_20	111.2(8)
F7_17–C4_17–C1_17	111.9(9)	O1_20–C1_20–C4_20	111.6(7)
F9_17–C4_17–C1_17	108.8(8)	C3_20–C1_20–C4_20	108.4(7)
F8_17–C4_17–C1_17	112.2(8)	O1_20–C1_20–C2_20	106.0(7)
C1_18–O1_18–Al14	144.8(8)	C3_20–C1_20–C2_20	109.9(7)
O1_18–C1_18–C4_18	114.0(10)	C4_20–C1_20–C2_20	109.7(7)
O1_18–C1_18–C2_18	112.9(9)	F3_20–C2_20–F1_20	111.1(9)
C4_18–C1_18–C2_18	109.5(8)	F3_20–C2_20–F2_20	103.7(8)
O1_18–C1_18–C3_18	106.4(8)	F1_20–C2_20–F2_20	109.6(8)
C4_18–C1_18–C3_18	107.9(8)	F3_20–C2_20–C1_20	109.7(8)
C2_18–C1_18–C3_18	105.7(8)	F1_20–C2_20–C1_20	110.7(7)
F1_18–C2_18–F2_18	109.6(10)	F2_20–C2_20–C1_20	111.9(8)
F1_18–C2_18–F3_18	103.8(10)	F6_20–C3_20–F5_20	103.9(9)
F2_18–C2_18–F3_18	109.8(10)	F6_20–C3_20–F4_20	113.0(10)
F1_18–C2_18–C1_18	111.2(9)	F5_20–C3_20–F4_20	107.8(9)
F2_18–C2_18–C1_18	111.9(10)	F6_20–C3_20–C1_20	112.0(9)
F3_18–C2_18–C1_18	110.1(9)	F5_20–C3_20–C1_20	112.0(8)
F5_18–C3_18–F4_18	105.9(10)	F4_20–C3_20–C1_20	108.1(8)
F5_18–C3_18–F6_18	109.5(11)	F9_20–C4_20–F8_20	108.9(9)
F4_18–C3_18–F6_18	115.9(12)	F9_20–C4_20–F7_20	108.1(8)
F5_18–C3_18–C1_18	108.8(9)	F8_20–C4_20–F7_20	108.3(8)

F9_20–C4_20–C1_20	109.6(8)	O1_23–C1_23–C4_23	108.9(11)
F8_20–C4_20–C1_20	111.1(8)	C2_23–C1_23–C4_23	109.5(9)
F7_20–C4_20–C1_20	110.8(8)	O1_23–C1_23–C3_23	109.6(11)
C1_21–O1_21–Al12	147.8(9)	C2_23–C1_23–C3_23	108.5(8)
O1_21–C1_21–C3_21	112.5(9)	C4_23–C1_23–C3_23	109.0(8)
O1_21–C1_21–C4_21	108.5(9)	F3_23–C2_23–F2_23	107.5(13)
C3_21–C1_21–C4_21	108.9(9)	F3_23–C2_23–F1_23	106.5(12)
O1_21–C1_21–C2_21	109.8(9)	F2_23–C2_23–F1_23	106.3(11)
C3_21–C1_21–C2_21	107.2(9)	F3_23–C2_23–C1_23	110.9(12)
C4_21–C1_21–C2_21	109.9(9)	F2_23–C2_23–C1_23	113.6(12)
F1_21–C2_21–F2_21	110.3(11)	F1_23–C2_23–C1_23	111.7(10)
F1_21–C2_21–F3_21	105.8(12)	F6_23–C3_23–F5_23	108.0(10)
F2_21–C2_21–F3_21	109.4(12)	F6_23–C3_23–F4_23	110.3(10)
F1_21–C2_21–C1_21	110.4(10)	F5_23–C3_23–F4_23	103.7(10)
F2_21–C2_21–C1_21	111.7(11)	F6_23–C3_23–C1_23	113.1(9)
F3_21–C2_21–C1_21	109.1(10)	F5_23–C3_23–C1_23	111.8(9)
F4_21–C3_21–F5_21	104.6(11)	F4_23–C3_23–C1_23	109.6(9)
F4_21–C3_21–F6_21	108.0(10)	F9_23–C4_23–F7_23	103.7(11)
F5_21–C3_21–F6_21	107.6(10)	F9_23–C4_23–F8_23	108.9(10)
F4_21–C3_21–C1_21	111.0(9)	F7_23–C4_23–F8_23	110.4(12)
F5_21–C3_21–C1_21	112.3(9)	F9_23–C4_23–C1_23	111.2(9)
F6_21–C3_21–C1_21	113.0(10)	F7_23–C4_23–C1_23	110.7(10)
F9_21–C4_21–F7_21	107.0(12)	F8_23–C4_23–C1_23	111.7(9)
F9_21–C4_21–F8_21	106.9(10)	C1_24–O1_24–Al11	150.1(6)
F7_21–C4_21–F8_21	107.5(12)	O1_24–C1_24–C3_24	104.6(6)
F9_21–C4_21–C1_21	110.6(9)	O1_24–C1_24–C4_24	110.1(6)
F7_21–C4_21–C1_21	113.0(12)	C3_24–C1_24–C4_24	111.0(6)
F8_21–C4_21–C1_21	111.6(10)	O1_24–C1_24–C2_24	114.8(7)
C1_22–O1_22–Al12	151.8(12)	C3_24–C1_24–C2_24	109.1(6)
O1_22–C1_22–C3_22	113.0(11)	C4_24–C1_24–C2_24	107.3(6)
O1_22–C1_22–C2_22	108.9(10)	F1_24–C2_24–F3_24	107.9(7)
C3_22–C1_22–C2_22	107.8(10)	F1_24–C2_24–F2_24	107.7(6)
O1_22–C1_22–C4_22	106.4(10)	F3_24–C2_24–F2_24	107.3(7)
C3_22–C1_22–C4_22	111.3(10)	F1_24–C2_24–C1_24	111.9(6)
C2_22–C1_22–C4_22	109.5(10)	F3_24–C2_24–C1_24	109.2(7)
F2_22–C2_22–F1_22	108.7(11)	F2_24–C2_24–C1_24	112.6(6)
F2_22–C2_22–F3_22	109.4(11)	F6_24–C3_24–F4_24	102.8(7)
F1_22–C2_22–F3_22	104.1(11)	F6_24–C3_24–F5_24	108.6(7)
F2_22–C2_22–C1_22	111.6(10)	F4_24–C3_24–F5_24	109.3(7)
F1_22–C2_22–C1_22	109.1(10)	F6_24–C3_24–C1_24	113.1(7)
F3_22–C2_22–C1_22	113.7(10)	F4_24–C3_24–C1_24	114.4(7)
F4_22–C3_22–F6_22	104.3(14)	F5_24–C3_24–C1_24	108.5(7)
F4_22–C3_22–F5_22	105.5(15)	F9_24–C4_24–F8_24	108.8(7)
F6_22–C3_22–F5_22	108.6(13)	F9_24–C4_24–F7_24	108.9(7)
F4_22–C3_22–C1_22	114.9(13)	F8_24–C4_24–F7_24	105.2(7)
F6_22–C3_22–C1_22	113.4(14)	F9_24–C4_24–C1_24	112.6(7)
F5_22–C3_22–C1_22	109.7(11)	F8_24–C4_24–C1_24	112.1(6)
F8_22–C4_22–F9_22	108.8(13)	F7_24–C4_24–C1_24	108.9(7)
F8_22–C4_22–F7_22	109.2(13)	C1_25–O1_25–Al11	146.7(4)
F9_22–C4_22–F7_22	105.7(14)	O1_25–C1_25–C4_25	106.8(5)
F8_22–C4_22–C1_22	112.5(12)	O1_25–C1_25–C2_25	109.6(5)
F9_22–C4_22–C1_22	112.6(12)	C4_25–C1_25–C2_25	110.0(5)
F7_22–C4_22–C1_22	107.7(12)	O1_25–C1_25–C3_25	112.1(5)
C1_23–O1_23–Al12	148.6(17)	C4_25–C1_25–C3_25	109.9(6)
O1_23–C1_23–C2_23	111.3(12)	C2_25–C1_25–C3_25	108.4(6)

F3_25–C2_25–F1_25	107.4(7)	F1_27–C2_27–C1_27	111.9(8)
F3_25–C2_25–F2_25	108.0(6)	F4_27–C3_27–F6_27	109.5(9)
F1_25–C2_25–F2_25	106.6(6)	F4_27–C3_27–F5_27	106.7(10)
F3_25–C2_25–C1_25	112.4(5)	F6_27–C3_27–F5_27	107.2(9)
F1_25–C2_25–C1_25	110.9(6)	F4_27–C3_27–C1_27	112.3(8)
F2_25–C2_25–C1_25	111.4(6)	F6_27–C3_27–C1_27	110.7(9)
F4_25–C3_25–F6_25	109.8(7)	F5_27–C3_27–C1_27	110.2(8)
F4_25–C3_25–F5_25	105.8(6)	F9_27–C4_27–F8_27	107.6(10)
F6_25–C3_25–F5_25	106.8(6)	F9_27–C4_27–F7_27	108.6(9)
F4_25–C3_25–C1_25	109.6(6)	F8_27–C4_27–F7_27	107.4(10)
F6_25–C3_25–C1_25	113.3(6)	F9_27–C4_27–C1_27	110.7(8)
F5_25–C3_25–C1_25	111.2(6)	F8_27–C4_27–C1_27	111.9(9)
F9_25–C4_25–F7_25	109.0(7)	F7_27–C4_27–C1_27	110.5(8)
F9_25–C4_25–F8_25	108.3(6)	C1_28–O1_28–Al10	152.4(9)
F7_25–C4_25–F8_25	105.4(7)	O1_28–C1_28–C4_28	109.1(8)
F9_25–C4_25–C1_25	112.2(6)	O1_28–C1_28–C3_28	109.5(9)
F7_25–C4_25–C1_25	109.1(6)	C4_28–C1_28–C3_28	109.6(8)
F8_25–C4_25–C1_25	112.7(6)	O1_28–C1_28–C2_28	110.2(9)
C1_26–O1_26–Al11	145.6(14)	C4_28–C1_28–C2_28	108.7(7)
O1_26–C1_26–C4_26	114.5(9)	C3_28–C1_28–C2_28	109.8(7)
O1_26–C1_26–C3_26	111.3(11)	F1_28–C2_28–F2_28	109.4(9)
C4_26–C1_26–C3_26	108.1(8)	F1_28–C2_28–F3_28	108.3(9)
O1_26–C1_26–C2_26	104.7(10)	F2_28–C2_28–F3_28	106.8(9)
C4_26–C1_26–C2_26	109.5(8)	F1_28–C2_28–C1_28	111.7(9)
C3_26–C1_26–C2_26	108.6(8)	F2_28–C2_28–C1_28	111.4(8)
F3_26–C2_26–F1_26	106.8(10)	F3_28–C2_28–C1_28	109.1(8)
F3_26–C2_26–F2_26	107.7(10)	F4_28–C3_28–F5_28	106.8(9)
F1_26–C2_26–F2_26	111.3(10)	F4_28–C3_28–F6_28	108.8(9)
F3_26–C2_26–C1_26	109.6(9)	F5_28–C3_28–F6_28	106.1(9)
F1_26–C2_26–C1_26	110.0(9)	F4_28–C3_28–C1_28	111.7(8)
F2_26–C2_26–C1_26	111.3(10)	F5_28–C3_28–C1_28	110.8(8)
F6_26–C3_26–F5_26	109.4(11)	F6_28–C3_28–C1_28	112.4(8)
F6_26–C3_26–F4_26	105.7(10)	F9_28–C4_28–F7_28	108.9(10)
F5_26–C3_26–F4_26	105.3(10)	F9_28–C4_28–F8_28	109.1(10)
F6_26–C3_26–C1_26	115.2(11)	F7_28–C4_28–F8_28	108.3(9)
F5_26–C3_26–C1_26	109.7(9)	F9_28–C4_28–C1_28	110.3(8)
F4_26–C3_26–C1_26	111.0(9)	F7_28–C4_28–C1_28	109.9(8)
F7_26–C4_26–F9_26	106.8(10)	F8_28–C4_28–C1_28	110.3(8)
F7_26–C4_26–F8_26	107.3(13)	C1_29–O1_29–Al10	152.7(8)
F9_26–C4_26–F8_26	106.4(12)	O1_29–C1_29–C4_29	109.6(8)
F7_26–C4_26–C1_26	111.3(9)	O1_29–C1_29–C2_29	109.5(8)
F9_26–C4_26–C1_26	112.3(9)	C4_29–C1_29–C2_29	110.5(8)
F8_26–C4_26–C1_26	112.3(11)	O1_29–C1_29–C3_29	108.6(8)
C1_27–O1_27–Al11	146.9(6)	C4_29–C1_29–C3_29	109.7(8)
O1_27–C1_27–C2_27	110.5(7)	C2_29–C1_29–C3_29	109.0(7)
O1_27–C1_27–C3_27	107.4(7)	F3_29–C2_29–F2_29	107.4(10)
C2_27–C1_27–C3_27	110.4(7)	F3_29–C2_29–F1_29	107.5(8)
O1_27–C1_27–C4_27	109.3(7)	F2_29–C2_29–F1_29	107.9(10)
C2_27–C1_27–C4_27	110.1(7)	F3_29–C2_29–C1_29	112.2(8)
C3_27–C1_27–C4_27	109.1(7)	F2_29–C2_29–C1_29	111.5(9)
F3_27–C2_27–F2_27	107.4(10)	F1_29–C2_29–C1_29	110.2(8)
F3_27–C2_27–F1_27	107.5(9)	F4_29–C3_29–F5_29	106.8(9)
F2_27–C2_27–F1_27	106.9(10)	F4_29–C3_29–F6_29	108.4(9)
F3_27–C2_27–C1_27	110.7(8)	F5_29–C3_29–F6_29	108.4(9)
F2_27–C2_27–C1_27	112.2(9)	F4_29–C3_29–C1_29	110.3(8)

F5_29–C3_29–C1_29	111.3(8)	F9_31–C4_31–C1_31	112.6(9)
F6_29–C3_29–C1_29	111.4(8)	F7_31–C4_31–C1_31	112.0(9)
F9_29–C4_29–F8_29	108.8(9)	F8_31–C4_31–C1_31	114.9(9)
F9_29–C4_29–F7_29	106.1(10)	C1_32–O1_32–Al13	147.5(16)
F8_29–C4_29–F7_29	106.5(10)	O1_32–C1_32–C3_32	109.3(11)
F9_29–C4_29–C1_29	111.4(8)	O1_32–C1_32–C2_32	110.9(11)
F8_29–C4_29–C1_29	111.9(9)	C3_32–C1_32–C2_32	111.2(9)
F7_29–C4_29–C1_29	111.9(9)	O1_32–C1_32–C4_32	110.1(12)
C1_30–O1_30–Al10	150.5(18)	C3_32–C1_32–C4_32	108.3(9)
O1_30–C1_30–C4_30	110.6(13)	C2_32–C1_32–C4_32	107.0(9)
O1_30–C1_30–C2_30	109.1(13)	F3_32–C2_32–F1_32	108.3(11)
C4_30–C1_30–C2_30	108.9(10)	F3_32–C2_32–F2_32	106.6(11)
O1_30–C1_30–C3_30	110.8(13)	F1_32–C2_32–F2_32	111.6(11)
C4_30–C1_30–C3_30	109.5(10)	F3_32–C2_32–C1_32	111.1(10)
C2_30–C1_30–C3_30	107.9(10)	F1_32–C2_32–C1_32	108.4(10)
F1_30–C2_30–F2_30	107.6(14)	F2_32–C2_32–C1_32	110.8(10)
F1_30–C2_30–F3_30	105.5(14)	F6_32–C3_32–F4_32	106.9(12)
F2_30–C2_30–F3_30	109.9(15)	F6_32–C3_32–F5_32	106.9(12)
F1_30–C2_30–C1_30	111.0(11)	F4_32–C3_32–F5_32	109.3(11)
F2_30–C2_30–C1_30	112.8(14)	F6_32–C3_32–C1_32	112.9(11)
F3_30–C2_30–C1_30	109.8(12)	F4_32–C3_32–C1_32	110.8(9)
F5_30–C3_30–F4_30	107.7(13)	F5_32–C3_32–C1_32	110.0(10)
F5_30–C3_30–F6_30	106.0(13)	F8_32–C4_32–F9_32	106.9(11)
F4_30–C3_30–F6_30	107.7(14)	F8_32–C4_32–F7_32	109.8(11)
F5_30–C3_30–C1_30	113.4(12)	F9_32–C4_32–F7_32	106.3(11)
F4_30–C3_30–C1_30	109.7(11)	F8_32–C4_32–C1_32	113.3(11)
F6_30–C3_30–C1_30	112.0(12)	F9_32–C4_32–C1_32	112.0(10)
F9_30–C4_30–F8_30	107.4(13)	F7_32–C4_32–C1_32	108.3(9)
F9_30–C4_30–F7_30	107.8(15)	C1_33–O1_33–Al11	152.7(17)
F8_30–C4_30–F7_30	110.0(15)	O1_33–C1_33–C4_33	112.5(11)
F9_30–C4_30–C1_30	111.5(11)	O1_33–C1_33–C2_33	106.1(11)
F8_30–C4_30–C1_30	110.1(12)	C4_33–C1_33–C2_33	107.8(9)
F7_30–C4_30–C1_30	110.0(13)	O1_33–C1_33–C3_33	109.9(12)
C1_31–O1_31–Al13	148.2(8)	C4_33–C1_33–C3_33	110.4(9)
O1_31–C1_31–C2_31	111.1(9)	C2_33–C1_33–C3_33	110.0(9)
O1_31–C1_31–C4_31	111.3(8)	F2_33–C2_33–F3_33	108.4(14)
C2_31–C1_31–C4_31	110.8(8)	F2_33–C2_33–F1_33	109.7(15)
O1_31–C1_31–C3_31	106.7(9)	F3_33–C2_33–F1_33	106.5(12)
C2_31–C1_31–C3_31	106.7(8)	F2_33–C2_33–C1_33	112.6(13)
C4_31–C1_31–C3_31	110.0(8)	F3_33–C2_33–C1_33	106.8(10)
F1_31–C2_31–F3_31	107.4(10)	F1_33–C2_33–C1_33	112.5(10)
F1_31–C2_31–F2_31	107.9(10)	F5_33–C3_33–F6_33	109.3(13)
F3_31–C2_31–F2_31	103.8(9)	F5_33–C3_33–F4_33	108.2(12)
F1_31–C2_31–C1_31	113.5(9)	F6_33–C3_33–F4_33	107.2(13)
F3_31–C2_31–C1_31	112.9(8)	F5_33–C3_33–C1_33	110.9(10)
F2_31–C2_31–C1_31	110.7(9)	F6_33–C3_33–C1_33	113.6(12)
F5_31–C3_31–F6_31	105.7(10)	F4_33–C3_33–C1_33	107.4(10)
F5_31–C3_31–F4_31	109.1(11)	C3_33–F5_33–F4_54	136.6(18)
F6_31–C3_31–F4_31	106.3(11)	F7_33–C4_33–F9_33	106.5(12)
F5_31–C3_31–C1_31	113.3(10)	F7_33–C4_33–F8_33	107.0(12)
F6_31–C3_31–C1_31	110.6(10)	F9_33–C4_33–F8_33	106.9(12)
F4_31–C3_31–C1_31	111.4(9)	F7_33–C4_33–C1_33	111.0(11)
F9_31–C4_31–F7_31	104.7(10)	F9_33–C4_33–C1_33	113.0(10)
F9_31–C4_31–F8_31	105.0(9)	F8_33–C4_33–C1_33	112.0(11)
F7_31–C4_31–F8_31	106.9(10)	C1_34–O1_34–Al11	146.9(12)

O1_34–C1_34–C4_34	111.2(11)	C2_36–C1_36–C4_36	108.8(9)
O1_34–C1_34–C3_34	110.6(11)	F2_36–C2_36–F1_36	105.7(12)
C4_34–C1_34–C3_34	108.8(10)	F2_36–C2_36–F3_36	110.7(11)
O1_34–C1_34–C2_34	106.0(11)	F1_36–C2_36–F3_36	104.7(12)
C4_34–C1_34–C2_34	109.8(10)	F2_36–C2_36–C1_36	113.6(10)
C3_34–C1_34–C2_34	110.3(10)	F1_36–C2_36–C1_36	111.2(11)
F2_34–C2_34–F3_34	106.9(16)	F3_36–C2_36–C1_36	110.5(11)
F2_34–C2_34–F1_34	109.1(17)	F4_36–C3_36–F6_36	108.3(11)
F3_34–C2_34–F1_34	108.1(15)	F4_36–C3_36–F5_36	103.5(14)
F2_34–C2_34–C1_34	111.0(14)	F6_36–C3_36–F5_36	106.3(13)
F3_34–C2_34–C1_34	111.9(12)	F4_36–C3_36–C1_36	115.3(11)
F1_34–C2_34–C1_34	109.7(12)	F6_36–C3_36–C1_36	112.3(11)
F5_34–C3_34–F6_34	105.7(15)	F5_36–C3_36–C1_36	110.4(11)
F5_34–C3_34–F4_34	105.9(14)	F9_36–C4_36–F7_36	105.2(13)
F6_34–C3_34–F4_34	111.1(16)	F9_36–C4_36–F8_36	108.4(15)
F5_34–C3_34–C1_34	110.6(12)	F7_36–C4_36–F8_36	109.5(12)
F6_34–C3_34–C1_34	111.6(14)	F9_36–C4_36–C1_36	110.8(13)
F4_34–C3_34–C1_34	111.6(12)	F7_36–C4_36–C1_36	110.4(10)
F8_34–C4_34–F9_34	105.6(17)	F8_36–C4_36–C1_36	112.3(13)
F8_34–C4_34–F7_34	108.9(17)	C1_37–O1_37–Al13	146.7(11)
F9_34–C4_34–F7_34	107.7(15)	O1_37–C1_37–C2_37	111.2(9)
F8_34–C4_34–C1_34	112.0(15)	O1_37–C1_37–C3_37	109.9(10)
F9_34–C4_34–C1_34	112.5(13)	C2_37–C1_37–C3_37	110.7(9)
F7_34–C4_34–C1_34	110.0(12)	O1_37–C1_37–C4_37	104.8(9)
C1_35–O1_35–Al10	147.0(10)	C2_37–C1_37–C4_37	110.2(9)
O1_35–C1_35–C2_35	106.9(10)	C3_37–C1_37–C4_37	109.8(9)
O1_35–C1_35–C4_35	113.2(10)	F3_37–C2_37–F1_37	106.9(11)
C2_35–C1_35–C4_35	108.5(9)	F3_37–C2_37–F2_37	107.1(11)
O1_35–C1_35–C3_35	109.9(10)	F1_37–C2_37–F2_37	106.5(11)
C2_35–C1_35–C3_35	109.9(10)	F3_37–C2_37–C1_37	112.7(9)
C4_35–C1_35–C3_35	108.4(10)	F1_37–C2_37–C1_37	110.7(10)
F1_35–C2_35–F2_35	107.8(13)	F2_37–C2_37–C1_37	112.5(10)
F1_35–C2_35–F3_35	108.5(14)	F5_37–C3_37–F4_37	102.5(11)
F2_35–C2_35–F3_35	107.1(12)	F5_37–C3_37–F6_37	109.4(10)
F1_35–C2_35–C1_35	111.5(13)	F4_37–C3_37–F6_37	109.2(10)
F2_35–C2_35–C1_35	113.0(11)	F5_37–C3_37–C1_37	108.8(10)
F3_35–C2_35–C1_35	108.7(10)	F4_37–C3_37–C1_37	117.7(10)
F4_35–C3_35–F5_35	108.9(15)	F6_37–C3_37–C1_37	108.9(9)
F4_35–C3_35–F6_35	106.7(11)	F8_37–C4_37–F9_37	110.9(12)
F5_35–C3_35–F6_35	110.1(14)	F8_37–C4_37–F7_37	102.9(12)
F4_35–C3_35–C1_35	110.8(11)	F9_37–C4_37–F7_37	108.0(12)
F5_35–C3_35–C1_35	108.9(12)	F8_37–C4_37–C1_37	112.7(10)
F6_35–C3_35–C1_35	111.5(11)	F9_37–C4_37–C1_37	111.1(11)
F7_35–C4_35–F9_35	106.7(11)	F7_37–C4_37–C1_37	110.7(10)
F7_35–C4_35–F8_35	108.1(11)	C1_38–O1_38–Al13	147.0(13)
F9_35–C4_35–F8_35	107.8(12)	O1_38–C1_38–C2_38	113.2(11)
F7_35–C4_35–C1_35	111.8(10)	O1_38–C1_38–C4_38	109.8(11)
F9_35–C4_35–C1_35	110.3(10)	C2_38–C1_38–C4_38	108.4(9)
F8_35–C4_35–C1_35	112.0(11)	O1_38–C1_38–C3_38	106.6(10)
C1_36–O1_36–Al12	148(2)	C2_38–C1_38–C3_38	109.0(9)
O1_36–C1_36–C3_36	107.0(13)	C4_38–C1_38–C3_38	109.8(9)
O1_36–C1_36–C2_36	113.0(12)	F2_38–C2_38–F3_38	108.6(11)
C3_36–C1_36–C2_36	109.8(10)	F2_38–C2_38–F1_38	105.9(12)
O1_36–C1_36–C4_36	110.2(13)	F3_38–C2_38–F1_38	108.4(11)
C3_36–C1_36–C4_36	107.9(9)	F2_38–C2_38–C1_38	112.6(11)

F3_38–C2_38–C1_38	109.4(10)	F4_40–C3_40–C1_40	111.1(10)
F1_38–C2_38–C1_38	111.8(12)	F6_40–C3_40–C1_40	109.4(9)
F6_38–C3_38–F4_38	111.0(12)	F5_40–C3_40–C1_40	106.4(9)
F6_38–C3_38–F5_38	104.6(12)	F9_40–C4_40–F8_40	108.0(10)
F4_38–C3_38–F5_38	104.5(12)	F9_40–C4_40–F7_40	108.5(11)
F6_38–C3_38–C1_38	111.9(11)	F8_40–C4_40–F7_40	109.1(10)
F4_38–C3_38–C1_38	111.8(10)	F9_40–C4_40–C1_40	111.4(9)
F5_38–C3_38–C1_38	112.5(11)	F8_40–C4_40–C1_40	112.2(9)
F8_38–C4_38–F9_38	111.1(12)	F7_40–C4_40–C1_40	107.5(9)
F8_38–C4_38–F7_38	106.7(13)	F1_41–C1_41–C6_41	120.6(8)
F9_38–C4_38–F7_38	103.5(12)	F1_41–C1_41–C2_41	118.7(8)
F8_38–C4_38–C1_38	115.5(11)	C6_41–C1_41–C2_41	120.6(8)
F9_38–C4_38–C1_38	110.8(10)	F2_41–C2_41–C3_41	120.5(8)
F7_38–C4_38–C1_38	108.3(11)	F2_41–C2_41–C1_41	118.4(8)
C1_39–O1_39–Al13	151.6(14)	C3_41–C2_41–C1_41	121.1(8)
O1_39–C1_39–C2_39	114.9(12)	C2_41–C3_41–C4_41	118.3(8)
O1_39–C1_39–C3_39	106.2(11)	C2_41–C3_41–H3_41	120.8
C2_39–C1_39–C3_39	108.6(10)	C4_41–C3_41–H3_41	120.8
O1_39–C1_39–C4_39	106.6(11)	C5_41–C4_41–C3_41	120.9(9)
C2_39–C1_39–C4_39	108.4(10)	C5_41–C4_41–H4_41	119.6
C3_39–C1_39–C4_39	112.2(10)	C3_41–C4_41–H4_41	119.6
F3_39–C2_39–F1_39	107.0(15)	C4_41–C5_41–C6_41	120.2(8)
F3_39–C2_39–F2_39	106.6(15)	C4_41–C5_41–H5_41	119.9
F1_39–C2_39–F2_39	103.9(13)	C6_41–C5_41–H5_41	119.9
F3_39–C2_39–C1_39	113.8(13)	C1_41–C6_41–C5_41	118.8(8)
F1_39–C2_39–C1_39	112.5(12)	C1_41–C6_41–H6_41	120.6
F2_39–C2_39–C1_39	112.3(12)	C5_41–C6_41–H6_41	120.6
F4_39–C3_39–F6_39	101.7(13)	F1_42–C1_42–C6_42	122.3(13)
F4_39–C3_39–F5_39	108.2(13)	F1_42–C1_42–C2_42	117.4(12)
F6_39–C3_39–F5_39	105.6(13)	C6_42–C1_42–C2_42	120.3(12)
F4_39–C3_39–C1_39	113.8(12)	F2_42–C2_42–C3_42	122.3(12)
F6_39–C3_39–C1_39	111.9(12)	F2_42–C2_42–C1_42	119.5(12)
F5_39–C3_39–C1_39	114.6(12)	C3_42–C2_42–C1_42	118.3(11)
F8_39–C4_39–F9_39	100.7(13)	C2_42–C3_42–C4_42	122.1(13)
F8_39–C4_39–F7_39	110.2(14)	C2_42–C3_42–H3_42	118.9
F9_39–C4_39–F7_39	104.3(13)	C4_42–C3_42–H3_42	118.9
F8_39–C4_39–C1_39	116.0(13)	C3_42–C4_42–C5_42	119.8(13)
F9_39–C4_39–C1_39	114.4(12)	C3_42–C4_42–H4_42	120.1
F7_39–C4_39–C1_39	110.3(12)	C5_42–C4_42–H4_42	120.1
C1_40–O1_40–Al10	146.5(7)	C6_42–C5_42–C4_42	118.0(13)
O1_40–C1_40–C2_40	111.8(8)	C6_42–C5_42–H5_42	121.0
O1_40–C1_40–C4_40	108.0(8)	C4_42–C5_42–H5_42	121.0
C2_40–C1_40–C4_40	111.6(9)	C5_42–C6_42–C1_42	121.5(13)
O1_40–C1_40–C3_40	111.8(8)	C5_42–C6_42–H6_42	119.3
C2_40–C1_40–C3_40	106.3(9)	C1_42–C6_42–H6_42	119.3
C4_40–C1_40–C3_40	107.2(8)	C1_43–O1_43–Al10	154.4(16)
F3_40–C2_40–F2_40	109.9(10)	O1_43–C1_43–C4_43	110.7(14)
F3_40–C2_40–F1_40	103.6(12)	O1_43–C1_43–C3_43	107.9(13)
F2_40–C2_40–F1_40	103.1(12)	C4_43–C1_43–C3_43	110.0(10)
F3_40–C2_40–C1_40	113.4(9)	O1_43–C1_43–C2_43	111.2(13)
F2_40–C2_40–C1_40	116.1(9)	C4_43–C1_43–C2_43	108.8(10)
F1_40–C2_40–C1_40	109.5(10)	C3_43–C1_43–C2_43	108.2(10)
F4_40–C3_40–F6_40	110.9(12)	F3_43–C2_43–F1_43	104.5(14)
F4_40–C3_40–F5_40	107.1(12)	F3_43–C2_43–F2_43	110.4(14)
F6_40–C3_40–F5_40	111.8(11)	F1_43–C2_43–F2_43	107.5(14)

