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Tetra-*n*-butylammonium μ-fluorido-bis{tris[2,2,2-trifluoro-1,1-bis(trifluoromethyl)ethanolato-κO]aluminate(III)}

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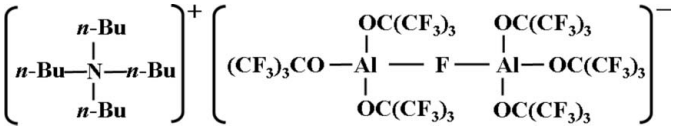
Key indicators: single-crystal X-ray study; T = 140 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.075; wR factor = 0.216; data-to-parameter ratio = 10.7.

The metathesis reaction of $Ag[(RO)_3Al-F-Al(OR)_3]$ and n-Bu_4NBr in CH_2Cl_2 yields nearly quantitatively n-Bu_4N^+.-$[(RO)_3Al-F-Al(OR)_3]^-$ [with R = $C(CF_3)_3$)] or $(C_{16}H_{36}N)$-$[Al_2(C_4F_9O)_6F]$. In the asymmetric unit, two entire cations and four half-anions (one is disordered over two positions) are found. The intramolecular distances are comparable to those found in other n-Bu_4N^+ or $[(RO)_3Al-F-Al(OR)_3]^-$ salts. Only weak interactions outside the sum of the van der Waals radii [r(F + H) = 2.6 Å] are found between the cations and anions. The title compound is considerably soluble in CH_2Cl_2, which makes this salt a possible candidate as supporting electrolyte for electrochemical applications in nonpolar solvents. In addition, the $[(RO)_3Al-F-Al(OR)_3]^-$ anion is very stable against oxidation. Two CF_3 groups of one anion are disordered over two positions; the site occupancy ratios are 0.64:0.36 and 0.78:0.22.

Related literature

For related literature, see: Bihlmeier *et al.* (2004); Krossing & Raabe (2004*a*,*b*); Raabe *et al.* (2007).



Experimental

Crystal data

$(C_{16}H_{36}N)[Al_2(C_4F_9O)_6F]$
M_r = 1725.66
Triclinic, $P\overline{1}$
a = 12.822 (3) Å
b = 19.230 (4) Å
c = 24.871 (5) Å
α = 88.35 (3)°
β = 86.72 (3)°
γ = 89.21 (3)°
V = 6119 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.26 mm^{-1}
T = 140 (2) K
0.5 × 0.5 × 0.2 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: none
55213 measured reflections
23694 independent reflections
16301 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.075
$wR(F^2)$ = 0.216
S = 1.06
23694 reflections
2215 parameters
149 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.48 e Å^{-3}
$\Delta\rho_{min}$ = −1.39 e Å^{-3}

Data collection: *XPOSE* (Stoe & Cie, 2003); cell refinement: *CELL* (Stoe & Cie, 2003); data reduction: *X-RED* (Stoe & Cie, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Crystal Impact, 2006); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2013).

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supplementary materials

Acta Cryst. (2007). E**63**, m2144 [**doi:10.1107/S1600536807033533**]

Tetra-*n*-butylammonium μ-fluorido-bis{tris[2,2,2-trifluoro-1,1-bis(trifluoromethyl)ethanolato-κ*O*]aluminate(III)}

I. Krossing and I. Raabe

Comment

$[n\text{-Bu}_4N]^+[(RO)_3Al—F—Al(OR)_3]^-$ (**I**) {with R = $C(CF_3)_3$)} has been prepared from $Ag[(RO)_3Al—F—Al(OR)_3]$ and $n\text{-Bu}_4NBr$ in CH_2Cl_2. The intramolecular distances in (**I**) ($d(Al—O)_{av}$ = 1.700 A, $d(Al—F)_{av}$ = 1.766 Å, d(C—N) = 1.525 Å are similar to those found in other $[n\text{-Bu}_4N]^+$ or $[(RO)_3Al—F—Al(OR)_3]^-$ salts (Bihlmeier *et al.*, 2004, Raabe *et al.*, 2007). Only weak interactions below the sum of the van-der-Waals radii (r(F+H) = 2.6 Å) are found between the cations and anions. (**I**) is considerably soluble in CH_2Cl_2, which makes this salt a possible candidate as supporting electrolyte for electrochemical applications in non-polar solvents. Besides, the $[(RO)_3Al—F—Al(OR)_3]^-$ anion is very stable against oxidation (Krossing and Raabe, 2004*a*,b).

Experimental

Solid $[Ag(CH_2Cl_2)][(RO)_3Al—F—Al(OR)_3]$ (0.566 g, 0.34 mmol) and solid $[n\text{-Bu}_4N]Br$ (0.109 g, 0.34 mmol) were weighed into a two-bulb frit plate Schlenk vessel equipped with two J. Young valves. CH_2Cl_2 (15 ml) was added on this solid mixture and the resulting colorless solution above the white precipitate (AgBr) was stirred for a few minutest at r.t.. The suspension was filtered, the filtrate was highly concentrated and stored for a few days at −30°C for crystallization. Colourless crystalline plates of **I** were isolated (yield: 86%).

Refinement

Refinement of F^2^ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2^, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2^. The threshold expression of F^2^ > 2sigma(F^2^) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2^ are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger. Refinement for su_max up to <0.001 was not possible even after many cycles due to disorder. All H atoms were positioned geometrically and refined using a riding model, with C—H distances of 0.98 \%A for methyl H atoms and 0.99 \%A for methylene H atoms, and with Uĩso~(H) = 1.5U~eq~(C) for methyl H atoms and 1.2U~eq~(C) for methylene H atoms. The disordered positions of the CF_3 groups of oneanion have been refined against each other using two free variables.

Figures

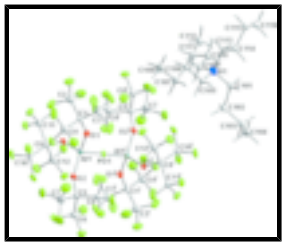


Fig. 1. A unit of [{(CF~3~)~3~CO}~3Ãl—F—Al{OC(CF~3~)~3~}~3~)]^-^ in I with displacement ellipsoids are drawn at the 25% probability level. [Symmetry code: (i) $1-x$, $1-y$, $-z$.]

Tetra-n-butylammonium μ-fluorido-bis{tris[2,2,2-trifluoro-1,1-bis(trifluoromethyl)ethanolato-κ*O*]aluminate(III)}

Crystal data

$(C_{16}H_{36}N)[Al_2(C_4F_9O)_6F]$	$Z = 4$
$M_r = 1725.66$	$F_{000} = 3408$
Triclinic, $P\bar{1}$	$D_x = 1.873$ Mg m^{-3}
Hall symbol: -p 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 12.822$ (3) Å	Cell parameters from 5000 reflections
$b = 19.230$ (4) Å	$\theta = 1.5$–26.0º
$c = 24.871$ (5) Å	$\mu = 0.26$ mm^{-1}
$\alpha = 88.35$ (3)º	$T = 140$ (2) K
$\beta = 86.72$ (3)º	Plate, colourless
$\gamma = 89.21$ (3)º	0.5 × 0.5 × 0.2 mm
$V = 6119$ (2) Å^3	

Data collection

Stoe IPDS II diffractometer	16301 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.041$
Monochromator: graphite	$\theta_{max} = 26.0$º
$T = 140(2)$ K	$\theta_{min} = 1.6$º
φ scans	$h = -15 \rightarrow 15$
Absorption correction: none	$k = -23 \rightarrow 23$
55213 measured reflections	$l = -30 \rightarrow 30$
23694 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.075$	H-atom parameters constrained
$wR(F^2) = 0.216$	$w = 1/[\sigma^2(F_o^2) + (0.105P)^2 + 10.4575P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
23694 reflections	$\Delta\rho_{max} = 1.48$ e Å^{-3}
2215 parameters	$\Delta\rho_{min} = -1.38$ e Å^{-3}
149 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Experimental. crystal mounted in PFE oil. ^{1}H NMR (250 MHz, CD_2Cl_2, 300 K): δ = 0.98, 1.37, 1.55, 3.01. $^{13}C\{^1H\}$ NMR (63 MHz, CD_2Cl_2, 300 K): δ = 13.3, 19.8, 24.0, 59.3, 121.0. ^{27}Al NMR (78 MHz, CD_2Cl_2, 300 K): δ =34.4 (ω1/2; = 2170 Hz).

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Al1	0.46494 (6)	0.50625 (4)	0.06957 (3)	0.02477 (17)	
F01	0.5000	0.5000	0.0000	0.0302 (5)	
F21	0.39513 (15)	0.66527 (10)	0.13747 (8)	0.0501 (5)	
F24	0.10193 (14)	0.63232 (10)	0.08817 (9)	0.0533 (5)	
F27	0.40438 (15)	0.66294 (11)	0.02918 (8)	0.0536 (5)	
O3	0.34302 (14)	0.54220 (10)	0.07363 (8)	0.0337 (5)	
F23	0.14730 (14)	0.54042 (10)	0.04544 (8)	0.0528 (5)	
F20	0.32413 (17)	0.57617 (10)	0.17651 (8)	0.0549 (5)	
O2	0.55328 (15)	0.55734 (10)	0.09701 (8)	0.0364 (5)	
F22	0.14336 (15)	0.53887 (11)	0.13157 (9)	0.0579 (6)	
O1	0.46612 (16)	0.42058 (10)	0.08835 (8)	0.0362 (5)	
F26	0.26678 (17)	0.71939 (9)	0.05718 (9)	0.0582 (6)	
F9	0.44784 (18)	0.45771 (10)	0.19018 (8)	0.0564 (6)	
F19	0.23194 (16)	0.66783 (11)	0.16221 (8)	0.0571 (5)	
F8	0.4136 (2)	0.35436 (12)	0.22164 (8)	0.0651 (6)	
F12	0.61813 (18)	0.69812 (10)	0.11680 (11)	0.0692 (7)	
F6	0.4818 (2)	0.25366 (10)	0.14968 (10)	0.0768 (8)	
F7	0.56871 (18)	0.37889 (13)	0.18728 (9)	0.0687 (7)	
F25	0.25739 (16)	0.64255 (11)	−0.00326 (8)	0.0565 (6)	
F15	0.57805 (18)	0.60080 (14)	0.19537 (9)	0.0701 (7)	
F18	0.82832 (15)	0.53504 (12)	0.09735 (11)	0.0689 (7)	
F5	0.58909 (19)	0.31146 (11)	0.09626 (10)	0.0734 (7)	

F3	0.26725 (17)	0.41524 (12)	0.15430 (11)	0.0731 (7)
F17	0.70552 (17)	0.46266 (10)	0.08750 (12)	0.0761 (8)
F16	0.73887 (18)	0.54087 (13)	0.02671 (10)	0.0734 (7)
F11	0.6297 (2)	0.66068 (13)	0.03632 (10)	0.0709 (7)
F10	0.76814 (17)	0.66957 (11)	0.07998 (11)	0.0697 (7)
F14	0.74522 (18)	0.61252 (14)	0.18159 (10)	0.0786 (7)
F2	0.28182 (19)	0.36705 (15)	0.07721 (10)	0.0824 (8)
F13	0.6785 (2)	0.51054 (14)	0.18684 (10)	0.0799 (8)
C12	0.3020 (2)	0.65759 (16)	0.04161 (13)	0.0408 (8)
F4	0.4456 (3)	0.27591 (11)	0.06693 (10)	0.0807 (8)
C11	0.1668 (2)	0.57767 (16)	0.08736 (13)	0.0401 (8)
C8	0.7327 (3)	0.52800 (18)	0.07970 (16)	0.0518 (9)
F1	0.2814 (2)	0.30329 (12)	0.14917 (11)	0.0793 (8)
C1	0.4345 (2)	0.37081 (14)	0.12581 (12)	0.0351 (7)
C10	0.3081 (2)	0.62761 (15)	0.14136 (12)	0.0393 (7)
C5	0.6508 (2)	0.57738 (14)	0.10707 (12)	0.0344 (7)
C4	0.4656 (3)	0.39041 (19)	0.18219 (14)	0.0515 (9)
C9	0.2828 (2)	0.59961 (14)	0.08572 (11)	0.0306 (6)
C7	0.6632 (3)	0.5756 (2)	0.16817 (15)	0.0557 (10)
C6	0.6677 (3)	0.65246 (17)	0.08399 (16)	0.0489 (9)
C3	0.4884 (3)	0.30158 (17)	0.10972 (15)	0.0588 (11)
C2	0.3144 (3)	0.3636 (2)	0.12630 (16)	0.0575 (10)
Al2	0.38351 (6)	0.45559 (4)	0.48895 (3)	0.02483 (17)
F02	0.5000	0.5000	0.5000	0.0295 (5)
O6	0.28906 (15)	0.49036 (10)	0.53111 (8)	0.0335 (5)
O5	0.36849 (15)	0.47845 (11)	0.42304 (8)	0.0370 (5)
O4	0.40546 (15)	0.37038 (10)	0.50346 (9)	0.0364 (5)
F49	0.08588 (15)	0.54858 (10)	0.62112 (9)	0.0611 (6)
F36	0.63343 (15)	0.35832 (11)	0.49363 (11)	0.0643 (7)
F45	0.26460 (17)	0.59721 (11)	0.41566 (9)	0.0615 (6)
F44	0.17445 (17)	0.56702 (12)	0.35115 (9)	0.0654 (6)
F48	0.08306 (15)	0.40952 (10)	0.61051 (9)	0.0640 (6)
F43	0.14597 (15)	0.52080 (14)	0.43043 (9)	0.0671 (7)
F35	0.54401 (18)	0.36223 (13)	0.42127 (9)	0.0710 (7)
F42	0.3996 (2)	0.57093 (13)	0.33107 (10)	0.0765 (7)
F34	0.60870 (17)	0.26465 (11)	0.44676 (10)	0.0689 (7)
F33	0.52281 (19)	0.34166 (15)	0.58462 (10)	0.0780 (8)
F41	0.3120 (2)	0.49868 (19)	0.28683 (9)	0.0946 (10)
F40	0.45166 (18)	0.46457 (15)	0.32419 (9)	0.0725 (7)
C21	0.2227 (2)	0.48256 (14)	0.57568 (12)	0.0322 (7)
F30	0.30270 (17)	0.25428 (12)	0.49576 (14)	0.0891 (9)
F32	0.5702 (2)	0.24037 (15)	0.55594 (11)	0.0895 (8)
F39	0.21330 (19)	0.38828 (13)	0.42292 (12)	0.0844 (8)
C13	0.4639 (2)	0.31089 (14)	0.49985 (13)	0.0353 (7)
F50	0.2217 (2)	0.60136 (12)	0.59653 (13)	0.1173 (11)
F46	0.0788 (2)	0.44250 (17)	0.53041 (12)	0.1234 (11)
F31	0.4059 (2)	0.25967 (14)	0.58344 (11)	0.0897 (8)
C17	0.3016 (2)	0.48513 (17)	0.38273 (12)	0.0383 (7)
F38	0.1611 (2)	0.42504 (15)	0.34650 (12)	0.0962 (8)