F3_43–C2_43–C1_43	112.2(12)	F6_45–C3_45–F5_45	107.4(13)
F1_43–C2_43–C1_43	110.8(13)	F4_45–C3_45–C1_45	112.9(12)
F2_43–C2_43–C1_43	111.2(12)	F6_45–C3_45–C1_45	112.3(11)
F6_43–C3_43–F4_43	108.0(14)	F5_45–C3_45–C1_45	107.6(11)
F6_43–C3_43–F5_43	109.2(15)	F9_45–C4_45–F7_45	105.6(12)
F4_43–C3_43–F5_43	109.0(15)	F9_45–C4_45–F8_45	109.5(13)
F6_43–C3_43–C1_43	112.4(12)	F7_45–C4_45–F8_45	106.4(11)
F4_43–C3_43–C1_43	110.1(12)	F9_45–C4_45–C1_45	112.9(11)
F5_43–C3_43–C1_43	108.1(14)	F7_45–C4_45–C1_45	111.6(10)
F9_43–C4_43–F8_43	107.7(14)	F8_45–C4_45–C1_45	110.5(10)
F9_43–C4_43–F7_43	111.1(16)	C1_46–O1_46–Al10	148.2(12)
F8_43–C4_43–F7_43	103.8(14)	O1_46–C1_46–C4_46	108.5(11)
F9_43–C4_43–C1_43	110.0(12)	O1_46–C1_46–C3_46	109.1(11)
F8_43–C4_43–C1_43	113.4(13)	C4_46–C1_46–C3_46	110.5(10)
F7_43–C4_43–C1_43	110.7(13)	O1_46–C1_46–C2_46	110.8(11)
C1_44–O1_44–Al13	157.6(19)	C4_46–C1_46–C2_46	108.8(10)
O1_44–C1_44–C2_44	112.3(14)	C3_46–C1_46–C2_46	109.1(11)
O1_44–C1_44–C4_44	110.1(13)	F1_46–C2_46–F3_46	108.4(14)
C2_44–C1_44–C4_44	114.1(11)	F1_46–C2_46–F2_46	106.8(14)
O1_44–C1_44–C3_44	110.3(13)	F3_46–C2_46–F2_46	108.4(14)
C2_44–C1_44–C3_44	104.3(10)	F1_46–C2_46–C1_46	111.6(12)
C4_44–C1_44–C3_44	105.4(10)	F3_46–C2_46–C1_46	110.3(11)
F1_44–C2_44–F3_44	103.6(14)	F2_46–C2_46–C1_46	111.1(13)
F1_44–C2_44–F2_44	115.3(14)	F6_46–C3_46–F5_46	111.2(16)
F3_44–C2_44–F2_44	108.8(12)	F6_46–C3_46–F4_46	105.9(15)
F1_44–C2_44–C1_44	108.8(13)	F5_46–C3_46–F4_46	110.5(16)
F3_44–C2_44–C1_44	109.8(12)	F6_46–C3_46–C1_46	111.4(13)
F2_44–C2_44–C1_44	110.3(11)	F5_46–C3_46–C1_46	107.8(13)
F6_44–C3_44–F5_44	107.6(16)	F4_46–C3_46–C1_46	110.0(13)
F6_44–C3_44–F4_44	109.7(15)	F9_46–C4_46–F8_46	108.7(14)
F5_44–C3_44–F4_44	108.9(15)	F9_46–C4_46–F7_46	110.1(15)
F6_44–C3_44–C1_44	113.5(13)	F8_46–C4_46–F7_46	106.0(13)
F5_44–C3_44–C1_44	108.3(14)	F9_46–C4_46–C1_46	108.3(12)
F4_44–C3_44–C1_44	108.8(12)	F8_46–C4_46–C1_46	112.5(13)
F9_44–C4_44–F8_44	109.5(13)	F7_46–C4_46–C1_46	111.2(12)
F9_44–C4_44–F7_44	102.3(14)	C1_47–O1_47–Al14	157.6(15)
F8_44–C4_44–F7_44	108.1(14)	O1_47–C1_47–C4_47	112.9(12)
F9_44–C4_44–C1_44	116.0(12)	O1_47–C1_47–C3_47	110.8(13)
F8_44–C4_44–C1_44	111.7(11)	C4_47–C1_47–C3_47	108.7(10)
F7_44–C4_44–C1_44	108.7(13)	O1_47–C1_47–C2_47	106.7(12)
C1_45–O1_45–Al10	149.7(10)	C4_47–C1_47–C2_47	108.3(10)
O1_45–C1_45–C2_45	112.3(9)	C3_47–C1_47–C2_47	109.5(11)
O1_45–C1_45–C3_45	109.2(10)	F2_47–C2_47–F1_47	106.5(14)
C2_45–C1_45–C3_45	110.1(10)	F2_47–C2_47–F3_47	107.0(14)
O1_45–C1_45–C4_45	108.2(10)	F1_47–C2_47–F3_47	104.6(13)
C2_45–C1_45–C4_45	110.5(9)	F2_47–C2_47–C1_47	111.5(12)
C3_45–C1_45–C4_45	106.4(9)	F1_47–C2_47–C1_47	116.5(13)
F2_45–C2_45–F1_45	101.8(14)	F3_47–C2_47–C1_47	110.2(12)
F2_45–C2_45–F3_45	112.6(12)	F4_47–C3_47–F6_47	104.5(14)
F1_45–C2_45–F3_45	102.1(14)	F4_47–C3_47–F5_47	109.0(15)
F2_45–C2_45–C1_45	115.4(11)	F6_47–C3_47–F5_47	105.6(13)
F1_45–C2_45–C1_45	114.3(12)	F4_47–C3_47–C1_47	112.4(13)
F3_45–C2_45–C1_45	109.7(10)	F6_47–C3_47–C1_47	114.7(13)
F4_45–C3_45–F6_45	108.8(14)	F5_47–C3_47–C1_47	110.2(12)
F4_45–C3_45–F5_45	107.6(14)	F8_47–C4_47–F7_47	103.1(13)

F8_47–C4_47–F9_47	105.8(14)
F7_47–C4_47–F9_47	115.1(14)
F8_47–C4_47–C1_47	111.4(12)
F7_47–C4_47–C1_47	114.1(12)
F9_47–C4_47–C1_47	107.0(11)
C1_48–O1_48–Al14	166.7(14)
O1_48–C1_48–C2_48	112.9(11)
O1_48–C1_48–C3_48	110.8(12)
C2_48–C1_48–C3_48	110.1(10)
O1_48–C1_48–C4_48	105.3(12)
C2_48–C1_48–C4_48	109.4(10)
C3_48–C1_48–C4_48	108.1(9)
F3_48–C2_48–F1_48	110.3(13)
F3_48–C2_48–F2_48	102.3(14)
F1_48–C2_48–F2_48	102.1(14)
F3_48–C2_48–C1_48	116.2(12)
F1_48–C2_48–C1_48	108.5(11)
F2_48–C2_48–C1_48	116.5(14)
F4_48–C3_48–F6_48	106.6(12)
F4_48–C3_48–F5_48	103.8(11)
F6_48–C3_48–F5_48	108.0(12)
F4_48–C3_48–C1_48	114.0(10)
F6_48–C3_48–C1_48	112.9(11)
F5_48–C3_48–C1_48	111.1(11)
F8_48–C4_48–F9_48	107.5(12)
F8_48–C4_48–F7_48	117.1(13)
F9_48–C4_48–F7_48	105.6(12)
F8_48–C4_48–C1_48	111.3(12)
F9_48–C4_48–C1_48	107.9(11)
F7_48–C4_48–C1_48	107.0(10)
C1_49–O1_49–Al13	164.7(17)
O1_49–C1_49–C3_49	108.5(13)
O1_49–C1_49–C2_49	108.7(13)
C3_49–C1_49–C2_49	108.7(11)
O1_49–C1_49–C4_49	108.4(12)
C3_49–C1_49–C4_49	109.0(11)
C2_49–C1_49–C4_49	113.4(11)
F1_49–C2_49–F2_49	115.2(18)
F1_49–C2_49–F3_49	106.3(16)
F2_49–C2_49–F3_49	103.4(13)
F1_49–C2_49–C1_49	104.6(13)
F2_49–C2_49–C1_49	110.4(13)
F3_49–C2_49–C1_49	117.3(13)
F6_49–C3_49–F4_49	101.0(15)
F6_49–C3_49–F5_49	111.9(17)
F4_49–C3_49–F5_49	110.5(16)
F6_49–C3_49–C1_49	109.8(14)
F4_49–C3_49–C1_49	115.8(14)
F5_49–C3_49–C1_49	107.9(13)
F7_49–C4_49–F8_49	108.8(15)
F7_49–C4_49–F9_49	112.8(16)
F8_49–C4_49–F9_49	100.6(15)
F7_49–C4_49–C1_49	104.2(11)
F8_49–C4_49–C1_49	115.5(14)
F9_49–C4_49–C1_49	115.2(13)
C1_50–O1_50–Al13	154(2)
O1_50–C1_50–C3_50	111.2(16)
O1_50–C1_50–C4_50	110.2(15)
C3_50–C1_50–C4_50	109.2(11)
O1_50–C1_50–C2_50	108.3(15)
C3_50–C1_50–C2_50	110.3(11)
C4_50–C1_50–C2_50	107.5(11)
F2_50–C2_50–F3_50	107.6(15)
F2_50–C2_50–F1_50	106.5(15)
F3_50–C2_50–F1_50	113.7(15)
F2_50–C2_50–C1_50	112.5(13)
F3_50–C2_50–C1_50	109.5(12)
F1_50–C2_50–C1_50	107.2(13)
F6_50–C3_50–F4_50	113.4(15)
F6_50–C3_50–F5_50	106.6(15)
F4_50–C3_50–F5_50	110.8(15)
F6_50–C3_50–C1_50	109.8(13)
F4_50–C3_50–C1_50	110.4(12)
F5_50–C3_50–C1_50	105.6(13)
F8_50–C4_50–F9_50	109.1(15)
F8_50–C4_50–F7_50	104.4(15)
F9_50–C4_50–F7_50	116.4(16)
F8_50–C4_50–C1_50	113.7(14)
F9_50–C4_50–C1_50	107.1(12)
F7_50–C4_50–C1_50	106.4(13)
Al3_52–Tl1_52–Al2_52	65.93(9)
Al3_52–Tl1_52–Al1_52	68.03(9)
Al2_52–Tl1_52–Al1_52	68.61(8)
C5B_52–Al2_52–C1B_52	37.6(2)
C5B_52–Al2_52–C4B_52	37.6(2)
C1B_52–Al2_52–C4B_52	62.6(2)
C5B_52–Al2_52–C2B_52	62.5(2)
C1B_52–Al2_52–C2B_52	37.2(2)
C4B_52–Al2_52–C2B_52	62.2(2)
C5B_52–Al2_52–C3B_52	62.3(2)
C1B_52–Al2_52–C3B_52	62.1(2)
C4B_52–Al2_52–C3B_52	37.0(2)
C2B_52–Al2_52–C3B_52	37.1(2)
C5B_52–Al2_52–Tl1_52	147.77(18)
C1B_52–Al2_52–Tl1_52	121.68(17)
C4B_52–Al2_52–Tl1_52	174.58(18)

C2B_52–Al2_52–Tl1_52	118.75(18)	C1A_52–Al1_52–Tl1_52	172.52(18)
C3B_52–Al2_52–Tl1_52	140.43(18)	C2A_52–Al1_52–Tl1_52	148.46(19)
C5C_52–Al3_52–C4C_52	37.0(2)	C3A_52–Al1_52–Tl1_52	120.1(2)
C5C_52–Al3_52–C2C_52	62.0(2)	C5A_52–Al1_52–Tl1_52	136.28(18)
C4C_52–Al3_52–C2C_52	61.4(2)	C4A_52–Al1_52–Tl1_52	114.83(19)
C5C_52–Al3_52–C1C_52	37.3(2)	C5A_52–C1A_52–C2A_52	107.7(5)
C4C_52–Al3_52–C1C_52	62.0(2)	C5A_52–C1A_52–C6A_52	126.8(6)
C2C_52–Al3_52–C1C_52	37.4(2)	C2A_52–C1A_52–C6A_52	125.3(6)
C5C_52–Al3_52–C3C_52	61.7(2)	C5A_52–C1A_52–Al1_52	72.2(3)
C4C_52–Al3_52–C3C_52	36.8(2)	C2A_52–C1A_52–Al1_52	71.6(4)
C2C_52–Al3_52–C3C_52	36.6(2)	C6A_52–C1A_52–Al1_52	125.3(5)
C1C_52–Al3_52–C3C_52	61.9(2)	C3A_52–C2A_52–C1A_52	107.9(5)
C5C_52–Al3_52–Tl1_52	160.4(2)	C3A_52–C2A_52–C7A_52	126.1(6)
C4C_52–Al3_52–Tl1_52	160.2(2)	C1A_52–C2A_52–C7A_52	125.9(6)
C2C_52–Al3_52–Tl1_52	113.1(2)	C3A_52–C2A_52–Al1_52	72.0(4)
C1C_52–Al3_52–Tl1_52	126.7(2)	C1A_52–C2A_52–Al1_52	71.3(3)
C3C_52–Al3_52–Tl1_52	127.1(2)	C7A_52–C2A_52–Al1_52	125.9(5)
C1A_52–Al1_52–C2A_52	37.1(2)	C2A_52–C3A_52–C4A_52	108.6(5)
C1A_52–Al1_52–C3A_52	61.5(2)	C2A_52–C3A_52–C8A_52	124.9(7)
C2A_52–Al1_52–C3A_52	36.7(2)	C4A_52–C3A_52–C8A_52	126.5(7)
C1A_52–Al1_52–C5A_52	36.9(2)	C2A_52–C3A_52–Al1_52	71.3(4)
C2A_52–Al1_52–C5A_52	61.5(2)	C4A_52–C3A_52–Al1_52	72.3(4)
C3A_52–Al1_52–C5A_52	61.2(2)	C8A_52–C3A_52–Al1_52	124.3(5)
C1A_52–Al1_52–C4A_52	61.5(2)	C3A_52–C4A_52–C5A_52	107.5(5)
C2A_52–Al1_52–C4A_52	61.4(2)	C3A_52–C4A_52–C9A_52	126.9(6)
C3A_52–Al1_52–C4A_52	36.6(2)	C5A_52–C4A_52–C9A_52	125.6(6)
C5A_52–Al1_52–C4A_52	36.6(2)	C3A_52–C4A_52–Al1_52	71.0(3)

C5A_52–C4A_52–Al1_52	71.1(3)	C2A_52–C7A_52–H7AB_52	109.5
C9A_52–C4A_52–Al1_52	123.8(5)	H7AA_52–C7A_52–H7AB_52	109.5
C1A_52–C5A_52–C4A_52	108.4(5)	C2A_52–C7A_52–H7AC_52	109.5
C1A_52–C5A_52–C10A_52	126.8(6)	H7AA_52–C7A_52–H7AC_52	109.5
C4A_52–C5A_52–C10A_52	124.7(6)	H7AB_52–C7A_52–H7AC_52	109.5
C1A_52–C5A_52–Al1_52	71.0(3)	C1A_52–C6A_52–H6AA_52	109.5
C4A_52–C5A_52–Al1_52	72.2(3)	C1A_52–C6A_52–H6AB_52	109.5
C10A_52–C5A_52–Al1_52	125.9(5)	H6AA_52–C6A_52–H6AB_52	109.5
C5A_52–C10A_52–H10A_52	109.5	C1A_52–C6A_52–H6AC_52	109.5
C5A_52–C10A_52–H10B_52	109.5	H6AA_52–C6A_52–H6AC_52	109.5
H10A_52–C10A_52–H10B_52	109.5	H6AB_52–C6A_52–H6AC_52	109.5
C5A_52–C10A_52–H10C_52	109.5	C2B_52–C1B_52–C5B_52	107.9(5)
H10A_52–C10A_52–H10C_52	109.5	C2B_52–C1B_52–C6B_52	127.0(6)
H10B_52–C10A_52–H10C_52	109.5	C5B_52–C1B_52–C6B_52	125.1(6)
C4A_52–C9A_52–H9AA_52	109.5	C2B_52–C1B_52–Al2_52	72.0(3)
C4A_52–C9A_52–H9AB_52	109.5	C5B_52–C1B_52–Al2_52	70.6(3)
H9AA_52–C9A_52–H9AB_52	109.5	C6B_52–C1B_52–Al2_52	121.4(4)
C4A_52–C9A_52–H9AC_52	109.5	C1B_52–C2B_52–C3B_52	107.8(5)
H9AA_52–C9A_52–H9AC_52	109.5	C1B_52–C2B_52–C7B_52	127.3(5)
H9AB_52–C9A_52–H9AC_52	109.5	C3B_52–C2B_52–C7B_52	124.8(6)
C3A_52–C8A_52–H8AA_52	109.5	C1B_52–C2B_52–Al2_52	70.8(3)
C3A_52–C8A_52–H8AB_52	109.5	C3B_52–C2B_52–Al2_52	71.4(3)
H8AA_52–C8A_52–H8AB_52	109.5	C7B_52–C2B_52–Al2_52	124.0(4)
C3A_52–C8A_52–H8AC_52	109.5	C4B_52–C3B_52–C2B_52	108.6(5)
H8AA_52–C8A_52–H8AC_52	109.5	C4B_52–C3B_52–C8B_52	127.0(5)
H8AB_52–C8A_52–H8AC_52	109.5	C2B_52–C3B_52–C8B_52	124.3(6)
C2A_52–C7A_52–H7AA_52	109.5	C4B_52–C3B_52–Al2_52	70.9(3)

C2B_52–C3B_52–Al2_52	71.5(3)	C3B_52–C8B_52–H8BB_52	109.5
C8B_52–C3B_52–Al2_52	127.0(5)	H8BA_52–C8B_52–H8BB_52	109.5
C3B_52–C4B_52–C5B_52	107.8(5)	C3B_52–C8B_52–H8BC_52	109.5
C3B_52–C4B_52–C9B_52	127.7(6)	H8BA_52–C8B_52–H8BC_52	109.5
C5B_52–C4B_52–C9B_52	124.4(6)	H8BB_52–C8B_52–H8BC_52	109.5
C3B_52–C4B_52–Al2_52	72.1(3)	C2B_52–C7B_52–H7BA_52	109.5
C5B_52–C4B_52–Al2_52	70.6(3)	C2B_52–C7B_52–H7BB_52	109.5
C9B_52–C4B_52–Al2_52	125.9(4)	H7BA_52–C7B_52–H7BB_52	109.5
C1B_52–C5B_52–C4B_52	107.9(5)	C2B_52–C7B_52–H7BC_52	109.5
C1B_52–C5B_52–C10B_52	125.3(6)	H7BA_52–C7B_52–H7BC_52	109.5
C4B_52–C5B_52–C10B_52	126.8(6)	H7BB_52–C7B_52–H7BC_52	109.5
C1B_52–C5B_52–Al2_52	71.8(3)	C1B_52–C6B_52–H6BA_52	109.5
C4B_52–C5B_52–Al2_52	71.7(3)	C1B_52–C6B_52–H6BB_52	109.5
C10B_52–C5B_52–Al2_52	124.7(5)	H6BA_52–C6B_52–H6BB_52	109.5
C5B_52–C10B_52–H10D_52	109.5	C1B_52–C6B_52–H6BC_52	109.5
C5B_52–C10B_52–H10E_52	109.5	H6BA_52–C6B_52–H6BC_52	109.5
H10D_52–C10B_52–H10E_52	109.5	H6BB_52–C6B_52–H6BC_52	109.5
C5B_52–C10B_52–H10F_52	109.5	C5C_52–C1C_52–C2C_52	106.8(5)
H10D_52–C10B_52–H10F_52	109.5	C5C_52–C1C_52–C6C_52	126.1(7)
H10E_52–C10B_52–H10F_52	109.5	C2C_52–C1C_52–C6C_52	127.1(7)
C4B_52–C9B_52–H9BA_52	109.5	C5C_52–C1C_52–Al3_52	70.9(3)
C4B_52–C9B_52–H9BB_52	109.5	C2C_52–C1C_52–Al3_52	71.2(3)
H9BA_52–C9B_52–H9BB_52	109.5	C6C_52–C1C_52–Al3_52	122.2(5)
C4B_52–C9B_52–H9BC_52	109.5	C3C_52–C2C_52–C1C_52	108.6(5)
H9BA_52–C9B_52–H9BC_52	109.5	C3C_52–C2C_52–C7C_52	125.9(7)
H9BB_52–C9B_52–H9BC_52	109.5	C1C_52–C2C_52–C7C_52	125.5(7)
C3B_52–C8B_52–H8BA_52	109.5	C3C_52–C2C_52–Al3_52	72.1(3)

C1C_52–C2C_52–Al3_52	71.4(3)	C4C_52–C9C_52–H9CB_52	109.5
C7C_52–C2C_52–Al3_52	124.1(5)	H9CA_52–C9C_52–H9CB_52	109.5
C2C_52–C3C_52–C4C_52	108.0(5)	C4C_52–C9C_52–H9CC_52	109.5
C2C_52–C3C_52–C8C_52	125.7(7)	H9CA_52–C9C_52–H9CC_52	109.5
C4C_52–C3C_52–C8C_52	126.2(7)	H9CB_52–C9C_52–H9CC_52	109.5
C2C_52–C3C_52–Al3_52	71.2(3)	C3C_52–C8C_52–H8CA_52	109.5
C4C_52–C3C_52–Al3_52	71.0(3)	C3C_52–C8C_52–H8CB_52	109.5
C8C_52–C3C_52–Al3_52	125.1(5)	H8CA_52–C8C_52–H8CB_52	109.5
C3C_52–C4C_52–C5C_52	108.5(5)	C3C_52–C8C_52–H8CC_52	109.5
C3C_52–C4C_52–C9C_52	125.9(6)	H8CA_52–C8C_52–H8CC_52	109.5
C5C_52–C4C_52–C9C_52	125.3(6)	H8CB_52–C8C_52–H8CC_52	109.5
C3C_52–C4C_52–Al3_52	72.2(3)	C2C_52–C7C_52–H7CA_52	109.5
C5C_52–C4C_52–Al3_52	71.3(3)	C2C_52–C7C_52–H7CB_52	109.5
C9C_52–C4C_52–Al3_52	127.0(5)	H7CA_52–C7C_52–H7CB_52	109.5
C4C_52–C5C_52–C1C_52	108.1(5)	C2C_52–C7C_52–H7CC_52	109.5
C4C_52–C5C_52–C10C_52	124.5(6)	H7CA_52–C7C_52–H7CC_52	109.5
C1C_52–C5C_52–C10C_52	127.2(6)	H7CB_52–C7C_52–H7CC_52	109.5
C4C_52–C5C_52–Al3_52	71.7(3)	C1C_52–C6C_52–H6CA_52	109.5
C1C_52–C5C_52–Al3_52	71.7(3)	C1C_52–C6C_52–H6CB_52	109.5
C10C_52–C5C_52–Al3_52	126.5(5)	H6CA_52–C6C_52–H6CB_52	109.5
C5C_52–C10C_52–H10G_52	109.5	C1C_52–C6C_52–H6CC_52	109.5
C5C_52–C10C_52–H10H_52	109.5	H6CA_52–C6C_52–H6CC_52	109.5
H10G_52–C10C_52–H10H_52	109.5	H6CB_52–C6C_52–H6CC_52	109.5
C5C_52–C10C_52–H10I_52	109.5	Al3_13–Tl1_13–Al1_13	66.8(4)
		Al3_13–Tl1_13–Al2_13	67.3(6)
H10G_52–C10C_52–H10I_52	109.5	Al1_13–Tl1_13–Al2_13	66.9(4)
H10H_52–C10C_52–H10I_52	109.5	C3B_13–Al2_13–C2B_13	37.1(4)
C4C_52–C9C_52–H9CA_52	109.5	C3B_13–Al2_13–C4B_13	36.8(5)
		C2B_13–Al2_13–C4B_13	61.1(6)

C3B_13–Al2_13–C1B_13	62.5(7)
C2B_13–Al2_13–C1B_13	37.8(4)
C4B_13–Al2_13–C1B_13	60.9(6)
C3B_13–Al2_13–C5B_13	62.6(6)
C2B_13–Al2_13–C5B_13	62.4(6)
C4B_13–Al2_13–C5B_13	36.8(4)
C1B_13–Al2_13–C5B_13	36.8(4)
C3B_13–Al2_13–Tl1_13	143.5(10)
C2B_13–Al2_13–Tl1_13	117.4(9)
C4B_13–Al2_13–Tl1_13	177.0(11)
C1B_13–Al2_13–Tl1_13	116.3(10)
C5B_13–Al2_13–Tl1_13	140.5(11)
C3B_13–Al2_13–Al1_13	153.6(10)
C2B_13–Al2_13–Al1_13	168.8(10)
C4B_13–Al2_13–Al1_13	125.4(9)
C1B_13–Al2_13–Al1_13	134.3(10)
C5B_13–Al2_13–Al1_13	116.3(9)
Tl1_13–Al2_13–Al1_13	55.7(3)
C4C_13–Al3_13–C5C_13	37.1(4)
C4C_13–Al3_13–C3C_13	36.8(5)
C5C_13–Al3_13–C3C_13	62.0(6)
C4C_13–Al3_13–C2C_13	61.4(7)
C5C_13–Al3_13–C2C_13	61.7(6)
C3C_13–Al3_13–C2C_13	37.0(4)
C4C_13–Al3_13–C1C_13	61.8(6)
C5C_13–Al3_13–C1C_13	37.0(4)
C3C_13–Al3_13–C1C_13	62.2(6)
C2C_13–Al3_13–C1C_13	37.2(4)
C4C_13–Al3_13–Tl1_13	163.1(10)
C5C_13–Al3_13–Tl1_13	158.3(11)
C3C_13–Al3_13–Tl1_13	129.8(9)
C2C_13–Al3_13–Tl1_13	114.9(9)
C1C_13–Al3_13–Tl1_13	126.6(10)
C4C_13–Al3_13–Al1_13	132.9(10)
C5C_13–Al3_13–Al1_13	117.9(9)
C3C_13–Al3_13–Al1_13	164.2(11)
C2C_13–Al3_13–Al1_13	158.6(11)
C1C_13–Al3_13–Al1_13	128.5(10)
Tl1_13–Al3_13–Al1_13	56.6(3)
C3A_13–Al1_13–C4A_13	36.7(4)
C3A_13–Al1_13–C2A_13	36.8(4)
C4A_13–Al1_13–C2A_13	61.5(6)
C3A_13–Al1_13–C5A_13	61.1(6)
C4A_13–Al1_13–C5A_13	36.7(4)
C2A_13–Al1_13–C5A_13	61.2(6)
C3A_13–Al1_13–C1A_13	61.0(6)
C4A_13–Al1_13–C1A_13	61.2(6)
C2A_13–Al1_13–C1A_13	36.5(4)
C5A_13–Al1_13–C1A_13	36.6(4)
C3A_13–Al1_13–Tl1_13	127.2(9)
C4A_13–Al1_13–Tl1_13	116.0(9)
C2A_13–Al1_13–Tl1_13	158.1(9)
C5A_13–Al1_13–Tl1_13	131.5(9)
C1A_13–Al1_13–Tl1_13	164.4(9)
C3A_13–Al1_13–Al3_13	121.4(9)
C4A_13–Al1_13–Al3_13	151.4(10)

C2A_13–Al1_13–Al3_13	113.8(9)
C5A_13–Al1_13–Al3_13	169.4(10)
C1A_13–Al1_13–Al3_13	133.7(9)
Tl1_13–Al1_13–Al3_13	56.7(3)
C3A_13–Al1_13–Al2_13	175.3(9)
C4A_13–Al1_13–Al2_13	143.0(10)
C2A_13–Al1_13–Al2_13	139.0(10)
C5A_13–Al1_13–Al2_13	116.0(9)
C1A_13–Al1_13–Al2_13	114.4(9)
Tl1_13–Al1_13–Al2_13	57.4(3)
Al3_13–Al1_13–Al2_13	60.7(5)
C2A_13–C1A_13–C5A_13	108.3(12)
C2A_13–C1A_13–C6A_13	126.7(19)
C5A_13–C1A_13–C6A_13	124.9(19)
C2A_13–C1A_13–Al1_13	71.6(7)
C5A_13–C1A_13–Al1_13	71.5(7)
C6A_13–C1A_13–Al1_13	123(2)
C1A_13–C2A_13–C3A_13	107.4(12)
C1A_13–C2A_13–C7A_13	126(2)
C3A_13–C2A_13–C7A_13	126.2(19)
C1A_13–C2A_13–Al1_13	71.9(7)
C3A_13–C2A_13–Al1_13	71.1(7)
C7A_13–C2A_13–Al1_13	121(2)
C4A_13–C3A_13–C2A_13	108.4(12)
C4A_13–C3A_13–C8A_13	128(2)
C2A_13–C3A_13–C8A_13	123(2)
C4A_13–C3A_13–Al1_13	71.6(7)
C2A_13–C3A_13–Al1_13	72.0(7)
C8A_13–C3A_13–Al1_13	123(2)
C3A_13–C4A_13–C5A_13	107.8(12)
C3A_13–C4A_13–C9A_13	127(2)
C5A_13–C4A_13–C9A_13	126(2)
C3A_13–C4A_13–Al1_13	71.6(7)
C5A_13–C4A_13–Al1_13	72.0(7)
C9A_13–C4A_13–Al1_13	121(2)
C4A_13–C5A_13–C1A_13	108.0(12)
C4A_13–C5A_13–C10A_13	126(2)
C1A_13–C5A_13–C10A_13	126(2)
C4A_13–C5A_13–Al1_13	71.3(7)
C1A_13–C5A_13–Al1_13	71.9(7)
C10A_13–C5A_13–Al1_13	124(2)
C5A_13–C10A_13–H10A_13	109.5
C5A_13–C10A_13–H10B_13	109.5
H10A_13–C10A_13–H10B_13	109.5
C5A_13–C10A_13–H10C_13	109.5
H10A_13–C10A_13–H10C_13	109.5
H10B_13–C10A_13–H10C_13	109.5
C4A_13–C9A_13–H9AA_13	109.5
C4A_13–C9A_13–H9AB_13	109.5
H9AA_13–C9A_13–H9AB_13	109.5
C4A_13–C9A_13–H9AC_13	109.5
H9AA_13–C9A_13–H9AC_13	109.5
H9AB_13–C9A_13–H9AC_13	109.5
C3A_13–C8A_13–H8AA_13	109.5
C3A_13–C8A_13–H8AB_13	109.5

H8AA_13–C8A_13–H8AB_13	109.5	C7B_13–C2B_13–Al2_13	127(2)
C3A_13–C8A_13–H8AC_13	109.5	C4B_13–C3B_13–C2B_13	106.6(12)
H8AA_13–C8A_13–H8AC_13	109.5	C4B_13–C3B_13–C8B_13	124(2)
H8AB_13–C8A_13–H8AC_13	109.5	C2B_13–C3B_13–C8B_13	129(2)
C2A_13–C7A_13–H7AA_13	109.5	C4B_13–C3B_13–Al2_13	72.8(7)
C2A_13–C7A_13–H7AB_13	109.5	C2B_13–C3B_13–Al2_13	70.6(7)
H7AA_13–C7A_13–H7AB_13	109.5	C8B_13–C3B_13–Al2_13	124(2)
C2A_13–C7A_13–H7AC_13	109.5	C3B_13–C4B_13–C5B_13	110.1(12)
H7AA_13–C7A_13–H7AC_13	109.5	C3B_13–C4B_13–C9B_13	126(2)
H7AB_13–C7A_13–H7AC_13	109.5	C5B_13–C4B_13–C9B_13	124(2)
C1A_13–C6A_13–H6AA_13	109.5	C3B_13–C4B_13–Al2_13	70.4(7)
C1A_13–C6A_13–H6AB_13	109.5	C5B_13–C4B_13–Al2_13	71.2(7)
H6AA_13–C6A_13–H6AB_13	109.5	C9B_13–C4B_13–Al2_13	120(2)
C1A_13–C6A_13–H6AC_13	109.5	C1B_13–C5B_13–C4B_13	106.4(12)
H6AA_13–C6A_13–H6AC_13	109.5	C1B_13–C5B_13–C10B_13	126(2)
H6AB_13–C6A_13–H6AC_13	109.5	C4B_13–C5B_13–C10B_13	127(2)
C5B_13–C1B_13–C2B_13	108.5(12)	C1B_13–C5B_13–Al2_13	70.5(7)
C5B_13–C1B_13–C6B_13	130(2)	C4B_13–C5B_13–Al2_13	72.0(7)
C2B_13–C1B_13–C6B_13	121.4(19)	C10B_13–C5B_13–Al2_13	120(2)
C5B_13–C1B_13–Al2_13	72.7(7)	C5B_13–C10B_13–H10D_13	109.5
C2B_13–C1B_13–Al2_13	70.6(7)	C5B_13–C10B_13–H10E_13	109.5
C6B_13–C1B_13–Al2_13	123(2)	H10D_13–C10B_13–H10E_13	109.5
C3B_13–C2B_13–C1B_13	108.3(12)	C5B_13–C10B_13–H10F_13	109.5
C3B_13–C2B_13–C7B_13	126.8(19)	H10D_13–C10B_13–H10F_13	109.5
C1B_13–C2B_13–C7B_13	124.5(19)	H10E_13–C10B_13–H10F_13	109.5
C3B_13–C2B_13–Al2_13	72.2(7)	C4B_13–C9B_13–H9BA_13	109.4
C1B_13–C2B_13–Al2_13	71.7(7)	C4B_13–C9B_13–H9BB_13	109.5