C20	0.2199 (2)	0.54427 (19)	0.39539 (14)	0.0461 (8)
F52	0.2294 (2)	0.46896 (16)	0.67115 (9)	0.0888 (9)
C23	0.1602 (2)	0.55156 (17)	0.58252 (12)	0.0491 (9)
F29	0.4014 (2)	0.26593 (16)	0.42027 (12)	0.0936 (9)
C22	0.1437 (2)	0.42351 (16)	0.56794 (12)	0.0505 (9)
C16	0.5655 (3)	0.3234 (2)	0.46432 (16)	0.0562 (10)
C19	0.3676 (3)	0.5066 (2)	0.33022 (14)	0.0607 (11)
F28	0.4399 (2)	0.19072 (12)	0.48635 (17)	0.1128 (13)
F37	0.3114 (3)	0.37080 (13)	0.35035 (13)	0.0976 (9)
C24	0.2827 (2)	0.46735 (16)	0.62591 (14)	0.0521 (9)
C15	0.4933 (3)	0.2879 (2)	0.55688 (18)	0.0668 (12)
C18	0.2455 (3)	0.4167 (2)	0.37542 (19)	0.0705 (12)
C14	0.3993 (3)	0.2543 (2)	0.4762 (3)	0.0872 (18)
Al3	0.88156 (6)	0.04630 (4)	0.49375 (3)	0.03129 (19)
F03	1.0000	0.0000	0.5000	0.0281 (5)
O7	0.85112 (15)	0.02531 (10)	0.43052 (8)	0.0365 (5)
C29	0.9486 (2)	0.19135 (15)	0.50695 (12)	0.0348 (7)
C33	0.74441 (19)	0.00148 (12)	0.58789 (12)	0.0415 (8)
C25	0.7786 (2)	0.02815 (16)	0.39304 (12)	0.0413 (8)
Al4	0.01488 (6)	0.99251 (4)	−0.07053 (3)	0.02861 (18)
F04	0.0000	1.0000	0.0000	0.0420 (6)
O12	−0.10346 (17)	0.96708 (11)	−0.08943 (10)	0.0475 (6)
F90	0.28021 (19)	0.99770 (12)	−0.14736 (10)	0.0714 (7)
O10	0.11013 (17)	0.93282 (11)	−0.08051 (11)	0.0519 (7)
F89	0.2728 (2)	1.00999 (12)	−0.06385 (10)	0.0754 (7)
F96	0.0962 (2)	1.23932 (11)	−0.15339 (10)	0.0790 (8)
F87	0.15408 (19)	0.81440 (11)	−0.03208 (10)	0.0700 (7)
O11	0.04457 (18)	1.07394 (11)	−0.09428 (9)	0.0459 (6)
F99	0.0257 (2)	1.14673 (13)	−0.22584 (9)	0.0769 (8)
F107	−0.35831 (16)	0.90372 (14)	−0.09235 (11)	0.0816 (8)
F106	−0.2987 (2)	0.98756 (15)	−0.05184 (10)	0.1033 (9)
F84	0.1500 (2)	0.80608 (12)	−0.13768 (11)	0.0843 (8)
F88	0.38497 (17)	0.93934 (14)	−0.09950 (12)	0.0813 (8)
F105	−0.22262 (18)	0.80438 (12)	−0.05771 (10)	0.0785 (7)
F102	−0.2255 (2)	0.84316 (12)	−0.16528 (10)	0.0766 (7)
F98	0.0375 (2)	1.04034 (12)	−0.19650 (10)	0.0778 (8)
F93	−0.14119 (19)	1.10034 (15)	−0.15888 (12)	0.0870 (8)
F104	−0.07122 (18)	0.84164 (14)	−0.04104 (13)	0.0993 (10)
F97	0.1684 (2)	1.10831 (14)	−0.19468 (12)	0.0863 (8)
F95	0.1855 (2)	1.17204 (13)	−0.10291 (12)	0.0881 (8)
F94	0.0438 (3)	1.21865 (13)	−0.07091 (10)	0.1009 (11)
C41	0.0267 (3)	1.12639 (15)	−0.13020 (13)	0.0398 (8)
F86	0.2633 (2)	0.88877 (16)	−0.00624 (10)	0.0917 (9)
F101	−0.0682 (2)	0.83729 (16)	−0.14669 (14)	0.1180 (12)
F85	0.3133 (2)	0.81239 (14)	−0.06352 (15)	0.1030 (10)
F92	−0.1075 (2)	1.20860 (14)	−0.15018 (14)	0.0998 (10)
F83	0.1503 (3)	0.90257 (16)	−0.18317 (10)	0.0964 (9)
C37	0.2053 (2)	0.90540 (14)	−0.09393 (12)	0.0338 (7)
F91	−0.1327 (2)	1.14136 (18)	−0.08055 (13)	0.1071 (10)

F82	0.2949 (2)	0.85234 (15)	−0.16913 (12)	0.1020 (9)
C44	0.0640 (3)	1.10551 (19)	−0.18779 (16)	0.0583 (10)
C45	−0.1722 (2)	0.91579 (16)	−0.09612 (13)	0.0407 (8)
C48	−0.2835 (3)	0.94965 (16)	−0.09365 (11)	0.0497 (9)
C47	−0.1672 (2)	0.86004 (17)	−0.05026 (16)	0.0580 (11)
C40	0.2887 (3)	0.96358 (18)	−0.10017 (15)	0.0500 (9)
C46	−0.1498 (3)	0.88115 (18)	−0.15021 (16)	0.0688 (12)
C43	0.0905 (4)	1.18955 (18)	−0.11425 (17)	0.0633 (12)
C39	0.2348 (3)	0.8537 (2)	−0.04831 (17)	0.0596 (11)
C42	−0.0906 (3)	1.1453 (2)	−0.12958 (19)	0.0673 (12)
C38	0.2015 (3)	0.8668 (2)	−0.14708 (16)	0.0620 (11)
N1	0.51284 (18)	0.84210 (11)	0.23133 (9)	0.0316 (5)
C106	0.5267 (2)	0.86130 (15)	0.12808 (12)	0.0349 (7)
H10A	0.5950	0.8367	0.1254	0.042*
H10B	0.5396	0.9117	0.1305	0.042*
C113	0.5477 (2)	0.91627 (13)	0.23929 (12)	0.0310 (6)
H11A	0.5696	0.9195	0.2767	0.037*
H11B	0.6100	0.9253	0.2148	0.037*
C105	0.4636 (2)	0.83557 (15)	0.17793 (11)	0.0333 (7)
H10C	0.3961	0.8614	0.1798	0.040*
H10D	0.4477	0.7859	0.1733	0.040*
C114	0.4674 (2)	0.97363 (14)	0.22962 (13)	0.0350 (7)
H11C	0.4530	0.9767	0.1909	0.042*
H11D	0.4011	0.9628	0.2504	0.042*
C101	0.4307 (2)	0.82305 (15)	0.27598 (12)	0.0387 (7)
H10E	0.4579	0.8353	0.3109	0.046*
H10F	0.3676	0.8521	0.2707	0.046*
C109	0.6073 (2)	0.79356 (15)	0.23334 (12)	0.0357 (7)
H10G	0.5833	0.7451	0.2307	0.043*
H10H	0.6546	0.8038	0.2013	0.043*
C115	0.5090 (2)	1.04267 (14)	0.24705 (12)	0.0352 (7)
H11E	0.5177	1.0404	0.2864	0.042*
H11F	0.5786	1.0508	0.2287	0.042*
C110	0.6692 (3)	0.79799 (16)	0.28309 (12)	0.0407 (8)
H11G	0.6219	0.7921	0.3157	0.049*
H11H	0.7015	0.8444	0.2839	0.049*
C116	0.4364 (3)	1.10302 (16)	0.23379 (16)	0.0503 (9)
H11I	0.4658	1.1464	0.2456	0.075*
H11J	0.3679	1.0956	0.2524	0.075*
H11K	0.4287	1.1060	0.1948	0.075*
C107	0.4664 (2)	0.84796 (18)	0.07836 (12)	0.0429 (8)
H10I	0.4532	0.7975	0.0766	0.052*
H10J	0.3978	0.8722	0.0818	0.052*
C102	0.3982 (3)	0.74699 (16)	0.27973 (15)	0.0525 (9)
H10K	0.4530	0.7185	0.2966	0.063*
H10L	0.3899	0.7297	0.2431	0.063*
C111	0.7541 (3)	0.74165 (16)	0.28296 (13)	0.0421 (8)
H11L	0.7213	0.6954	0.2878	0.050*
H11M	0.7941	0.7429	0.2477	0.050*

C112	0.8279 (3)	0.75163 (18)	0.32735 (14)	0.0495 (9)
H11N	0.8821	0.7151	0.3259	0.074*
H11O	0.7889	0.7489	0.3624	0.074*
H11P	0.8607	0.7973	0.3225	0.074*
C103	0.2946 (3)	0.74007 (19)	0.31348 (16)	0.0572 (10)
H10M	0.2829	0.6902	0.3226	0.069*
H10N	0.3006	0.7645	0.3476	0.069*
C108	0.5235 (3)	0.8722 (2)	0.02678 (14)	0.0625 (11)
H10O	0.4815	0.8624	−0.0038	0.094*
H10P	0.5908	0.8476	0.0227	0.094*
H10Q	0.5354	0.9223	0.0279	0.094*
C104	0.2011 (3)	0.7687 (2)	0.28606 (18)	0.0719 (12)
H10R	0.1385	0.7631	0.3102	0.108*
H10S	0.1924	0.7435	0.2530	0.108*
H10T	0.2114	0.8182	0.2771	0.108*
N2	0.06563 (17)	0.64387 (12)	0.77218 (9)	0.0300 (5)
C213	−0.0003 (2)	0.58229 (14)	0.75861 (11)	0.0303 (6)
H21A	−0.0702	0.5878	0.7771	0.036*
H21P	−0.0099	0.5844	0.7194	0.036*
C210	0.0020 (2)	0.63873 (15)	0.87244 (11)	0.0348 (7)
H21B	−0.0397	0.5965	0.8683	0.042*
H21C	−0.0437	0.6799	0.8667	0.042*
C201	0.0026 (2)	0.71075 (15)	0.76268 (12)	0.0351 (7)
H20A	−0.0669	0.7056	0.7817	0.042*
H20B	0.0382	0.7494	0.7794	0.042*
C209	0.0928 (2)	0.64001 (15)	0.83094 (11)	0.0326 (6)
H20C	0.1359	0.5976	0.8366	0.039*
H20D	0.1365	0.6805	0.8377	0.039*
C214	0.0420 (2)	0.51068 (14)	0.77322 (12)	0.0323 (6)
H21D	0.0396	0.5041	0.8129	0.039*
H21E	0.1157	0.5063	0.7594	0.039*
C206	0.2395 (2)	0.70328 (16)	0.74265 (13)	0.0393 (7)
H20E	0.2680	0.7007	0.7788	0.047*
H20F	0.2009	0.7479	0.7390	0.047*
C215	−0.0232 (2)	0.45524 (15)	0.74886 (13)	0.0379 (7)
H21F	−0.0973	0.4616	0.7613	0.045*
H21G	−0.0183	0.4612	0.7091	0.045*
C211	0.0411 (3)	0.63911 (18)	0.92902 (12)	0.0436 (8)
H21H	0.0853	0.5973	0.9348	0.052*
H21I	0.0850	0.6805	0.9324	0.052*
C202	−0.0134 (3)	0.73133 (17)	0.70424 (12)	0.0426 (8)
H20G	−0.0382	0.6908	0.6851	0.051*
H20H	0.0537	0.7465	0.6863	0.051*
C205	0.1657 (2)	0.64295 (15)	0.73671 (12)	0.0358 (7)
H20I	0.1469	0.6423	0.6987	0.043*
H20J	0.2039	0.5991	0.7445	0.043*
C216	0.0127 (3)	0.38215 (16)	0.76423 (16)	0.0494 (9)
H21J	−0.0315	0.3482	0.7480	0.074*
H21K	0.0072	0.3758	0.8035	0.074*