H9BA_13–C9B_13–H9BB_13	109.5	C6C_13–C1C_13–Al3_13	123(2)
C4B_13–C9B_13–H9BC_13	109.5	C3C_13–C2C_13–C1C_13	108.8(12)
H9BA_13–C9B_13–H9BC_13	109.5	C3C_13–C2C_13–C7C_13	124.1(19)
H9BB_13–C9B_13–H9BC_13	109.5	C1C_13–C2C_13–C7C_13	126.7(19)
C3B_13–C8B_13–H8BA_13	109.5	C3C_13–C2C_13–Al3_13	71.9(7)
C3B_13–C8B_13–H8BB_13	109.5	C1C_13–C2C_13–Al3_13	71.4(7)
H8BA_13–C8B_13–H8BB_13	109.5	C7C_13–C2C_13–Al3_13	128(2)
C3B_13–C8B_13–H8BC_13	109.5	C4C_13–C3C_13–C2C_13	107.2(12)
H8BA_13–C8B_13–H8BC_13	109.5	C4C_13–C3C_13–C8C_13	128(2)
H8BB_13–C8B_13–H8BC_13	109.5	C2C_13–C3C_13–C8C_13	125(2)
C2B_13–C7B_13–H7BA_13	109.5	C4C_13–C3C_13–Al3_13	71.5(7)
C2B_13–C7B_13–H7BB_13	109.5	C2C_13–C3C_13–Al3_13	71.0(7)
H7BA_13–C7B_13–H7BB_13	109.5	C8C_13–C3C_13–Al3_13	124(2)
C2B_13–C7B_13–H7BC_13	109.5	C3C_13–C4C_13–C5C_13	108.7(12)
H7BA_13–C7B_13–H7BC_13	109.5	C3C_13–C4C_13–C9C_13	124(2)
H7BB_13–C7B_13–H7BC_13	109.5	C5C_13–C4C_13–C9C_13	127(2)
C1B_13–C6B_13–H6BA_13	109.5	C3C_13–C4C_13–Al3_13	71.7(7)
C1B_13–C6B_13–H6BB_13	109.5	C5C_13–C4C_13–Al3_13	71.1(7)
H6BA_13–C6B_13–H6BB_13	109.5	C9C_13–C4C_13–Al3_13	125(2)
C1B_13–C6B_13–H6BC_13	109.5	C1C_13–C5C_13–C4C_13	107.8(12)
H6BA_13–C6B_13–H6BC_13	109.5	C1C_13–C5C_13–C10C_13	125.6(19)
H6BB_13–C6B_13–H6BC_13	109.5	C4C_13–C5C_13–C10C_13	126.6(19)
C5C_13–C1C_13–C2C_13	107.5(12)	C1C_13–C5C_13–Al3_13	71.4(7)
C5C_13–C1C_13–C6C_13	129(2)	C4C_13–C5C_13–Al3_13	71.8(7)
C2C_13–C1C_13–C6C_13	123.3(19)	C10C_13–C5C_13–Al3_13	124(2)
C5C_13–C1C_13–Al3_13	71.5(7)	C5C_13–C10C_13–H10G_13	109.5
C2C_13–C1C_13–Al3_13	71.5(7)	C5C_13–C10C_13–H10H_13	109.5

H10G_13–C10C_13–H10H_13	109.5
C5C_13–C10C_13–H10I_13	109.5
H10G_13–C10C_13–H10I_13	109.5
H10H_13–C10C_13–H10I_13	109.5
C4C_13–C9C_13–H9CA_13	109.5
C4C_13–C9C_13–H9CB_13	109.5
H9CA_13–C9C_13–H9CB_13	109.5
C4C_13–C9C_13–H9CC_13	109.5
H9CA_13–C9C_13–H9CC_13	109.5
H9CB_13–C9C_13–H9CC_13	109.5
C3C_13–C8C_13–H8CA_13	109.5
C3C_13–C8C_13–H8CB_13	109.5
H8CA_13–C8C_13–H8CB_13	109.5
C3C_13–C8C_13–H8CC_13	109.5
H8CA_13–C8C_13–H8CC_13	109.5
H8CB_13–C8C_13–H8CC_13	109.5
C2C_13–C7C_13–H7CA_13	109.5
C2C_13–C7C_13–H7CB_13	109.5
H7CA_13–C7C_13–H7CB_13	109.5
C2C_13–C7C_13–H7CC_13	109.5
H7CA_13–C7C_13–H7CC_13	109.5
H7CB_13–C7C_13–H7CC_13	109.5
C1C_13–C6C_13–H6CA_13	109.5
C1C_13–C6C_13–H6CB_13	109.5
H6CA_13–C6C_13–H6CB_13	109.5
C1C_13–C6C_13–H6CC_13	109.5
H6CA_13–C6C_13–H6CC_13	109.5
H6CB_13–C6C_13–H6CC_13	109.5
Al1_14–Tl1_14–Al3_14	67.06(13)
Al1_14–Tl1_14–Al2_14	67.10(14)
Al3_14–Tl1_14–Al2_14	69.36(9)
C5B_14–Al2_14–C4B_14	37.3(2)
C5B_14–Al2_14–C3B_14	61.8(2)
C4B_14–Al2_14–C3B_14	36.7(2)
C5B_14–Al2_14–C1B_14	37.0(2)
C4B_14–Al2_14–C1B_14	61.8(3)
C3B_14–Al2_14–C1B_14	61.6(2)
C5B_14–Al2_14–C2B_14	62.0(2)
C4B_14–Al2_14–C2B_14	61.6(3)
C3B_14–Al2_14–C2B_14	36.8(2)
C1B_14–Al2_14–C2B_14	37.1(2)
C5B_14–Al2_14–Tl1_14	151.6(2)
C4B_14–Al2_14–Tl1_14	164.5(2)
C3B_14–Al2_14–Tl1_14	128.2(2)
C1B_14–Al2_14–Tl1_14	118.8(2)
C2B_14–Al2_14–Tl1_14	108.6(2)
C4C_14–Al3_14–C5C_14	37.7(2)
C4C_14–Al3_14–C2C_14	62.6(2)
C5C_14–Al3_14–C2C_14	62.1(2)
C4C_14–Al3_14–C1C_14	62.9(2)
C5C_14–Al3_14–C1C_14	37.3(2)
C2C_14–Al3_14–C1C_14	37.2(2)
C4C_14–Al3_14–C3C_14	37.3(2)
C5C_14–Al3_14–C3C_14	62.3(2)
C2C_14–Al3_14–C3C_14	37.5(2)
C1C_14–Al3_14–C3C_14	62.5(2)

C4C_14–Al3_14–Tl1_14	154.5(2)	C3A_14–C2A_14–C7A_14	126.0(7)
C5C_14–Al3_14–Tl1_14	167.3(2)	C1A_14–C2A_14–C7A_14	125.8(7)
C2C_14–Al3_14–Tl1_14	116.5(2)	C3A_14–C2A_14–Al1_14	72.7(4)
C1C_14–Al3_14–Tl1_14	133.7(2)	C1A_14–C2A_14–Al1_14	71.0(4)
C3C_14–Al3_14–Tl1_14	125.3(2)	C7A_14–C2A_14–Al1_14	125.9(5)
C1A_14–Al1_14–C5A_14	37.1(2)	C4A_14–C3A_14–C2A_14	108.3(5)
C1A_14–Al1_14–C2A_14	37.3(2)	C4A_14–C3A_14–C8A_14	125.6(7)
C5A_14–Al1_14–C2A_14	61.8(3)	C2A_14–C3A_14–C8A_14	126.1(7)
C1A_14–Al1_14–C3A_14	61.7(3)	C4A_14–C3A_14–Al1_14	72.1(4)
C5A_14–Al1_14–C3A_14	61.2(3)	C2A_14–C3A_14–Al1_14	70.5(4)
C2A_14–Al1_14–C3A_14	36.8(2)	C8A_14–C3A_14–Al1_14	122.8(5)
C1A_14–Al1_14–C4A_14	61.7(3)	C3A_14–C4A_14–C5A_14	107.7(6)
C5A_14–Al1_14–C4A_14	36.8(2)	C3A_14–C4A_14–C9A_14	127.4(7)
C2A_14–Al1_14–C4A_14	61.4(3)	C5A_14–C4A_14–C9A_14	124.8(7)
C3A_14–Al1_14–C4A_14	36.4(3)	C3A_14–C4A_14–Al1_14	71.5(4)
C1A_14–Al1_14–Tl1_14	168.0(3)	C5A_14–C4A_14–Al1_14	70.4(3)
C5A_14–Al1_14–Tl1_14	132.7(3)	C9A_14–C4A_14–Al1_14	122.2(5)
C2A_14–Al1_14–Tl1_14	152.7(3)	C1A_14–C5A_14–C4A_14	108.5(5)
C3A_14–Al1_14–Tl1_14	122.5(3)	C1A_14–C5A_14–C10A_14	126.5(6)
C4A_14–Al1_14–Tl1_14	114.1(3)	C4A_14–C5A_14–C10A_14	125.0(6)
C5A_14–C1A_14–C2A_14	107.4(5)	C1A_14–C5A_14–Al1_14	71.0(4)
C5A_14–C1A_14–C6A_14	125.3(6)	C4A_14–C5A_14–Al1_14	72.9(4)
C2A_14–C1A_14–C6A_14	127.2(6)	C10A_14–C5A_14–Al1_14	123.6(5)
C5A_14–C1A_14–Al1_14	71.9(4)	C5A_14–C10A_14–H10A_14	109.5
C2A_14–C1A_14–Al1_14	71.7(4)	C5A_14–C10A_14–H10B_14	109.5
C6A_14–C1A_14–Al1_14	123.7(5)	H10A_14–C10A_14–H10B_14	109.5
C3A_14–C2A_14–C1A_14	108.0(6)	C5A_14–C10A_14–H10C_14	109.5

H10A_14–C10A_14–H10C_14	109.5	C5B_14–C1B_14–C6B_14	126.1(6)
H10B_14–C10A_14–H10C_14	109.5	C2B_14–C1B_14–C6B_14	126.0(7)
C4A_14–C9A_14–H9AA_14	109.5	C5B_14–C1B_14–Al2_14	70.7(4)
C4A_14–C9A_14–H9AB_14	109.5	C2B_14–C1B_14–Al2_14	71.6(3)
H9AA_14–C9A_14–H9AB_14	109.5	C6B_14–C1B_14–Al2_14	123.8(5)
C4A_14–C9A_14–H9AC_14	109.5	C3B_14–C2B_14–C1B_14	107.4(5)
H9AA_14–C9A_14–H9AC_14	109.5	C3B_14–C2B_14–C7B_14	125.3(7)
H9AB_14–C9A_14–H9AC_14	109.5	C1B_14–C2B_14–C7B_14	127.2(7)
C3A_14–C8A_14–H8AA_14	109.5	C3B_14–C2B_14–Al2_14	71.1(3)
C3A_14–C8A_14–H8AB_14	109.5	C1B_14–C2B_14–Al2_14	71.3(3)
H8AA_14–C8A_14–H8AB_14	109.5	C7B_14–C2B_14–Al2_14	123.3(5)
C3A_14–C8A_14–H8AC_14	109.5	C4B_14–C3B_14–C2B_14	108.7(5)
H8AA_14–C8A_14–H8AC_14	109.5	C4B_14–C3B_14–C8B_14	125.5(7)
H8AB_14–C8A_14–H8AC_14	109.5	C2B_14–C3B_14–C8B_14	125.8(7)
C2A_14–C7A_14–H7AA_14	109.5	C4B_14–C3B_14–Al2_14	71.3(3)
C2A_14–C7A_14–H7AB_14	109.5	C2B_14–C3B_14–Al2_14	72.1(3)
H7AA_14–C7A_14–H7AB_14	109.5	C8B_14–C3B_14–Al2_14	123.5(5)
C2A_14–C7A_14–H7AC_14	109.5	C3B_14–C4B_14–C5B_14	108.2(5)
H7AA_14–C7A_14–H7AC_14	109.5	C3B_14–C4B_14–C9B_14	127.0(6)
H7AB_14–C7A_14–H7AC_14	109.5	C5B_14–C4B_14–C9B_14	124.7(7)
C1A_14–C6A_14–H6AA_14	109.5	C3B_14–C4B_14–Al2_14	72.0(4)
C1A_14–C6A_14–H6AB_14	109.5	C5B_14–C4B_14–Al2_14	71.3(4)
H6AA_14–C6A_14–H6AB_14	109.5	C9B_14–C4B_14–Al2_14	126.4(5)
C1A_14–C6A_14–H6AC_14	109.5	C1B_14–C5B_14–C4B_14	107.8(5)
H6AA_14–C6A_14–H6AC_14	109.5	C1B_14–C5B_14–C10B_14	126.9(6)
H6AB_14–C6A_14–H6AC_14	109.5	C4B_14–C5B_14–C10B_14	125.0(6)
C5B_14–C1B_14–C2B_14	107.9(5)	C1B_14–C5B_14–Al2_14	72.3(4)

C4B_14–C5B_14–Al2_14	71.4(3)	C1B_14–C6B_14–H6BB_14	109.5
C10B_14–C5B_14–Al2_14	126.6(5)	H6BA_14–C6B_14–H6BB_14	109.5
C5B_14–C10B_14–H10D_14	109.5	C1B_14–C6B_14–H6BC_14	109.5
C5B_14–C10B_14–H10E_14	109.5	H6BA_14–C6B_14–H6BC_14	109.5
H10D_14–C10B_14–H10E_14	109.5	H6BB_14–C6B_14–H6BC_14	109.5
C5B_14–C10B_14–H10F_14	109.5	C5C_14–C1C_14–C2C_14	107.5(5)
H10D_14–C10B_14–H10F_14	109.5	C5C_14–C1C_14–C6C_14	127.8(6)
H10E_14–C10B_14–H10F_14	109.5	C2C_14–C1C_14–C6C_14	124.7(6)
C4B_14–C9B_14–H9BA_14	109.5	C5C_14–C1C_14–Al3_14	71.0(3)
C4B_14–C9B_14–H9BB_14	109.5	C2C_14–C1C_14–Al3_14	71.2(3)
H9BA_14–C9B_14–H9BB_14	109.5	C6C_14–C1C_14–Al3_14	124.8(5)
C4B_14–C9B_14–H9BC_14	109.5	C1C_14–C2C_14–C3C_14	108.4(5)
H9BA_14–C9B_14–H9BC_14	109.5	C1C_14–C2C_14–C7C_14	126.3(6)
H9BB_14–C9B_14–H9BC_14	109.5	C3C_14–C2C_14–C7C_14	125.3(6)
C3B_14–C8B_14–H8BA_14	109.5	C1C_14–C2C_14–Al3_14	71.5(3)
C3B_14–C8B_14–H8BB_14	109.5	C3C_14–C2C_14–Al3_14	71.3(3)
H8BA_14–C8B_14–H8BB_14	109.5	C7C_14–C2C_14–Al3_14	124.7(5)
C3B_14–C8B_14–H8BC_14	109.5	C4C_14–C3C_14–C2C_14	107.8(5)
H8BA_14–C8B_14–H8BC_14	109.5	C4C_14–C3C_14–C8C_14	126.8(6)
H8BB_14–C8B_14–H8BC_14	109.5	C2C_14–C3C_14–C8C_14	125.4(6)
C2B_14–C7B_14–H7BA_14	109.5	C4C_14–C3C_14–Al3_14	70.4(3)
C2B_14–C7B_14–H7BB_14	109.5	C2C_14–C3C_14–Al3_14	71.2(3)
H7BA_14–C7B_14–H7BB_14	109.5	C8C_14–C3C_14–Al3_14	123.3(5)
C2B_14–C7B_14–H7BC_14	109.5	C3C_14–C4C_14–C5C_14	107.9(5)
H7BA_14–C7B_14–H7BC_14	109.5	C3C_14–C4C_14–C9C_14	127.3(6)
H7BB_14–C7B_14–H7BC_14	109.5	C5C_14–C4C_14–C9C_14	124.8(6)
C1B_14–C6B_14–H6BA_14	109.5	C3C_14–C4C_14–Al3_14	72.3(4)

C5C_14–C4C_14–Al3_14	71.8(4)
C9C_14–C4C_14–Al3_14	123.8(5)
C1C_14–C5C_14–C4C_14	108.4(5)
C1C_14–C5C_14–C10C_14	126.5(6)
C4C_14–C5C_14–C10C_14	125.0(6)
C1C_14–C5C_14–Al3_14	71.7(4)
C4C_14–C5C_14–Al3_14	70.5(3)
C10C_14–C5C_14–Al3_14	126.8(6)
C5C_14–C10C_14–H10G_14	109.5
C5C_14–C10C_14–H10H_14	109.5
H10G_14–C10C_14–H10H_14	109.5
C5C_14–C10C_14–H10I_14	109.5
H10G_14–C10C_14–H10I_14	109.5
H10H_14–C10C_14–H10I_14	109.5
C4C_14–C9C_14–H9CA_14	109.5
C4C_14–C9C_14–H9CB_14	109.5
H9CA_14–C9C_14–H9CB_14	109.5
C4C_14–C9C_14–H9CC_14	109.5
H9CA_14–C9C_14–H9CC_14	109.5
H9CB_14–C9C_14–H9CC_14	109.5
C3C_14–C8C_14–H8CA_14	109.5
C3C_14–C8C_14–H8CB_14	109.5
H8CA_14–C8C_14–H8CB_14	109.5
C3C_14–C8C_14–H8CC_14	109.5
H8CA_14–C8C_14–H8CC_14	109.5
H8CB_14–C8C_14–H8CC_14	109.5
C2C_14–C7C_14–H7CA_14	109.5
C2C_14–C7C_14–H7CB_14	109.5
H7CA_14–C7C_14–H7CB_14	109.5
C2C_14–C7C_14–H7CC_14	109.5
H7CA_14–C7C_14–H7CC_14	109.5
H7CB_14–C7C_14–H7CC_14	109.5
C1C_14–C6C_14–H6CA_14	109.5
C1C_14–C6C_14–H6CB_14	109.5
H6CA_14–C6C_14–H6CB_14	109.5
C1C_14–C6C_14–H6CC_14	109.5
H6CA_14–C6C_14–H6CC_14	109.5
H6CB_14–C6C_14–H6CC_14	109.5
Al1_1–Tl1_1–Al2_1	68.5(4)
Al1_1–Tl1_1–Al3_1	67.3(3)
Al2_1–Tl1_1–Al3_1	68.4(6)
C1B_1–Al2_1–C5B_1	37.7(4)
C1B_1–Al2_1–C2B_1	37.0(4)
C5B_1–Al2_1–C2B_1	62.6(6)
C1B_1–Al2_1–C4B_1	62.4(7)
C5B_1–Al2_1–C4B_1	37.2(4)
C2B_1–Al2_1–C4B_1	62.7(6)
C1B_1–Al2_1–C3B_1	61.2(7)
C5B_1–Al2_1–C3B_1	61.4(6)
C2B_1–Al2_1–C3B_1	37.1(4)
C4B_1–Al2_1–C3B_1	36.8(4)
C1B_1–Al2_1–Tl1_1	137.1(11)
C5B_1–Al2_1–Tl1_1	167.3(10)
C2B_1–Al2_1–Tl1_1	121.0(10)
C4B_1–Al2_1–Tl1_1	155.3(10)
C3B_1–Al2_1–Tl1_1	129.7(9)
C3C_1–Al3_1–C2C_1	37.1(4)
C3C_1–Al3_1–C4C_1	37.1(5)
C2C_1–Al3_1–C4C_1	62.2(6)
C3C_1–Al3_1–C5C_1	61.5(6)
C2C_1–Al3_1–C5C_1	61.9(6)
C4C_1–Al3_1–C5C_1	36.8(4)
C3C_1–Al3_1–C1C_1	61.1(7)
C2C_1–Al3_1–C1C_1	36.9(4)
C4C_1–Al3_1–C1C_1	61.1(6)
C5C_1–Al3_1–C1C_1	36.4(4)
C3C_1–Al3_1–Tl1_1	136.7(9)
C2C_1–Al3_1–Tl1_1	117.0(9)
C4C_1–Al3_1–Tl1_1	171.0(9)
C5C_1–Al3_1–Tl1_1	151.8(9)
C1C_1–Al3_1–Tl1_1	124.4(9)

C2A_1–Al1_1–C3A_1	36.5(4)
C2A_1–Al1_1–C1A_1	36.7(4)
C3A_1–Al1_1–C1A_1	61.2(6)
C2A_1–Al1_1–C4A_1	60.5(6)
C3A_1–Al1_1–C4A_1	36.4(4)
C1A_1–Al1_1–C4A_1	60.8(6)
C2A_1–Al1_1–C5A_1	60.4(6)
C3A_1–Al1_1–C5A_1	60.7(6)
C1A_1–Al1_1–C5A_1	36.1(4)
C4A_1–Al1_1–C5A_1	36.4(4)
C2A_1–Al1_1–Tl1_1	159.8(8)
C3A_1–Al1_1–Tl1_1	126.3(7)
C1A_1–Al1_1–Tl1_1	159.8(8)
C4A_1–Al1_1–Tl1_1	112.5(7)
C5A_1–Al1_1–Tl1_1	126.8(8)
C5A_1–C1A_1–C2A_1	107.3(11)
C5A_1–C1A_1–C6A_1	127.9(19)
C2A_1–C1A_1–C6A_1	124.7(19)
C5A_1–C1A_1–Al1_1	72.5(7)
C2A_1–C1A_1–Al1_1	71.2(7)
C6A_1–C1A_1–Al1_1	119.6(18)
C3A_1–C2A_1–C1A_1	108.7(12)
C3A_1–C2A_1–C7A_1	127.7(18)
C1A_1–C2A_1–C7A_1	123.4(18)
C3A_1–C2A_1–Al1_1	72.0(7)
C1A_1–C2A_1–Al1_1	72.1(7)
C7A_1–C2A_1–Al1_1	126(2)
C2A_1–C3A_1–C4A_1	107.7(12)
C2A_1–C3A_1–C8A_1	127.3(19)
C4A_1–C3A_1–C8A_1	125.0(18)
C2A_1–C3A_1–Al1_1	71.5(7)
C4A_1–C3A_1–Al1_1	72.5(7)
C8A_1–C3A_1–Al1_1	121.3(18)
C3A_1–C4A_1–C5A_1	107.8(11)
C3A_1–C4A_1–C9A_1	123.7(18)
C5A_1–C4A_1–C9A_1	128.5(19)
C3A_1–C4A_1–Al1_1	71.1(7)
C5A_1–C4A_1–Al1_1	71.8(7)
C9A_1–C4A_1–Al1_1	123.7(18)
C1A_1–C5A_1–C4A_1	108.6(12)
C1A_1–C5A_1–C10A_1	127.1(18)
C4A_1–C5A_1–C10A_1	124.3(18)
C1A_1–C5A_1–Al1_1	71.4(7)
C4A_1–C5A_1–Al1_1	71.8(7)
C10A_1–C5A_1–Al1_1	122.9(18)
C5A_1–C10A_1–H10A_1	109.5
C5A_1–C10A_1–H10B_1	109.5
H10A_1–C10A_1–H10B_1	109.5
C5A_1–C10A_1–H10C_1	109.5
H10A_1–C10A_1–H10C_1	109.5
H10B_1–C10A_1–H10C_1	109.5
C4A_1–C9A_1–H9AA_1	109.5
C4A_1–C9A_1–H9AB_1	109.5
H9AA_1–C9A_1–H9AB_1	109.5
C4A_1–C9A_1–H9AC_1	109.5
H9AA_1–C9A_1–H9AC_1	109.5
H9AB_1–C9A_1–H9AC_1	109.5
C3A_1–C8A_1–H8AA_1	109.5
C3A_1–C8A_1–H8AB_1	109.5
H8AA_1–C8A_1–H8AB_1	109.5
C3A_1–C8A_1–H8AC_1	109.5
H8AA_1–C8A_1–H8AC_1	109.5
H8AB_1–C8A_1–H8AC_1	109.5
C2A_1–C7A_1–H7AA_1	109.5
C2A_1–C7A_1–H7AB_1	109.5
H7AA_1–C7A_1–H7AB_1	109.5
C2A_1–C7A_1–H7AC_1	109.5
H7AA_1–C7A_1–H7AC_1	109.5
H7AB_1–C7A_1–H7AC_1	109.5
C1A_1–C6A_1–H6AA_1	109.5
C1A_1–C6A_1–H6AB_1	109.5
H6AA_1–C6A_1–H6AB_1	109.5
C1A_1–C6A_1–H6AC_1	109.5
H6AA_1–C6A_1–H6AC_1	109.5
H6AB_1–C6A_1–H6AC_1	109.5
C2B_1–C1B_1–C5B_1	108.8(12)
C2B_1–C1B_1–C6B_1	129.4(19)
C5B_1–C1B_1–C6B_1	121.8(18)
C2B_1–C1B_1–Al2_1	72.1(7)
C5B_1–C1B_1–Al2_1	71.2(7)

C6B_1–C1B_1–Al2_1	123(2)
C1B_1–C2B_1–C3B_1	106.4(12)
C1B_1–C2B_1–C7B_1	126.7(19)
C3B_1–C2B_1–C7B_1	126.8(19)
C1B_1–C2B_1–Al2_1	70.9(7)
C3B_1–C2B_1–Al2_1	72.0(7)
C7B_1–C2B_1–Al2_1	125(2)
C4B_1–C3B_1–C2B_1	109.8(12)
C4B_1–C3B_1–C8B_1	127.9(19)
C2B_1–C3B_1–C8B_1	122.2(19)
C4B_1–C3B_1–Al2_1	71.0(7)
C2B_1–C3B_1–Al2_1	70.9(7)
C8B_1–C3B_1–Al2_1	122(2)
C3B_1–C4B_1–C5B_1	107.0(12)
C3B_1–C4B_1–C9B_1	125.4(19)
C5B_1–C4B_1–C9B_1	127.6(19)
C3B_1–C4B_1–Al2_1	72.2(7)
C5B_1–C4B_1–Al2_1	70.9(7)
C9B_1–C4B_1–Al2_1	123(2)
C4B_1–C5B_1–C1B_1	107.8(12)
C4B_1–C5B_1–C10B_1	126.1(18)
C1B_1–C5B_1–C10B_1	126.0(18)
C4B_1–C5B_1–Al2_1	72.0(7)
C1B_1–C5B_1–Al2_1	71.1(7)
C10B_1–C5B_1–Al2_1	124(2)
C5B_1–C10B_1–H10D_1	109.5
C5B_1–C10B_1–H10E_1	109.5
H10D_1–C10B_1–H10E_1	109.5
C5B_1–C10B_1–H10F_1	109.5
H10D_1–C10B_1–H10F_1	109.5
H10E_1–C10B_1–H10F_1	109.5
C4B_1–C9B_1–H9BA_1	109.5
C4B_1–C9B_1–H9BB_1	109.5
H9BA_1–C9B_1–H9BB_1	109.5
C4B_1–C9B_1–H9BC_1	109.5
H9BA_1–C9B_1–H9BC_1	109.5
H9BB_1–C9B_1–H9BC_1	109.5
C3B_1–C8B_1–H8BA_1	109.5
C3B_1–C8B_1–H8BB_1	109.5
H8BA_1–C8B_1–H8BB_1	109.5
C3B_1–C8B_1–H8BC_1	109.5
H8BA_1–C8B_1–H8BC_1	109.5
H8BB_1–C8B_1–H8BC_1	109.5
C2B_1–C7B_1–H7BA_1	109.5
C2B_1–C7B_1–H7BB_1	109.5
H7BA_1–C7B_1–H7BB_1	109.5
C2B_1–C7B_1–H7BC_1	109.5
H7BA_1–C7B_1–H7BC_1	109.5
H7BB_1–C7B_1–H7BC_1	109.5
C1B_1–C6B_1–H6BA_1	109.5
C1B_1–C6B_1–H6BB_1	109.5
H6BA_1–C6B_1–H6BB_1	109.5
C1B_1–C6B_1–H6BC_1	109.5
H6BA_1–C6B_1–H6BC_1	109.5
H6BB_1–C6B_1–H6BC_1	109.5
C5C_1–C1C_1–C2C_1	108.8(12)
C5C_1–C1C_1–C6C_1	128(2)
C2C_1–C1C_1–C6C_1	123.4(19)
C5C_1–C1C_1–Al3_1	71.6(7)
C2C_1–C1C_1–Al3_1	70.0(7)
C6C_1–C1C_1–Al3_1	123(2)
C3C_1–C2C_1–C1C_1	106.9(12)
C3C_1–C2C_1–C7C_1	127(2)
C1C_1–C2C_1–C7C_1	126(2)
C3C_1–C2C_1–Al3_1	71.3(7)
C1C_1–C2C_1–Al3_1	73.1(7)
C7C_1–C2C_1–Al3_1	124(2)
C2C_1–C3C_1–C4C_1	108.9(12)
C2C_1–C3C_1–C8C_1	128.1(19)
C4C_1–C3C_1–C8C_1	121.9(19)
C2C_1–C3C_1–Al3_1	71.5(7)
C4C_1–C3C_1–Al3_1	72.2(7)
C8C_1–C3C_1–Al3_1	131(2)
C3C_1–C4C_1–C5C_1	107.5(12)
C3C_1–C4C_1–C9C_1	125.9(19)
C5C_1–C4C_1–C9C_1	126.5(19)
C3C_1–C4C_1–Al3_1	70.8(7)
C5C_1–C4C_1–Al3_1	72.3(7)
C9C_1–C4C_1–Al3_1	122(2)
C1C_1–C5C_1–C4C_1	107.8(12)
C1C_1–C5C_1–C10C_1	127(2)
C4C_1–C5C_1–C10C_1	125.1(19)
C1C_1–C5C_1–Al3_1	72.0(7)
C4C_1–C5C_1–Al3_1	70.8(7)
C10C_1–C5C_1–Al3_1	122(2)
C5C_1–C10C_1–H10G_1	109.5

C5C_1–C10C_1–H10H_1	109.5
H10G_1–C10C_1–H10H_1	109.5
C5C_1–C10C_1–H10I_1	109.5
H10G_1–C10C_1–H10I_1	109.5
H10H_1–C10C_1–H10I_1	109.5
C4C_1–C9C_1–H9CA_1	109.5
C4C_1–C9C_1–H9CB_1	109.5
H9CA_1–C9C_1–H9CB_1	109.5
C4C_1–C9C_1–H9CC_1	109.5
H9CA_1–C9C_1–H9CC_1	109.5
H9CB_1–C9C_1–H9CC_1	109.5
C3C_1–C8C_1–H8CA_1	109.5
C3C_1–C8C_1–H8CB_1	109.5
H8CA_1–C8C_1–H8CB_1	109.5
C3C_1–C8C_1–H8CC_1	109.5
H8CA_1–C8C_1–H8CC_1	109.5
H8CB_1–C8C_1–H8CC_1	109.5
C2C_1–C7C_1–H7CA_1	109.5
C2C_1–C7C_1–H7CB_1	109.5
H7CA_1–C7C_1–H7CB_1	109.5
C2C_1–C7C_1–H7CC_1	109.5
H7CA_1–C7C_1–H7CC_1	109.5
H7CB_1–C7C_1–H7CC_1	109.5
C1C_1–C6C_1–H6CA_1	109.5
C1C_1–C6C_1–H6CB_1	109.5
H6CA_1–C6C_1–H6CB_1	109.5
C1C_1–C6C_1–H6CC_1	109.5
H6CA_1–C6C_1–H6CC_1	109.5
H6CB_1–C6C_1–H6CC_1	109.5
C1_2–O1_2–Al12	152(3)
O1_2–C1_2–C4_2	109.4(17)
O1_2–C1_2–C3_2	112.0(17)
C4_2–C1_2–C3_2	114.1(13)
O1_2–C1_2–C2_2	106.0(16)
C4_2–C1_2–C2_2	108.1(12)
C3_2–C1_2–C2_2	106.9(12)
F1_2–C2_2–F3_2	105.2(17)
F1_2–C2_2–F2_2	112.7(18)
F3_2–C2_2–F2_2	108.7(17)
F1_2–C2_2–C1_2	113.9(16)
F3_2–C2_2–C1_2	106.9(15)
F2_2–C2_2–C1_2	109.1(15)
F6_2–C3_2–F4_2	106.9(17)
F6_2–C3_2–F5_2	108.5(18)
F4_2–C3_2–F5_2	106.5(18)
F6_2–C3_2–C1_2	111.6(16)
F4_2–C3_2–C1_2	114.6(17)
F5_2–C3_2–C1_2	108.6(16)
F9_2–C4_2–F7_2	111.4(18)
F9_2–C4_2–F8_2	108.2(18)
F7_2–C4_2–F8_2	106.9(18)
F9_2–C4_2–C1_2	111.9(17)
F7_2–C4_2–C1_2	108.4(15)
F8_2–C4_2–C1_2	109.9(16)
C1_3–O1_3–Al14	149(2)
O1_3–C1_3–C4_3	117.8(17)
O1_3–C1_3–C3_3	107.8(16)
C4_3–C1_3–C3_3	108.7(13)
O1_3–C1_3–C2_3	107.4(16)
C4_3–C1_3–C2_3	104.7(13)
C3_3–C1_3–C2_3	110.2(14)
F2_3–C2_3–F3_3	105.4(18)
F2_3–C2_3–F1_3	105.1(19)
F3_3–C2_3–F1_3	109.9(19)
F2_3–C2_3–C1_3	116.1(18)
F3_3–C2_3–C1_3	111.2(17)
F1_3–C2_3–C1_3	108.9(17)
F6_3–C3_3–F5_3	111.0(19)
F6_3–C3_3–F4_3	104.2(18)
F5_3–C3_3–F4_3	107.4(19)
F6_3–C3_3–C1_3	111.4(16)
F5_3–C3_3–C1_3	108.8(15)
F4_3–C3_3–C1_3	113.9(18)
F9_3–C4_3–F7_3	106.8(18)
F9_3–C4_3–F8_3	106.5(19)
F7_3–C4_3–F8_3	106.2(19)
F9_3–C4_3–C1_3	118.0(17)
F7_3–C4_3–C1_3	115.5(17)
F8_3–C4_3–C1_3	102.7(15)
C1_15–O1_15–Al14	151.9(18)
O1_15–C1_15–C3_15	109.3(14)
O1_15–C1_15–C2_15	108.0(13)
C3_15–C1_15–C2_15	110.5(12)
O1_15–C1_15–C4_15	112.3(14)
C3_15–C1_15–C4_15	108.8(12)
C2_15–C1_15–C4_15	108.0(12)
F1_15–C2_15–F3_15	111.1(17)
F1_15–C2_15–F2_15	109.0(17)
F3_15–C2_15–F2_15	106.6(17)
F1_15–C2_15–C1_15	108.4(13)
F3_15–C2_15–C1_15	111.7(14)
F2_15–C2_15–C1_15	109.9(14)
F4_15–C3_15–F5_15	112.9(18)

F4_15–C3_15–F6_15	104.0(16)	F7_53–C4_53–F8_53	108.6(17)
F5_15–C3_15–F6_15	108.2(18)	F7_53–C4_53–F9_53	115.2(17)
F4_15–C3_15–C1_15	111.3(14)	F8_53–C4_53–F9_53	104.5(15)
F5_15–C3_15–C1_15	109.4(16)	F7_53–C4_53–C1_53	109.4(15)
F6_15–C3_15–C1_15	110.9(15)	F8_53–C4_53–C1_53	110.4(15)
F9_15–C4_15–F7_15	110.0(17)	F9_53–C4_53–C1_53	108.5(14)
F9_15–C4_15–F8_15	109.7(17)	C1_54–O1_54–Al11	147(2)
F7_15–C4_15–F8_15	109.3(17)	O1_54–C1_54–C2_54	117.6(17)
F9_15–C4_15–C1_15	109.1(14)	O1_54–C1_54–C3_54	111.8(16)
F7_15–C4_15–C1_15	108.2(13)	C2_54–C1_54–C3_54	108.2(14)
F8_15–C4_15–C1_15	110.5(15)	O1_54–C1_54–C4_54	102.5(16)
C1_51–O1_51–Al13	156.3(19)	C2_54–C1_54–C4_54	108.0(14)
O1_51–C1_51–C4_51	111.5(14)	C3_54–C1_54–C4_54	108.2(14)
O1_51–C1_51–C2_51	112.0(14)	F3_54–C2_54–F1_54	109(2)
C4_51–C1_51–C2_51	111.3(11)	F3_54–C2_54–F2_54	107.2(19)
O1_51–C1_51–C3_51	106.5(13)	F1_54–C2_54–F2_54	106.8(19)
C4_51–C1_51–C3_51	107.4(11)	F3_54–C2_54–C1_54	111.3(18)
C2_51–C1_51–C3_51	107.8(11)	F1_54–C2_54–C1_54	113.3(17)
F3_51–C2_51–F1_51	104.1(14)	F2_54–C2_54–C1_54	109.3(17)
F3_51–C2_51–F2_51	113.7(16)	F5_54–C3_54–F6_54	108(2)
F1_51–C2_51–F2_51	108.2(15)	F5_54–C3_54–F4_54	109.4(19)
F3_51–C2_51–C1_51	109.8(13)	F6_54–C3_54–F4_54	106(2)
F1_51–C2_51–C1_51	114.1(14)	F5_54–C3_54–C1_54	107.6(16)
F2_51–C2_51–C1_51	107.1(13)	F6_54–C3_54–C1_54	110.3(18)
F5_51–C3_51–F6_51	110.4(16)	F4_54–C3_54–C1_54	114.7(18)
F5_51–C3_51–F4_51	105.8(15)	C3_54–F4_54–F5_33	147(3)
F6_51–C3_51–F4_51	107.6(15)	F8_54–C4_54–F7_54	112(2)
F5_51–C3_51–C1_51	111.7(14)	F8_54–C4_54–F9_54	113(2)
F6_51–C3_51–C1_51	112.1(13)	F7_54–C4_54–F9_54	110(2)
F4_51–C3_51–C1_51	109.0(13)	F8_54–C4_54–C1_54	111.3(18)
F8_51–C4_51–F9_51	110.8(15)	F7_54–C4_54–C1_54	105.8(17)
F8_51–C4_51–F7_51	105.3(15)	F9_54–C4_54–C1_54	104.2(17)
F9_51–C4_51–F7_51	107.0(15)	C1_55–O1_55–Al12	148.6(10)
F8_51–C4_51–C1_51	112.3(13)	O1_55–C1_55–C3_55	112.6(10)
F9_51–C4_51–C1_51	110.7(13)	O1_55–C1_55–C4_55	107.2(10)
F7_51–C4_51–C1_51	110.5(13)	C3_55–C1_55–C4_55	107.5(10)
C1_53–O1_53–Al14	152(3)	O1_55–C1_55–C2_55	106.8(9)
O1_53–C1_53–C3_53	111.9(17)	C3_55–C1_55–C2_55	110.1(9)
O1_53–C1_53–C2_53	109.4(18)	C4_55–C1_55–C2_55	112.7(10)
C3_53–C1_53–C2_53	109.4(12)	F2_55–C2_55–F3_55	110.4(13)
O1_53–C1_53–C4_53	107.4(17)	F2_55–C2_55–F1_55	107.3(11)
C3_53–C1_53–C4_53	112.2(12)	F3_55–C2_55–F1_55	107.5(12)
C2_53–C1_53–C4_53	106.4(12)	F2_55–C2_55–C1_55	110.7(10)
F3_53–C2_53–F2_53	108.6(17)	F3_55–C2_55–C1_55	110.2(10)
F3_53–C2_53–F1_53	110.0(17)	F1_55–C2_55–C1_55	110.7(11)
F2_53–C2_53–F1_53	110.1(17)	F4_55–C3_55–F5_55	109.8(12)
F3_53–C2_53–C1_53	110.4(15)	F4_55–C3_55–F6_55	107.7(13)
F2_53–C2_53–C1_53	109.7(14)	F5_55–C3_55–F6_55	105.5(12)
F1_53–C2_53–C1_53	107.9(15)	F4_55–C3_55–C1_55	107.8(10)
F4_53–C3_53–F6_53	108.2(17)	F5_55–C3_55–C1_55	113.4(11)
F4_53–C3_53–F5_53	108.9(16)	F6_55–C3_55–C1_55	112.5(13)
F6_53–C3_53–F5_53	107.4(17)	F8_55–C4_55–F9_55	109.2(12)
F4_53–C3_53–C1_53	109.2(15)	F8_55–C4_55–F7_55	108.1(11)
F6_53–C3_53–C1_53	112.5(17)	F9_55–C4_55–F7_55	106.2(13)
F5_53–C3_53–C1_53	110.6(14)	F8_55–C4_55–C1_55	111.3(12)

F9_55–C4_55–C1_55	109.5(12)	C1_57–C5_57–Al1	73.7(14)
F7_55–C4_55–C1_55	112.4(12)	C6_57–C5_57–Al1	119(2)
C1_56–O1_56–Al12	168(4)	C5_57–C6_57–H6A_57	109.5
O1_56–C1_56–C2_56	108.8(19)	C5_57–C6_57–H6B_57	109.5
O1_56–C1_56–C3_56	108.9(19)	H6A_57–C6_57–H6B_57	109.5
C2_56–C1_56–C3_56	110.7(15)		
O1_56–C1_56–C4_56	106.2(18)	C5_57–C6_57–H6C_57	109.5
C2_56–C1_56–C4_56	112.8(16)	H6A_57–C6_57–H6C_57	109.5
C3_56–C1_56–C4_56	109.4(15)		
F1_56–C2_56–F2_56	108(2)	H6B_57–C6_57–H6C_57	109.5
F1_56–C2_56–F3_56	108(2)		
F2_56–C2_56–F3_56	106(2)	C4_57–C7_57–H7A_57	109.5
F1_56–C2_56–C1_56	111.7(19)	C4_57–C7_57–H7B_57	109.5
F2_56–C2_56–C1_56	113.1(19)	H7A_57–C7_57–H7B_57	109.5
F3_56–C2_56–C1_56	110.7(19)		
F5_56–C3_56–F6_56	109(2)	C4_57–C7_57–H7C_57	109.5
F5_56–C3_56–F4_56	109(2)	H7A_57–C7_57–H7C_57	109.5
F6_56–C3_56–F4_56	107(2)		
F5_56–C3_56–C1_56	108.9(18)	H7B_57–C7_57–H7C_57	109.5
F6_56–C3_56–C1_56	112(2)		
F4_56–C3_56–C1_56	111.6(19)	C3_57–C8_57–H8A_57	109.5
F8_56–C4_56–F7_56	106(2)	C3_57–C8_57–H8B_57	109.5
F8_56–C4_56–F9_56	109(2)	H8A_57–C8_57–H8B_57	109.5
F7_56–C4_56–F9_56	109(2)		
F8_56–C4_56–C1_56	114(2)	C3_57–C8_57–H8C_57	109.5
F7_56–C4_56–C1_56	110.8(19)	H8A_57–C8_57–H8C_57	109.5
F9_56–C4_56–C1_56	107.8(19)		
C5_57–C1_57–C2_57	107.8(12)	H8B_57–C8_57–H8C_57	109.5
C5_57–C1_57–C10_57	128.6(18)		
C2_57–C1_57–C10_57	123.6(17)	C2_57–C9_57–H9A_57	109.5
C5_57–C1_57–Al1	69.6(15)	C2_57–C9_57–H9B_57	109.5
C2_57–C1_57–Al1	77.2(9)	H9A_57–C9_57–H9B_57	109.5
C10_57–C1_57–Al1	120.0(17)		
C3_57–C2_57–C1_57	108.4(12)	C2_57–C9_57–H9C_57	109.5
C3_57–C2_57–C9_57	125.0(17)	H9A_57–C9_57–H9C_57	109.5
C1_57–C2_57–C9_57	126.6(17)		
C3_57–C2_57–Al1	74.5(9)	H9B_57–C9_57–H9C_57	109.5
C1_57–C2_57–Al1	67.7(9)		
C9_57–C2_57–Al1	126.3(16)	C1_57–C10_57–H10A_57	109.5
C2_57–C3_57–C4_57	107.7(12)		
C2_57–C3_57–C8_57	127.0(17)	C1_57–C10_57–H10B_57	109.5
C4_57–C3_57–C8_57	125.3(17)		
C2_57–C3_57–Al1	71.6(9)	H10A_57–C10_57–H10B_57	109.5
C4_57–C3_57–Al1	68.2(14)		
C8_57–C3_57–Al1	125.3(15)	C1_57–C10_57–H10C_57	109.5
C5_57–C4_57–C3_57	108.2(11)		
C5_57–C4_57–C7_57	126.0(17)	H10A_57–C10_57–H10C_57	109.5
C3_57–C4_57–C7_57	125.7(17)		
C5_57–C4_57–Al1	68.1(17)	H10B_57–C10_57–H10C_57	109.5
C3_57–C4_57–Al1	77.2(13)		
C7_57–C4_57–Al1	122(2)	C1_58–O1_58–Al13	140.9(16)
C4_57–C5_57–C1_57	108.0(12)	O1_58–C1_58–C4_58	115.6(14)
C4_57–C5_57–C6_57	126.3(17)	O1_58–C1_58–C2_58	106.5(13)
C1_57–C5_57–C6_57	125.6(17)	C4_58–C1_58–C2_58	109.5(12)
C4_57–C5_57–Al1	75.7(17)	O1_58–C1_58–C3_58	104.7(12)

C4_58–C1_58–C3_58	110.9(12)	F1_60–C2_60–C1_60	109.0(16)
C2_58–C1_58–C3_58	109.4(12)	F3_60–C2_60–C1_60	107.7(14)
F2_58–C2_58–F3_58	107.2(17)	F2_60–C2_60–C1_60	111.1(17)
F2_58–C2_58–F1_58	106.6(18)	F6_60–C3_60–F5_60	117.9(19)
F3_58–C2_58–F1_58	107.1(17)	F6_60–C3_60–F4_60	104.5(18)
F2_58–C2_58–C1_58	112.8(17)	F5_60–C3_60–F4_60	105.6(17)
F3_58–C2_58–C1_58	113.6(15)	F6_60–C3_60–C1_60	109.2(15)
F1_58–C2_58–C1_58	109.1(15)	F5_60–C3_60–C1_60	110.7(15)
F4_58–C3_58–F5_58	109.7(16)	F4_60–C3_60–C1_60	108.4(14)
F4_58–C3_58–F6_58	109.1(16)	F7_60–C4_60–F8_60	101.9(17)
F5_58–C3_58–F6_58	104.9(16)	F7_60–C4_60–F9_60	110.8(19)
F4_58–C3_58–C1_58	108.3(14)	F8_60–C4_60–F9_60	113.3(18)
F5_58–C3_58–C1_58	109.0(13)	F7_60–C4_60–C1_60	110.2(17)
F6_58–C3_58–C1_58	115.8(15)	F8_60–C4_60–C1_60	109.0(15)
F7_58–C4_58–F9_58	107.8(16)	F9_60–C4_60–C1_60	111.3(16)
F7_58–C4_58–F8_58	100.7(16)	C1_61–O1_61–Al14	140(3)
F9_58–C4_58–F8_58	108.9(16)	O1_61–C1_61–C2_61	106.5(16)
F7_58–C4_58–C1_58	112.6(15)	O1_61–C1_61–C3_61	110.9(17)
F9_58–C4_58–C1_58	118.8(14)	C2_61–C1_61–C3_61	108.1(12)
F8_58–C4_58–C1_58	106.5(14)	O1_61–C1_61–C4_61	110.7(17)
C1_59–O1_59–Al10	154(3)	C2_61–C1_61–C4_61	112.3(12)
O1_59–C1_59–C2_59	110.7(17)	C3_61–C1_61–C4_61	108.3(12)
O1_59–C1_59–C3_59	109.6(16)	F1_61–C2_61–F2_61	117.5(18)
C2_59–C1_59–C3_59	108.2(11)	F1_61–C2_61–F3_61	97.1(16)
O1_59–C1_59–C4_59	109.7(17)	F2_61–C2_61–F3_61	107.5(17)
C2_59–C1_59–C4_59	109.0(12)	F1_61–C2_61–C1_61	108.4(14)
C3_59–C1_59–C4_59	109.6(12)	F2_61–C2_61–C1_61	111.7(14)
F1_59–C2_59–F3_59	105.3(16)	F3_61–C2_61–C1_61	114.1(15)
F1_59–C2_59–F2_59	107.9(17)	F5_61–C3_61–F6_61	108.5(16)
F3_59–C2_59–F2_59	106.8(16)	F5_61–C3_61–F4_61	108.8(17)
F1_59–C2_59–C1_59	111.0(13)	F6_61–C3_61–F4_61	112.2(17)
F3_59–C2_59–C1_59	114.2(15)	F5_61–C3_61–C1_61	107.2(14)
F2_59–C2_59–C1_59	111.3(15)	F6_61–C3_61–C1_61	113.6(15)
F5_59–C3_59–F6_59	108.2(17)	F4_61–C3_61–C1_61	106.4(14)
F5_59–C3_59–F4_59	109.1(16)	F8_61–C4_61–F9_61	104.5(16)
F6_59–C3_59–F4_59	108.9(17)	F8_61–C4_61–F7_61	102.8(17)
F5_59–C3_59–C1_59	110.5(13)	F9_61–C4_61–F7_61	115.4(17)
F6_59–C3_59–C1_59	111.2(16)	F8_61–C4_61–C1_61	112.6(16)
F4_59–C3_59–C1_59	108.9(13)	F9_61–C4_61–C1_61	111.4(14)
F7_59–C4_59–F9_59	104.4(16)	F7_61–C4_61–C1_61	109.8(15)
F7_59–C4_59–F8_59	106.1(16)	C1_62–O1_62–Al12	151.4(11)
F9_59–C4_59–F8_59	109.7(16)	O1_62–C1_62–C3_62	112.1(10)
F7_59–C4_59–C1_59	113.5(14)	O1_62–C1_62–C4_62	107.2(10)
F9_59–C4_59–C1_59	109.7(13)	C3_62–C1_62–C4_62	109.5(10)
F8_59–C4_59–C1_59	113.0(15)	O1_62–C1_62–C2_62	109.4(10)
C1_60–O1_60–Al13	150(3)	C3_62–C1_62–C2_62	110.0(10)
O1_60–C1_60–C4_60	110.8(17)	C4_62–C1_62–C2_62	108.5(9)
O1_60–C1_60–C2_60	113.1(16)	F3_62–C2_62–F1_62	104.8(14)
C4_60–C1_60–C2_60	109.1(12)	F3_62–C2_62–F2_62	108.8(12)
O1_60–C1_60–C3_60	107.7(16)	F1_62–C2_62–F2_62	108.4(14)
C4_60–C1_60–C3_60	108.1(12)	F3_62–C2_62–C1_62	112.0(11)
C2_60–C1_60–C3_60	107.9(12)	F1_62–C2_62–C1_62	110.3(13)
F1_60–C2_60–F3_60	116.0(19)	F2_62–C2_62–C1_62	112.3(11)
F1_60–C2_60–F2_60	106.0(18)	F6_62–C3_62–F5_62	103.9(12)
F3_60–C2_60–F2_60	107.1(19)	F6_62–C3_62–F4_62	107.9(13)

F5_62–C3_62–F4_62	109.3(13)
F6_62–C3_62–C1_62	115.2(12)
F5_62–C3_62–C1_62	109.9(11)
F4_62–C3_62–C1_62	110.3(11)
F9_62–C4_62–F7_62	108.4(11)
F9_62–C4_62–F8_62	104.3(11)
F7_62–C4_62–F8_62	106.5(11)
F9_62–C4_62–C1_62	113.2(10)
F7_62–C4_62–C1_62	112.3(10)
F8_62–C4_62–C1_62	111.6(10)

S-Table 11: Bond lengths and angles for **4**

Atom–Atom	Length [Å]
Al1–N2	2.1420(16)
Al1–N3	2.1518(15)
Al1–N1	2.1650(15)
Al1–Al4	2.7553(12)
Al1–Al3	2.7598(10)
Al1–Al2	2.7800(10)
Al2–C4_6	2.3148(18)
Al2–C5_6	2.3262(17)
Al2–C3_6	2.3569(17)
Al2–C1_6	2.3747(17)
Al2–C2_6	2.3904(17)
Al2–Al4	2.7356(9)
Al2–Al3	2.7895(8)
Al3–C5_5	2.2795(17)
Al3–C4_5	2.3006(18)
Al3–C1_5	2.3747(17)
Al3–C3_5	2.4208(18)
Al3–C2_5	2.4680(18)
Al3–Al4	2.7358(9)
Al4–C4_7	2.3128(18)
Al4–C3_7	2.3570(17)
Al4–C5_7	2.3807(17)
Al4–C2_7	2.4528(17)
Al4–C1_7	2.4691(18)
Al5–O1_4	1.7207(13)
Al5–O1_1	1.7263(12)
Al5–O1_2	1.7269(12)
Al5–O1_3	1.7269(13)
N1–C1	1.482(2)
N1–C2	1.490(2)
N1–C9	1.493(2)
N2–C4	1.484(2)
N2–C5	1.485(2)
N2–C3	1.491(2)
N3–C7	1.480(2)
N3–C8	1.488(2)
N3–C6	1.494(2)
C1–H1A	0.9800
C1–H1B	0.9800
C1–H1C	0.9800
C2–C3	1.512(2)
C2–H2A	0.9900
C2–H2B	0.9900
C3–H3A	0.9900
C3–H3B	0.9900
C4–H4A	0.9800
C4–H4B	0.9800
C4–H4C	0.9800
C5–C6	1.517(3)
C5–H5A	0.9900
C5–H5B	0.9900
C6–H6A	0.9900
C6–H6B	0.9900
C7–H7A	0.9800
C7–H7B	0.9800
C7–H7C	0.9800
C8–C9	1.516(3)
C8–H8A	0.9900
C8–H8B	0.9900
C9–H9A	0.9900
C9–H9B	0.9900
O1_1–C1_1	1.3495(19)
C1_1–C3_1	1.554(2)
C1_1–C2_1	1.554(2)
C1_1–C4_1	1.555(2)
C2_1–F1_1	1.330(2)
C2_1–F3_1	1.336(2)
C2_1–F2_1	1.340(2)
C3_1–F4_1	1.324(2)
C3_1–F5_1	1.336(2)
C3_1–F6_1	1.344(2)
C4_1–F9_1	1.325(2)
C4_1–F7_1	1.338(2)
C4_1–F8_1	1.340(2)
O1_2–C1_2	1.3517(19)
C1_2–C3_2	1.550(2)
C1_2–C2_2	1.555(2)
C1_2–C4_2	1.559(2)
C2_2–F3_2	1.329(2)
C2_2–F1_2	1.332(2)
C2_2–F2_2	1.343(2)
C3_2–F4_2	1.330(2)
C3_2–F5_2	1.337(2)
C3_2–F6_2	1.340(2)
C4_2–F9_2	1.324(2)
C4_2–F7_2	1.331(2)
C4_2–F8_2	1.3458(19)
O1_3–C1_3	1.350(2)
C1_3–C3_3	1.546(3)
C1_3–C2_3	1.550(3)
C1_3–C4_3	1.556(3)
C2_3–F3_3	1.327(2)
C2_3–F1_3	1.327(2)
C2_3–F2_3	1.346(2)
C3_3–F4_3	1.328(3)
C3_3–F6_3	1.334(2)
C3_3–F5_3	1.342(3)
C4_3–F7_3	1.326(3)
C4_3–F9_3	1.329(3)
C4_3–F8_3	1.334(2)
O1_4–C1_4	1.353(2)
C1_4–C3_4	1.550(2)
C1_4–C2_4	1.554(2)
C1_4–C4_4	1.555(3)
C2_4–F3_4	1.325(2)
C2_4–F1_4	1.332(3)
C2_4–F2_4	1.340(2)

C3_4–F4_4	1.328(2)
C3_4–F5_4	1.334(2)
C3_4–F6_4	1.340(2)
C4_4–F9_4	1.330(2)
C4_4–F7_4	1.333(2)
C4_4–F8_4	1.338(2)
C1_5–C2_5	1.415(2)
C1_5–C5_5	1.421(2)
C1_5–C10_5	1.501(3)
C2_5–C3_5	1.409(3)
C2_5–C9_5	1.504(3)
C3_5–C4_5	1.412(3)
C3_5–C8_5	1.500(3)
C4_5–C5_5	1.421(3)
C4_5–C7_5	1.501(3)
C5_5–C6_5	1.502(2)
C6_5–H6A_5	0.9800
C6_5–H6B_5	0.9800
C6_5–H6C_5	0.9800
C7_5–H7A_5	0.9800
C7_5–H7B_5	0.9800
C7_5–H7C_5	0.9800
C8_5–H8A_5	0.9800
C8_5–H8B_5	0.9800
C8_5–H8C_5	0.9800
C9_5–H9A_5	0.9800
C9_5–H9B_5	0.9800
C9_5–H9C_5	0.9800
C10_5–H10A_5	0.9800
C10_5–H10B_5	0.9800
C10_5–H10C_5	0.9800
C1_6–C2_6	1.415(2)
C1_6–C5_6	1.416(2)
C1_6–C10_6	1.505(2)
C2_6–C3_6	1.421(2)
C2_6–C9_6	1.502(2)
C3_6–C4_6	1.418(2)
C3_6–C8_6	1.501(2)
C4_6–C5_6	1.419(2)
C4_6–C7_6	1.501(2)
C5_6–C6_6	1.498(2)
C6_6–H6A_6	0.9800
C6_6–H6B_6	0.9800
C6_6–H6C_6	0.9800
C7_6–H7A_6	0.9800
C7_6–H7B_6	0.9800
C7_6–H7C_6	0.9800
C8_6–H8A_6	0.9800
C8_6–H8B_6	0.9800
C8_6–H8C_6	0.9800
C9_6–H9A_6	0.9800
C9_6–H9B_6	0.9800
C9_6–H9C_6	0.9800
C10_6–H10A_6	0.9800
C10_6–H10B_6	0.9800
C10_6–H10C_6	0.9800
C1_7–C2_7	1.413(2)
C1_7–C5_7	1.421(2)
C1_7–C10_7	1.503(2)
C2_7–C3_7	1.421(2)
C2_7–C9_7	1.501(2)
C3_7–C4_7	1.423(2)
C3_7–C8_7	1.496(2)
C4_7–C5_7	1.426(2)
C4_7–C7_7	1.501(2)
C5_7–C6_7	1.503(2)
C6_7–H6A_7	0.9800
C6_7–H6B_7	0.9800
C6_7–H6C_7	0.9800
C7_7–H7A_7	0.9800
C7_7–H7B_7	0.9800
C7_7–H7C_7	0.9800
C8_7–H8A_7	0.9800
C8_7–H8B_7	0.9800
C8_7–H8C_7	0.9800
C9_7–H9A_7	0.9800
C9_7–H9B_7	0.9800
C9_7–H9C_7	0.9800
C10_7–H10A_7	0.9800
C10_7–H10B_7	0.9800
C10_7–H10C_7	0.9800

Atom–Atom–Atom	**Angle [°]**
N2–Al1–N3	80.77(6)
N2–Al1–N1	80.26(6)
N3–Al1–N1	80.85(6)
N2–Al1–Al4	164.43(5)
N3–Al1–Al4	108.78(4)
N1–Al1–Al4	112.88(4)
N2–Al1–Al3	106.33(5)
N3–Al1–Al3	107.87(5)
N1–Al1–Al3	169.60(4)
Al4–Al1–Al3	59.48(2)
N2–Al1–Al2	109.37(5)
N3–Al1–Al2	165.88(4)
N1–Al1–Al2	110.03(5)
Al4–Al1–Al2	59.23(2)
Al3–Al1–Al2	60.47(3)
C4_6–Al2–C5_6	35.60(6)
C4_6–Al2–C3_6	35.33(6)
C5_6–Al2–C3_6	58.65(6)
C4_6–Al2–C1_6	58.68(6)
C5_6–Al2–C1_6	35.04(6)
C3_6–Al2–C1_6	58.16(6)
C4_6–Al2–C2_6	58.31(6)
C5_6–Al2–C2_6	57.99(6)
C3_6–Al2–C2_6	34.83(6)
C1_6–Al2–C2_6	34.56(6)
C4_6–Al2–Al4	133.89(5)
C5_6–Al2–Al4	115.24(5)