H21L	0.0855	0.3752	0.7511	0.074*	
C207	0.3287 (3)	0.69989 (18)	0.69935 (14)	0.0479 (9)	
H20K	0.3624	0.6533	0.7010	0.057*	
H20L	0.2999	0.7062	0.6634	0.057*	
C212	−0.0465 (3)	0.6401 (2)	0.97214 (13)	0.0486 (9)	
H21M	−0.0172	0.6401	1.0077	0.073*	
H21N	−0.0898	0.5989	0.9694	0.073*	
H21O	−0.0895	0.6821	0.9673	0.073*	
C203	−0.0939 (3)	0.79066 (17)	0.70200 (14)	0.0513 (9)	
H20M	−0.0767	0.8259	0.7282	0.062*	
H20N	−0.0881	0.8131	0.6657	0.062*	
C208	0.4100 (3)	0.75476 (19)	0.70601 (16)	0.0557 (10)	
H20O	0.4655	0.7507	0.6775	0.084*	
H20P	0.4398	0.7481	0.7412	0.084*	
H20Q	0.3773	0.8010	0.7036	0.084*	
C204	−0.2049 (3)	0.7685 (2)	0.71392 (18)	0.0632 (11)	
H20R	−0.2515	0.8092	0.7119	0.095*	
H20S	−0.2120	0.7471	0.7502	0.095*	
H20T	−0.2237	0.7346	0.6875	0.095*	
F47	0.1901 (2)	0.36806 (12)	0.55364 (15)	0.1538 (12)	
F51	0.1222 (3)	0.57268 (17)	0.53856 (11)	0.1484 (11)	
F53	0.3196 (3)	0.40359 (17)	0.62570 (12)	0.1518 (13)	
F54	0.3614 (2)	0.5052 (2)	0.62822 (13)	0.1935 (15)	
F100	−0.1251 (3)	0.92545 (16)	−0.18831 (11)	0.1490 (14)	
F103	−0.2058 (2)	0.88515 (16)	−0.00346 (10)	0.0940 (10)	
F108	−0.2938 (2)	0.98838 (15)	−0.13744 (11)	0.0933 (9)	
F56	0.69148 (18)	0.11210 (12)	0.44572 (10)	0.0853 (8)	
O9	0.7966 (2)	0.00107 (15)	0.53958 (12)	0.0336 (8)	0.6388 (16)
C36	0.6651 (3)	0.0631 (2)	0.59326 (15)	0.0473 (14)	0.6388 (16)
C35	0.6762 (3)	−0.0655 (2)	0.59359 (15)	0.0518 (14)	0.6388 (16)
C34	0.8139 (3)	0.0017 (2)	0.63656 (17)	0.0541 (17)	0.6388 (16)
F73	0.7655 (3)	0.0175 (2)	0.68274 (13)	0.0715 (12)	0.6388 (16)
F74	0.8581 (3)	−0.05976 (18)	0.64336 (18)	0.0864 (13)	0.6388 (16)
F75	0.8898 (3)	0.04607 (18)	0.62673 (16)	0.0688 (11)	0.6388 (16)
F76	0.7294 (3)	−0.12082 (15)	0.57906 (16)	0.0984 (13)	0.6388 (16)
F77	0.6346 (2)	−0.08051 (16)	0.64245 (12)	0.0650 (9)	0.6388 (16)
F78	0.5950 (3)	−0.0614 (2)	0.56248 (15)	0.0841 (13)	0.6388 (16)
F79	0.5912 (3)	0.05809 (17)	0.63230 (13)	0.0642 (10)	0.6388 (16)
F80	0.6178 (3)	0.0768 (2)	0.54863 (15)	0.0802 (12)	0.6388 (16)
F81	0.7153 (3)	0.12137 (15)	0.60332 (15)	0.0721 (11)	0.6388 (16)
O9A	0.8015 (5)	0.0385 (4)	0.5484 (2)	0.057 (2)	0.3612 (16)
F73A	0.7751 (6)	−0.0224 (4)	0.6802 (3)	0.070 (2)	0.3612 (16)
F74A	0.9036 (6)	0.0153 (9)	0.6301 (5)	0.157 (6)	0.3612 (16)
F75A	0.7778 (10)	0.0867 (4)	0.6528 (4)	0.126 (4)	0.3612 (16)
F76A	0.7691 (6)	−0.0871 (4)	0.5259 (2)	0.126 (4)	0.3612 (16)
F77A	0.8754 (4)	−0.0891 (4)	0.5906 (3)	0.102 (3)	0.3612 (16)
F78A	0.7117 (6)	−0.1095 (4)	0.6078 (3)	0.132 (4)	0.3612 (16)
F79A	0.5921 (5)	0.0132 (4)	0.6339 (2)	0.112 (4)	0.3612 (16)
F80A	0.5920 (5)	0.0004 (4)	0.5485 (2)	0.132 (4)	0.3612 (16)

F81A	0.6344 (8)	0.0988 (3)	0.5790 (3)	0.126 (3)	0.3612 (16)
C34A	0.8044 (7)	0.0234 (6)	0.6366 (3)	0.059 (3)	0.3612 (16)
C35A	0.7794 (4)	−0.0744 (3)	0.5770 (2)	0.089 (5)	0.3612 (16)
C36A	0.6337 (4)	0.0323 (3)	0.5871 (2)	0.080 (5)	0.3612 (16)
O8	0.8907 (2)	0.12944 (14)	0.51118 (12)	0.0317 (7)	0.6418 (15)
F66	1.0474 (4)	0.2576 (2)	0.44219 (17)	0.0813 (13)	0.6418 (15)
F64	0.8826 (4)	0.2402 (2)	0.42947 (18)	0.0902 (14)	0.6418 (15)
F65	0.9973 (3)	0.1567 (2)	0.41895 (14)	0.0856 (12)	0.6418 (15)
C31	1.0511 (3)	0.17322 (18)	0.53466 (16)	0.0468 (13)	0.6418 (15)
F67	1.0322 (3)	0.13709 (16)	0.58040 (13)	0.0568 (10)	0.6418 (15)
F68	1.0977 (2)	0.23323 (16)	0.54613 (14)	0.0622 (10)	0.6418 (15)
F69	1.1171 (2)	0.13745 (15)	0.50165 (14)	0.0578 (9)	0.6418 (15)
C32	0.8849 (3)	0.2449 (2)	0.53886 (17)	0.0554 (17)	0.6418 (15)
F70	0.8873 (2)	0.23221 (16)	0.59115 (12)	0.0595 (9)	0.6418 (15)
F71	0.7866 (2)	0.24442 (16)	0.52528 (17)	0.0709 (12)	0.6418 (15)
F72	0.9226 (3)	0.30725 (14)	0.52708 (17)	0.0740 (12)	0.6418 (15)
C30	0.9704 (6)	0.2108 (4)	0.4469 (3)	0.070 (2)	0.6418 (15)
O8A	0.9301 (5)	0.1312 (2)	0.4883 (3)	0.0560 (18)	0.3582 (15)
F64A	1.0845 (6)	0.2268 (4)	0.4414 (4)	0.097 (3)	0.3582 (15)
F66A	1.0160 (6)	0.3114 (3)	0.4782 (3)	0.076 (2)	0.3582 (15)
C30A	0.9898 (11)	0.2415 (7)	0.4642 (5)	0.080 (4)	0.3582 (15)
F65A	0.9217 (9)	0.2621 (5)	0.4238 (3)	0.107 (3)	0.3582 (15)
F67A	1.0201 (5)	0.2543 (3)	0.5790 (3)	0.090 (2)	0.3582 (15)
F68A	1.0077 (7)	0.1499 (3)	0.5855 (3)	0.159 (4)	0.3582 (15)
F69A	1.1191 (5)	0.1931 (4)	0.5350 (4)	0.179 (6)	0.3582 (15)
C32A	0.8468 (5)	0.2281 (2)	0.5257 (2)	0.058 (3)	0.3582 (15)
F70A	0.8123 (6)	0.1971 (3)	0.5709 (2)	0.119 (3)	0.3582 (15)
F71A	0.7740 (5)	0.2174 (4)	0.4923 (3)	0.148 (4)	0.3582 (15)
F72A	0.8376 (6)	0.2945 (2)	0.5355 (3)	0.093 (3)	0.3582 (15)
C31A	1.0248 (5)	0.1993 (3)	0.5524 (2)	0.071 (3)	0.3582 (15)
C26	0.7137 (3)	0.0953 (2)	0.39514 (14)	0.0528 (12)	0.7758 (19)
F55	0.7703 (3)	0.14518 (17)	0.37076 (16)	0.1016 (13)	0.7758 (19)
F57	0.6255 (2)	0.09144 (15)	0.37026 (13)	0.0743 (10)	0.7758 (19)
C27	0.8318 (3)	0.0153 (2)	0.33735 (16)	0.0641 (15)	0.7758 (19)
F58	0.7678 (2)	0.0300 (2)	0.29802 (11)	0.0896 (12)	0.7758 (19)
F59	0.9147 (2)	0.05603 (19)	0.32944 (13)	0.0818 (11)	0.7758 (19)
F60	0.8668 (2)	−0.05026 (16)	0.33128 (12)	0.0768 (10)	0.7758 (19)
C28	0.6991 (3)	−0.03436 (18)	0.40579 (14)	0.0479 (11)	0.7758 (19)
F61	0.6407 (2)	−0.04697 (15)	0.36473 (11)	0.0648 (8)	0.7758 (19)
F62	0.6325 (2)	−0.01927 (17)	0.44679 (12)	0.0672 (9)	0.7758 (19)
F63	0.7470 (2)	−0.09272 (14)	0.41893 (14)	0.0733 (10)	0.7758 (19)
C26A	0.6755 (5)	0.0623 (3)	0.4114 (2)	0.069 (5)	0.2242 (19)
F55A	0.6328 (9)	0.0074 (4)	0.4366 (3)	0.196 (12)	0.2242 (19)
F57A	0.6160 (6)	0.0861 (4)	0.3728 (3)	0.066 (4)	0.2242 (19)
C27A	0.8231 (4)	0.0879 (3)	0.3555 (3)	0.086 (6)	0.2242 (19)
F58A	0.7932 (6)	0.0918 (5)	0.3031 (3)	0.081 (4)	0.2242 (19)
F59A	0.9296 (5)	0.0922 (6)	0.3457 (4)	0.106 (5)	0.2242 (19)
F60A	0.8028 (9)	0.1560 (4)	0.3691 (4)	0.111 (7)	0.2242 (19)
C28A	0.7841 (4)	−0.0385 (3)	0.3568 (2)	0.085 (7)	0.2242 (19)