C3_6–Al2–Al4	168.55(5)	C3_7–Al4–Al2	148.59(5)
C1_6–Al2–Al4	123.48(5)	C5_7–Al4–Al2	114.11(5)
C2_6–Al2–Al4	152.76(5)	C2_7–Al4–Al2	169.29(5)
C4_6–Al2–Al1	163.45(5)	C1_7–Al4–Al2	135.94(5)
C5_6–Al2–Al1	156.53(5)	C4_7–Al4–Al3	126.90(5)
C3_6–Al2–Al1	129.87(5)	C3_7–Al4–Al3	114.27(5)
C1_6–Al2–Al1	125.29(5)	C5_7–Al4–Al3	159.74(5)
C2_6–Al2–Al1	114.44(5)	C2_7–Al4–Al3	129.30(5)
Al4–Al2–Al1	59.93(3)	C1_7–Al4–Al3	160.90(5)
C4_6–Al2–Al3	116.39(5)	Al2–Al4–Al3	61.31(2)
C5_6–Al2–Al3	140.91(5)	C4_7–Al4–Al1	172.38(5)
C3_6–Al2–Al3	118.16(5)	C3_7–Al4–Al1	147.59(5)
C1_6–Al2–Al3	175.07(5)	C5_7–Al4–Al1	137.07(5)
C2_6–Al2–Al3	144.25(5)	C2_7–Al4–Al1	120.91(5)
Al4–Al2–Al3	59.352(19)	C1_7–Al4–Al1	116.76(5)
Al1–Al2–Al3	59.408(19)	Al2–Al4–Al1	60.83(2)
C5_5–Al3–C4_5	36.14(6)	Al3–Al4–Al1	60.34(3)
C5_5–Al3–C1_5	35.48(6)	O1_4–Al5–O1_1	107.45(6)
C4_5–Al3–C1_5	58.75(6)	O1_4–Al5–O1_2	108.61(6)
C5_5–Al3–C3_5	58.31(6)	O1_1–Al5–O1_2	112.81(6)
C4_5–Al3–C3_5	34.68(6)	O1_4–Al5–O1_3	115.17(6)
C1_5–Al3–C3_5	57.07(6)	O1_1–Al5–O1_3	106.47(6)
C5_5–Al3–C2_5	57.51(6)	O1_2–Al5–O1_3	106.48(6)
C4_5–Al3–C2_5	57.07(6)	C1–N1–C2	108.61(13)
C1_5–Al3–C2_5	33.91(6)	C1–N1–C9	110.35(14)
C3_5–Al3–C2_5	33.47(6)	C2–N1–C9	111.40(14)
C5_5–Al3–Al4	119.50(5)	C1–N1–Al1	111.09(11)
C4_5–Al3–Al4	147.70(5)	C2–N1–Al1	104.53(10)
C1_5–Al3–Al4	116.65(5)	C9–N1–Al1	110.73(11)
C3_5–Al3–Al4	172.63(5)	C4–N2–C5	108.86(13)
C2_5–Al3–Al4	139.16(5)	C4–N2–C3	109.57(13)
C5_5–Al3–Al1	170.15(5)	C5–N2–C3	112.07(14)
C4_5–Al3–Al1	148.43(5)	C4–N2–Al1	110.18(10)
C1_5–Al3–Al1	134.79(5)	C5–N2–Al1	103.84(10)
C3_5–Al3–Al1	120.57(5)	C3–N2–Al1	112.16(10)
C2_5–Al3–Al1	115.49(5)	C7–N3–C8	109.10(13)
Al4–Al3–Al1	60.18(3)	C7–N3–C6	109.56(13)
C5_5–Al3–Al2	129.10(5)	C8–N3–C6	112.15(14)
C4_5–Al3–Al2	114.39(5)	C7–N3–Al1	111.11(10)
C1_5–Al3–Al2	162.66(5)	C8–N3–Al1	103.97(10)
C3_5–Al3–Al2	127.87(5)	C6–N3–Al1	110.84(10)
C2_5–Al3–Al2	158.81(5)	N1–C1–H1A	109.5
Al4–Al3–Al2	59.343(19)	N1–C1–H1B	109.5
Al1–Al3–Al2	60.13(2)	H1A–C1–H1B	109.5
C4_7–Al4–C3_7	35.47(6)	N1–C1–H1C	109.5
C4_7–Al4–C5_7	35.33(6)	H1A–C1–H1C	109.5
C3_7–Al4–C5_7	58.10(6)	H1B–C1–H1C	109.5
C4_7–Al4–C2_7	57.66(6)	N1–C2–C3	110.31(14)
C3_7–Al4–C2_7	34.29(6)	N1–C2–H2A	109.6
C5_7–Al4–C2_7	56.71(6)	C3–C2–H2A	109.6
C4_7–Al4–C1_7	57.43(6)	N1–C2–H2B	109.6
C3_7–Al4–C1_7	56.72(6)	C3–C2–H2B	109.6
C5_7–Al4–C1_7	34.02(6)	H2A–C2–H2B	108.1
C2_7–Al4–C1_7	33.36(6)	N2–C3–C2	109.76(14)
C4_7–Al4–Al2	119.00(5)	N2–C3–H3A	109.7

C2–C3–H3A	109.7	F5_1–C3_1–F6_1	106.97(14)
N2–C3–H3B	109.7	F4_1–C3_1–C1_1	111.02(14)
C2–C3–H3B	109.7	F5_1–C3_1–C1_1	110.96(13)
H3A–C3–H3B	108.2	F6_1–C3_1–C1_1	112.86(14)
N2–C4–H4A	109.5	F9_1–C4_1–F7_1	107.44(14)
N2–C4–H4B	109.5	F9_1–C4_1–F8_1	108.06(14)
H4A–C4–H4B	109.5	F7_1–C4_1–F8_1	106.94(14)
N2–C4–H4C	109.5	F9_1–C4_1–C1_1	110.66(14)
H4A–C4–H4C	109.5	F7_1–C4_1–C1_1	110.72(14)
H4B–C4–H4C	109.5	F8_1–C4_1–C1_1	112.79(14)
N2–C5–C6	109.96(14)	C1_2–O1_2–Al5	145.15(11)
N2–C5–H5A	109.7	O1_2–C1_2–C3_2	110.92(13)
C6–C5–H5A	109.7	O1_2–C1_2–C2_2	107.83(13)
N2–C5–H5B	109.7	C3_2–C1_2–C2_2	109.54(14)
C6–C5–H5B	109.7	O1_2–C1_2–C4_2	110.51(13)
H5A–C5–H5B	108.2	C3_2–C1_2–C4_2	109.05(13)
N3–C6–C5	109.64(13)	C2_2–C1_2–C4_2	108.95(14)
N3–C6–H6A	109.7	F3_2–C2_2–F1_2	107.79(15)
C5–C6–H6A	109.7	F3_2–C2_2–F2_2	107.32(15)
N3–C6–H6B	109.7	F1_2–C2_2–F2_2	107.75(15)
C5–C6–H6B	109.7	F3_2–C2_2–C1_2	110.79(15)
H6A–C6–H6B	108.2	F1_2–C2_2–C1_2	110.64(15)
N3–C7–H7A	109.5	F2_2–C2_2–C1_2	112.35(15)
N3–C7–H7B	109.5	F4_2–C3_2–F5_2	107.37(14)
H7A–C7–H7B	109.5	F4_2–C3_2–F6_2	107.67(14)
N3–C7–H7C	109.5	F5_2–C3_2–F6_2	107.43(14)
H7A–C7–H7C	109.5	F4_2–C3_2–C1_2	110.67(14)
H7B–C7–H7C	109.5	F5_2–C3_2–C1_2	110.59(14)
N3–C8–C9	110.70(14)	F6_2–C3_2–C1_2	112.88(14)
N3–C8–H8A	109.5	F9_2–C4_2–F7_2	107.53(14)
C9–C8–H8A	109.5	F9_2–C4_2–F8_2	107.89(14)
N3–C8–H8B	109.5	F7_2–C4_2–F8_2	107.12(14)
C9–C8–H8B	109.5	F9_2–C4_2–C1_2	110.95(14)
H8A–C8–H8B	108.1	F7_2–C4_2–C1_2	111.06(14)
N1–C9–C8	110.09(14)	F8_2–C4_2–C1_2	112.09(14)
N1–C9–H9A	109.6	C1_3–O1_3–Al5	147.60(12)
C8–C9–H9A	109.6	O1_3–C1_3–C3_3	107.39(16)
N1–C9–H9B	109.6	O1_3–C1_3–C2_3	111.18(15)
C8–C9–H9B	109.6	C3_3–C1_3–C2_3	109.10(16)
H9A–C9–H9B	108.2	O1_3–C1_3–C4_3	110.82(15)
C1_1–O1_1–Al5	149.27(11)	C3_3–C1_3–C4_3	109.33(17)
O1_1–C1_1–C3_1	107.81(13)	C2_3–C1_3–C4_3	108.98(16)
O1_1–C1_1–C2_1	112.24(13)	F3_3–C2_3–F1_3	107.46(17)
C3_1–C1_1–C2_1	109.10(13)	F3_3–C2_3–F2_3	107.29(16)
O1_1–C1_1–C4_1	109.33(13)	F1_3–C2_3–F2_3	106.95(17)
C3_1–C1_1–C4_1	109.46(13)	F3_3–C2_3–C1_3	111.09(17)
C2_1–C1_1–C4_1	108.85(13)	F1_3–C2_3–C1_3	111.47(16)
F1_1–C2_1–F3_1	107.30(14)	F2_3–C2_3–C1_3	112.32(16)
F1_1–C2_1–F2_1	107.74(14)	F4_3–C3_3–F6_3	107.76(19)
F3_1–C2_1–F2_1	107.43(14)	F4_3–C3_3–F5_3	107.5(2)
F1_1–C2_1–C1_1	111.23(14)	F6_3–C3_3–F5_3	106.53(18)
F3_1–C2_1–C1_1	110.71(13)	F4_3–C3_3–C1_3	111.28(17)
F2_1–C2_1–C1_1	112.20(14)	F6_3–C3_3–C1_3	112.90(19)
F4_1–C3_1–F5_1	107.19(14)	F5_3–C3_3–C1_3	110.55(18)
F4_1–C3_1–F6_1	107.57(14)	F7_3–C4_3–F9_3	107.55(17)

F7_3–C4_3–F8_3	107.69(17)	C4_5–C5_5–C6_5	125.00(17)
F9_3–C4_3–F8_3	107.88(19)	C1_5–C5_5–C6_5	127.27(17)
F7_3–C4_3–C1_3	111.03(19)	C4_5–C5_5–Al3	72.74(10)
F9_3–C4_3–C1_3	110.15(16)	C1_5–C5_5–Al3	75.92(10)
F8_3–C4_3–C1_3	112.35(16)	C6_5–C5_5–Al3	119.34(12)
C1_4–O1_4–Al5	148.63(11)	C5_5–C6_5–H6A_5	109.5
O1_4–C1_4–C3_4	109.99(14)	C5_5–C6_5–H6B_5	109.5
O1_4–C1_4–C2_4	108.00(14)	H6A_5–C6_5–H6B_5	109.5
C3_4–C1_4–C2_4	109.40(15)	C5_5–C6_5–H6C_5	109.5
O1_4–C1_4–C4_4	111.51(14)	H6A_5–C6_5–H6C_5	109.5
C3_4–C1_4–C4_4	108.68(14)	H6B_5–C6_5–H6C_5	109.5
C2_4–C1_4–C4_4	109.23(15)	C4_5–C7_5–H7A_5	109.5
F3_4–C2_4–F1_4	107.57(17)	C4_5–C7_5–H7B_5	109.5
F3_4–C2_4–F2_4	107.97(17)	H7A_5–C7_5–H7B_5	109.5
F1_4–C2_4–F2_4	107.48(16)	C4_5–C7_5–H7C_5	109.5
F3_4–C2_4–C1_4	110.87(16)	H7A_5–C7_5–H7C_5	109.5
F1_4–C2_4–C1_4	110.48(17)	H7B_5–C7_5–H7C_5	109.5
F2_4–C2_4–C1_4	112.28(15)	C3_5–C8_5–H8A_5	109.5
F4_4–C3_4–F5_4	107.47(16)	C3_5–C8_5–H8B_5	109.5
F4_4–C3_4–F6_4	107.75(16)	H8A_5–C8_5–H8B_5	109.5
F5_4–C3_4–F6_4	107.24(15)	C3_5–C8_5–H8C_5	109.5
F4_4–C3_4–C1_4	110.70(15)	H8A_5–C8_5–H8C_5	109.5
F5_4–C3_4–C1_4	111.21(15)	H8B_5–C8_5–H8C_5	109.5
F6_4–C3_4–C1_4	112.27(15)	C2_5–C9_5–H9A_5	109.5
F9_4–C4_4–F7_4	106.97(16)	C2_5–C9_5–H9B_5	109.5
F9_4–C4_4–F8_4	107.78(16)	H9A_5–C9_5–H9B_5	109.5
F7_4–C4_4–F8_4	107.30(16)	C2_5–C9_5–H9C_5	109.5
F9_4–C4_4–C1_4	110.40(15)	H9A_5–C9_5–H9C_5	109.5
F7_4–C4_4–C1_4	111.18(15)	H9B_5–C9_5–H9C_5	109.5
F8_4–C4_4–C1_4	112.95(16)	C1_5–C10_5–H10A_5	109.5
C2_5–C1_5–C5_5	107.70(16)	C1_5–C10_5–H10B_5	109.5
C2_5–C1_5–C10_5	125.09(17)	H10A_5–C10_5–H10B_5	109.5
C5_5–C1_5–C10_5	126.99(17)		
C2_5–C1_5–Al3	76.66(10)	C1_5–C10_5–H10C_5	109.5
C5_5–C1_5–Al3	68.60(9)	H10A_5–C10_5–H10C_5	109.5
C10_5–C1_5–Al3	124.61(12)		
C3_5–C2_5–C1_5	108.47(16)	H10B_5–C10_5–H10C_5	109.5
C3_5–C2_5–C9_5	126.23(18)		
C1_5–C2_5–C9_5	124.72(19)	C2_6–C1_6–C5_6	107.73(15)
C3_5–C2_5–Al3	71.42(10)	C2_6–C1_6–C10_6	125.82(17)
C1_5–C2_5–Al3	69.43(9)	C5_6–C1_6–C10_6	126.27(17)
C9_5–C2_5–Al3	131.79(13)	C2_6–C1_6–Al2	73.33(9)
C2_5–C3_5–C4_5	108.05(16)	C5_6–C1_6–Al2	70.61(9)
C2_5–C3_5–C8_5	125.8(2)	C10_6–C1_6–Al2	125.45(12)
C4_5–C3_5–C8_5	125.8(2)	C1_6–C2_6–C3_6	108.33(15)
C2_5–C3_5–Al3	75.10(10)	C1_6–C2_6–C9_6	125.32(17)
C4_5–C3_5–Al3	68.00(10)	C3_6–C2_6–C9_6	125.65(17)
C8_5–C3_5–Al3	127.83(13)	C1_6–C2_6–Al2	72.12(10)
C3_5–C4_5–C5_5	108.11(16)	C3_6–C2_6–Al2	71.30(9)
C3_5–C4_5–C7_5	124.77(18)	C9_6–C2_6–Al2	129.85(12)
C5_5–C4_5–C7_5	126.74(18)	C4_6–C3_6–C2_6	107.72(15)
C3_5–C4_5–Al3	77.32(10)	C4_6–C3_6–C8_6	126.57(16)
C5_5–C4_5–Al3	71.12(10)	C2_6–C3_6–C8_6	125.53(16)
C7_5–C4_5–Al3	123.16(13)	C4_6–C3_6–Al2	70.71(9)
C4_5–C5_5–C1_5	107.67(15)	C2_6–C3_6–Al2	73.87(10)

C8_6–C3_6–Al2	124.72(12)	C1_7–C2_7–Al4	73.95(9)
C3_6–C4_6–C5_6	107.89(15)	C3_7–C2_7–Al4	69.16(9)
C3_6–C4_6–C7_6	128.06(16)	C9_7–C2_7–Al4	124.90(11)
C5_6–C4_6–C7_6	123.92(16)	C2_7–C3_7–C4_7	108.03(14)
C3_6–C4_6–Al2	73.95(9)	C2_7–C3_7–C8_7	126.96(16)
C5_6–C4_6–Al2	72.64(10)	C4_7–C3_7–C8_7	124.64(15)
C7_6–C4_6–Al2	122.41(12)	C2_7–C3_7–Al4	76.55(9)
C1_6–C5_6–C4_6	108.33(15)	C4_7–C3_7–Al4	70.57(9)
C1_6–C5_6–C6_6	127.65(17)	C8_7–C3_7–Al4	124.08(11)
C4_6–C5_6–C6_6	123.76(17)	C3_7–C4_7–C5_7	107.71(14)
C1_6–C5_6–Al2	74.35(10)	C3_7–C4_7–C7_7	124.34(15)
C4_6–C5_6–Al2	71.76(10)	C5_7–C4_7–C7_7	127.87(15)
C6_6–C5_6–Al2	124.25(12)	C3_7–C4_7–Al4	73.96(9)
C5_6–C6_6–H6A_6	109.5	C5_7–C4_7–Al4	74.94(9)
C5_6–C6_6–H6B_6	109.5	C7_7–C4_7–Al4	119.63(11)
H6A_6–C6_6–H6B_6	109.5	C1_7–C5_7–C4_7	107.87(14)
C5_6–C6_6–H6C_6	109.5	C1_7–C5_7–C6_7	125.15(15)
H6A_6–C6_6–H6C_6	109.5	C4_7–C5_7–C6_7	126.87(15)
H6B_6–C6_6–H6C_6	109.5	C1_7–C5_7–Al4	76.40(9)
C4_6–C7_6–H7A_6	109.5	C4_7–C5_7–Al4	69.73(9)
C4_6–C7_6–H7B_6	109.5	C6_7–C5_7–Al4	122.66(11)
H7A_6–C7_6–H7B_6	109.5	C5_7–C6_7–H6A_7	109.5
C4_6–C7_6–H7C_6	109.5	C5_7–C6_7–H6B_7	109.5
H7A_6–C7_6–H7C_6	109.5	H6A_7–C6_7–H6B_7	109.5
H7B_6–C7_6–H7C_6	109.5	C5_7–C6_7–H6C_7	109.5
C3_6–C8_6–H8A_6	109.5	H6A_7–C6_7–H6C_7	109.5
C3_6–C8_6–H8B_6	109.5	H6B_7–C6_7–H6C_7	109.5
H8A_6–C8_6–H8B_6	109.5	C4_7–C7_7–H7A_7	109.5
C3_6–C8_6–H8C_6	109.5	C4_7–C7_7–H7B_7	109.5
H8A_6–C8_6–H8C_6	109.5	H7A_7–C7_7–H7B_7	109.5
H8B_6–C8_6–H8C_6	109.5	C4_7–C7_7–H7C_7	109.5
C2_6–C9_6–H9A_6	109.5	H7A_7–C7_7–H7C_7	109.5
C2_6–C9_6–H9B_6	109.5	H7B_7–C7_7–H7C_7	109.5
H9A_6–C9_6–H9B_6	109.5	C3_7–C8_7–H8A_7	109.5
C2_6–C9_6–H9C_6	109.5	C3_7–C8_7–H8B_7	109.5
H9A_6–C9_6–H9C_6	109.5	H8A_7–C8_7–H8B_7	109.5
H9B_6–C9_6–H9C_6	109.5	C3_7–C8_7–H8C_7	109.5
C1_6–C10_6–H10A_6	109.5	H8A_7–C8_7–H8C_7	109.5
C1_6–C10_6–H10B_6	109.5	H8B_7–C8_7–H8C_7	109.5
H10A_6–C10_6–H10B_6	109.5	C2_7–C9_7–H9A_7	109.5
		C2_7–C9_7–H9B_7	109.5
C1_6–C10_6–H10C_6	109.5	H9A_7–C9_7–H9B_7	109.5
H10A_6–C10_6–H10C_6	109.5	C2_7–C9_7–H9C_7	109.5
		H9A_7–C9_7–H9C_7	109.5
H10B_6–C10_6–H10C_6	109.5	H9B_7–C9_7–H9C_7	109.5
		C1_7–C10_7–H10A_7	109.5
C2_7–C1_7–C5_7	108.24(14)	C1_7–C10_7–H10B_7	109.5
C2_7–C1_7–C10_7	125.14(16)	H10A_7–C10_7–H10B_7	109.5
C5_7–C1_7–C10_7	126.43(16)		
C2_7–C1_7–Al4	72.69(9)	C1_7–C10_7–H10C_7	109.5
C5_7–C1_7–Al4	69.58(9)	H10A_7–C10_7–H10C_7	109.5
C10_7–C1_7–Al4	127.31(11)		
C1_7–C2_7–C3_7	108.15(14)	H10B_7–C10_7–H10C_7	109.5
C1_7–C2_7–C9_7	124.90(16)		
C3_7–C2_7–C9_7	126.89(16)		

S-Table 12: Bond lengths and angles for **5**

Atom–Atom	Length [Å]
Ga1–C1_5	2.440(4)
Ga1–Al2	2.7242(16)
Ga1–Al3	2.7276(16)
Ga1–Al1	2.8208(17)
Al3–C5_6	2.312(3)
Al3–C1_6	2.318(3)
Al3–C4_6	2.350(3)
Al3–C2_6	2.356(3)
Al3–C3_6	2.378(3)
Al3–Al2	2.826(2)
Al3–Al1	2.8375(18)
Al1–N1	2.108(3)
Al1–N3	2.132(3)
Al1–N2	2.141(3)
Al1–Al2	2.7997(19)
Al2–C4_7	2.241(6)
Al2–C3_7	2.261(5)
Al2–C5_7	2.314(5)
Al2–C2_7	2.344(4)
Al2–C3_10	2.37(2)
Al2–C4_10	2.39(3)
Al2–C1_7	2.391(4)
Al2–C2_10	2.438(17)
Al2–C5_10	2.49(2)
Al2–C1_10	2.519(17)
Al4–O1_9	1.612(9)
Al4–O1_3	1.707(3)
Al4–O1_4	1.708(8)
Al4–O1_1	1.711(3)
Al4–O1_2	1.743(3)
Al4–O1_13	1.746(10)
Al4–O1_12	1.746(15)
Al4–O1_8	1.779(12)
N1–C4	1.487(4)
N1–C1	1.489(5)
N1–C9	1.497(4)
N2–C3	1.481(5)
N2–C7	1.489(5)
N2–C8	1.498(4)
N3–C2	1.486(4)
N3–C5	1.488(4)
N3–C6	1.498(5)
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–H3A	0.9800
C3–H3B	0.9800
C3–H3C	0.9800
C4–C5	1.520(5)
C4–H4A	0.9900
C4–H4B	0.9900
C5–H5A	0.9900
C5–H5B	0.9900
C6–C7	1.515(6)
C6–H6A	0.9900
C6–H6B	0.9900
C7–H7A	0.9900
C7–H7B	0.9900
C8–C9	1.503(6)
C8–H8A	0.9900
C8–H8B	0.9900
C9–H9A	0.9900
C9–H9B	0.9900
O1_1–C1_1	1.346(4)
C1_1–C4_1	1.550(5)
C1_1–C2_1	1.556(5)
C1_1–C3_1	1.558(5)
C2_1–F3_1	1.325(4)
C2_1–F2_1	1.327(5)
C2_1–F1_1	1.340(5)
C3_1–F4_1	1.329(5)
C3_1–F5_1	1.331(5)
C3_1–F6_1	1.339(5)
C4_1–F9_1	1.321(5)
C4_1–F7_1	1.332(5)
C4_1–F8_1	1.346(5)
O1_2–C1_2	1.350(6)
C1_2–C3_2	1.515(8)
C1_2–C4_2	1.553(8)
C1_2–C2_2	1.570(7)
C2_2–F2_2	1.311(7)
C2_2–F3_2	1.316(7)
C2_2–F1_2	1.335(7)
C3_2–F6_2	1.336(9)
C3_2–F5_2	1.337(9)
C3_2–F4_2	1.346(9)
C4_2–F7_2	1.295(7)
C4_2–F9_2	1.313(8)
C4_2–F8_2	1.354(7)
O1_3–C1_3	1.359(4)
C1_3–C2_3	1.532(6)
C1_3–C3_3	1.546(5)
C1_3–C4_3	1.552(5)
C2_3–F3_3	1.318(6)
C2_3–F1_3	1.336(6)
C2_3–F2_3	1.347(5)
C3_3–F6_3	1.319(5)
C3_3–F4_3	1.326(6)
C3_3–F5_3	1.330(5)
C4_3–F9_3	1.309(5)
C4_3–F7_3	1.327(6)
C4_3–F8_3	1.345(5)
O1_4–C1_4	1.352(9)
C1_4–C3_4	1.543(8)

C1_4–C4_4	1.547(9)	C9_6–H9A_6	0.9800
C1_4–C2_4	1.549(9)	C9_6–H9B_6	0.9800
C2_4–F2_4	1.316(8)	C9_6–H9C_6	0.9800
C2_4–F3_4	1.322(9)	C10_6–H10A_6	0.9800
C2_4–F1_4	1.326(9)	C10_6–H10B_6	0.9800
C3_4–F6_4	1.328(10)	C10_6–H10C_6	0.9800
C3_4–F5_4	1.333(9)	C1_7–C2_7	1.396(7)
C3_4–F4_4	1.334(10)	C1_7–C5_7	1.413(6)
C4_4–F9_4	1.322(8)	C1_7–C10_7	1.522(6)
C4_4–F7_4	1.328(9)	C2_7–C3_7	1.417(6)
C4_4–F8_4	1.340(8)	C2_7–C9_7	1.521(6)
C1_5–C2_5	1.424(5)	C3_7–C4_7	1.424(7)
C1_5–C5_5	1.426(5)	C3_7–C8_7	1.496(7)
C1_5–C10_5	1.511(5)	C4_7–C5_7	1.414(7)
C2_5–C3_5	1.416(5)	C4_7–C7_7	1.500(6)
C2_5–C9_5	1.511(5)	C5_7–C6_7	1.502(7)
C3_5–C4_5	1.407(4)	C6_7–H6A_7	0.9800
C3_5–C8_5	1.507(5)	C6_7–H6B_7	0.9800
C4_5–C5_5	1.411(5)	C6_7–H6C_7	0.9800
C4_5–C7_5	1.510(5)	C7_7–H7A_7	0.9800
C5_5–C6_5	1.505(5)	C7_7–H7B_7	0.9800
C6_5–H6A_5	0.9800	C7_7–H7C_7	0.9800
C6_5–H6B_5	0.9800	C8_7–H8A_7	0.9800
C6_5–H6C_5	0.9800	C8_7–H8B_7	0.9800
C7_5–H7A_5	0.9800	C8_7–H8C_7	0.9800
C7_5–H7B_5	0.9800	C9_7–H9A_7	0.9800
C7_5–H7C_5	0.9800	C9_7–H9B_7	0.9800
C8_5–H8A_5	0.9800	C9_7–H9C_7	0.9800
C8_5–H8B_5	0.9800	C10_7–H10A_7	0.9800
C8_5–H8C_5	0.9800	C10_7–H10B_7	0.9800
C9_5–H9A_5	0.9800	C10_7–H10C_7	0.9800
C9_5–H9B_5	0.9800	O1_8–C1_8	1.346(11)
C9_5–H9C_5	0.9800	C1_8–C4_8	1.549(10)
C10_5–H10A_5	0.9800	C1_8–C2_8	1.553(11)
C10_5–H10B_5	0.9800	C1_8–C3_8	1.559(11)
C10_5–H10C_5	0.9800	C2_8–F1_8	1.324(11)
C1_6–C5_6	1.414(5)	C2_8–F3_8	1.338(11)
C1_6–C2_6	1.419(4)	C2_8–F2_8	1.343(11)
C1_6–C10_6	1.504(5)	C3_8–F6_8	1.324(10)
C2_6–C3_6	1.424(4)	C3_8–F4_8	1.329(10)
C2_6–C9_6	1.504(5)	C3_8–F5_8	1.336(10)
C3_6–C4_6	1.420(4)	C4_8–F8_8	1.325(9)
C3_6–C8_6	1.504(4)	C4_8–F7_8	1.343(11)
C4_6–C5_6	1.421(4)	C4_8–F9_8	1.345(10)
C4_6–C7_6	1.507(5)	O1_9–C1_9	1.365(13)
C5_6–C6_6	1.503(4)	C1_9–C4_9	1.531(12)
C6_6–H6A_6	0.9800	C1_9–C3_9	1.540(12)
C6_6–H6B_6	0.9800	C1_9–C2_9	1.550(12)
C6_6–H6C_6	0.9800	C2_9–F1_9	1.304(13)
C7_6–H7A_6	0.9800	C2_9–F2_9	1.325(13)
C7_6–H7B_6	0.9800	C2_9–F3_9	1.338(13)
C7_6–H7C_6	0.9800	C3_9–F6_9	1.304(13)
C8_6–H8A_6	0.9800	C3_9–F5_9	1.317(13)
C8_6–H8B_6	0.9800	C3_9–F4_9	1.334(13)
C8_6–H8C_6	0.9800	C4_9–F8_9	1.309(12)

C4_9–F7_9	1.323(13)
C4_9–F9_9	1.323(12)
O1_12–C1_12	1.356(13)
C1_12–C3_12	1.539(12)
C1_12–C4_12	1.553(12)
C1_12–C2_12	1.556(12)
C2_12–F1_12	1.328(13)
C2_12–F3_12	1.333(13)
C2_12–F2_12	1.337(12)
C3_12–F4_12	1.331(13)
C3_12–F6_12	1.331(13)
C3_12–F5_12	1.333(13)
C4_12–F8_12	1.328(12)
C4_12–F9_12	1.331(13)
C4_12–F7_12	1.332(13)
F1_11–C1_11	1.364(18)
C1_11–C6_11	1.379(13)
C1_11–C2_11	1.384(13)
C2_11–C3_11	1.377(14)
C2_11–H2_11	0.9500
C3_11–C4_11	1.392(14)
C3_11–H3_11	0.9500
C4_11–C5_11	1.398(14)
C4_11–H4_11	0.9500
C5_11–C6_11	1.359(12)
C5_11–H5_11	0.9500
C6_11–H6_11	0.9500
C1_10–C5_10	1.410(12)
C1_10–C2_10	1.410(12)
C1_10–C10_10	1.515(13)
C2_10–C3_10	1.413(13)
C2_10–C9_10	1.501(13)
C3_10–C4_10	1.409(12)
C3_10–C8_10	1.508(13)
C4_10–C5_10	1.426(13)
C4_10–C7_10	1.513(13)
C5_10–C6_10	1.505(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_13–C1_13	1.380(12)
C1_13–C4_13	1.543(11)
C1_13–C3_13	1.550(12)
C1_13–C2_13	1.565(11)
C2_13–F2_13	1.325(11)
C2_13–F3_13	1.332(12)
C2_13–F1_13	1.332(11)
C3_13–F5_13	1.330(12)
C3_13–F6_13	1.330(13)
C3_13–F4_13	1.332(12)
C4_13–F9_13	1.344(13)
C4_13–F8_13	1.354(13)
C4_13–F7_13	1.357(13)

Atom–Atom–Atom	**Angle [°]**
C1_5–Ga1–Al2	131.05(9)
C1_5–Ga1–Al3	137.39(9)
Al2–Ga1–Al3	62.45(5)
C1_5–Ga1–Al1	159.10(9)
Al2–Ga1–Al1	60.62(4)
Al3–Ga1–Al1	61.49(4)
C5_6–Al3–C1_6	35.58(12)
C5_6–Al3–C4_6	35.48(11)
C1_6–Al3–C4_6	58.95(11)
C5_6–Al3–C2_6	58.95(12)
C1_6–Al3–C2_6	35.34(11)
C4_6–Al3–C2_6	58.64(12)
C5_6–Al3–C3_6	58.53(11)
C1_6–Al3–C3_6	58.46(11)
C4_6–Al3–C3_6	34.96(11)
C2_6–Al3–C3_6	35.00(11)
C5_6–Al3–Ga1	112.06(10)
C1_6–Al3–Ga1	134.32(9)
C4_6–Al3–Ga1	117.85(9)
C2_6–Al3–Ga1	169.61(9)
C3_6–Al3–Ga1	147.20(9)
C5_6–Al3–Al2	136.52(9)
C1_6–Al3–Al2	116.78(9)
C4_6–Al3–Al2	171.32(9)
C2_6–Al3–Al2	123.10(9)
C3_6–Al3–Al2	151.31(10)
Ga1–Al3–Al2	58.72(4)
C5_6–Al3–Al1	159.15(10)
C1_6–Al3–Al1	162.05(10)
C4_6–Al3–Al1	127.37(9)
C2_6–Al3–Al1	129.43(9)
C3_6–Al3–Al1	115.44(9)
Ga1–Al3–Al1	60.87(4)
Al2–Al3–Al1	59.25(4)
N1–Al1–N3	81.79(11)
N1–Al1–N2	81.29(11)
N3–Al1–N2	81.21(12)
N1–Al1–Al2	109.68(9)
N3–Al1–Al2	106.53(10)
N2–Al1–Al2	167.11(9)
N1–Al1–Ga1	163.24(9)
N3–Al1–Ga1	111.72(8)
N2–Al1–Ga1	109.82(9)

Al2–Al1–Ga1	57.98(4)	O1_12–Al4–O1_8	123.4(8)
N1–Al1–Al3	107.18(9)	C4–N1–C1	109.9(3)
N3–Al1–Al3	165.61(9)	C4–N1–C9	111.2(3)
N2–Al1–Al3	110.86(10)	C1–N1–C9	108.4(3)
Al2–Al1–Al3	60.17(5)	C4–N1–Al1	111.3(2)
Ga1–Al1–Al3	57.64(3)	C1–N1–Al1	110.7(2)
C4_7–Al2–C3_7	36.89(18)	C9–N1–Al1	105.2(2)
C4_7–Al2–C5_7	36.12(17)	C3–N2–C7	110.6(3)
C3_7–Al2–C5_7	59.93(17)	C3–N2–C8	109.8(3)
C4_7–Al2–C2_7	59.78(16)	C7–N2–C8	111.6(3)
C3_7–Al2–C2_7	35.78(16)	C3–N2–Al1	109.8(2)
C5_7–Al2–C2_7	58.11(17)	C7–N2–Al1	103.8(2)
C3_10–Al2–C4_10	34.5(4)	C8–N2–Al1	111.1(2)
C4_7–Al2–C1_7	59.47(16)	C2–N3–C5	108.8(3)
C3_7–Al2–C1_7	59.06(16)	C2–N3–C6	109.8(3)
C5_7–Al2–C1_7	34.92(15)	C5–N3–C6	112.6(3)
C2_7–Al2–C1_7	34.28(16)	C2–N3–Al1	111.0(2)
C3_10–Al2–C2_10	34.2(4)	C5–N3–Al1	103.2(2)
C4_10–Al2–C2_10	56.4(6)	C6–N3–Al1	111.4(2)
C3_10–Al2–C5_10	56.3(5)	N1–C1–H1A	109.5
C4_10–Al2–C5_10	33.9(4)	N1–C1–H1B	109.5
C2_10–Al2–C5_10	55.2(5)	H1A–C1–H1B	109.5
C3_10–Al2–C1_10	55.8(5)	N1–C1–H1C	109.5
C4_10–Al2–C1_10	55.5(5)	H1A–C1–H1C	109.5
C2_10–Al2–C1_10	33.0(3)	H1B–C1–H1C	109.5
C5_10–Al2–C1_10	32.7(3)	N3–C2–H2A	109.5
C4_7–Al2–Ga1	122.30(15)	N3–C2–H2B	109.5
C3_7–Al2–Ga1	156.35(14)	H2A–C2–H2B	109.5
C5_7–Al2–Ga1	110.94(14)	N3–C2–H2C	109.5
C2_7–Al2–Ga1	160.78(14)	H2A–C2–H2C	109.5
C3_10–Al2–Ga1	117.8(4)	H2B–C2–H2C	109.5
C4_10–Al2–Ga1	115.9(5)	N2–C3–H3A	109.5
C1_7–Al2–Ga1	127.55(14)	N2–C3–H3B	109.5
C2_10–Al2–Ga1	144.8(4)	H3A–C3–H3B	109.5
C5_10–Al2–Ga1	140.1(4)	N2–C3–H3C	109.5
C1_10–Al2–Ga1	171.4(4)	H3A–C3–H3C	109.5
C4_7–Al2–Al1	175.90(16)	H3B–C3–H3C	109.5
C3_7–Al2–Al1	139.08(14)	N1–C4–C5	109.7(3)
C5_7–Al2–Al1	146.08(14)	N1–C4–H4A	109.7
C2_7–Al2–Al1	117.47(12)	C5–C4–H4A	109.7
C3_10–Al2–Al1	139.0(5)	N1–C4–H4B	109.7
C4_10–Al2–Al1	172.3(5)	C5–C4–H4B	109.7
C1_7–Al2–Al1	120.35(12)	H4A–C4–H4B	108.2
C2_10–Al2–Al1	121.0(4)	N3–C5–C4	110.2(3)
C5_10–Al2–Al1	152.4(4)	N3–C5–H5A	109.6
C1_10–Al2–Al1	127.1(4)	C4–C5–H5A	109.6
Ga1–Al2–Al1	61.40(4)	N3–C5–H5B	109.6
O1_3–Al4–O1_4	109.6(4)	C4–C5–H5B	109.6
O1_3–Al4–O1_1	109.31(16)	H5A–C5–H5B	108.1
O1_4–Al4–O1_1	108.1(4)	N3–C6–C7	109.1(3)
O1_3–Al4–O1_2	111.48(16)	N3–C6–H6A	109.9
O1_4–Al4–O1_2	112.0(4)	C7–C6–H6A	109.9
O1_1–Al4–O1_2	106.10(19)	N3–C6–H6B	109.9
O1_9–Al4–O1_12	111.6(7)	C7–C6–H6B	109.9
O1_9–Al4–O1_8	71.5(6)	H6A–C6–H6B	108.3

N2–C7–C6	110.4(3)	F1_2–C2_2–C1_2	108.1(5)
N2–C7–H7A	109.6	F6_2–C3_2–F5_2	110.2(8)
C6–C7–H7A	109.6	F6_2–C3_2–F4_2	106.5(7)
N2–C7–H7B	109.6	F5_2–C3_2–F4_2	105.6(8)
C6–C7–H7B	109.6	F6_2–C3_2–C1_2	111.3(7)
H7A–C7–H7B	108.1	F5_2–C3_2–C1_2	111.7(6)
N2–C8–C9	109.4(3)	F4_2–C3_2–C1_2	111.3(7)
N2–C8–H8A	109.8	F7_2–C4_2–F9_2	107.0(7)
C9–C8–H8A	109.8	F7_2–C4_2–F8_2	106.7(6)
N2–C8–H8B	109.8	F9_2–C4_2–F8_2	108.5(6)
C9–C8–H8B	109.8	F7_2–C4_2–C1_2	114.5(6)
H8A–C8–H8B	108.2	F9_2–C4_2–C1_2	111.5(5)
N1–C9–C8	110.6(3)	F8_2–C4_2–C1_2	108.4(6)
N1–C9–H9A	109.5	C1_3–O1_3–Al4	151.5(2)
C8–C9–H9A	109.5	O1_3–C1_3–C2_3	110.9(3)
N1–C9–H9B	109.5	O1_3–C1_3–C3_3	111.3(3)
C8–C9–H9B	109.5	C2_3–C1_3–C3_3	108.5(4)
H9A–C9–H9B	108.1	O1_3–C1_3–C4_3	107.3(3)
C1_1–O1_1–Al4	148.0(3)	C2_3–C1_3–C4_3	110.0(4)
O1_1–C1_1–C4_1	107.7(3)	C3_3–C1_3–C4_3	108.8(3)
O1_1–C1_1–C2_1	111.5(3)	F3_3–C2_3–F1_3	109.0(4)
C4_1–C1_1–C2_1	109.6(3)	F3_3–C2_3–F2_3	107.5(5)
O1_1–C1_1–C3_1	109.5(3)	F1_3–C2_3–F2_3	106.6(4)
C4_1–C1_1–C3_1	109.7(3)	F3_3–C2_3–C1_3	110.8(4)
C2_1–C1_1–C3_1	108.9(3)	F1_3–C2_3–C1_3	109.6(4)
F3_1–C2_1–F2_1	108.5(4)	F2_3–C2_3–C1_3	113.2(4)
F3_1–C2_1–F1_1	107.4(4)	F6_3–C3_3–F4_3	107.9(4)
F2_1–C2_1–F1_1	107.0(4)	F6_3–C3_3–F5_3	108.2(4)
F3_1–C2_1–C1_1	110.8(3)	F4_3–C3_3–F5_3	105.7(4)
F2_1–C2_1–C1_1	112.8(3)	F6_3–C3_3–C1_3	113.4(4)
F1_1–C2_1–C1_1	110.1(4)	F4_3–C3_3–C1_3	110.2(4)
F4_1–C3_1–F5_1	107.9(4)	F5_3–C3_3–C1_3	111.1(4)
F4_1–C3_1–F6_1	107.4(3)	F9_3–C4_3–F7_3	106.9(5)
F5_1–C3_1–F6_1	107.8(4)	F9_3–C4_3–F8_3	108.3(4)
F4_1–C3_1–C1_1	110.8(3)	F7_3–C4_3–F8_3	107.1(4)
F5_1–C3_1–C1_1	110.7(3)	F9_3–C4_3–C1_3	111.5(3)
F6_1–C3_1–C1_1	112.1(3)	F7_3–C4_3–C1_3	110.8(4)
F9_1–C4_1–F7_1	106.8(4)	F8_3–C4_3–C1_3	111.9(4)
F9_1–C4_1–F8_1	106.9(4)	C1_4–O1_4–Al4	149.4(9)
F7_1–C4_1–F8_1	107.3(3)	O1_4–C1_4–C3_4	111.8(7)
F9_1–C4_1–C1_1	111.5(3)	O1_4–C1_4–C4_4	111.9(7)
F7_1–C4_1–C1_1	111.8(3)	C3_4–C1_4–C4_4	111.0(6)
F8_1–C4_1–C1_1	112.1(3)	O1_4–C1_4–C2_4	104.6(7)
C1_2–O1_2–Al4	149.5(4)	C3_4–C1_4–C2_4	109.6(7)
O1_2–C1_2–C3_2	111.8(5)	C4_4–C1_4–C2_4	107.6(6)
O1_2–C1_2–C4_2	107.0(5)	F2_4–C2_4–F3_4	110.0(8)
C3_2–C1_2–C4_2	107.9(6)	F2_4–C2_4–F1_4	108.8(7)
O1_2–C1_2–C2_2	110.7(4)	F3_4–C2_4–F1_4	108.4(8)
C3_2–C1_2–C2_2	109.6(5)	F2_4–C2_4–C1_4	111.4(8)
C4_2–C1_2–C2_2	109.9(5)	F3_4–C2_4–C1_4	105.6(8)
F2_2–C2_2–F3_2	107.7(6)	F1_4–C2_4–C1_4	112.5(8)
F2_2–C2_2–F1_2	108.9(6)	F6_4–C3_4–F5_4	106.0(10)
F3_2–C2_2–F1_2	106.7(5)	F6_4–C3_4–F4_4	107.0(11)
F2_2–C2_2–C1_2	114.1(5)	F5_4–C3_4–F4_4	106.8(8)
F3_2–C2_2–C1_2	111.0(5)	F6_4–C3_4–C1_4	115.0(10)

F5_4–C3_4–C1_4	111.8(7)
F4_4–C3_4–C1_4	109.7(8)
F9_4–C4_4–F7_4	109.6(8)
F9_4–C4_4–F8_4	106.3(6)
F7_4–C4_4–F8_4	108.5(7)
F9_4–C4_4–C1_4	111.3(6)
F7_4–C4_4–C1_4	109.2(7)
F8_4–C4_4–C1_4	111.8(7)
C2_5–C1_5–C5_5	107.3(3)
C2_5–C1_5–C10_5	125.1(3)
C5_5–C1_5–C10_5	127.2(3)
C2_5–C1_5–Ga1	78.22(18)
C5_5–C1_5–Ga1	83.2(2)
C10_5–C1_5–Ga1	111.1(2)
C3_5–C2_5–C1_5	107.9(3)
C3_5–C2_5–C9_5	124.9(3)
C1_5–C2_5–C9_5	126.7(3)
C4_5–C3_5–C2_5	108.3(3)
C4_5–C3_5–C8_5	126.1(3)
C2_5–C3_5–C8_5	125.5(3)
C3_5–C4_5–C5_5	108.3(3)
C3_5–C4_5–C7_5	126.2(3)
C5_5–C4_5–C7_5	125.4(3)
C4_5–C5_5–C1_5	108.1(3)
C4_5–C5_5–C6_5	125.0(3)
C1_5–C5_5–C6_5	126.7(3)
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
C5_6–C1_6–C2_6	108.3(3)
C5_6–C1_6–C10_6	124.5(3)
C2_6–C1_6–C10_6	127.0(3)
C5_6–C1_6–Al3	71.99(18)
C2_6–C1_6–Al3	73.83(18)
C10_6–C1_6–Al3	123.3(2)
C1_6–C2_6–C3_6	107.5(3)
C1_6–C2_6–C9_6	125.2(3)
C3_6–C2_6–C9_6	127.0(3)
C1_6–C2_6–Al3	70.84(18)
C3_6–C2_6–Al3	73.32(18)
C9_6–C2_6–Al3	125.3(2)
C4_6–C3_6–C2_6	108.3(3)
C4_6–C3_6–C8_6	126.0(3)
C2_6–C3_6–C8_6	125.4(3)
C4_6–C3_6–Al3	71.45(17)
C2_6–C3_6–Al3	71.68(17)
C8_6–C3_6–Al3	127.9(2)
C3_6–C4_6–C5_6	107.7(3)
C3_6–C4_6–C7_6	126.4(3)
C5_6–C4_6–C7_6	125.9(3)
C3_6–C4_6–Al3	73.59(17)
C5_6–C4_6–Al3	70.80(17)
C7_6–C4_6–Al3	123.6(2)
C1_6–C5_6–C4_6	108.2(3)
C1_6–C5_6–C6_6	124.7(3)
C4_6–C5_6–C6_6	127.0(3)
C1_6–C5_6–Al3	72.43(18)
C4_6–C5_6–Al3	73.72(18)
C6_6–C5_6–Al3	121.5(2)
C5_6–C6_6–H6A_6	109.5
C5_6–C6_6–H6B_6	109.5
H6A_6–C6_6–H6B_6	109.5
C5_6–C6_6–H6C_6	109.5
H6A_6–C6_6–H6C_6	109.5
H6B_6–C6_6–H6C_6	109.5
C4_6–C7_6–H7A_6	109.5
C4_6–C7_6–H7B_6	109.5
H7A_6–C7_6–H7B_6	109.5
C4_6–C7_6–H7C_6	109.5
H7A_6–C7_6–H7C_6	109.5
H7B_6–C7_6–H7C_6	109.5
C3_6–C8_6–H8A_6	109.5
C3_6–C8_6–H8B_6	109.5
H8A_6–C8_6–H8B_6	109.5
C3_6–C8_6–H8C_6	109.5
H8A_6–C8_6–H8C_6	109.5
H8B_6–C8_6–H8C_6	109.5
C2_6–C9_6–H9A_6	109.5
C2_6–C9_6–H9B_6	109.5
H9A_6–C9_6–H9B_6	109.5

C2_6–C9_6–H9C_6	109.5	C3_7–C8_7–H8B_7	109.5
H9A_6–C9_6–H9C_6	109.5	H8A_7–C8_7–H8B_7	109.5
H9B_6–C9_6–H9C_6	109.5	C3_7–C8_7–H8C_7	109.5
C1_6–C10_6–H10A_6	109.5	H8A_7–C8_7–H8C_7	109.5
C1_6–C10_6–H10B_6	109.5	H8B_7–C8_7–H8C_7	109.5
H10A_6–C10_6–H10B_6	109.5	C2_7–C9_7–H9A_7	109.5
		C2_7–C9_7–H9B_7	109.5
C1_6–C10_6–H10C_6	109.5	H9A_7–C9_7–H9B_7	109.5
H10A_6–C10_6–H10C_6	109.5	C2_7–C9_7–H9C_7	109.5
		H9A_7–C9_7–H9C_7	109.5
H10B_6–C10_6–H10C_6	109.5	H9B_7–C9_7–H9C_7	109.5
		C1_7–C10_7–H10A_7	109.5
C2_7–C1_7–C5_7	107.3(4)	C1_7–C10_7–H10B_7	109.5
C2_7–C1_7–C10_7	125.5(5)	H10A_7–C10_7–H10B_7	109.5
C5_7–C1_7–C10_7	127.1(5)		
C2_7–C1_7–Al2	71.0(2)	C1_7–C10_7–H10C_7	109.5
C5_7–C1_7–Al2	69.6(2)	H10A_7–C10_7–H10C_7	109.5
C10_7–C1_7–Al2	128.2(3)		
C1_7–C2_7–C3_7	109.4(4)	H10B_7–C10_7–H10C_7	109.5
C1_7–C2_7–C9_7	125.5(5)		
C3_7–C2_7–C9_7	124.7(5)	C1_8–O1_8–Al4	152.7(11)
C1_7–C2_7–Al2	74.7(2)	O1_8–C1_8–C4_8	111.8(8)
C3_7–C2_7–Al2	68.9(2)	O1_8–C1_8–C2_8	110.0(10)
C9_7–C2_7–Al2	128.2(3)	C4_8–C1_8–C2_8	108.9(8)
C2_7–C3_7–C4_7	107.2(4)	O1_8–C1_8–C3_8	110.5(9)
C2_7–C3_7–C8_7	125.4(5)	C4_8–C1_8–C3_8	108.6(7)
C4_7–C3_7–C8_7	127.3(5)	C2_8–C1_8–C3_8	107.0(7)
C2_7–C3_7–Al2	75.3(3)	F1_8–C2_8–F3_8	106.4(11)
C4_7–C3_7–Al2	70.8(3)	F1_8–C2_8–F2_8	108.6(11)
C8_7–C3_7–Al2	122.0(3)	F3_8–C2_8–F2_8	110.5(12)
C5_7–C4_7–C3_7	107.3(4)	F1_8–C2_8–C1_8	111.0(8)
C5_7–C4_7–C7_7	125.0(5)	F3_8–C2_8–C1_8	110.2(11)
C3_7–C4_7–C7_7	127.7(5)	F2_8–C2_8–C1_8	110.1(10)
C5_7–C4_7–Al2	74.8(3)	F6_8–C3_8–F4_8	107.4(9)
C3_7–C4_7–Al2	72.3(3)	F6_8–C3_8–F5_8	107.9(8)
C7_7–C4_7–Al2	119.5(4)	F4_8–C3_8–F5_8	107.4(9)
C1_7–C5_7–C4_7	108.9(4)	F6_8–C3_8–C1_8	112.3(8)
C1_7–C5_7–C6_7	124.3(5)	F4_8–C3_8–C1_8	111.1(8)
C4_7–C5_7–C6_7	126.7(5)	F5_8–C3_8–C1_8	110.5(8)
C1_7–C5_7–Al2	75.5(3)	F8_8–C4_8–F7_8	107.9(11)
C4_7–C5_7–Al2	69.1(3)	F8_8–C4_8–F9_8	109.0(8)
C6_7–C5_7–Al2	124.8(4)	F7_8–C4_8–F9_8	105.9(10)
C5_7–C6_7–H6A_7	109.5	F8_8–C4_8–C1_8	114.5(7)
C5_7–C6_7–H6B_7	109.5	F7_8–C4_8–C1_8	109.1(9)
H6A_7–C6_7–H6B_7	109.5	F9_8–C4_8–C1_8	110.1(8)
C5_7–C6_7–H6C_7	109.5	C1_9–O1_9–Al4	148.6(11)
H6A_7–C6_7–H6C_7	109.5	O1_9–C1_9–C4_9	112.7(11)
H6B_7–C6_7–H6C_7	109.5	O1_9–C1_9–C3_9	106.0(10)
C4_7–C7_7–H7A_7	109.5	C4_9–C1_9–C3_9	114.2(11)
C4_7–C7_7–H7B_7	109.5	O1_9–C1_9–C2_9	103.8(11)
H7A_7–C7_7–H7B_7	109.5	C4_9–C1_9–C2_9	108.4(11)
C4_7–C7_7–H7C_7	109.5	C3_9–C1_9–C2_9	111.2(11)
H7A_7–C7_7–H7C_7	109.5	F1_9–C2_9–F2_9	116.9(16)
H7B_7–C7_7–H7C_7	109.5	F1_9–C2_9–F3_9	104.6(15)
C3_7–C8_7–H8A_7	109.5	F2_9–C2_9–F3_9	104.7(14)

F1_9–C2_9–C1_9	106.3(14)	C5_11–C6_11–C1_11	120.8(12)
F2_9–C2_9–C1_9	113.4(13)	C5_11–C6_11–H6_11	119.6
F3_9–C2_9–C1_9	110.5(12)	C1_11–C6_11–H6_11	119.6
F6_9–C3_9–F5_9	113.5(15)	C5_10–C1_10–C2_10	108.1(11)
F6_9–C3_9–F4_9	104.5(15)	C5_10–C1_10–C10_10	127.3(15)
F5_9–C3_9–F4_9	104.0(15)	C2_10–C1_10–C10_10	124.6(15)
F6_9–C3_9–C1_9	116.0(14)	C5_10–C1_10–Al2	72.5(10)
F5_9–C3_9–C1_9	108.4(12)	C2_10–C1_10–Al2	70.3(7)
F4_9–C3_9–C1_9	109.7(12)	C10_10–C1_10–Al2	124.1(11)
F8_9–C4_9–F7_9	110.0(15)	C1_10–C2_10–C3_10	108.3(11)
F8_9–C4_9–F9_9	107.6(14)	C1_10–C2_10–C9_10	126.3(16)
F7_9–C4_9–F9_9	95.6(14)	C3_10–C2_10–C9_10	125.1(16)
F8_9–C4_9–C1_9	112.7(13)	C1_10–C2_10–Al2	76.6(7)
F7_9–C4_9–C1_9	114.5(12)	C3_10–C2_10–Al2	70.2(7)
F9_9–C4_9–C1_9	115.0(13)	C9_10–C2_10–Al2	123.0(13)
C1_12–O1_12–Al4	147.1(13)	C4_10–C3_10–C2_10	107.9(11)
O1_12–C1_12–C3_12	113.8(13)	C4_10–C3_10–C8_10	128.2(16)
O1_12–C1_12–C4_12	108.9(11)	C2_10–C3_10–C8_10	124.0(16)
C3_12–C1_12–C4_12	109.1(11)	C4_10–C3_10–Al2	73.7(14)
O1_12–C1_12–C2_12	108.9(12)	C2_10–C3_10–Al2	75.7(7)
C3_12–C1_12–C2_12	108.5(11)	C8_10–C3_10–Al2	117.3(13)
C4_12–C1_12–C2_12	107.4(11)	C3_10–C4_10–C5_10	108.0(11)
F1_12–C2_12–F3_12	109.0(15)	C3_10–C4_10–C7_10	127.7(16)
F1_12–C2_12–F2_12	110.9(15)	C5_10–C4_10–C7_10	124.2(16)
F3_12–C2_12–F2_12	107.9(14)	C3_10–C4_10–Al2	71.9(13)
F1_12–C2_12–C1_12	109.8(13)	C5_10–C4_10–Al2	76.8(14)
F3_12–C2_12–C1_12	108.8(12)	C7_10–C4_10–Al2	119.5(19)
F2_12–C2_12–C1_12	110.3(13)	C1_10–C5_10–C4_10	107.7(11)
F4_12–C3_12–F6_12	107.2(15)	C1_10–C5_10–C6_10	124.9(16)
F4_12–C3_12–F5_12	107.3(16)	C4_10–C5_10–C6_10	127.3(16)
F6_12–C3_12–F5_12	106.1(16)	C1_10–C5_10–Al2	74.8(10)
F4_12–C3_12–C1_12	112.2(15)	C4_10–C5_10–Al2	69.3(14)
F6_12–C3_12–C1_12	112.2(14)	C6_10–C5_10–Al2	124.8(16)
F5_12–C3_12–C1_12	111.4(15)	C5_10–C6_10–H6A_10	109.5
F8_12–C4_12–F9_12	109.0(14)	C5_10–C6_10–H6B_10	109.5
F8_12–C4_12–F7_12	108.4(14)	H6A_10–C6_10–H6B_10	109.5
F9_12–C4_12–F7_12	107.2(14)		
F8_12–C4_12–C1_12	112.0(13)	C5_10–C6_10–H6C_10	109.5
F9_12–C4_12–C1_12	109.6(12)	H6A_10–C6_10–H6C_10	109.5
F7_12–C4_12–C1_12	110.4(12)		
F1_11–C1_11–C6_11	120.0(12)	H6B_10–C6_10–H6C_10	109.5
F1_11–C1_11–C2_11	118.7(13)		
C6_11–C1_11–C2_11	121.3(12)	C4_10–C7_10–H7A_10	109.5
C3_11–C2_11–C1_11	117.3(12)	C4_10–C7_10–H7B_10	109.5
C3_11–C2_11–H2_11	121.4	H7A_10–C7_10–H7B_10	109.5
C1_11–C2_11–H2_11	121.4		
C2_11–C3_11–C4_11	122.6(13)	C4_10–C7_10–H7C_10	109.5
C2_11–C3_11–H3_11	118.7	H7A_10–C7_10–H7C_10	109.5
C4_11–C3_11–H3_11	118.7		
C3_11–C4_11–C5_11	118.2(13)	H7B_10–C7_10–H7C_10	109.5
C3_11–C4_11–H4_11	120.9		
C5_11–C4_11–H4_11	120.9	C3_10–C8_10–H8A_10	109.5
C6_11–C5_11–C4_11	119.8(13)	C3_10–C8_10–H8B_10	109.5
C6_11–C5_11–H5_11	120.1	H8A_10–C8_10–H8B_10	109.5
C4_11–C5_11–H5_11	120.1		

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
C1_13–O1_13–Al4	151.2(9)
O1_13–C1_13–C4_13	113.3(11)
O1_13–C1_13–C3_13	110.2(10)
C4_13–C1_13–C3_13	110.1(10)
O1_13–C1_13–C2_13	105.6(10)
C4_13–C1_13–C2_13	112.6(10)
C3_13–C1_13–C2_13	104.7(9)
F2_13–C2_13–F3_13	105.4(12)
F2_13–C2_13–F1_13	106.9(11)
F3_13–C2_13–F1_13	107.5(12)
F2_13–C2_13–C1_13	111.2(11)
F3_13–C2_13–C1_13	113.4(11)
F1_13–C2_13–C1_13	112.1(10)
F5_13–C3_13–F6_13	107.4(18)
F5_13–C3_13–F4_13	105.5(12)
F6_13–C3_13–F4_13	108.7(18)
F5_13–C3_13–C1_13	113.7(12)
F6_13–C3_13–C1_13	111.2(17)
F4_13–C3_13–C1_13	110.0(11)
F9_13–C4_13–F8_13	103.3(14)
F9_13–C4_13–F7_13	104.2(15)
F8_13–C4_13–F7_13	99.4(13)
F9_13–C4_13–C1_13	112.5(15)
F8_13–C4_13–C1_13	113.7(13)
F7_13–C4_13–C1_13	121.6(14)

S-Table 13: Bond lengths and angles for **6**

Atom–Atom	Length [Å]
Ga1–N4	2.305(6)
Ga1–N3	2.306(5)
Ga1–N1	2.350(7)
Ga1–Al1	2.736(2)
Ga1–Al3	2.744(3)
Ga1–Al2	2.759(2)
Ga2–N2	2.317(6)
Ga2–N5	2.328(7)
Ga2–N6	2.343(7)
Ga2–Al6	2.726(3)
Ga2–Al5	2.728(2)
Ga2–Al4	2.759(3)
Al1–C2_16	2.309(6)
Al1–C3_16	2.338(6)
Al1–C1_16	2.365(6)
Al1–C4_16	2.411(7)
Al1–C5_16	2.421(7)
Al1–Al3	2.765(3)
Al1–Al2	2.783(3)
Al2–C5_15	2.316(8)
Al2–C4_15	2.317(7)
Al2–C3_15	2.332(7)
Al2–C2_15	2.367(7)
Al2–C1_15	2.368(8)
Al2–Al3	2.823(3)
Al3–C3_17	2.288(8)
Al3–C4_17	2.321(8)
Al3–C2_17	2.325(7)
Al3–C5_17	2.393(8)
Al3–C1_17	2.399(7)
Al4–C1_18	2.280(7)
Al4–C5_18	2.315(8)
Al4–C2_18	2.325(6)
Al4–C4_18	2.363(8)
Al4–C3_18	2.367(7)
Al4–Al5	2.788(3)
Al4–Al6	2.833(3)
Al5–C2_19	2.325(6)
Al5–C1_19	2.338(7)
Al5–C3_19	2.380(6)
Al5–C5_19	2.396(6)
Al5–C4_19	2.424(7)
Al5–Al6	2.769(3)
Al6–C1_20	2.286(7)
Al6–C2_20	2.293(7)
Al6–C5_20	2.328(8)
Al6–C3_20	2.378(7)
Al6–C4_20	2.400(9)
Al7–O1_8	1.710(5)
Al7–O1_6	1.719(12)
Al7–O1_5	1.722(5)
Al7–O1_12	1.73(3)
Al7–O1_7	1.739(6)
Al7–O1_14	1.88(3)
Al8–O1_9	1.52(3)
Al8–O1_13	1.618(14)
Al8–O1_4	1.685(18)
Al8–O1_3	1.695(16)
Al8–O1_10	1.70(3)
Al8–O1_2	1.703(9)
Al8–O1_11	1.749(15)
Al8–O1_1	1.756(7)
Al8–O1_21	1.80(2)
N1–C1	1.448(10)
N1–C2	1.474(10)
N1–C9	1.486(10)
N2–C13	1.475(11)
N2–C17	1.482(9)
N2–C12	1.489(11)
C1–H1A	0.9800
C1–H1B	0.9800
C1–H1C	0.9800
C2–C3	1.524(11)
C2–H2A	0.9900
C2–H2B	0.9900
N3–C3	1.453(10)
N3–C5	1.475(8)
N3–C4	1.484(10)
N4–C6	1.466(10)
N4–C8	1.482(10)
N4–C7	1.485(10)
N5–C10	1.471(11)
N5–C11	1.476(10)
N5–C18	1.495(12)
N6–C15	1.452(11)
N6–C14	1.464(10)
N6–C16	1.491(11)
C3–H3A	0.9900
C3–H3B	0.9900
C4–C6	1.531(12)
C4–H4A	0.9900
C4–H4B	0.9900
C5–H5A	0.9800
C5–H5B	0.9800
C5–H5C	0.9800
C6–H6A	0.9900
C6–H6B	0.9900
C7–H7A	0.9800
C7–H7B	0.9800
C7–H7C	0.9800
C8–C9	1.500(12)
C8–H8A	0.9900
C8–H8B	0.9900
C9–H9A	0.9900
C9–H9B	0.9900
C10–H10A	0.9800
C10–H10B	0.9800

C10–H10C	0.9800	C3_3–F4_3	1.328(12)
C11–C12	1.517(13)	C3_3–F5_3	1.334(12)
C11–H11A	0.9900	C3_3–F6_3	1.345(12)
C11–H11B	0.9900	C4_3–F8_3	1.301(12)
C12–H12A	0.9900	C4_3–F7_3	1.323(12)
C12–H12B	0.9900	C4_3–F9_3	1.338(12)
C13–C14	1.513(12)	O1_4–C1_4	1.368(12)
C13–H13A	0.9900	C1_4–C3_4	1.546(12)
C13–H13B	0.9900	C1_4–C2_4	1.549(12)
C14–H14A	0.9900	C1_4–C4_4	1.555(12)
C14–H14B	0.9900	C2_4–F3_4	1.319(13)
C15–H15A	0.9800	C2_4–F2_4	1.329(12)
C15–H15B	0.9800	C2_4–F1_4	1.345(13)
C15–H15C	0.9800	C3_4–F4_4	1.326(12)
C16–C18	1.487(13)	C3_4–F6_4	1.339(12)
C16–H16A	0.9900	C3_4–F5_4	1.339(13)
C16–H16B	0.9900	C4_4–F9_4	1.333(13)
C17–H17A	0.9800	C4_4–F8_4	1.336(12)
C17–H17B	0.9800	C4_4–F7_4	1.345(13)
C17–H17C	0.9800	O1_5–C1_5	1.345(7)
C18–H18A	0.9900	C1_5–C3_5	1.532(8)
C18–H18B	0.9900	C1_5–C4_5	1.558(9)
O1_1–C1_1	1.352(9)	C1_5–C2_5	1.566(9)
C1_1–C3_1	1.540(10)	C2_5–F1_5	1.316(8)
C1_1–C2_1	1.558(9)	C2_5–F2_5	1.326(8)
C1_1–C4_1	1.568(9)	C2_5–F3_5	1.346(9)
C2_1–F1_1	1.313(9)	C3_5–F6_5	1.317(8)
C2_1–F3_1	1.325(9)	C3_5–F4_5	1.332(8)
C2_1–F2_1	1.340(9)	C3_5–F5_5	1.350(9)
C3_1–F6_1	1.324(9)	C4_5–F9_5	1.304(9)
C3_1–F5_1	1.328(9)	C4_5–F7_5	1.345(9)
C3_1–F4_1	1.330(9)	C4_5–F8_5	1.355(8)
C4_1–F9_1	1.318(9)	O1_6–C1_6	1.340(10)
C4_1–F8_1	1.319(9)	C1_6–C4_6	1.544(11)
C4_1–F7_1	1.325(10)	C1_6–C2_6	1.551(11)
O1_2–C1_2	1.373(11)	C1_6–C3_6	1.565(11)
C1_2–C4_2	1.526(12)	C2_6–F1_6	1.320(11)
C1_2–C3_2	1.542(12)	C2_6–F3_6	1.338(11)
C1_2–C2_2	1.556(12)	C2_6–F2_6	1.344(11)
C2_2–F2_2	1.327(12)	C3_6–F6_6	1.319(11)
C2_2–F1_2	1.327(12)	C3_6–F4_6	1.334(11)
C2_2–F3_2	1.335(12)	C3_6–F5_6	1.345(11)
C3_2–F5_2	1.318(12)	C4_6–F8_6	1.338(11)
C3_2–F4_2	1.333(12)	C4_6–F9_6	1.339(11)
C3_2–F6_2	1.335(11)	C4_6–F7_6	1.349(11)
C4_2–F9_2	1.322(12)	O1_7–C1_7	1.367(7)
C4_2–F8_2	1.323(12)	C1_7–C4_7	1.539(9)
C4_2–F7_2	1.349(12)	C1_7–C2_7	1.540(9)
O1_3–C1_3	1.333(12)	C1_7–C3_7	1.560(9)
C1_3–C3_3	1.532(11)	C2_7–F1_7	1.324(8)
C1_3–C2_3	1.544(12)	C2_7–F2_7	1.335(8)
C1_3–C4_3	1.572(12)	C2_7–F3_7	1.340(9)
C2_3–F2_3	1.313(12)	C3_7–F4_7	1.331(8)
C2_3–F3_3	1.323(12)	C3_7–F6_7	1.337(8)
C2_3–F1_3	1.331(12)	C3_7–F5_7	1.337(9)