F61A	0.7103 (5)	−0.0330 (5)	0.3260 (3)	0.104 (4)	0.2242 (19)
F62A	0.7756 (6)	−0.0864 (4)	0.3915 (4)	0.076 (4)	0.2242 (19)
F63A	0.8731 (6)	−0.0308 (9)	0.3347 (5)	0.303 (11)	0.2242 (19)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Al1	0.0282 (3)	0.0237 (3)	0.0226 (4)	0.0020 (3)	−0.0026 (3)	−0.0024 (3)
F01	0.0341 (10)	0.0303 (10)	0.0261 (10)	0.0027 (9)	−0.0004 (9)	−0.0025 (9)
F21	0.0520 (10)	0.0462 (9)	0.0547 (11)	0.0029 (8)	−0.0169 (9)	−0.0212 (8)
F24	0.0369 (9)	0.0589 (11)	0.0651 (12)	0.0189 (8)	−0.0077 (9)	−0.0179 (10)
F27	0.0467 (10)	0.0602 (11)	0.0531 (11)	−0.0082 (9)	0.0005 (9)	0.0119 (9)
O3	0.0309 (9)	0.0318 (9)	0.0388 (11)	0.0054 (8)	−0.0027 (8)	−0.0105 (8)
F23	0.0375 (9)	0.0581 (11)	0.0648 (12)	−0.0003 (8)	−0.0074 (9)	−0.0272 (9)
F20	0.0732 (12)	0.0528 (11)	0.0392 (10)	0.0146 (10)	−0.0124 (9)	0.0013 (9)
O2	0.0320 (9)	0.0401 (10)	0.0387 (11)	0.0013 (8)	−0.0084 (8)	−0.0145 (9)
F22	0.0443 (10)	0.0612 (12)	0.0660 (13)	−0.0022 (9)	0.0142 (9)	0.0057 (10)
O1	0.0428 (10)	0.0307 (9)	0.0341 (10)	0.0037 (8)	0.0022 (9)	0.0055 (8)
F26	0.0716 (12)	0.0345 (9)	0.0686 (13)	0.0132 (9)	−0.0122 (11)	0.0047 (9)
F9	0.0793 (13)	0.0457 (10)	0.0445 (11)	0.0034 (10)	−0.0009 (10)	−0.0105 (9)
F19	0.0582 (11)	0.0668 (11)	0.0474 (10)	0.0263 (9)	−0.0055 (9)	−0.0280 (9)
F8	0.0921 (15)	0.0673 (13)	0.0338 (10)	0.0009 (12)	0.0085 (10)	0.0113 (9)
F12	0.0697 (13)	0.0379 (10)	0.1002 (17)	0.0062 (9)	0.0016 (13)	−0.0227 (11)
F6	0.124 (2)	0.0388 (10)	0.0639 (13)	0.0226 (12)	0.0123 (14)	0.0182 (10)
F7	0.0661 (12)	0.0769 (14)	0.0649 (13)	0.0062 (11)	−0.0277 (11)	0.0093 (11)
F25	0.0621 (11)	0.0725 (13)	0.0358 (10)	0.0019 (10)	−0.0148 (9)	0.0044 (9)
F15	0.0603 (12)	0.1006 (16)	0.0511 (12)	0.0043 (12)	−0.0064 (10)	−0.0305 (12)
F18	0.0319 (9)	0.0684 (13)	0.1080 (18)	0.0087 (9)	−0.0096 (11)	−0.0229 (13)
F5	0.0834 (14)	0.0573 (12)	0.0750 (15)	0.0354 (11)	0.0212 (12)	0.0094 (11)
F3	0.0500 (11)	0.0677 (13)	0.0976 (17)	0.0074 (10)	0.0213 (12)	0.0123 (13)
F17	0.0497 (11)	0.0401 (10)	0.138 (2)	0.0070 (9)	0.0054 (13)	−0.0275 (12)
F16	0.0581 (12)	0.0970 (16)	0.0652 (13)	−0.0019 (12)	0.0146 (11)	−0.0400 (12)
F11	0.0777 (14)	0.0732 (14)	0.0616 (13)	−0.0032 (12)	−0.0117 (12)	0.0204 (11)
F10	0.0515 (11)	0.0552 (11)	0.1022 (18)	−0.0190 (10)	0.0055 (12)	−0.0095 (12)
F14	0.0655 (12)	0.1062 (17)	0.0693 (14)	−0.0134 (13)	−0.0330 (11)	−0.0300 (13)
F2	0.0681 (13)	0.1131 (19)	0.0685 (15)	−0.0285 (13)	−0.0285 (12)	0.0183 (14)
F13	0.0782 (15)	0.0884 (16)	0.0743 (15)	0.0014 (13)	−0.0291 (12)	0.0254 (13)
C12	0.0450 (16)	0.0395 (15)	0.0386 (16)	0.0003 (13)	−0.0103 (13)	0.0014 (13)
F4	0.145 (2)	0.0427 (11)	0.0547 (13)	−0.0062 (13)	−0.0011 (15)	−0.0126 (10)
C11	0.0337 (14)	0.0424 (15)	0.0444 (17)	0.0070 (12)	−0.0007 (13)	−0.0096 (14)
C8	0.0342 (15)	0.0490 (18)	0.074 (2)	0.0025 (14)	−0.0053 (16)	−0.0208 (17)
F1	0.0832 (15)	0.0659 (13)	0.0872 (17)	−0.0324 (12)	0.0047 (13)	0.0191 (12)
C1	0.0443 (15)	0.0271 (12)	0.0331 (14)	0.0004 (11)	0.0005 (12)	0.0056 (11)
C10	0.0462 (16)	0.0368 (14)	0.0353 (15)	0.0107 (13)	−0.0043 (13)	−0.0105 (12)
C5	0.0319 (13)	0.0335 (13)	0.0393 (15)	0.0005 (11)	−0.0115 (12)	−0.0117 (12)
C4	0.063 (2)	0.0493 (18)	0.0415 (18)	0.0026 (16)	−0.0043 (16)	0.0076 (15)
C9	0.0323 (13)	0.0281 (12)	0.0318 (14)	0.0066 (10)	−0.0037 (11)	−0.0062 (11)
C7	0.0493 (18)	0.069 (2)	0.051 (2)	−0.0043 (17)	−0.0207 (16)	−0.0074 (18)

C6	0.0436 (16)	0.0419 (16)	0.062 (2)	−0.0020 (14)	−0.0051 (16)	−0.0067 (16)
C3	0.088 (3)	0.0349 (16)	0.051 (2)	0.0122 (17)	0.0118 (19)	0.0085 (15)
C2	0.058 (2)	0.0555 (19)	0.059 (2)	−0.0123 (17)	−0.0064 (17)	0.0154 (17)
Al2	0.0204 (3)	0.0280 (4)	0.0263 (4)	−0.0024 (3)	−0.0023 (3)	−0.0020 (3)
F02	0.0234 (9)	0.0343 (10)	0.0312 (11)	−0.0049 (8)	−0.0037 (8)	−0.0015 (9)
O6	0.0321 (9)	0.0317 (9)	0.0357 (10)	0.0002 (8)	0.0064 (8)	0.0016 (8)
O5	0.0299 (9)	0.0539 (12)	0.0279 (10)	−0.0015 (9)	−0.0073 (8)	−0.0001 (9)
O4	0.0277 (9)	0.0311 (9)	0.0494 (12)	0.0015 (8)	0.0052 (9)	0.0019 (9)
F49	0.0497 (10)	0.0542 (11)	0.0759 (14)	0.0064 (9)	0.0300 (10)	−0.0103 (10)
F36	0.0357 (9)	0.0576 (12)	0.1000 (17)	−0.0096 (9)	−0.0035 (11)	−0.0060 (12)
F45	0.0559 (11)	0.0613 (12)	0.0693 (13)	0.0091 (10)	−0.0152 (10)	−0.0201 (10)
F44	0.0614 (11)	0.0810 (14)	0.0557 (12)	0.0170 (11)	−0.0276 (10)	0.0047 (11)
F48	0.0496 (10)	0.0539 (11)	0.0844 (15)	−0.0125 (9)	0.0321 (10)	0.0008 (10)
F43	0.0354 (9)	0.1065 (17)	0.0579 (13)	0.0067 (11)	0.0021 (9)	0.0088 (12)
F35	0.0625 (12)	0.0854 (15)	0.0601 (13)	0.0204 (11)	0.0228 (10)	0.0254 (11)
F42	0.0723 (14)	0.0807 (15)	0.0735 (15)	−0.0064 (12)	0.0098 (12)	0.0255 (13)
F34	0.0665 (12)	0.0622 (12)	0.0748 (14)	0.0279 (10)	0.0220 (11)	−0.0115 (11)
F33	0.0652 (13)	0.1138 (19)	0.0572 (13)	0.0156 (13)	−0.0152 (11)	−0.0264 (13)
F41	0.0861 (16)	0.169 (3)	0.0295 (10)	0.0338 (17)	−0.0156 (11)	−0.0100 (14)
F40	0.0591 (12)	0.1173 (18)	0.0406 (11)	0.0297 (12)	−0.0006 (10)	−0.0113 (12)
C21	0.0279 (12)	0.0339 (13)	0.0340 (14)	0.0000 (11)	0.0066 (11)	−0.0014 (11)
F30	0.0417 (11)	0.0619 (13)	0.164 (3)	−0.0219 (10)	0.0069 (14)	−0.0277 (15)
F32	0.0803 (14)	0.1034 (17)	0.0816 (17)	0.0570 (13)	−0.0019 (13)	0.0177 (14)
F39	0.0692 (13)	0.0732 (14)	0.112 (2)	−0.0282 (12)	−0.0264 (14)	0.0279 (14)
C13	0.0296 (13)	0.0272 (13)	0.0486 (17)	0.0030 (11)	0.0012 (12)	−0.0024 (12)
F50	0.0976 (16)	0.0449 (11)	0.201 (3)	−0.0211 (12)	0.0847 (18)	−0.0417 (15)
F46	0.1241 (18)	0.158 (2)	0.094 (2)	−0.0935 (17)	−0.0459 (16)	0.0265 (18)
F31	0.0863 (16)	0.0905 (16)	0.0841 (15)	0.0202 (13)	0.0397 (13)	0.0436 (13)
C17	0.0335 (13)	0.0515 (17)	0.0311 (14)	−0.0004 (13)	−0.0118 (12)	−0.0022 (13)
F38	0.0851 (14)	0.0907 (17)	0.1218 (19)	−0.0153 (13)	−0.0717 (13)	−0.0198 (15)
C20	0.0363 (15)	0.0601 (19)	0.0427 (17)	0.0016 (14)	−0.0104 (13)	0.0000 (15)
F52	0.0720 (15)	0.157 (3)	0.0350 (11)	0.0162 (16)	0.0075 (11)	0.0042 (14)
C23	0.0454 (17)	0.0502 (18)	0.0499 (19)	0.0120 (15)	0.0117 (15)	−0.0047 (15)
F29	0.1012 (19)	0.1054 (19)	0.0793 (16)	0.0008 (16)	−0.0309 (15)	−0.0403 (15)
C22	0.0460 (17)	0.0506 (18)	0.054 (2)	−0.0151 (15)	0.0096 (16)	−0.0038 (16)
C16	0.0525 (19)	0.0533 (19)	0.061 (2)	0.0077 (16)	0.0099 (17)	0.0016 (17)
C19	0.056 (2)	0.095 (3)	0.0306 (16)	0.020 (2)	−0.0095 (15)	−0.0047 (18)
F28	0.0805 (17)	0.0342 (11)	0.224 (4)	−0.0029 (11)	−0.001 (2)	−0.0249 (17)
F37	0.121 (2)	0.0602 (13)	0.118 (2)	0.0143 (14)	−0.0477 (17)	−0.0387 (14)
C24	0.0369 (16)	0.071 (2)	0.0477 (19)	0.0043 (16)	0.0027 (14)	0.0074 (17)
C15	0.061 (2)	0.067 (2)	0.070 (3)	0.0174 (19)	0.005 (2)	0.015 (2)
C18	0.066 (2)	0.064 (2)	0.086 (3)	−0.0114 (19)	−0.042 (2)	−0.004 (2)
C14	0.050 (2)	0.0394 (18)	0.174 (5)	−0.0044 (17)	−0.012 (3)	−0.025 (3)
Al3	0.0268 (4)	0.0382 (4)	0.0296 (4)	0.0118 (3)	−0.0076 (3)	−0.0081 (3)
F03	0.0200 (9)	0.0335 (10)	0.0311 (11)	0.0036 (8)	−0.0038 (8)	−0.0017 (9)
O7	0.0337 (9)	0.0415 (10)	0.0356 (10)	0.0059 (8)	−0.0129 (8)	−0.0065 (9)
C29	0.0275 (12)	0.0421 (15)	0.0352 (15)	−0.0013 (11)	−0.0026 (11)	−0.0053 (12)
C33	0.0423 (15)	0.0358 (14)	0.0453 (17)	0.0075 (13)	0.0061 (14)	−0.0039 (13)
C25	0.0409 (15)	0.0484 (16)	0.0367 (15)	0.0105 (13)	−0.0195 (13)	−0.0104 (13)

Al4	0.0329 (4)	0.0278 (4)	0.0251 (4)	−0.0008 (3)	0.0009 (3)	−0.0045 (3)
F04	0.0567 (14)	0.0397 (12)	0.0295 (12)	−0.0113 (11)	0.0051 (11)	−0.0069 (10)
O12	0.0440 (11)	0.0427 (11)	0.0575 (14)	−0.0053 (9)	−0.0143 (10)	−0.0053 (10)
F90	0.0782 (14)	0.0658 (13)	0.0678 (14)	−0.0185 (11)	0.0110 (12)	0.0170 (11)
O10	0.0389 (11)	0.0382 (11)	0.0764 (16)	0.0068 (9)	0.0129 (11)	0.0011 (11)
F89	0.0918 (15)	0.0600 (12)	0.0753 (15)	−0.0313 (11)	0.0083 (13)	−0.0271 (11)
F96	0.130 (2)	0.0414 (10)	0.0657 (14)	−0.0172 (12)	−0.0125 (14)	0.0191 (10)
F87	0.0837 (15)	0.0594 (12)	0.0670 (14)	−0.0193 (11)	−0.0134 (12)	0.0254 (11)
O11	0.0555 (12)	0.0333 (10)	0.0494 (13)	−0.0057 (9)	−0.0116 (10)	0.0091 (9)
F99	0.1128 (19)	0.0745 (14)	0.0422 (12)	−0.0036 (14)	−0.0003 (12)	0.0108 (11)
F107	0.0383 (10)	0.1123 (19)	0.0953 (19)	−0.0100 (12)	−0.0065 (12)	−0.0110 (16)
F106	0.0751 (15)	0.147 (2)	0.0922 (17)	0.0519 (15)	−0.0238 (13)	−0.0705 (16)
F84	0.1109 (19)	0.0558 (12)	0.0882 (17)	−0.0263 (13)	−0.0035 (15)	−0.0273 (12)
F88	0.0388 (11)	0.0873 (16)	0.117 (2)	−0.0016 (11)	−0.0042 (13)	0.0043 (15)
F105	0.0845 (14)	0.0702 (13)	0.0826 (16)	−0.0404 (12)	−0.0163 (13)	0.0111 (12)
F102	0.1038 (17)	0.0654 (13)	0.0643 (14)	−0.0155 (13)	−0.0217 (13)	−0.0265 (11)
F98	0.118 (2)	0.0505 (12)	0.0632 (14)	−0.0065 (13)	0.0164 (14)	−0.0167 (11)
F93	0.0578 (13)	0.0938 (17)	0.111 (2)	−0.0037 (13)	−0.0299 (13)	0.0265 (16)
F104	0.0552 (13)	0.0906 (16)	0.150 (2)	−0.0012 (13)	−0.0150 (15)	0.0569 (17)
F97	0.0711 (14)	0.0786 (16)	0.1028 (19)	0.0076 (12)	0.0429 (13)	0.0093 (14)
F95	0.0926 (16)	0.0645 (13)	0.111 (2)	−0.0334 (12)	−0.0423 (15)	0.0279 (13)
F94	0.197 (3)	0.0503 (13)	0.0553 (14)	−0.0104 (17)	−0.0008 (18)	−0.0126 (11)
C41	0.0478 (16)	0.0322 (14)	0.0386 (16)	0.0055 (12)	0.0012 (13)	0.0051 (12)
F86	0.1057 (18)	0.119 (2)	0.0535 (13)	−0.0318 (16)	−0.0335 (13)	0.0078 (14)
F101	0.098 (2)	0.124 (2)	0.133 (3)	0.0340 (18)	0.0107 (19)	−0.0612 (19)
F85	0.0877 (17)	0.0723 (15)	0.147 (3)	0.0403 (13)	−0.0125 (18)	0.0219 (17)
F92	0.1008 (18)	0.0694 (14)	0.126 (2)	0.0486 (13)	−0.0051 (17)	0.0202 (15)
F83	0.137 (2)	0.1037 (19)	0.0510 (13)	−0.0348 (18)	−0.0329 (15)	0.0182 (13)
C37	0.0334 (13)	0.0291 (13)	0.0382 (15)	0.0042 (11)	0.0038 (12)	−0.0023 (12)
F91	0.0902 (17)	0.128 (2)	0.0953 (19)	0.0396 (17)	0.0492 (15)	0.0046 (17)
F82	0.1068 (18)	0.0944 (17)	0.1011 (17)	−0.0193 (15)	0.0567 (15)	−0.0526 (14)
C44	0.077 (2)	0.0453 (18)	0.050 (2)	0.0028 (18)	0.0137 (19)	0.0005 (16)
C45	0.0363 (14)	0.0424 (15)	0.0442 (17)	−0.0042 (12)	−0.0020 (13)	−0.0133 (13)
C48	0.0437 (17)	0.064 (2)	0.0424 (18)	0.0010 (16)	−0.0096 (14)	−0.0020 (16)
C47	0.0450 (18)	0.0517 (19)	0.077 (3)	−0.0013 (16)	−0.0065 (18)	0.0031 (19)
C40	0.0455 (17)	0.0494 (18)	0.055 (2)	−0.0027 (15)	−0.0006 (16)	−0.0046 (16)
C46	0.060 (2)	0.078 (2)	0.069 (2)	−0.006 (2)	0.0079 (19)	−0.038 (2)
C43	0.097 (3)	0.0347 (16)	0.058 (2)	−0.0073 (18)	−0.003 (2)	0.0098 (16)
C39	0.060 (2)	0.055 (2)	0.063 (2)	−0.0021 (18)	−0.0104 (19)	0.0072 (18)
C42	0.064 (2)	0.065 (2)	0.071 (3)	0.0208 (19)	0.007 (2)	0.011 (2)
C38	0.072 (2)	0.060 (2)	0.054 (2)	−0.0140 (19)	0.0020 (19)	−0.0189 (18)
N1	0.0371 (11)	0.0276 (10)	0.0300 (12)	0.0008 (9)	0.0008 (10)	−0.0028 (9)
C106	0.0348 (13)	0.0366 (14)	0.0333 (14)	−0.0023 (12)	−0.0009 (12)	−0.0015 (12)
C113	0.0330 (13)	0.0285 (12)	0.0319 (14)	0.0012 (11)	−0.0026 (11)	−0.0056 (11)
C105	0.0350 (13)	0.0335 (13)	0.0320 (14)	−0.0048 (11)	−0.0032 (11)	−0.0074 (11)
C114	0.0351 (13)	0.0297 (13)	0.0407 (15)	0.0001 (11)	−0.0058 (12)	−0.0033 (12)
C101	0.0442 (15)	0.0356 (14)	0.0351 (15)	−0.0013 (12)	0.0096 (13)	−0.0028 (12)
C109	0.0426 (15)	0.0328 (13)	0.0313 (14)	0.0062 (12)	−0.0003 (12)	−0.0016 (12)
C115	0.0378 (14)	0.0305 (13)	0.0375 (15)	−0.0021 (11)	−0.0031 (12)	−0.0043 (12)