C4_7–F7_7	1.338(9)	O1_12–C1_12	1.350(14)
C4_7–F9_7	1.340(9)	C1_12–C2_12	1.553(13)
C4_7–F8_7	1.352(8)	C1_12–C3_12	1.554(13)
O1_8–C1_8	1.358(8)	C1_12–C4_12	1.556(13)
C1_8–C4_8	1.542(8)	C2_12–F3_12	1.328(14)
C1_8–C2_8	1.545(8)	C2_12–F1_12	1.338(14)
C1_8–C3_8	1.568(8)	C2_12–F2_12	1.340(14)
C2_8–F3_8	1.318(8)	C3_12–F6_12	1.326(14)
C2_8–F1_8	1.328(8)	C3_12–F4_12	1.329(14)
C2_8–F2_8	1.355(8)	C3_12–F5_12	1.340(14)
C3_8–F6_8	1.308(8)	C4_12–F7_12	1.318(14)
C3_8–F4_8	1.330(7)	C4_12–F8_12	1.327(14)
C3_8–F5_8	1.344(8)	C4_12–F9_12	1.344(14)
C4_8–F9_8	1.325(8)	O1_14–C1_14	1.360(15)
C4_8–F8_8	1.330(8)	C1_14–C2_14	1.543(13)
C4_8–F7_8	1.342(7)	C1_14–C3_14	1.551(13)
O1_9–C1_9	1.366(14)	C1_14–C4_14	1.553(13)
C1_9–C3_9	1.542(13)	C2_14–F2_14	1.331(14)
C1_9–C4_9	1.547(13)	C2_14–F1_14	1.335(14)
C1_9–C2_9	1.556(13)	C2_14–F3_14	1.339(14)
C2_9–F3_9	1.328(14)	C3_14–F5_14	1.327(14)
C2_9–F2_9	1.329(14)	C3_14–F4_14	1.329(14)
C2_9–F1_9	1.339(14)	C3_14–F6_14	1.338(14)
C3_9–F5_9	1.330(14)	C4_14–F8_14	1.324(14)
C3_9–F4_9	1.335(14)	C4_14–F7_14	1.325(14)
C3_9–F6_9	1.343(14)	C4_14–F9_14	1.339(14)
C4_9–F9_9	1.327(14)	C1_15–C5_15	1.409(9)
C4_9–F7_9	1.329(14)	C1_15–C2_15	1.416(8)
C4_9–F8_9	1.329(14)	C1_15–C10_15	1.510(9)
O1_11–C1_11	1.340(12)	C2_15–C3_15	1.421(9)
C1_11–C4_11	1.536(12)	C2_15–C9_15	1.502(9)
C1_11–C3_11	1.547(12)	C3_15–C4_15	1.422(8)
C1_11–C2_11	1.555(12)	C3_15–C8_15	1.500(8)
C2_11–F1_11	1.305(12)	C4_15–C5_15	1.434(8)
C2_11–F2_11	1.322(12)	C4_15–C7_15	1.484(9)
C2_11–F3_11	1.323(12)	C5_15–C6_15	1.500(8)
C3_11–F4_11	1.320(12)	C6_15–H6A_15	0.9800
C3_11–F6_11	1.322(12)	C6_15–H6B_15	0.9800
C3_11–F5_11	1.326(12)	C6_15–H6C_15	0.9800
C4_11–F8_11	1.325(12)	C7_15–H7A_15	0.9800
C4_11–F9_11	1.325(12)	C7_15–H7B_15	0.9800
C4_11–F7_11	1.354(13)	C7_15–H7C_15	0.9800
O1_13–C1_13	1.350(13)	C8_15–H8A_15	0.9800
C1_13–C4_13	1.537(12)	C8_15–H8B_15	0.9800
C1_13–C3_13	1.539(12)	C8_15–H8C_15	0.9800
C1_13–C2_13	1.561(13)	C9_15–H9A_15	0.9800
C2_13–F2_13	1.319(13)	C9_15–H9B_15	0.9800
C2_13–F1_13	1.338(13)	C9_15–H9C_15	0.9800
C2_13–F3_13	1.339(13)	C10_15–H10A_15	0.9800
C3_13–F5_13	1.329(13)	C10_15–H10B_15	0.9800
C3_13–F4_13	1.338(13)	C10_15–H10C_15	0.9800
C3_13–F6_13	1.339(13)	C1_16–C5_16	1.419(8)
C4_13–F9_13	1.330(13)	C1_16–C2_16	1.422(8)
C4_13–F7_13	1.334(13)	C1_16–C10_16	1.510(8)
C4_13–F8_13	1.348(13)	C2_16–C3_16	1.425(8)

C2_16–C9_16	1.494(9)	C5_18–C6_18	1.486(9)
C3_16–C4_16	1.415(9)	C6_18–H6A_18	0.9800
C3_16–C8_16	1.494(8)	C6_18–H6B_18	0.9800
C4_16–C5_16	1.411(8)	C6_18–H6C_18	0.9800
C4_16–C7_16	1.495(9)	C7_18–H7A_18	0.9800
C5_16–C6_16	1.495(9)	C7_18–H7B_18	0.9800
C6_16–H6A_16	0.9800	C7_18–H7C_18	0.9800
C6_16–H6B_16	0.9800	C8_18–H8A_18	0.9800
C6_16–H6C_16	0.9800	C8_18–H8B_18	0.9800
C7_16–H7A_16	0.9800	C8_18–H8C_18	0.9800
C7_16–H7B_16	0.9800	C9_18–H9A_18	0.9800
C7_16–H7C_16	0.9800	C9_18–H9B_18	0.9800
C8_16–H8A_16	0.9800	C9_18–H9C_18	0.9800
C8_16–H8B_16	0.9800	C10_18–H10A_18	0.9800
C8_16–H8C_16	0.9800	C10_18–H10B_18	0.9800
C9_16–H9A_16	0.9800	C10_18–H10C_18	0.9800
C9_16–H9B_16	0.9800	C1_19–C5_19	1.412(8)
C9_16–H9C_16	0.9800	C1_19–C2_19	1.430(8)
C10_16–H10A_16	0.9800	C1_19–C10_19	1.499(9)
C10_16–H10B_16	0.9800	C2_19–C3_19	1.403(9)
C10_16–H10C_16	0.9800	C2_19–C9_19	1.503(8)
C1_17–C5_17	1.402(9)	C3_19–C4_19	1.423(9)
C1_17–C2_17	1.416(8)	C3_19–C8_19	1.516(9)
C1_17–C10_17	1.514(9)	C4_19–C5_19	1.415(8)
C2_17–C3_17	1.412(8)	C4_19–C7_19	1.495(9)
C2_17–C9_17	1.518(8)	C5_19–C6_19	1.504(8)
C3_17–C4_17	1.417(9)	C6_19–H6A_19	0.9800
C3_17–C8_17	1.498(8)	C6_19–H6B_19	0.9800
C4_17–C5_17	1.426(9)	C6_19–H6C_19	0.9800
C4_17–C7_17	1.479(9)	C7_19–H7A_19	0.9800
C5_17–C6_17	1.496(9)	C7_19–H7B_19	0.9800
C6_17–H6A_17	0.9800	C7_19–H7C_19	0.9800
C6_17–H6B_17	0.9800	C8_19–H8A_19	0.9800
C6_17–H6C_17	0.9800	C8_19–H8B_19	0.9800
C7_17–H7A_17	0.9800	C8_19–H8C_19	0.9800
C7_17–H7B_17	0.9800	C9_19–H9A_19	0.9800
C7_17–H7C_17	0.9800	C9_19–H9B_19	0.9800
C8_17–H8A_17	0.9800	C9_19–H9C_19	0.9800
C8_17–H8B_17	0.9800	C10_19–H10A_19	0.9800
C8_17–H8C_17	0.9800	C10_19–H10B_19	0.9800
C9_17–H9A_17	0.9800	C10_19–H10C_19	0.9800
C9_17–H9B_17	0.9800	C1_20–C5_20	1.410(9)
C9_17–H9C_17	0.9800	C1_20–C2_20	1.429(8)
C10_17–H10A_17	0.9800	C1_20–C10_20	1.503(9)
C10_17–H10B_17	0.9800	C2_20–C3_20	1.418(9)
C10_17–H10C_17	0.9800	C2_20–C9_20	1.508(9)
C1_18–C2_18	1.413(8)	C3_20–C4_20	1.415(9)
C1_18–C5_18	1.421(9)	C3_20–C8_20	1.501(9)
C1_18–C10_18	1.525(9)	C4_20–C5_20	1.429(9)
C2_18–C3_18	1.416(8)	C4_20–C7_20	1.496(9)
C2_18–C9_18	1.509(8)	C5_20–C6_20	1.500(9)
C3_18–C4_18	1.412(9)	C6_20–H6A_20	0.9800
C3_18–C8_18	1.512(9)	C6_20–H6B_20	0.9800
C4_18–C5_18	1.416(9)	C6_20–H6C_20	0.9800
C4_18–C7_18	1.502(9)	C7_20–H7A_20	0.9800

C7_20–H7B_20	0.9800
C7_20–H7C_20	0.9800
C8_20–H8A_20	0.9800
C8_20–H8B_20	0.9800
C8_20–H8C_20	0.9800
C9_20–H9A_20	0.9800
C9_20–H9B_20	0.9800
C9_20–H9C_20	0.9800
C10_20–H10A_20	0.9800
C10_20–H10B_20	0.9800
C10_20–H10C_20	0.9800
O1_10–C1_10	1.364(14)
C1_10–C4_10	1.542(13)
C1_10–C2_10	1.546(13)
C1_10–C3_10	1.564(13)
C2_10–F1_10	1.322(13)
C2_10–F2_10	1.329(14)
C2_10–F3_10	1.334(14)
C3_10–F4_10	1.328(13)
C3_10–F6_10	1.334(13)
C3_10–F5_10	1.338(13)
C4_10–F9_10	1.328(13)
C4_10–F8_10	1.330(14)
C4_10–F7_10	1.330(14)
O1_21–C1_21	1.358(14)
C1_21–C2_21	1.541(13)
C1_21–C3_21	1.552(13)
C1_21–C4_21	1.558(13)
C2_21–F1_21	1.323(14)
C2_21–F2_21	1.332(14)
C2_21–F3_21	1.340(14)
C3_21–F4_21	1.327(14)
C3_21–F5_21	1.334(14)
C3_21–F6_21	1.343(14)
C4_21–F8_21	1.299(14)
C4_21–F7_21	1.332(14)
C4_21–F9_21	1.346(14)

Atom–Atom–Atom	**Angle [°]**
N4–Ga1–N3	76.2(2)
N4–Ga1–N1	75.6(2)
N3–Ga1–N1	74.7(2)
N4–Ga1–Al1	111.06(16)
N3–Ga1–Al1	165.80(15)
N1–Ga1–Al1	118.44(16)
N4–Ga1–Al3	111.14(18)
N3–Ga1–Al3	105.67(16)
N1–Ga1–Al3	173.26(17)
Al1–Ga1–Al3	60.59(7)
N4–Ga1–Al2	170.80(17)
N3–Ga1–Al2	110.72(16)
N1–Ga1–Al2	111.70(17)
Al1–Ga1–Al2	60.86(7)
Al3–Ga1–Al2	61.72(7)
N2–Ga2–N5	75.8(2)
N2–Ga2–N6	75.6(2)
N5–Ga2–N6	76.0(2)
N2–Ga2–Al6	105.92(17)
N5–Ga2–Al6	173.3(2)
N6–Ga2–Al6	110.8(2)
N2–Ga2–Al5	166.30(16)
N5–Ga2–Al5	116.62(18)
N6–Ga2–Al5	111.87(17)
Al6–Ga2–Al5	61.03(7)
N2–Ga2–Al4	110.28(18)
N5–Ga2–Al4	111.1(2)
N6–Ga2–Al4	171.49(19)
Al6–Ga2–Al4	62.19(7)
Al5–Ga2–Al4	61.07(7)
C2_16–Al1–C3_16	35.7(2)
C2_16–Al1–C1_16	35.4(2)
C3_16–Al1–C1_16	58.5(2)
C2_16–Al1–C4_16	58.4(2)
C3_16–Al1–C4_16	34.6(2)
C1_16–Al1–C4_16	57.8(2)
C2_16–Al1–C5_16	57.8(2)
C3_16–Al1–C5_16	57.1(2)
C1_16–Al1–C5_16	34.5(2)
C4_16–Al1–C5_16	34.0(2)
C2_16–Al1–Ga1	132.93(18)
C3_16–Al1–Ga1	167.97(19)
C1_16–Al1–Ga1	114.96(16)
C4_16–Al1–Ga1	153.17(19)
C5_16–Al1–Ga1	124.36(17)
C2_16–Al1–Al3	164.02(18)
C3_16–Al1–Al3	130.43(17)
C1_16–Al1–Al3	157.02(19)
C4_16–Al1–Al3	115.44(19)
C5_16–Al1–Al3	126.83(19)
Ga1–Al1–Al3	59.84(6)
C2_16–Al1–Al2	113.98(18)
C3_16–Al1–Al2	117.02(19)
C1_16–Al1–Al2	138.5(2)
C4_16–Al1–Al2	144.30(19)
C5_16–Al1–Al2	171.75(18)
Ga1–Al1–Al2	59.96(7)
Al3–Al1–Al2	61.16(8)
C5_15–Al2–C4_15	36.1(2)
C5_15–Al2–C3_15	59.2(2)
C4_15–Al2–C3_15	35.6(2)
C5_15–Al2–C2_15	58.7(2)
C4_15–Al2–C2_15	59.1(2)
C3_15–Al2–C2_15	35.2(2)
C5_15–Al2–C1_15	35.0(2)
C4_15–Al2–C1_15	58.9(2)
C3_15–Al2–C1_15	58.3(2)
C2_15–Al2–C1_15	34.8(2)
C5_15–Al2–Ga1	155.3(2)
C4_15–Al2–Ga1	165.69(19)
C3_15–Al2–Ga1	132.02(19)

C2_15–Al2–Ga1	115.55(19)	C2_18–Al4–Ga2	132.65(19)
C1_15–Al2–Ga1	125.6(2)	C4_18–Al4–Ga2	125.6(2)
C5_15–Al2–Al1	114.9(2)	C3_18–Al4–Ga2	116.61(19)
C4_15–Al2–Al1	131.67(19)	C1_18–Al4–Al5	131.06(19)
C3_15–Al2–Al1	165.7(2)	C5_18–Al4–Al5	114.7(2)
C2_15–Al2–Al1	155.7(2)	C2_18–Al4–Al5	165.0(2)
C1_15–Al2–Al1	125.65(19)	C4_18–Al4–Al5	125.7(2)
Ga1–Al2–Al1	59.17(6)	C3_18–Al4–Al5	156.4(2)
C5_15–Al2–Al3	142.0(2)	Ga2–Al4–Al5	58.91(7)
C4_15–Al2–Al3	115.9(2)	C1_18–Al4–Al6	116.0(2)
C3_15–Al2–Al3	116.3(2)	C5_18–Al4–Al6	142.4(2)
C2_15–Al2–Al3	141.7(2)	C2_18–Al4–Al6	116.0(2)
C1_15–Al2–Al3	174.3(2)	C4_18–Al4–Al6	174.6(2)
Ga1–Al2–Al3	58.89(7)	C3_18–Al4–Al6	141.6(2)
Al1–Al2–Al3	59.09(8)	Ga2–Al4–Al6	58.32(8)
C3_17–Al3–C4_17	35.8(2)	Al5–Al4–Al6	59.02(8)
C3_17–Al3–C2_17	35.6(2)	C2_19–Al5–C1_19	35.7(2)
C4_17–Al3–C2_17	58.8(2)	C2_19–Al5–C3_19	34.7(2)
C3_17–Al3–C5_17	58.8(2)	C1_19–Al5–C3_19	58.0(2)
C4_17–Al3–C5_17	35.2(2)	C2_19–Al5–C5_19	58.0(2)
C2_17–Al3–C5_17	57.8(2)	C1_19–Al5–C5_19	34.7(2)
C3_17–Al3–C1_17	58.5(2)	C3_19–Al5–C5_19	57.0(2)
C4_17–Al3–C1_17	57.9(3)	C2_19–Al5–C4_19	57.9(2)
C2_17–Al3–C1_17	34.8(2)	C1_19–Al5–C4_19	57.8(2)
C5_17–Al3–C1_17	34.0(2)	C3_19–Al5–C4_19	34.5(2)
C3_17–Al3–Ga1	171.8(2)	C5_19–Al5–C4_19	34.1(2)
C4_17–Al3–Ga1	151.0(2)	C2_19–Al5–Ga2	169.6(2)
C2_17–Al3–Ga1	137.4(2)	C1_19–Al5–Ga2	134.19(18)
C5_17–Al3–Ga1	124.0(2)	C3_19–Al5–Ga2	151.1(2)
C1_17–Al3–Ga1	118.57(19)	C5_19–Al5–Ga2	115.44(16)
C3_17–Al3–Al1	116.28(19)	C4_19–Al5–Ga2	122.20(19)
C4_17–Al3–Al1	145.6(2)	C2_19–Al5–Al6	129.86(18)
C2_17–Al3–Al1	112.59(19)	C1_19–Al5–Al6	163.29(18)
C5_17–Al3–Al1	169.8(2)	C3_19–Al5–Al6	115.8(2)
C1_17–Al3–Al1	136.0(2)	C5_19–Al5–Al6	158.3(2)
Ga1–Al3–Al1	59.57(6)	C4_19–Al5–Al6	127.5(2)
C3_17–Al3–Al2	126.0(2)	Ga2–Al5–Al6	59.45(7)
C4_17–Al3–Al2	114.4(2)	C2_19–Al5–Al4	118.1(2)
C2_17–Al3–Al2	158.2(2)	C1_19–Al5–Al4	114.0(2)
C5_17–Al3–Al2	130.5(2)	C3_19–Al5–Al4	146.5(2)
C1_17–Al3–Al2	162.8(2)	C5_19–Al5–Al4	137.21(19)
Ga1–Al3–Al2	59.39(7)	C4_19–Al5–Al4	171.2(2)
Al1–Al3–Al2	59.75(8)	Ga2–Al5–Al4	60.02(7)
C1_18–Al4–C5_18	36.0(2)	Al6–Al5–Al4	61.30(8)
C1_18–Al4–C2_18	35.7(2)	C1_20–Al6–C2_20	36.4(2)
C5_18–Al4–C2_18	59.3(2)	C1_20–Al6–C5_20	35.6(2)
C1_18–Al4–C4_18	59.2(3)	C2_20–Al6–C5_20	59.2(2)
C5_18–Al4–C4_18	35.2(2)	C1_20–Al6–C3_20	59.3(2)
C2_18–Al4–C4_18	58.7(2)	C2_20–Al6–C3_20	35.3(2)
C1_18–Al4–C3_18	58.7(2)	C5_20–Al6–C3_20	58.1(2)
C5_18–Al4–C3_18	58.3(2)	C1_20–Al6–C4_20	59.1(3)
C2_18–Al4–C3_18	35.1(2)	C2_20–Al6–C4_20	58.6(3)
C4_18–Al4–C3_18	34.7(2)	C5_20–Al6–C4_20	35.1(2)
C1_18–Al4–Ga2	166.3(2)	C3_20–Al6–C4_20	34.4(2)
C5_18–Al4–Ga2	155.3(2)	C1_20–Al6–Ga2	170.1(2)

C2_20–Al6–Ga2	151.5(2)	C3–C2–H2A	109.3
C5_20–Al6–Ga2	135.9(2)	N1–C2–H2B	109.3
C3_20–Al6–Ga2	123.59(19)	C3–C2–H2B	109.3
C4_20–Al6–Ga2	117.0(2)	H2A–C2–H2B	108.0
C1_20–Al6–Al5	116.2(2)	C3–N3–C5	110.2(6)
C2_20–Al6–Al5	145.1(2)	C3–N3–C4	113.4(6)
C5_20–Al6–Al5	113.7(2)	C5–N3–C4	108.2(6)
C3_20–Al6–Al5	171.4(2)	C3–N3–Ga1	114.0(4)
C4_20–Al6–Al5	137.3(2)	C5–N3–Ga1	107.6(4)
Ga2–Al6–Al5	59.52(7)	C4–N3–Ga1	103.0(4)
C1_20–Al6–Al4	127.5(2)	C6–N4–C8	113.7(7)
C2_20–Al6–Al4	114.3(2)	C6–N4–C7	111.7(6)
C5_20–Al6–Al4	160.3(2)	C8–N4–C7	109.2(6)
C3_20–Al6–Al4	128.9(2)	C6–N4–Ga1	110.8(5)
C4_20–Al6–Al4	160.7(2)	C8–N4–Ga1	103.5(5)
Ga2–Al6–Al4	59.48(8)	C7–N4–Ga1	107.5(5)
Al5–Al6–Al4	59.68(9)	C10–N5–C11	109.0(7)
O1_8–Al7–O1_6	112.7(5)	C10–N5–C18	110.7(7)
O1_8–Al7–O1_5	107.2(3)	C11–N5–C18	112.5(7)
O1_6–Al7–O1_5	110.8(5)	C10–N5–Ga2	109.3(5)
O1_8–Al7–O1_7	109.0(3)	C11–N5–Ga2	103.3(5)
O1_6–Al7–O1_7	104.7(5)	C18–N5–Ga2	111.8(5)
O1_5–Al7–O1_7	112.5(3)	C15–N6–C14	111.1(7)
O1_9–Al8–O1_13	123.2(15)	C15–N6–C16	110.9(7)
O1_4–Al8–O1_3	106.2(11)	C14–N6–C16	112.3(7)
O1_4–Al8–O1_2	108.4(9)	C15–N6–Ga2	108.3(5)
O1_3–Al8–O1_2	107.7(9)	C14–N6–Ga2	111.1(5)
O1_9–Al8–O1_11	98.1(15)	C16–N6–Ga2	102.7(5)
O1_13–Al8–O1_11	108.5(10)	N3–C3–C2	111.1(6)
O1_4–Al8–O1_1	109.0(9)	N3–C3–H3A	109.4
O1_3–Al8–O1_1	113.9(7)	C2–C3–H3A	109.4
O1_2–Al8–O1_1	111.3(6)	N3–C3–H3B	109.4
O1_9–Al8–O1_21	110.6(16)	C2–C3–H3B	109.4
O1_13–Al8–O1_21	99.7(12)	H3A–C3–H3B	108.0
O1_11–Al8–O1_21	118.0(12)	N3–C4–C6	109.4(6)
C1–N1–C2	110.3(7)	N3–C4–H4A	109.8
C1–N1–C9	110.7(6)	C6–C4–H4A	109.8
C2–N1–C9	112.2(7)	N3–C4–H4B	109.8
C1–N1–Ga1	108.6(5)	C6–C4–H4B	109.8
C2–N1–Ga1	103.9(5)	H4A–C4–H4B	108.2
C9–N1–Ga1	111.0(5)	N3–C5–H5A	109.5
C13–N2–C17	110.9(7)	N3–C5–H5B	109.5
C13–N2–C12	114.7(7)	H5A–C5–H5B	109.5
C17–N2–C12	109.0(7)	N3–C5–H5C	109.5
C13–N2–Ga2	103.2(5)	H5A–C5–H5C	109.5
C17–N2–Ga2	106.7(4)	H5B–C5–H5C	109.5
C12–N2–Ga2	111.9(5)	N4–C6–C4	112.8(6)
N1–C1–H1A	109.5	N4–C6–H6A	109.0
N1–C1–H1B	109.5	C4–C6–H6A	109.0
H1A–C1–H1B	109.5	N4–C6–H6B	109.0
N1–C1–H1C	109.5	C4–C6–H6B	109.0
H1A–C1–H1C	109.5	H6A–C6–H6B	107.8
H1B–C1–H1C	109.5	N4–C7–H7A	109.5
N1–C2–C3	111.5(7)	N4–C7–H7B	109.5
N1–C2–H2A	109.3	H7A–C7–H7B	109.5

N4–C7–H7C	109.5	N6–C16–H16B	108.8
H7A–C7–H7C	109.5	H16A–C16–H16B	107.7
H7B–C7–H7C	109.5	N2–C17–H17A	109.5
N4–C8–C9	112.0(7)	N2–C17–H17B	109.5
N4–C8–H8A	109.2	H17A–C17–H17B	109.5
C9–C8–H8A	109.2	N2–C17–H17C	109.5
N4–C8–H8B	109.2	H17A–C17–H17C	109.5
C9–C8–H8B	109.2	H17B–C17–H17C	109.5
H8A–C8–H8B	107.9	C16–C18–N5	111.2(7)
N1–C9–C8	110.8(7)	C16–C18–H18A	109.4
N1–C9–H9A	109.5	N5–C18–H18A	109.4
C8–C9–H9A	109.5	C16–C18–H18B	109.4
N1–C9–H9B	109.5	N5–C18–H18B	109.4
C8–C9–H9B	109.5	H18A–C18–H18B	108.0
H9A–C9–H9B	108.1	C1_1–O1_1–Al8	148.4(6)
N5–C10–H10A	109.5	O1_1–C1_1–C3_1	107.7(6)
N5–C10–H10B	109.5	O1_1–C1_1–C2_1	110.6(7)
H10A–C10–H10B	109.5	C3_1–C1_1–C2_1	108.9(6)
N5–C10–H10C	109.5	O1_1–C1_1–C4_1	111.4(7)
H10A–C10–H10C	109.5	C3_1–C1_1–C4_1	109.8(7)
H10B–C10–H10C	109.5	C2_1–C1_1–C4_1	108.3(6)
N5–C11–C12	112.4(7)	F1_1–C2_1–F3_1	107.9(8)
N5–C11–H11A	109.1	F1_1–C2_1–F2_1	108.0(7)
C12–C11–H11A	109.1	F3_1–C2_1–F2_1	106.5(8)
N5–C11–H11B	109.1	F1_1–C2_1–C1_1	111.6(7)
C12–C11–H11B	109.1	F3_1–C2_1–C1_1	111.2(7)
H11A–C11–H11B	107.9	F2_1–C2_1–C1_1	111.4(7)
N2–C12–C11	111.5(7)	F6_1–C3_1–F5_1	107.5(7)
N2–C12–H12A	109.3	F6_1–C3_1–F4_1	107.3(7)
C11–C12–H12A	109.3	F5_1–C3_1–F4_1	106.5(7)
N2–C12–H12B	109.3	F6_1–C3_1–C1_1	114.1(7)
C11–C12–H12B	109.3	F5_1–C3_1–C1_1	111.3(7)
H12A–C12–H12B	108.0	F4_1–C3_1–C1_1	109.8(7)
N2–C13–C14	112.0(7)	F9_1–C4_1–F8_1	109.9(8)
N2–C13–H13A	109.2	F9_1–C4_1–F7_1	107.4(8)
C14–C13–H13A	109.2	F8_1–C4_1–F7_1	106.8(8)
N2–C13–H13B	109.2	F9_1–C4_1–C1_1	110.3(7)
C14–C13–H13B	109.2	F8_1–C4_1–C1_1	111.5(7)
H13A–C13–H13B	107.9	F7_1–C4_1–C1_1	110.8(7)
N6–C14–C13	111.9(7)	C1_2–O1_2–Al8	149.2(9)
N6–C14–H14A	109.2	O1_2–C1_2–C4_2	114.1(11)
C13–C14–H14A	109.2	O1_2–C1_2–C3_2	112.1(9)
N6–C14–H14B	109.2	C4_2–C1_2–C3_2	109.8(9)
C13–C14–H14B	109.2	O1_2–C1_2–C2_2	101.4(9)
H14A–C14–H14B	107.9	C4_2–C1_2–C2_2	109.8(9)
N6–C15–H15A	109.5	C3_2–C1_2–C2_2	109.2(9)
N6–C15–H15B	109.5	F2_2–C2_2–F1_2	109.6(12)
H15A–C15–H15B	109.5	F2_2–C2_2–F3_2	106.3(12)
N6–C15–H15C	109.5	F1_2–C2_2–F3_2	107.9(12)
H15A–C15–H15C	109.5	F2_2–C2_2–C1_2	112.5(11)
H15B–C15–H15C	109.5	F1_2–C2_2–C1_2	111.7(10)
C18–C16–N6	113.6(7)	F3_2–C2_2–C1_2	108.5(10)
C18–C16–H16A	108.8	F5_2–C3_2–F4_2	109.3(11)
N6–C16–H16A	108.8	F5_2–C3_2–F6_2	107.7(11)
C18–C16–H16B	108.8	F4_2–C3_2–F6_2	107.9(11)

F5_2–C3_2–C1_2	113.1(10)	F8_4–C4_4–F7_4	109.3(13)
F4_2–C3_2–C1_2	106.8(9)	F9_4–C4_4–C1_4	115.2(12)
F6_2–C3_2–C1_2	111.9(11)	F8_4–C4_4–C1_4	108.9(12)
F9_2–C4_2–F8_2	106.1(12)	F7_4–C4_4–C1_4	111.9(12)
F9_2–C4_2–F7_2	104.2(12)	C1_5–O1_5–Al7	150.1(5)
F8_2–C4_2–F7_2	109.1(12)	O1_5–C1_5–C3_5	111.2(6)
F9_2–C4_2–C1_2	111.9(11)	O1_5–C1_5–C4_5	107.8(6)
F8_2–C4_2–C1_2	112.0(11)	C3_5–C1_5–C4_5	109.2(6)
F7_2–C4_2–C1_2	113.0(11)	O1_5–C1_5–C2_5	109.9(6)
C1_3–O1_3–Al8	156.5(17)	C3_5–C1_5–C2_5	110.3(6)
O1_3–C1_3–C3_3	111.2(12)	C4_5–C1_5–C2_5	108.3(6)
O1_3–C1_3–C2_3	107.2(11)	F1_5–C2_5–F2_5	109.3(6)
C3_3–C1_3–C2_3	110.1(9)	F1_5–C2_5–F3_5	108.6(6)
O1_3–C1_3–C4_3	110.8(12)	F2_5–C2_5–F3_5	107.6(7)
C3_3–C1_3–C4_3	108.1(9)	F1_5–C2_5–C1_5	111.0(6)
C2_3–C1_3–C4_3	109.4(9)	F2_5–C2_5–C1_5	111.4(6)
F2_3–C2_3–F3_3	112.3(12)	F3_5–C2_5–C1_5	108.9(6)
F2_3–C2_3–F1_3	102.4(11)	F6_5–C3_5–F4_5	108.8(7)
F3_3–C2_3–F1_3	107.3(11)	F6_5–C3_5–F5_5	107.8(7)
F2_3–C2_3–C1_3	112.7(10)	F4_5–C3_5–F5_5	105.1(7)
F3_3–C2_3–C1_3	110.7(10)	F6_5–C3_5–C1_5	112.9(6)
F1_3–C2_3–C1_3	111.0(10)	F4_5–C3_5–C1_5	111.0(6)
F4_3–C3_3–F5_3	105.7(12)	F5_5–C3_5–C1_5	110.9(6)
F4_3–C3_3–F6_3	107.1(12)	F9_5–C4_5–F7_5	107.5(7)
F5_3–C3_3–F6_3	105.5(12)	F9_5–C4_5–F8_5	107.9(7)
F4_3–C3_3–C1_3	113.1(12)	F7_5–C4_5–F8_5	106.1(7)
F5_3–C3_3–C1_3	112.1(10)	F9_5–C4_5–C1_5	112.2(6)
F6_3–C3_3–C1_3	112.8(10)	F7_5–C4_5–C1_5	111.2(7)
F8_3–C4_3–F7_3	114.1(13)	F8_5–C4_5–C1_5	111.6(7)
F8_3–C4_3–F9_3	105.6(12)	C1_6–O1_6–Al7	146.2(11)
F7_3–C4_3–F9_3	105.6(12)	O1_6–C1_6–C4_6	113.2(9)
F8_3–C4_3–C1_3	112.7(11)	O1_6–C1_6–C2_6	107.1(9)
F7_3–C4_3–C1_3	108.9(11)	C4_6–C1_6–C2_6	108.2(8)
F9_3–C4_3–C1_3	109.4(10)	O1_6–C1_6–C3_6	110.2(9)
C1_4–O1_4–Al8	152.3(19)	C4_6–C1_6–C3_6	108.7(8)
O1_4–C1_4–C3_4	112.8(13)	C2_6–C1_6–C3_6	109.4(8)
O1_4–C1_4–C2_4	109.7(13)	F1_6–C2_6–F3_6	106.7(9)
C3_4–C1_4–C2_4	110.4(10)	F1_6–C2_6–F2_6	110.7(10)
O1_4–C1_4–C4_4	103.9(13)	F3_6–C2_6–F2_6	104.1(9)
C3_4–C1_4–C4_4	109.4(10)	F1_6–C2_6–C1_6	110.9(9)
C2_4–C1_4–C4_4	110.6(10)	F3_6–C2_6–C1_6	111.5(9)
F3_4–C2_4–F2_4	107.4(12)	F2_6–C2_6–C1_6	112.7(9)
F3_4–C2_4–F1_4	107.2(13)	F6_6–C3_6–F4_6	109.4(9)
F2_4–C2_4–F1_4	105.3(12)	F6_6–C3_6–F5_6	108.3(9)
F3_4–C2_4–C1_4	111.5(11)	F4_6–C3_6–F5_6	105.6(9)
F2_4–C2_4–C1_4	115.5(12)	F6_6–C3_6–C1_6	113.4(9)
F1_4–C2_4–C1_4	109.5(12)	F4_6–C3_6–C1_6	110.2(8)
F4_4–C3_4–F6_4	111.3(13)	F5_6–C3_6–C1_6	109.6(8)
F4_4–C3_4–F5_4	107.7(13)	F8_6–C4_6–F9_6	109.7(10)
F6_4–C3_4–F5_4	107.5(13)	F8_6–C4_6–F7_6	105.6(10)
F4_4–C3_4–C1_4	110.2(12)	F9_6–C4_6–F7_6	107.3(10)
F6_4–C3_4–C1_4	110.3(11)	F8_6–C4_6–C1_6	112.6(9)
F5_4–C3_4–C1_4	109.8(12)	F9_6–C4_6–C1_6	109.7(9)
F9_4–C4_4–F8_4	106.6(12)	F7_6–C4_6–C1_6	111.8(9)
F9_4–C4_4–F7_4	104.6(13)	C1_7–O1_7–Al7	150.0(5)

O1_7–C1_7–C4_7	108.4(6)	C4_9–C1_9–C2_9	109.5(14)
O1_7–C1_7–C2_7	111.3(6)	F3_9–C2_9–F2_9	108.3(19)
C4_7–C1_7–C2_7	109.5(6)	F3_9–C2_9–F1_9	107(2)
O1_7–C1_7–C3_7	110.1(6)	F2_9–C2_9–F1_9	108(2)
C4_7–C1_7–C3_7	108.3(6)	F3_9–C2_9–C1_9	112.1(17)
C2_7–C1_7–C3_7	109.1(6)	F2_9–C2_9–C1_9	113.4(18)
F1_7–C2_7–F2_7	108.4(7)	F1_9–C2_9–C1_9	107.0(18)
F1_7–C2_7–F3_7	105.2(6)	F5_9–C3_9–F4_9	108(2)
F2_7–C2_7–F3_7	108.2(7)	F5_9–C3_9–F6_9	106(2)
F1_7–C2_7–C1_7	111.1(6)	F4_9–C3_9–F6_9	105.8(19)
F2_7–C2_7–C1_7	113.5(6)	F5_9–C3_9–C1_9	113(2)
F3_7–C2_7–C1_7	110.1(6)	F4_9–C3_9–C1_9	112.1(18)
F4_7–C3_7–F6_7	106.7(6)	F6_9–C3_9–C1_9	112.1(18)
F4_7–C3_7–F5_7	107.8(7)	F9_9–C4_9–F7_9	105.4(19)
F6_7–C3_7–F5_7	108.0(7)	F9_9–C4_9–F8_9	109(2)
F4_7–C3_7–C1_7	111.6(6)	F7_9–C4_9–F8_9	105.0(19)
F6_7–C3_7–C1_7	111.4(6)	F9_9–C4_9–C1_9	111.6(17)
F5_7–C3_7–C1_7	111.0(6)	F7_9–C4_9–C1_9	112.7(17)
F7_7–C4_7–F9_7	108.3(7)	F8_9–C4_9–C1_9	112.4(17)
F7_7–C4_7–F8_7	108.0(7)	C1_11–O1_11–Al8	144.1(13)
F9_7–C4_7–F8_7	106.8(7)	O1_11–C1_11–C4_11	112.4(11)
F7_7–C4_7–C1_7	110.1(7)	O1_11–C1_11–C3_11	105.2(12)
F9_7–C4_7–C1_7	110.8(6)	C4_11–C1_11–C3_11	108.4(9)
F8_7–C4_7–C1_7	112.7(7)	O1_11–C1_11–C2_11	109.5(11)
C1_8–O1_8–Al7	146.7(5)	C4_11–C1_11–C2_11	113.6(10)
O1_8–C1_8–C4_8	110.8(5)	C3_11–C1_11–C2_11	107.3(9)
O1_8–C1_8–C2_8	107.0(6)	F1_11–C2_11–F2_11	111.5(12)
C4_8–C1_8–C2_8	109.9(5)	F1_11–C2_11–F3_11	105.8(14)
O1_8–C1_8–C3_8	111.1(5)	F2_11–C2_11–F3_11	105.5(13)
C4_8–C1_8–C3_8	109.1(5)	F1_11–C2_11–C1_11	109.6(11)
C2_8–C1_8–C3_8	108.8(5)	F2_11–C2_11–C1_11	110.6(11)
F3_8–C2_8–F1_8	107.0(7)	F3_11–C2_11–C1_11	113.6(12)
F3_8–C2_8–F2_8	108.2(6)	F4_11–C3_11–F6_11	105.0(12)
F1_8–C2_8–F2_8	106.9(6)	F4_11–C3_11–F5_11	108.6(12)
F3_8–C2_8–C1_8	111.5(6)	F6_11–C3_11–F5_11	107.5(12)
F1_8–C2_8–C1_8	111.3(6)	F4_11–C3_11–C1_11	111.6(10)
F2_8–C2_8–C1_8	111.7(6)	F6_11–C3_11–C1_11	113.7(10)
F6_8–C3_8–F4_8	108.5(6)	F5_11–C3_11–C1_11	110.2(12)
F6_8–C3_8–F5_8	108.2(6)	F8_11–C4_11–F9_11	109.9(11)
F4_8–C3_8–F5_8	106.2(6)	F8_11–C4_11–F7_11	98.9(12)
F6_8–C3_8–C1_8	113.8(6)	F9_11–C4_11–F7_11	106.2(12)
F4_8–C3_8–C1_8	110.2(5)	F8_11–C4_11–C1_11	115.6(11)
F5_8–C3_8–C1_8	109.5(6)	F9_11–C4_11–C1_11	113.7(11)
F9_8–C4_8–F8_8	107.7(6)	F7_11–C4_11–C1_11	111.2(10)
F9_8–C4_8–F7_8	107.6(6)	C1_13–O1_13–Al8	169.0(18)
F8_8–C4_8–F7_8	106.1(6)	O1_13–C1_13–C4_13	108.9(12)
F9_8–C4_8–C1_8	110.7(6)	O1_13–C1_13–C3_13	112.5(12)
F8_8–C4_8–C1_8	113.6(5)	C4_13–C1_13–C3_13	110.2(11)
F7_8–C4_8–C1_8	110.8(5)	O1_13–C1_13–C2_13	104.4(13)
C1_9–O1_9–Al8	149(3)	C4_13–C1_13–C2_13	111.3(11)
O1_9–C1_9–C3_9	111.0(17)	C3_13–C1_13–C2_13	109.5(11)
O1_9–C1_9–C4_9	108.3(17)	F2_13–C2_13–F1_13	110.0(14)
C3_9–C1_9–C4_9	109.9(14)	F2_13–C2_13–F3_13	107.3(13)
O1_9–C1_9–C2_9	106.2(16)	F1_13–C2_13–F3_13	105.8(14)
C3_9–C1_9–C2_9	111.7(14)	F2_13–C2_13–C1_13	114.5(13)

F1_13–C2_13–C1_13	106.4(13)	F5_14–C3_14–C1_14	112.5(18)
F3_13–C2_13–C1_13	112.6(12)	F4_14–C3_14–C1_14	111.5(18)
F5_13–C3_13–F4_13	107.0(14)	F6_14–C3_14–C1_14	111.0(18)
F5_13–C3_13–F6_13	103.7(13)	F8_14–C4_14–F7_14	108(2)
F4_13–C3_13–F6_13	104.6(13)	F8_14–C4_14–F9_14	109(2)
F5_13–C3_13–C1_13	112.1(12)	F7_14–C4_14–F9_14	104(2)
F4_13–C3_13–C1_13	116.6(13)	F8_14–C4_14–C1_14	111.5(18)
F6_13–C3_13–C1_13	111.8(12)	F7_14–C4_14–C1_14	113.3(19)
F9_13–C4_13–F7_13	106.2(14)	F9_14–C4_14–C1_14	111.3(18)
F9_13–C4_13–F8_13	106.6(14)	C5_15–C1_15–C2_15	108.6(6)
F7_13–C4_13–F8_13	107.4(14)	C5_15–C1_15–C10_15	125.8(7)
F9_13–C4_13–C1_13	116.6(13)	C2_15–C1_15–C10_15	125.5(7)
F7_13–C4_13–C1_13	110.2(12)	C5_15–C1_15–Al2	70.5(4)
F8_13–C4_13–C1_13	109.4(12)	C2_15–C1_15–Al2	72.6(4)
C1_12–O1_12–Al7	146(3)	C10_15–C1_15–Al2	125.5(5)
O1_12–C1_12–C2_12	112.4(19)	C1_15–C2_15–C3_15	107.6(6)
O1_12–C1_12–C3_12	106.5(18)	C1_15–C2_15–C9_15	126.5(7)
C2_12–C1_12–C3_12	108.4(13)	C3_15–C2_15–C9_15	125.3(7)
O1_12–C1_12–C4_12	111.6(18)	C1_15–C2_15–Al2	72.6(4)
C2_12–C1_12–C4_12	106.8(12)	C3_15–C2_15–Al2	71.0(4)
C3_12–C1_12–C4_12	111.2(13)	C9_15–C2_15–Al2	128.9(5)
F3_12–C2_12–F1_12	115.7(19)	C2_15–C3_15–C4_15	108.6(6)
F3_12–C2_12–F2_12	104.8(17)	C2_15–C3_15–C8_15	124.6(6)
F1_12–C2_12–F2_12	106.8(18)	C4_15–C3_15–C8_15	126.7(6)
F3_12–C2_12–C1_12	109.1(15)	C2_15–C3_15–Al2	73.7(4)
F1_12–C2_12–C1_12	108.1(17)	C4_15–C3_15–Al2	71.6(4)
F2_12–C2_12–C1_12	112.4(17)	C8_15–C3_15–Al2	124.1(5)
F6_12–C3_12–F4_12	115(2)	C3_15–C4_15–C5_15	107.0(6)
F6_12–C3_12–F5_12	106.9(19)	C3_15–C4_15–C7_15	128.6(6)
F4_12–C3_12–F5_12	105.3(17)	C5_15–C4_15–C7_15	124.3(6)
F6_12–C3_12–C1_12	110.8(18)	C3_15–C4_15–Al2	72.8(4)
F4_12–C3_12–C1_12	109.4(15)	C5_15–C4_15–Al2	71.9(4)
F5_12–C3_12–C1_12	109.4(16)	C7_15–C4_15–Al2	122.5(5)
F7_12–C4_12–F8_12	111.4(18)	C1_15–C5_15–C4_15	108.2(6)
F7_12–C4_12–F9_12	109.6(18)	C1_15–C5_15–C6_15	127.8(7)
F8_12–C4_12–F9_12	104.8(18)	C4_15–C5_15–C6_15	123.5(7)
F7_12–C4_12–C1_12	109.6(16)	C1_15–C5_15–Al2	74.5(4)
F8_12–C4_12–C1_12	111.9(16)	C4_15–C5_15–Al2	72.0(4)
F9_12–C4_12–C1_12	109.5(15)	C6_15–C5_15–Al2	126.1(6)
C1_14–O1_14–Al7	162(3)	C5_15–C6_15–H6A_15	109.5
O1_14–C1_14–C2_14	110.1(17)	C5_15–C6_15–H6B_15	109.5
O1_14–C1_14–C3_14	107.5(17)	H6A_15–C6_15–H6B_15	109.5
C2_14–C1_14–C3_14	110.2(14)		
O1_14–C1_14–C4_14	106.4(17)	C5_15–C6_15–H6C_15	109.5
C2_14–C1_14–C4_14	113.1(14)	H6A_15–C6_15–H6C_15	109.5
C3_14–C1_14–C4_14	109.4(14)		
F2_14–C2_14–F1_14	106.4(19)	H6B_15–C6_15–H6C_15	109.5
F2_14–C2_14–F3_14	104.4(19)		
F1_14–C2_14–F3_14	105.0(19)	C4_15–C7_15–H7A_15	109.5
F2_14–C2_14–C1_14	114.0(18)	C4_15–C7_15–H7B_15	109.5
F1_14–C2_14–C1_14	114.5(19)	H7A_15–C7_15–H7B_15	109.5
F3_14–C2_14–C1_14	111.7(18)		
F5_14–C3_14–F4_14	108(2)	C4_15–C7_15–H7C_15	109.5
F5_14–C3_14–F6_14	107(2)	H7A_15–C7_15–H7C_15	109.5
F4_14–C3_14–F6_14	106(2)		

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
C5_16–C1_16–C2_16	107.3(5)
C5_16–C1_16–C10_16	126.5(6)
C2_16–C1_16–C10_16	125.9(6)
C5_16–C1_16–Al1	75.0(4)
C2_16–C1_16–Al1	70.1(3)
C10_16–C1_16–Al1	125.8(4)
C1_16–C2_16–C3_16	107.7(6)
C1_16–C2_16–C9_16	124.8(6)
C3_16–C2_16–C9_16	127.4(6)
C1_16–C2_16–Al1	74.5(3)
C3_16–C2_16–Al1	73.3(3)
C9_16–C2_16–Al1	121.2(4)
C4_16–C3_16–C2_16	108.6(5)
C4_16–C3_16–C8_16	124.8(6)
C2_16–C3_16–C8_16	126.6(7)
C4_16–C3_16–Al1	75.5(4)
C2_16–C3_16–Al1	71.0(3)
C8_16–C3_16–Al1	120.8(4)
C5_16–C4_16–C3_16	107.3(6)
C5_16–C4_16–C7_16	126.7(7)
C3_16–C4_16–C7_16	125.6(7)
C5_16–C4_16–Al1	73.4(4)
C3_16–C4_16–Al1	69.8(4)
C7_16–C4_16–Al1	127.5(5)
C4_16–C5_16–C1_16	109.2(6)
C4_16–C5_16–C6_16	125.5(7)
C1_16–C5_16–C6_16	125.1(6)
C4_16–C5_16–Al1	72.6(4)
C1_16–C5_16–Al1	70.6(4)
C6_16–C5_16–Al1	126.6(5)
C5_16–C6_16–H6A_16	109.5
C5_16–C6_16–H6B_16	109.5
H6A_16–C6_16–H6B_16	109.5
C5_16–C6_16–H6C_16	109.5
H6A_16–C6_16–H6C_16	109.5
H6B_16–C6_16–H6C_16	109.5
C4_16–C7_16–H7A_16	109.5
C4_16–C7_16–H7B_16	109.5
H7A_16–C7_16–H7B_16	109.5
C4_16–C7_16–H7C_16	109.5
H7A_16–C7_16–H7C_16	109.5
H7B_16–C7_16–H7C_16	109.5
C3_16–C8_16–H8A_16	109.5
C3_16–C8_16–H8B_16	109.5
H8A_16–C8_16–H8B_16	109.5
C3_16–C8_16–H8C_16	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
C2_16–C9_16–H9B_16	109.5
H9A_16–C9_16–H9B_16	109.5
C2_16–C9_16–H9C_16	109.5
H9A_16–C9_16–H9C_16	109.5
H9B_16–C9_16–H9C_16	109.5
C1_16–C10_16–H10A_16	109.5
C1_16–C10_16–H10B_16	109.5
H10A_16–C10_16–H10B_16	109.5
C1_16–C10_16–H10C_16	109.5
H10A_16–C10_16–H10C_16	109.5
H10B_16–C10_16–H10C_16	109.5

C5_17–C1_17–C2_17	108.2(6)
C5_17–C1_17–C10_17	126.7(7)
C2_17–C1_17–C10_17	124.9(7)
C5_17–C1_17–Al3	72.8(4)
C2_17–C1_17–Al3	69.7(3)
C10_17–C1_17–Al3	127.9(5)
C3_17–C2_17–C1_17	108.4(6)
C3_17–C2_17–C9_17	126.4(6)
C1_17–C2_17–C9_17	125.0(6)
C3_17–C2_17–Al3	70.8(4)
C1_17–C2_17–Al3	75.4(4)
C9_17–C2_17–Al3	123.4(5)
C2_17–C3_17–C4_17	107.5(6)
C2_17–C3_17–C8_17	127.3(7)
C4_17–C3_17–C8_17	125.1(7)
C2_17–C3_17–Al3	73.6(4)
C4_17–C3_17–Al3	73.4(4)
C8_17–C3_17–Al3	120.7(5)
C3_17–C4_17–C5_17	107.9(6)
C3_17–C4_17–C7_17	127.3(8)
C5_17–C4_17–C7_17	124.6(7)
C3_17–C4_17–Al3	70.8(4)
C5_17–C4_17–Al3	75.2(4)
C7_17–C4_17–Al3	123.2(6)
C1_17–C5_17–C4_17	107.9(6)
C1_17–C5_17–C6_17	125.8(8)
C4_17–C5_17–C6_17	126.0(8)
C1_17–C5_17–Al3	73.2(4)
C4_17–C5_17–Al3	69.6(4)
C6_17–C5_17–Al3	126.9(6)
C5_17–C6_17–H6A_17	109.5
C5_17–C6_17–H6B_17	109.5
H6A_17–C6_17–H6B_17	109.5
C5_17–C6_17–H6C_17	109.5
H6A_17–C6_17–H6C_17	109.5
H6B_17–C6_17–H6C_17	109.5
C4_17–C7_17–H7A_17	109.5
C4_17–C7_17–H7B_17	109.5
H7A_17–C7_17–H7B_17	109.5
C4_17–C7_17–H7C_17	109.5
H7A_17–C7_17–H7C_17	109.5
H7B_17–C7_17–H7C_17	109.5
C3_17–C8_17–H8A_17	109.5
C3_17–C8_17–H8B_17	109.5
H8A_17–C8_17–H8B_17	109.5
C3_17–C8_17–H8C_17	109.5
H8A_17–C8_17–H8C_17	109.5
H8B_17–C8_17–H8C_17	109.5
C2_17–C9_17–H9A_17	109.5
C2_17–C9_17–H9B_17	109.5
H9A_17–C9_17–H9B_17	109.5
C2_17–C9_17–H9C_17	109.5
H9A_17–C9_17–H9C_17	109.5
H9B_17–C9_17–H9C_17	109.5
C1_17–C10_17–H10A_17	109.5
C1_17–C10_17–H10B_17	109.5
H10A_17–C10_17–H10B_17	109.5
C1_17–C10_17–H10C_17	109.5
H10A_17–C10_17–H10C_17	109.5
H10B_17–C10_17–H10C_17	109.5
C2_18–C1_18–C5_18	108.3(6)
C2_18–C1_18–C10_18	127.7(7)
C5_18–C1_18–C10_18	123.8(7)
C2_18–C1_18–Al4	73.9(3)
C5_18–C1_18–Al4	73.3(4)
C10_18–C1_18–Al4	122.9(5)
C1_18–C2_18–C3_18	107.4(6)
C1_18–C2_18–C9_18	127.0(6)
C3_18–C2_18–C9_18	125.5(6)
C1_18–C2_18–Al4	70.4(3)
C3_18–C2_18–Al4	74.1(3)
C9_18–C2_18–Al4	124.7(5)
C4_18–C3_18–C2_18	108.8(6)
C4_18–C3_18–C8_18	125.7(7)
C2_18–C3_18–C8_18	125.0(6)
C4_18–C3_18–Al4	72.5(4)
C2_18–C3_18–Al4	70.8(3)
C8_18–C3_18–Al4	129.0(5)
C3_18–C4_18–C5_18	107.6(6)
C3_18–C4_18–C7_18	127.1(7)
C5_18–C4_18–C7_18	125.2(7)
C3_18–C4_18–Al4	72.8(4)
C5_18–C4_18–Al4	70.5(4)
C7_18–C4_18–Al4	125.7(6)
C4_18–C5_18–C1_18	107.9(6)
C4_18–C5_18–C6_18	127.8(7)
C1_18–C5_18–C6_18	124.1(7)
C4_18–C5_18–Al4	74.2(5)
C1_18–C5_18–Al4	70.6(4)
C6_18–C5_18–Al4	124.4(6)
C5_18–C6_18–H6A_18	109.5
C5_18–C6_18–H6B_18	109.5

H6A_18–C6_18–H6B_18	109.5
C5_18–C6_18–H6C_18	109.5
H6A_18–C6_18–H6C_18	109.5
H6B_18–C6_18–H6C_18	109.5
C4_18–C7_18–H7A_18	109.5
C4_18–C7_18–H7B_18	109.5
H7A_18–C7_18–H7B_18	109.5
C4_18–C7_18–H7C_18	109.5
H7A_18–C7_18–H7C_18	109.5
H7B_18–C7_18–H7C_18	109.5
C3_18–C8_18–H8A_18	109.5
C3_18–C8_18–H8B_18	109.5
H8A_18–C8_18–H8B_18	109.5
C3_18–C8_18–H8C_18	109.5
H8A_18–C8_18–H8C_18	109.5
H8B_18–C8_18–H8C_18	109.5
C2_18–C9_18–H9A_18	109.5
C2_18–C9_18–H9B_18	109.5
H9A_18–C9_18–H9B_18	109.5
C2_18–C9_18–H9C_18	109.5
H9A_18–C9_18–H9C_18	109.5
H9B_18–C9_18–H9C_18	109.5
C1_18–C10_18–H10A_18	109.5
C1_18–C10_18–H10B_18	109.5
H10A_18–C10_18–H10B_18	109.5
C1_18–C10_18–H10C_18	109.5
H10A_18–C10_18–H10C_18	109.5
H10B_18–C10_18–H10C_18	109.5
C5_19–C1_19–C2_19	107.3(6)
C5_19–C1_19–C10_19	125.6(6)
C2_19–C1_19–C10_19	127.0(6)
C5_19–C1_19–Al5	74.9(4)
C2_19–C1_19–Al5	71.7(3)
C10_19–C1_19–Al5	121.9(5)
C3_19–C2_19–C1_19	107.8(6)
C3_19–C2_19–C9_19	125.5(7)
C1_19–C2_19–C9_19	126.6(7)
C3_19–C2_19–Al5	74.8(4)
C1_19–C2_19–Al5	72.6(3)
C9_19–C2_19–Al5	122.0(4)
C2_19–C3_19–C4_19	109.0(6)
C2_19–C3_19–C8_19	125.0(8)
C4_19–C3_19–C8_19	125.7(8)
C2_19–C3_19–Al5	70.6(3)
C4_19–C3_19–Al5	74.5(4)
C8_19–C3_19–Al5	125.9(5)
C5_19–C4_19–C3_19	106.8(6)
C5_19–C4_19–C7_19	126.9(7)
C3_19–C4_19–C7_19	126.2(7)
C5_19–C4_19–Al5	71.8(4)
C3_19–C4_19–Al5	71.1(4)
C7_19–C4_19–Al5	124.9(5)
C1_19–C5_19–C4_19	109.1(6)
C1_19–C5_19–C6_19	125.9(6)
C4_19–C5_19–C6_19	124.8(6)
C1_19–C5_19–Al5	70.4(4)
C4_19–C5_19–Al5	74.0(4)
C6_19–C5_19–Al5	125.5(5)
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	H7A_20–C7_20–H7B_20	109.5
C1_19–C10_19–H10A_19	109.5	C4_20–C7_20–H7C_20	109.5
C1_19–C10_19–H10B_19	109.5	H7A_20–C7_20–H7C_20	109.5
H10A_19–C10_19–H10B_19	109.5	H7B_20–C7_20–H7C_20	109.5
C1_19–C10_19–H10C_19	109.5	C3_20–C8_20–H8A_20	109.5
H10A_19–C10_19–H10C_19	109.5	C3_20–C8_20–H8B_20	109.5
H10B_19–C10_19–H10C_19	109.5	H8A_20–C8_20–H8B_20	109.5
C5_20–C1_20–C2_20	107.0(6)	C3_20–C8_20–H8C_20	109.5
C5_20–C1_20–C10_20	127.9(7)	H8A_20–C8_20–H8C_20	109.5
C2_20–C1_20–C10_20	125.2(7)	H8B_20–C8_20–H8C_20	109.5
C5_20–C1_20–Al6	73.9(4)	C2_20–C9_20–H9A_20	109.5
C2_20–C1_20–Al6	72.1(3)	C2_20–C9_20–H9B_20	109.5
C10_20–C1_20–Al6	120.5(5)	H9A_20–C9_20–H9B_20	109.5
C3_20–C2_20–C1_20	108.3(6)	C2_20–C9_20–H9C_20	109.5
C3_20–C2_20–C9_20	125.7(7)	H9A_20–C9_20–H9C_20	109.5
C1_20–C2_20–C9_20	125.5(7)	H9B_20–C9_20–H9C_20	109.5
C3_20–C2_20–Al6	75.6(4)	C1_20–C10_20–H10A_20	109.5
C1_20–C2_20–Al6	71.5(4)	C1_20–C10_20–H10B_20	109.5
C9_20–C2_20–Al6	124.8(5)	H10A_20–C10_20–H10B_20	109.5
C4_20–C3_20–C2_20	108.5(6)	C1_20–C10_20–H10C_20	109.5
C4_20–C3_20–C8_20	127.0(8)	H10A_20–C10_20–H10C_20	109.5
C2_20–C3_20–C8_20	124.2(7)	H10B_20–C10_20–H10C_20	109.5
C4_20–C3_20–Al6	73.7(4)	C1_10–O1_10–Al8	142(3)
C2_20–C3_20–Al6	69.1(4)	O1_10–C1_10–C4_10	111.0(17)
C8_20–C3_20–Al6	127.6(6)	O1_10–C1_10–C2_10	111.2(17)
C3_20–C4_20–C5_20	107.0(6)	C4_10–C1_10–C2_10	113.6(13)
C3_20–C4_20–C7_20	127.8(7)	O1_10–C1_10–C3_10	106.5(17)
C5_20–C4_20–C7_20	124.6(7)	C4_10–C1_10–C3_10	108.7(12)
C3_20–C4_20–Al6	71.9(4)	C2_10–C1_10–C3_10	105.5(12)
C5_20–C4_20–Al6	69.7(5)	F1_10–C2_10–F2_10	107.2(16)
C7_20–C4_20–Al6	130.4(6)	F1_10–C2_10–F3_10	107.4(17)
C1_20–C5_20–C4_20	109.2(6)	F2_10–C2_10–F3_10	105.6(15)
C1_20–C5_20–C6_20	126.0(7)	F1_10–C2_10–C1_10	113.8(15)
C4_20–C5_20–C6_20	124.7(7)	F2_10–C2_10–C1_10	111.0(14)
C1_20–C5_20–Al6	70.6(4)	F3_10–C2_10–C1_10	111.3(14)
C4_20–C5_20–Al6	75.2(5)	F4_10–C3_10–F6_10	107.3(16)
C6_20–C5_20–Al6	122.5(6)	F4_10–C3_10–F5_10	112.5(18)
C5_20–C6_20–H6A_20	109.5	F6_10–C3_10–F5_10	110.6(17)
C5_20–C6_20–H6B_20	109.5	F4_10–C3_10–C1_10	107.6(15)
H6A_20–C6_20–H6B_20	109.5	F6_10–C3_10–C1_10	109.2(15)
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		

F5_10–C3_10–C1_10	109.5(15)
F9_10–C4_10–F8_10	106.6(16)
F9_10–C4_10–F7_10	108.7(17)
F8_10–C4_10–F7_10	106.3(16)
F9_10–C4_10–C1_10	113.2(15)
F8_10–C4_10–C1_10	110.0(15)
F7_10–C4_10–C1_10	111.7(15)
C1_21–O1_21–Al8	154(2)
O1_21–C1_21–C2_21	110.5(15)
O1_21–C1_21–C3_21	112.6(16)
C2_21–C1_21–C3_21	109.9(13)
O1_21–C1_21–C4_21	104.1(15)
C2_21–C1_21–C4_21	112.6(13)
C3_21–C1_21–C4_21	107.0(13)
F1_21–C2_21–F2_21	107.8(18)
F1_21–C2_21–F3_21	108.8(18)
F2_21–C2_21–F3_21	107.6(17)
F1_21–C2_21–C1_21	111.2(16)
F2_21–C2_21–C1_21	111.5(16)
F3_21–C2_21–C1_21	109.9(16)
F4_21–C3_21–F5_21	107.4(18)
F4_21–C3_21–F6_21	107.0(17)
F5_21–C3_21–F6_21	111.1(18)
F4_21–C3_21–C1_21	113.5(16)
F5_21–C3_21–C1_21	108.1(16)
F6_21–C3_21–C1_21	109.8(16)
F8_21–C4_21–F7_21	112.2(18)
F8_21–C4_21–F9_21	106.5(17)
F7_21–C4_21–F9_21	110.2(18)
F8_21–C4_21–C1_21	114.1(17)
F7_21–C4_21–C1_21	107.5(16)
F9_21–C4_21–C1_21	106.2(15)

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