C110	0.0501 (17)	0.0391 (15)	0.0323 (15)	0.0119 (13)	−0.0005 (13)	−0.0013 (12)
C116	0.0519 (17)	0.0303 (14)	0.071 (2)	0.0034 (13)	−0.0191 (17)	−0.0046 (15)
C107	0.0395 (15)	0.0551 (18)	0.0346 (16)	−0.0044 (14)	−0.0044 (13)	−0.0016 (14)
C102	0.066 (2)	0.0332 (15)	0.055 (2)	−0.0028 (15)	0.0223 (17)	−0.0007 (14)
C111	0.0514 (17)	0.0374 (15)	0.0369 (16)	0.0148 (13)	−0.0020 (14)	−0.0004 (13)
C112	0.0564 (18)	0.0493 (18)	0.0426 (18)	0.0156 (15)	−0.0077 (15)	0.0014 (15)
C103	0.070 (2)	0.0449 (17)	0.054 (2)	−0.0140 (16)	0.0187 (18)	−0.0004 (16)
C108	0.0512 (19)	0.101 (3)	0.0356 (18)	−0.017 (2)	−0.0068 (15)	0.0002 (19)
C104	0.062 (2)	0.094 (3)	0.062 (2)	−0.030 (2)	0.0025 (19)	−0.022 (2)
N2	0.0308 (11)	0.0324 (11)	0.0273 (11)	0.0004 (9)	−0.0027 (9)	−0.0069 (9)
C213	0.0295 (12)	0.0325 (13)	0.0294 (13)	−0.0005 (11)	−0.0049 (11)	−0.0041 (11)
C210	0.0364 (14)	0.0375 (14)	0.0307 (14)	0.0019 (12)	−0.0035 (12)	−0.0026 (12)
C201	0.0421 (15)	0.0318 (13)	0.0314 (14)	0.0067 (12)	−0.0020 (12)	−0.0028 (11)
C209	0.0347 (13)	0.0348 (13)	0.0291 (13)	0.0003 (11)	−0.0065 (11)	−0.0065 (11)
C214	0.0303 (13)	0.0337 (13)	0.0333 (14)	−0.0006 (11)	−0.0037 (11)	−0.0054 (11)
C206	0.0412 (15)	0.0382 (15)	0.0392 (16)	−0.0048 (12)	−0.0046 (13)	−0.0040 (13)
C215	0.0339 (14)	0.0400 (15)	0.0404 (16)	−0.0049 (12)	−0.0043 (12)	−0.0089 (13)
C211	0.0430 (16)	0.0555 (18)	0.0326 (15)	0.0053 (14)	−0.0069 (13)	−0.0025 (14)
C202	0.0544 (17)	0.0431 (16)	0.0297 (15)	0.0089 (14)	0.0003 (13)	0.0013 (13)
C205	0.0339 (13)	0.0403 (14)	0.0331 (14)	−0.0020 (12)	0.0029 (12)	−0.0088 (12)
C216	0.0449 (17)	0.0383 (15)	0.065 (2)	−0.0035 (14)	0.0011 (16)	−0.0127 (15)
C207	0.0460 (17)	0.0539 (18)	0.0438 (18)	−0.0151 (15)	0.0024 (14)	−0.0042 (15)
C212	0.0519 (18)	0.063 (2)	0.0309 (15)	0.0067 (16)	−0.0044 (14)	−0.0016 (15)
C203	0.077 (2)	0.0423 (16)	0.0337 (16)	0.0164 (16)	−0.0042 (16)	0.0028 (14)
C208	0.0534 (19)	0.0561 (19)	0.058 (2)	−0.0196 (16)	−0.0077 (17)	0.0072 (17)
C204	0.066 (2)	0.056 (2)	0.068 (2)	0.0220 (18)	−0.014 (2)	−0.0119 (19)
F47	0.1048 (15)	0.0592 (12)	0.286 (3)	−0.0481 (12)	0.1323 (18)	−0.0797 (16)
F51	0.207 (2)	0.172 (2)	0.0625 (17)	0.1551 (19)	−0.0105 (18)	−0.0083 (16)
F53	0.185 (2)	0.200 (3)	0.0661 (18)	0.146 (2)	−0.0099 (18)	0.0031 (18)
F54	0.165 (2)	0.320 (4)	0.1036 (19)	−0.169 (2)	−0.0935 (17)	0.109 (2)
F100	0.273 (4)	0.117 (2)	0.0545 (15)	−0.103 (2)	0.056 (2)	−0.0316 (14)
F103	0.128 (2)	0.105 (2)	0.0500 (14)	0.0087 (18)	−0.0172 (15)	0.0030 (14)
F108	0.0620 (14)	0.116 (2)	0.1012 (19)	0.0077 (14)	−0.0241 (13)	0.0441 (16)
F56	0.0777 (14)	0.0900 (15)	0.0920 (17)	0.0490 (12)	−0.0316 (13)	−0.0413 (13)
O9	0.0356 (15)	0.0293 (14)	0.0352 (16)	0.0026 (12)	0.0115 (13)	−0.0180 (13)
C36	0.031 (2)	0.054 (3)	0.056 (3)	0.000 (2)	0.010 (2)	−0.002 (3)
C35	0.058 (3)	0.045 (3)	0.052 (3)	−0.017 (2)	0.017 (3)	−0.008 (2)
C34	0.059 (3)	0.053 (3)	0.049 (3)	−0.008 (3)	0.000 (3)	0.015 (3)
F73	0.073 (2)	0.097 (3)	0.0439 (19)	−0.013 (2)	0.0097 (17)	−0.0040 (19)
F74	0.085 (3)	0.078 (2)	0.095 (3)	0.023 (2)	−0.013 (2)	0.016 (2)
F75	0.063 (2)	0.071 (2)	0.074 (2)	−0.0353 (17)	−0.0057 (18)	−0.0085 (18)
F76	0.114 (2)	0.0273 (14)	0.145 (3)	−0.0275 (16)	0.089 (2)	−0.0272 (17)
F77	0.0682 (18)	0.0492 (16)	0.072 (2)	−0.0178 (15)	0.0445 (16)	−0.0039 (15)
F78	0.067 (2)	0.101 (3)	0.087 (3)	−0.036 (2)	0.001 (2)	−0.022 (2)
F79	0.0600 (19)	0.0543 (18)	0.075 (2)	0.0092 (15)	0.0281 (17)	−0.0184 (16)
F80	0.067 (2)	0.091 (3)	0.083 (3)	0.0409 (19)	−0.017 (2)	−0.005 (2)
F81	0.073 (2)	0.0385 (16)	0.102 (3)	0.0031 (16)	0.021 (2)	−0.0139 (17)
O9A	0.046 (3)	0.085 (5)	0.037 (3)	0.039 (3)	0.009 (3)	−0.018 (3)
F73A	0.083 (4)	0.085 (5)	0.042 (3)	−0.018 (4)	−0.002 (3)	0.018 (3)

F74A	0.034 (4)	0.314 (17)	0.120 (8)	−0.018 (7)	−0.011 (4)	0.066 (10)
F75A	0.240 (11)	0.045 (4)	0.099 (6)	0.000 (5)	−0.068 (6)	−0.024 (4)
F76A	0.254 (12)	0.052 (4)	0.076 (5)	−0.007 (6)	−0.021 (7)	−0.018 (4)
F77A	0.106 (5)	0.081 (4)	0.113 (6)	0.050 (4)	0.018 (5)	0.017 (4)
F78A	0.249 (12)	0.064 (5)	0.078 (6)	−0.058 (6)	0.044 (7)	−0.006 (4)
F79A	0.030 (3)	0.231 (11)	0.071 (5)	−0.010 (5)	0.026 (3)	0.022 (6)
F80A	0.064 (4)	0.256 (11)	0.077 (5)	−0.074 (5)	−0.038 (3)	0.061 (6)
F81A	0.185 (8)	0.093 (5)	0.107 (6)	0.078 (5)	−0.076 (6)	−0.025 (5)
C34A	0.039 (5)	0.072 (7)	0.064 (7)	0.006 (5)	0.011 (5)	0.021 (6)
C35A	0.113 (11)	0.082 (9)	0.068 (8)	0.011 (8)	0.020 (8)	−0.004 (7)
C36A	0.024 (4)	0.173 (14)	0.042 (6)	−0.009 (7)	0.014 (4)	0.008 (8)
O8	0.0287 (14)	0.0325 (15)	0.0334 (16)	0.0043 (12)	0.0072 (12)	−0.0115 (13)
F66	0.104 (3)	0.080 (3)	0.058 (2)	−0.025 (2)	0.008 (2)	0.013 (2)
F64	0.112 (3)	0.076 (2)	0.085 (2)	−0.018 (2)	−0.052 (2)	0.042 (2)
F65	0.120 (3)	0.092 (2)	0.0433 (17)	−0.046 (2)	0.0322 (19)	−0.0292 (17)
C31	0.041 (2)	0.044 (2)	0.057 (3)	−0.018 (2)	0.001 (2)	−0.021 (2)
F67	0.0512 (16)	0.0601 (19)	0.060 (2)	0.0025 (15)	−0.0226 (15)	0.0190 (16)
F68	0.0509 (16)	0.0614 (18)	0.077 (2)	−0.0306 (15)	−0.0162 (16)	−0.0007 (17)
F69	0.0310 (13)	0.0537 (16)	0.089 (2)	0.0056 (12)	0.0068 (15)	−0.0276 (16)
C32	0.047 (3)	0.030 (2)	0.090 (4)	−0.008 (2)	−0.002 (3)	−0.014 (3)
F70	0.0626 (18)	0.0619 (18)	0.0528 (17)	−0.0101 (15)	0.0216 (15)	−0.0261 (15)
F71	0.0454 (16)	0.0455 (17)	0.123 (3)	0.0215 (14)	−0.0189 (19)	−0.0138 (19)
F72	0.064 (2)	0.0279 (14)	0.128 (3)	−0.0024 (14)	0.012 (2)	−0.0081 (18)
C30	0.102 (5)	0.065 (4)	0.044 (3)	−0.029 (4)	−0.002 (3)	−0.012 (3)
O8A	0.068 (4)	0.040 (3)	0.064 (4)	0.036 (3)	−0.029 (3)	−0.044 (3)
F64A	0.091 (4)	0.059 (4)	0.129 (6)	−0.012 (4)	0.077 (4)	0.012 (4)
F66A	0.115 (5)	0.035 (3)	0.077 (4)	−0.014 (3)	0.008 (4)	−0.001 (3)
C30A	0.078 (8)	0.106 (10)	0.055 (7)	0.014 (8)	0.009 (7)	−0.024 (7)
F65A	0.176 (9)	0.101 (6)	0.047 (4)	−0.033 (6)	−0.043 (5)	0.039 (4)
F67A	0.100 (5)	0.082 (4)	0.093 (5)	−0.008 (4)	−0.058 (4)	−0.020 (4)
F68A	0.247 (11)	0.125 (7)	0.115 (7)	−0.100 (7)	−0.116 (7)	0.074 (5)
F69A	0.046 (4)	0.271 (14)	0.219 (12)	−0.033 (7)	−0.042 (6)	0.125 (11)
C32A	0.060 (6)	0.032 (5)	0.082 (8)	0.008 (5)	0.000 (6)	−0.019 (5)
F70A	0.119 (6)	0.084 (5)	0.142 (7)	0.013 (5)	0.084 (5)	−0.002 (5)
F71A	0.054 (3)	0.235 (9)	0.165 (7)	0.081 (5)	−0.060 (4)	−0.121 (7)
F72A	0.095 (5)	0.039 (3)	0.143 (7)	0.027 (3)	0.016 (5)	−0.024 (4)
C31A	0.134 (9)	0.037 (5)	0.046 (5)	−0.015 (6)	−0.058 (6)	0.009 (4)
C26	0.048 (2)	0.046 (2)	0.067 (3)	0.0095 (19)	−0.030 (2)	−0.001 (2)
F55	0.102 (2)	0.0555 (18)	0.152 (3)	−0.0110 (17)	−0.068 (2)	0.0391 (19)
F57	0.0618 (15)	0.0587 (17)	0.108 (2)	0.0218 (14)	−0.0552 (16)	−0.0030 (16)
C27	0.052 (2)	0.107 (4)	0.035 (2)	−0.003 (3)	−0.016 (2)	−0.002 (3)
F58	0.0725 (19)	0.161 (4)	0.0371 (15)	−0.001 (2)	−0.0243 (14)	0.0016 (19)
F59	0.0610 (17)	0.133 (3)	0.0510 (17)	−0.0192 (19)	−0.0095 (14)	0.0164 (19)
F60	0.080 (2)	0.100 (2)	0.0524 (15)	0.0330 (17)	−0.0128 (15)	−0.0427 (15)
C28	0.044 (2)	0.047 (2)	0.056 (2)	0.0050 (18)	−0.0260 (19)	−0.0108 (19)
F61	0.0533 (13)	0.0733 (17)	0.0726 (17)	−0.0038 (13)	−0.0354 (13)	−0.0224 (14)
F62	0.0401 (13)	0.092 (2)	0.0703 (19)	−0.0165 (14)	−0.0012 (13)	−0.0150 (16)
F63	0.0647 (16)	0.0483 (15)	0.110 (3)	−0.0047 (13)	−0.0347 (17)	0.0094 (16)
C26A	0.058 (9)	0.059 (10)	0.093 (13)	−0.009 (8)	−0.045 (9)	0.017 (10)

F55A	0.068 (10)	0.34 (3)	0.167 (17)	−0.019 (15)	0.013 (11)	0.116 (19)
F57A	0.022 (4)	0.139 (11)	0.038 (5)	−0.012 (6)	−0.004 (4)	0.011 (6)
C27A	0.075 (10)	0.089 (14)	0.099 (14)	0.013 (10)	−0.058 (10)	0.009 (11)
F58A	0.087 (7)	0.120 (9)	0.034 (5)	0.033 (7)	−0.012 (5)	0.005 (6)
F59A	0.084 (9)	0.152 (13)	0.081 (9)	−0.034 (9)	0.011 (7)	0.025 (9)
F60A	0.207 (18)	0.044 (6)	0.082 (9)	−0.022 (9)	−0.015 (10)	0.030 (6)
C28A	0.078 (12)	0.082 (14)	0.101 (15)	0.005 (11)	−0.049 (11)	−0.007 (12)
F61A	0.125 (8)	0.068 (6)	0.132 (8)	0.018 (6)	−0.099 (7)	−0.049 (6)
F62A	0.103 (8)	0.026 (4)	0.103 (9)	0.003 (5)	−0.042 (7)	−0.002 (5)
F63A	0.163 (14)	0.44 (2)	0.32 (2)	0.190 (16)	−0.043 (16)	−0.276 (18)

Geometric parameters (Å, °)

Al1—O2	1.695 (2)	C47—F103	1.339 (4)
Al1—O3	1.699 (2)	C46—F100	1.285 (4)
Al1—O1	1.700 (2)	N1—C105	1.512 (4)
Al1—F01	1.7696 (9)	N1—C109	1.521 (4)
F01—Al1^{i}	1.7696 (9)	N1—C113	1.522 (3)
F21—C10	1.336 (4)	N1—C101	1.526 (4)
F24—C11	1.331 (4)	C106—C105	1.516 (4)
F27—C12	1.336 (4)	C106—C107	1.525 (4)
O3—C9	1.369 (3)	C106—H10A	0.9900
F23—C11	1.319 (4)	C106—H10B	0.9900
F20—C10	1.323 (4)	C113—C114	1.522 (4)
O2—C5	1.353 (3)	C113—H11A	0.9900
F22—C11	1.333 (4)	C113—H11B	0.9900
O1—C1	1.365 (3)	C105—H10C	0.9900
F26—C12	1.326 (4)	C105—H10D	0.9900
F9—C4	1.330 (4)	C114—C115	1.522 (4)
F19—C10	1.328 (4)	C114—H11C	0.9900
F8—C4	1.337 (4)	C114—H11D	0.9900
F12—C6	1.344 (4)	C101—C102	1.525 (4)
F6—C3	1.336 (4)	C101—H10E	0.9900
F7—C4	1.350 (4)	C101—H10F	0.9900
F25—C12	1.324 (4)	C109—C110	1.512 (4)
F15—C7	1.343 (4)	C109—H10G	0.9900
F18—C8	1.336 (4)	C109—H10H	0.9900
F5—C3	1.330 (5)	C115—C116	1.518 (4)
F3—C2	1.345 (5)	C115—H11E	0.9900
F17—C8	1.314 (4)	C115—H11F	0.9900
F16—C8	1.332 (5)	C110—C111	1.525 (4)
F11—C6	1.312 (4)	C110—H11G	0.9900
F10—C6	1.331 (4)	C110—H11H	0.9900
F14—C7	1.340 (4)	C116—H11I	0.9800
F2—C2	1.312 (5)	C116—H11J	0.9800
F13—C7	1.338 (5)	C116—H11K	0.9800
C12—C9	1.554 (4)	C107—C108	1.506 (5)
F4—C3	1.335 (5)	C107—H10I	0.9900
C11—C9	1.550 (4)	C107—H10J	0.9900

C8—C5	1.548 (4)	C102—C103	1.535 (5)
F1—C2	1.341 (4)	C102—H10K	0.9900
C1—C4	1.538 (5)	C102—H10L	0.9900
C1—C3	1.544 (4)	C111—C112	1.513 (5)
C1—C2	1.548 (5)	C111—H11L	0.9900
C10—C9	1.552 (4)	C111—H11M	0.9900
C5—C7	1.536 (5)	C112—H11N	0.9800
C5—C6	1.552 (4)	C112—H11O	0.9800
Al2—O4	1.691 (2)	C112—H11P	0.9800
Al2—O6	1.699 (2)	C103—C104	1.503 (6)
Al2—O5	1.706 (2)	C103—H10M	0.9900
Al2—F02	1.7696 (9)	C103—H10N	0.9900
F02—Al2^{ii}	1.7696 (9)	C108—H10O	0.9800
O6—C21	1.364 (3)	C108—H10P	0.9800
O5—C17	1.358 (4)	C108—H10Q	0.9800
O4—C13	1.361 (3)	C104—H10R	0.9800
F49—C23	1.314 (3)	C104—H10S	0.9800
F36—C16	1.363 (5)	C104—H10T	0.9800
F45—C20	1.303 (4)	N2—C205	1.515 (4)
F44—C20	1.334 (4)	N2—C209	1.521 (4)
F48—C22	1.302 (3)	N2—C213	1.521 (3)
F43—C20	1.325 (4)	N2—C201	1.529 (4)
F35—C16	1.328 (5)	C213—C214	1.515 (4)
F42—C19	1.309 (5)	C213—H21A	0.9900
F34—C16	1.325 (4)	C213—H21P	0.9900
F33—C15	1.330 (5)	C210—C209	1.511 (4)
F41—C19	1.341 (4)	C210—C211	1.520 (4)
F40—C19	1.343 (5)	C210—H21B	0.9900
C21—C24	1.524 (4)	C210—H21C	0.9900
C21—C23	1.549 (4)	C201—C202	1.520 (4)
C21—C22	1.555 (4)	C201—H20A	0.9900
F30—C14	1.305 (5)	C201—H20B	0.9900
F32—C15	1.335 (5)	C209—H20C	0.9900
F39—C18	1.333 (5)	C209—H20D	0.9900
C13—C14	1.528 (5)	C214—C215	1.524 (4)
C13—C15	1.539 (5)	C214—H21D	0.9900
C13—C16	1.550 (5)	C214—H21E	0.9900
F50—C23	1.316 (4)	C206—C205	1.523 (4)
F46—C22	1.326 (4)	C206—C207	1.528 (4)
F31—C15	1.378 (5)	C206—H20E	0.9900
C17—C18	1.530 (5)	C206—H20F	0.9900
C17—C20	1.562 (5)	C215—C216	1.518 (4)
C17—C19	1.564 (5)	C215—H21F	0.9900
F38—C18	1.338 (5)	C215—H21G	0.9900
F52—C24	1.284 (4)	C211—C212	1.508 (5)
C23—F51	1.276 (4)	C211—H21H	0.9900
F29—C14	1.400 (7)	C211—H21I	0.9900
C22—F47	1.263 (4)	C202—C203	1.530 (5)
F28—C14	1.345 (5)	C202—H20G	0.9900

F37—C18	1.353 (5)	C202—H20H	0.9900
C24—F54	1.257 (4)	C205—H20I	0.9900
C24—F53	1.308 (4)	C205—H20J	0.9900
Al3—O9A	1.660 (5)	C216—H21J	0.9800
Al3—O8	1.676 (3)	C216—H21K	0.9800
Al3—O7	1.703 (2)	C216—H21L	0.9800
Al3—O9	1.752 (3)	C207—C208	1.512 (5)
Al3—O8A	1.754 (5)	C207—H20K	0.9900
Al3—F03	1.7620 (9)	C207—H20L	0.9900
F03—Al3^{iii}	1.7620 (9)	C212—H21M	0.9800
O7—C25	1.353 (4)	C212—H21N	0.9800
C29—O8A	1.289 (6)	C212—H21O	0.9800
C29—O8	1.410 (4)	C203—C204	1.503 (6)
C29—C30A	1.494 (12)	C203—H20M	0.9900
C29—C32	1.519 (5)	C203—H20N	0.9900
C29—C32A	1.531 (7)	C208—H20O	0.9800
C29—C30	1.540 (7)	C208—H20P	0.9800
C29—C31A	1.549 (7)	C208—H20Q	0.9800
C29—C31	1.550 (5)	C204—H20R	0.9800
C33—O9	1.341 (4)	C204—H20S	0.9800
C33—O9A	1.378 (7)	C204—H20T	0.9800
C33—C36A	1.531 (6)	F56—C26	1.322 (4)
C33—C34	1.543 (5)	F56—C26A	1.326 (5)
C33—C34A	1.544 (7)	C36—F80	1.313 (5)
C33—C35A	1.547 (6)	C36—F79	1.320 (4)
C33—C36	1.554 (4)	C36—F81	1.337 (5)
C33—C35	1.565 (4)	C35—F76	1.304 (5)
C25—C26A	1.520 (7)	C35—F77	1.325 (4)
C25—C26	1.527 (5)	C35—F78	1.333 (5)
C25—C27	1.534 (5)	C34—F75	1.312 (5)
C25—C27A	1.552 (7)	C34—F74	1.314 (5)
C25—C28A	1.588 (7)	C34—F73	1.315 (5)
C25—C28	1.600 (5)	F73A—C34A	1.415 (12)
Al4—O10	1.677 (2)	F74A—C34A	1.280 (12)
Al4—O12	1.696 (2)	F75A—C34A	1.327 (14)
Al4—O11	1.698 (2)	F76A—C35A	1.315 (6)
Al4—F04	1.7635 (9)	F77A—C35A	1.320 (6)
F04—Al4^{iv}	1.7635 (9)	F78A—C35A	1.307 (7)
O12—C45	1.352 (4)	F79A—C36A	1.298 (6)
F90—C40	1.337 (4)	F80A—C36A	1.298 (6)
O10—C37	1.350 (4)	F81A—C36A	1.289 (6)
F89—C40	1.294 (4)	F66—C30	1.343 (8)
F96—C43	1.345 (4)	F64—C30	1.341 (9)
F87—C39	1.327 (5)	F65—C30	1.300 (8)
O11—C41	1.354 (4)	C31—F67	1.328 (4)
F99—C44	1.329 (5)	C31—F69	1.342 (4)
F107—C48	1.311 (4)	C31—F68	1.352 (4)
F106—C48	1.291 (4)	C32—F72	1.318 (4)

F84—C38	1.358 (5)	C32—F70	1.319 (5)
F88—C40	1.315 (4)	C32—F71	1.324 (4)
F105—C47	1.317 (4)	F64A—C30A	1.340 (15)
F102—C46	1.301 (4)	F66A—C30A	1.446 (15)
F98—C44	1.330 (4)	C30A—F65A	1.414 (17)
F93—C42	1.344 (5)	F67A—C31A	1.262 (6)
F104—C47	1.306 (4)	F68A—C31A	1.251 (7)
F97—C44	1.342 (5)	F69A—C31A	1.267 (7)
F95—C43	1.303 (5)	C32A—F71A	1.307 (7)
F94—C43	1.336 (5)	C32A—F72A	1.310 (6)
C41—C42	1.542 (5)	C32A—F70A	1.313 (6)
C41—C44	1.546 (5)	C26—F55	1.322 (4)
C41—C43	1.547 (5)	C26—F57	1.324 (4)
F86—C39	1.332 (5)	C27—F59	1.331 (4)
F101—C46	1.340 (4)	C27—F58	1.335 (4)
F85—C39	1.319 (5)	C27—F60	1.341 (5)
F92—C42	1.327 (5)	C28—F63	1.313 (4)
F83—C38	1.315 (5)	C28—F62	1.328 (4)
C37—C38	1.538 (5)	C28—F61	1.330 (4)
C37—C39	1.547 (5)	C26A—F55A	1.322 (7)
C37—C40	1.557 (4)	C26A—F57A	1.327 (7)
F91—C42	1.306 (5)	C27A—F59A	1.378 (8)
F82—C38	1.318 (5)	C27A—F58A	1.378 (7)
C45—C46	1.529 (5)	C27A—F60A	1.381 (8)
C45—C47	1.546 (5)	C28A—F62A	1.246 (7)
C45—C48	1.559 (5)	C28A—F63A	1.247 (8)
C48—F108	1.313 (4)	C28A—F61A	1.252 (7)
O2—Al1—O3	111.84 (10)	F91—C42—F93	107.1 (4)
O2—Al1—O1	116.75 (11)	F92—C42—F93	107.3 (4)
O3—Al1—O1	112.74 (11)	F91—C42—C41	110.6 (4)
O2—Al1—F01	108.10 (8)	F92—C42—C41	112.3 (3)
O3—Al1—F01	106.04 (8)	F93—C42—C41	110.3 (3)
O1—Al1—F01	100.01 (8)	F83—C38—F82	107.3 (3)
Al1—F01—Al1^{i}	180.00 (5)	F83—C38—F84	106.8 (3)
C9—O3—Al1	146.80 (18)	F82—C38—F84	108.1 (3)
C5—O2—Al1	154.47 (19)	F83—C38—C37	112.1 (3)
C1—O1—Al1	147.09 (19)	F82—C38—C37	113.1 (3)
F25—C12—F26	108.3 (3)	F84—C38—C37	109.2 (3)
F25—C12—F27	107.0 (3)	C105—N1—C109	109.5 (2)
F26—C12—F27	107.8 (3)	C105—N1—C113	111.2 (2)
F25—C12—C9	111.2 (2)	C109—N1—C113	108.9 (2)
F26—C12—C9	112.7 (3)	C105—N1—C101	107.9 (2)
F27—C12—C9	109.6 (2)	C109—N1—C101	110.9 (2)
F23—C11—F24	108.0 (3)	C113—N1—C101	108.5 (2)
F23—C11—F22	107.5 (3)	C105—C106—C107	109.2 (2)
F24—C11—F22	107.3 (2)	C105—C106—H10A	109.8
F23—C11—C9	111.5 (2)	C107—C106—H10A	109.8
F24—C11—C9	112.1 (2)	C105—C106—H10B	109.8

F22—C11—C9	110.3 (3)	C107—C106—H10B	109.8
F17—C8—F16	107.3 (3)	H10A—C106—H10B	108.3
F17—C8—F18	108.1 (3)	C114—C113—N1	116.4 (2)
F16—C8—F18	107.5 (3)	C114—C113—H11A	108.2
F17—C8—C5	110.9 (3)	N1—C113—H11A	108.2
F16—C8—C5	109.7 (3)	C114—C113—H11B	108.2
F18—C8—C5	113.1 (3)	N1—C113—H11B	108.2
O1—C1—C4	110.6 (2)	H11A—C113—H11B	107.3
O1—C1—C3	107.7 (2)	N1—C105—C106	116.9 (2)
C4—C1—C3	109.8 (3)	N1—C105—H10C	108.1
O1—C1—C2	109.4 (3)	C106—C105—H10C	108.1
C4—C1—C2	109.3 (3)	N1—C105—H10D	108.1
C3—C1—C2	110.1 (3)	C106—C105—H10D	108.1
F20—C10—F19	107.7 (3)	H10C—C105—H10D	107.3
F20—C10—F21	106.7 (3)	C115—C114—C113	109.4 (2)
F19—C10—F21	107.4 (2)	C115—C114—H11C	109.8
F20—C10—C9	111.3 (2)	C113—C114—H11C	109.8
F19—C10—C9	112.4 (2)	C115—C114—H11D	109.8
F21—C10—C9	111.0 (2)	C113—C114—H11D	109.8
O2—C5—C7	109.5 (3)	H11C—C114—H11D	108.2
O2—C5—C8	110.1 (2)	C102—C101—N1	116.1 (2)
C7—C5—C8	109.5 (3)	C102—C101—H10E	108.3
O2—C5—C6	108.8 (2)	N1—C101—H10E	108.3
C7—C5—C6	109.8 (3)	C102—C101—H10F	108.3
C8—C5—C6	109.2 (3)	N1—C101—H10F	108.3
F9—C4—F8	107.9 (3)	H10E—C101—H10F	107.4
F9—C4—F7	106.9 (3)	C110—C109—N1	115.5 (2)
F8—C4—F7	107.9 (3)	C110—C109—H10G	108.4
F9—C4—C1	110.7 (3)	N1—C109—H10G	108.4
F8—C4—C1	112.7 (3)	C110—C109—H10H	108.4
F7—C4—C1	110.5 (3)	N1—C109—H10H	108.4
O3—C9—C11	107.7 (2)	H10G—C109—H10H	107.5
O3—C9—C10	110.8 (2)	C116—C115—C114	111.9 (3)
C11—C9—C10	109.4 (2)	C116—C115—H11E	109.2
O3—C9—C12	110.1 (2)	C114—C115—H11E	109.2
C11—C9—C12	109.3 (2)	C116—C115—H11F	109.2
C10—C9—C12	109.5 (2)	C114—C115—H11F	109.2
F13—C7—F14	106.7 (3)	H11E—C115—H11F	107.9
F13—C7—F15	107.0 (3)	C109—C110—C111	110.2 (3)
F14—C7—F15	107.6 (3)	C109—C110—H11G	109.6
F13—C7—C5	111.2 (3)	C111—C110—H11G	109.6
F14—C7—C5	112.2 (3)	C109—C110—H11H	109.6
F15—C7—C5	111.9 (3)	C111—C110—H11H	109.6
F11—C6—F10	108.4 (3)	H11G—C110—H11H	108.1
F11—C6—F12	107.6 (3)	C115—C116—H11I	109.5
F10—C6—F12	107.2 (3)	C115—C116—H11J	109.5
F11—C6—C5	111.4 (3)	H11I—C116—H11J	109.5
F10—C6—C5	112.3 (3)	C115—C116—H11K	109.5
F12—C6—C5	109.7 (3)	H11I—C116—H11K	109.5

F5—C3—F4	107.2 (3)	H11J—C116—H11K	109.5
F5—C3—F6	107.9 (3)	C108—C107—C106	112.8 (3)
F4—C3—F6	108.3 (3)	C108—C107—H10I	109.0
F5—C3—C1	110.5 (3)	C106—C107—H10I	109.0
F4—C3—C1	110.6 (3)	C108—C107—H10J	109.0
F6—C3—C1	112.1 (3)	C106—C107—H10J	109.0
F2—C2—F1	107.5 (3)	H10I—C107—H10J	107.8
F2—C2—F3	108.0 (3)	C101—C102—C103	109.8 (3)
F1—C2—F3	107.4 (3)	C101—C102—H10K	109.7
F2—C2—C1	111.1 (3)	C103—C102—H10K	109.7
F1—C2—C1	112.4 (3)	C101—C102—H10L	109.7
F3—C2—C1	110.2 (3)	C103—C102—H10L	109.7
O4—Al2—O6	112.05 (10)	H10K—C102—H10L	108.2
O4—Al2—O5	116.98 (11)	C112—C111—C110	111.4 (3)
O6—Al2—O5	112.67 (11)	C112—C111—H11L	109.3
O4—Al2—F02	107.09 (8)	C110—C111—H11L	109.3
O6—Al2—F02	106.40 (8)	C112—C111—H11M	109.3
O5—Al2—F02	100.23 (8)	C110—C111—H11M	109.3
Al2—F02—Al2^{ii}	180.00 (4)	H11L—C111—H11M	108.0
C21—O6—Al2	148.51 (18)	C111—C112—H11N	109.5
C17—O5—Al2	146.50 (19)	C111—C112—H11O	109.5
C13—O4—Al2	152.32 (19)	H11N—C112—H11O	109.5
O6—C21—C24	111.1 (2)	C111—C112—H11P	109.5
O6—C21—C23	107.6 (2)	H11N—C112—H11P	109.5
C24—C21—C23	109.2 (2)	H11O—C112—H11P	109.5
O6—C21—C22	110.5 (2)	C104—C103—C102	114.3 (3)
C24—C21—C22	110.1 (2)	C104—C103—H10M	108.7
C23—C21—C22	108.1 (2)	C102—C103—H10M	108.7
O4—C13—C14	109.1 (3)	C104—C103—H10N	108.7
O4—C13—C15	108.5 (3)	C102—C103—H10N	108.7
C14—C13—C15	109.5 (3)	H10M—C103—H10N	107.6
O4—C13—C16	110.7 (2)	C107—C108—H10O	109.5
C14—C13—C16	110.3 (3)	C107—C108—H10P	109.5
C15—C13—C16	108.7 (3)	H10O—C108—H10P	109.5
O5—C17—C18	110.6 (3)	C107—C108—H10Q	109.5
O5—C17—C20	110.0 (3)	H10O—C108—H10Q	109.5
C18—C17—C20	109.9 (3)	H10P—C108—H10Q	109.5
O5—C17—C19	107.3 (2)	C103—C104—H10R	109.5
C18—C17—C19	110.7 (3)	C103—C104—H10S	109.5
C20—C17—C19	108.3 (3)	H10R—C104—H10S	109.5
F45—C20—F43	108.9 (3)	C103—C104—H10T	109.5
F45—C20—F44	107.6 (3)	H10R—C104—H10T	109.5
F43—C20—F44	108.1 (3)	H10S—C104—H10T	109.5
F45—C20—C17	110.6 (3)	C205—N2—C209	109.0 (2)
F43—C20—C17	109.8 (3)	C205—N2—C213	108.7 (2)
F44—C20—C17	111.7 (3)	C209—N2—C213	111.0 (2)
F51—C23—F49	109.8 (3)	C205—N2—C201	111.2 (2)
F51—C23—F50	106.0 (3)	C209—N2—C201	108.4 (2)
F49—C23—F50	104.6 (3)	C213—N2—C201	108.5 (2)

F51—C23—C21	111.8 (3)	C214—C213—N2	116.5 (2)
F49—C23—C21	113.7 (3)	C214—C213—H21A	108.2
F50—C23—C21	110.5 (2)	N2—C213—H21A	108.2
F47—C22—F48	108.4 (3)	C214—C213—H21P	108.2
F47—C22—F46	108.3 (3)	N2—C213—H21P	108.2
F48—C22—F46	104.4 (3)	H21A—C213—H21P	107.3
F47—C22—C21	111.4 (3)	C209—C210—C211	110.5 (2)
F48—C22—C21	113.9 (3)	C209—C210—H21B	109.5
F46—C22—C21	110.1 (3)	C211—C210—H21B	109.5
F34—C16—F35	107.2 (3)	C209—C210—H21C	109.5
F34—C16—F36	110.6 (3)	C211—C210—H21C	109.5
F35—C16—F36	108.8 (3)	H21B—C210—H21C	108.1
F34—C16—C13	112.4 (3)	C202—C201—N2	116.1 (2)
F35—C16—C13	109.5 (3)	C202—C201—H20A	108.3
F36—C16—C13	108.4 (3)	N2—C201—H20A	108.3
F42—C19—F41	109.4 (3)	C202—C201—H20B	108.3
F42—C19—F40	108.4 (3)	N2—C201—H20B	108.3
F41—C19—F40	106.5 (3)	H20A—C201—H20B	107.4
F42—C19—C17	112.2 (3)	C210—C209—N2	116.5 (2)
F41—C19—C17	110.4 (3)	C210—C209—H20C	108.2
F40—C19—C17	109.8 (3)	N2—C209—H20C	108.2
F54—C24—F52	108.9 (3)	C210—C209—H20D	108.2
F54—C24—F53	105.1 (3)	N2—C209—H20D	108.2
F52—C24—F53	102.5 (3)	H20C—C209—H20D	107.3
F54—C24—C21	112.7 (3)	C213—C214—C215	109.7 (2)
F52—C24—C21	116.2 (3)	C213—C214—H21D	109.7
F53—C24—C21	110.3 (3)	C215—C214—H21D	109.7
F33—C15—F32	108.4 (4)	C213—C214—H21E	109.7
F33—C15—F31	108.1 (3)	C215—C214—H21E	109.7
F32—C15—F31	108.9 (3)	H21D—C214—H21E	108.2
F33—C15—C13	111.4 (3)	C205—C206—C207	109.6 (3)
F32—C15—C13	112.1 (3)	C205—C206—H20E	109.7
F31—C15—C13	107.9 (3)	C207—C206—H20E	109.7
F39—C18—F38	107.1 (3)	C205—C206—H20F	109.7
F39—C18—F37	107.9 (4)	C207—C206—H20F	109.7
F38—C18—F37	108.5 (4)	H20E—C206—H20F	108.2
F39—C18—C17	110.9 (3)	C216—C215—C214	112.1 (3)
F38—C18—C17	112.5 (3)	C216—C215—H21F	109.2
F37—C18—C17	109.9 (3)	C214—C215—H21F	109.2
F30—C14—F28	107.3 (4)	C216—C215—H21G	109.2
F30—C14—F29	109.6 (4)	C214—C215—H21G	109.2
F28—C14—F29	108.6 (4)	H21F—C215—H21G	107.9
F30—C14—C13	112.4 (4)	C212—C211—C210	112.8 (3)
F28—C14—C13	111.1 (4)	C212—C211—H21H	109.0
F29—C14—C13	107.8 (4)	C210—C211—H21H	109.0
O9A—Al3—O8	84.8 (3)	C212—C211—H21I	109.0
O9A—Al3—O7	124.9 (3)	C210—C211—H21I	109.0
O8—Al3—O7	121.24 (14)	H21H—C211—H21I	107.8
O9A—Al3—O9	25.7 (3)	C201—C202—C203	109.4 (3)

O8—Al3—O9	110.48 (15)	C201—C202—H20G	109.8
O7—Al3—O9	107.69 (13)	C203—C202—H20G	109.8
O9A—Al3—O8A	109.5 (4)	C201—C202—H20H	109.8
O8—Al3—O8A	24.8 (2)	C203—C202—H20H	109.8
O7—Al3—O8A	106.0 (2)	H20G—C202—H20H	108.2
O9—Al3—O8A	135.1 (2)	N2—C205—C206	116.2 (2)
O9A—Al3—F03	112.7 (2)	N2—C205—H20I	108.2
O8—Al3—F03	112.09 (11)	C206—C205—H20I	108.2
O7—Al3—F03	101.21 (8)	N2—C205—H20J	108.2
O9—Al3—F03	102.19 (11)	C206—C205—H20J	108.2
O8A—Al3—F03	99.3 (2)	H20I—C205—H20J	107.4
Al3—F03—Al3^{iii}	180.0	C215—C216—H21J	109.5
C25—O7—Al3	146.65 (19)	C215—C216—H21K	109.5
O8A—C29—O8	31.4 (3)	H21J—C216—H21K	109.5
O8A—C29—C30A	112.5 (6)	C215—C216—H21L	109.5
O8—C29—C30A	138.8 (6)	H21J—C216—H21L	109.5
O8A—C29—C32	135.0 (4)	H21K—C216—H21L	109.5
O8—C29—C32	106.2 (2)	C208—C207—C206	112.2 (3)
C30A—C29—C32	95.6 (6)	C208—C207—H20K	109.2
O8A—C29—C32A	110.8 (4)	C206—C207—H20K	109.2
O8—C29—C32A	86.0 (3)	C208—C207—H20L	109.2
C30A—C29—C32A	100.9 (6)	C206—C207—H20L	109.2
C32—C29—C32A	26.2 (2)	H20K—C207—H20L	107.9
O8A—C29—C30	82.9 (4)	C211—C212—H21M	109.5
O8—C29—C30	108.8 (3)	C211—C212—H21N	109.5
C30A—C29—C30	30.2 (5)	H21M—C212—H21N	109.5
C32—C29—C30	114.8 (4)	C211—C212—H21O	109.5
C32A—C29—C30	107.5 (4)	H21M—C212—H21O	109.5
O8A—C29—C31A	121.1 (4)	H21N—C212—H21O	109.5
O8—C29—C31A	113.9 (3)	C204—C203—C202	114.4 (3)
C30A—C29—C31A	103.1 (6)	C204—C203—H20M	108.7
C32—C29—C31A	82.7 (3)	C202—C203—H20M	108.7
C32A—C29—C31A	106.3 (3)	C204—C203—H20N	108.7
C30—C29—C31A	126.4 (4)	C202—C203—H20N	108.7
O8A—C29—C31	99.0 (4)	H20M—C203—H20N	107.6
O8—C29—C31	104.6 (3)	C207—C208—H20O	109.5
C30A—C29—C31	99.7 (6)	C207—C208—H20P	109.5
C32—C29—C31	110.5 (3)	H20O—C208—H20P	109.5
C32A—C29—C31	133.3 (3)	C207—C208—H20Q	109.5
C30—C29—C31	111.3 (4)	H20O—C208—H20Q	109.5
C31A—C29—C31	27.7 (2)	H20P—C208—H20Q	109.5
O9—C33—O9A	32.5 (3)	C203—C204—H20R	109.5
O9—C33—C36A	114.4 (3)	C203—C204—H20S	109.5
O9A—C33—C36A	105.0 (4)	H20R—C204—H20S	109.5
O9—C33—C34	115.0 (3)	C203—C204—H20T	109.5
O9A—C33—C34	103.6 (3)	H20R—C204—H20T	109.5
C36A—C33—C34	125.1 (3)	H20S—C204—H20T	109.5
O9—C33—C34A	117.7 (4)	C26—F56—C26A	38.9 (3)
O9A—C33—C34A	97.9 (5)	C33—O9—Al3	146.1 (2)

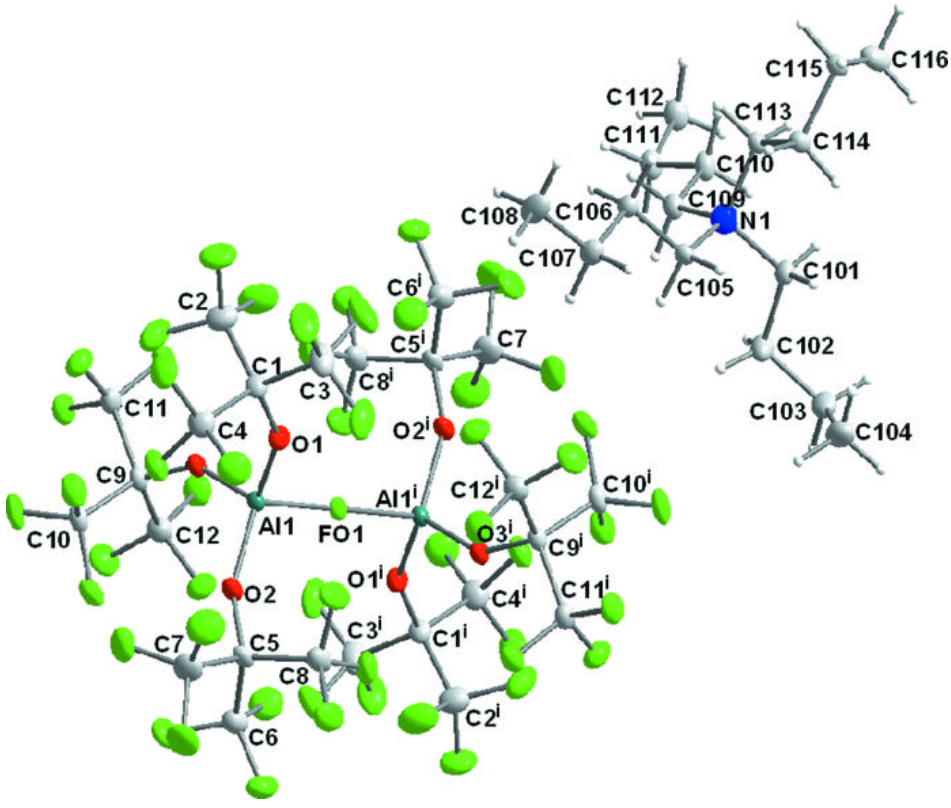
C36A—C33—C34A	113.6 (5)	F80—C36—F79	106.6 (3)
C34—C33—C34A	16.1 (5)	F80—C36—F81	105.3 (4)
O9—C33—C35A	72.2 (3)	F79—C36—F81	104.3 (3)
O9A—C33—C35A	102.3 (4)	F80—C36—C33	112.8 (3)
C36A—C33—C35A	127.6 (3)	F79—C36—C33	117.1 (3)
C34—C33—C35A	89.7 (3)	F81—C36—C33	109.8 (3)
C34A—C33—C35A	105.7 (5)	F76—C35—F77	105.7 (3)
O9—C33—C36	112.7 (3)	F76—C35—F78	106.2 (4)
O9A—C33—C36	90.0 (3)	F77—C35—F78	104.5 (3)
C36A—C33—C36	27.9 (2)	F76—C35—C33	111.8 (3)
C34—C33—C36	108.2 (3)	F77—C35—C33	116.1 (3)
C34A—C33—C36	93.3 (5)	F78—C35—C33	111.8 (3)
C35A—C33—C36	155.5 (3)	F75—C34—F74	106.6 (4)
O9—C33—C35	107.9 (3)	F75—C34—F73	107.9 (4)
O9A—C33—C35	138.8 (4)	F74—C34—F73	107.2 (4)
C36A—C33—C35	78.3 (3)	F75—C34—C33	109.3 (3)
C34—C33—C35	107.5 (3)	F74—C34—C33	110.1 (3)
C34A—C33—C35	118.7 (5)	F73—C34—C33	115.3 (3)
C35A—C33—C35	52.4 (3)	C33—O9A—Al3	154.1 (6)
C36—C33—C35	105.0 (2)	F74A—C34A—F75A	112.2 (12)
O7—C25—C26A	114.7 (3)	F74A—C34A—F73A	104.4 (10)
O7—C25—C26	112.3 (3)	F75A—C34A—F73A	105.8 (8)
C26A—C25—C26	33.6 (2)	F74A—C34A—C33	113.8 (9)
O7—C25—C27	109.4 (2)	F75A—C34A—C33	112.7 (8)
C26A—C25—C27	133.1 (3)	F73A—C34A—C33	107.2 (7)
C26—C25—C27	113.4 (3)	F78A—C35A—F76A	110.9 (5)
O7—C25—C27A	100.3 (3)	F78A—C35A—F77A	110.4 (5)
C26A—C25—C27A	98.7 (3)	F76A—C35A—F77A	110.7 (5)
C26—C25—C27A	65.8 (3)	F78A—C35A—C33	101.6 (5)
C27—C25—C27A	57.3 (3)	F76A—C35A—C33	109.2 (5)
O7—C25—C28A	111.9 (3)	F77A—C35A—C33	113.8 (5)
C26A—C25—C28A	122.2 (3)	F81A—C36A—F79A	113.5 (5)
C26—C25—C28A	135.8 (3)	F81A—C36A—F80A	112.2 (5)
C27—C25—C28A	48.3 (3)	F79A—C36A—F80A	111.4 (5)
C27A—C25—C28A	104.8 (4)	F81A—C36A—C33	111.9 (6)
O7—C25—C28	108.1 (2)	F79A—C36A—C33	103.0 (5)
C26A—C25—C28	74.4 (3)	F80A—C36A—C33	104.1 (5)
C26—C25—C28	106.7 (2)	C29—O8—Al3	147.4 (2)
C27—C25—C28	106.7 (3)	F67—C31—F69	109.9 (3)
C27A—C25—C28	151.2 (3)	F67—C31—F68	108.3 (3)
C28A—C25—C28	59.9 (3)	F69—C31—F68	108.0 (3)
O10—Al4—O12	113.88 (12)	F67—C31—C29	111.3 (3)
O10—Al4—O11	115.00 (12)	F69—C31—C29	110.7 (3)
O12—Al4—O11	111.87 (12)	F68—C31—C29	108.5 (3)
O10—Al4—F04	104.93 (11)	F72—C32—F70	109.4 (4)
O12—Al4—F04	105.13 (10)	F72—C32—F71	108.1 (3)
O11—Al4—F04	104.80 (9)	F70—C32—F71	108.9 (4)
$Al4^{iv}$—F04—Al4	180.0	F72—C32—C29	109.1 (3)
C45—O12—Al4	149.6 (2)	F70—C32—C29	111.4 (3)

C37—O10—Al4	159.7 (2)	F71—C32—C29	109.8 (3)
C41—O11—Al4	148.1 (2)	F65—C30—F64	110.8 (6)
O11—C41—C42	110.9 (3)	F65—C30—F66	109.4 (6)
O11—C41—C44	110.6 (3)	F64—C30—F66	109.1 (6)
C42—C41—C44	108.8 (3)	F65—C30—C29	111.7 (5)
O11—C41—C43	107.3 (3)	F64—C30—C29	106.9 (5)
C42—C41—C43	110.4 (3)	F66—C30—C29	108.8 (5)
C44—C41—C43	108.8 (3)	C29—O8A—Al3	153.4 (6)
O10—C37—C38	109.6 (3)	F64A—C30A—F65A	109.6 (10)
O10—C37—C39	108.2 (3)	F64A—C30A—F66A	94.7 (10)
C38—C37—C39	109.7 (3)	F65A—C30A—F66A	95.5 (9)
O10—C37—C40	110.5 (2)	F64A—C30A—C29	116.3 (10)
C38—C37—C40	109.7 (3)	F65A—C30A—C29	117.1 (11)
C39—C37—C40	109.1 (3)	F66A—C30A—C29	119.9 (9)
F99—C44—F98	108.6 (3)	F71A—C32A—F72A	103.8 (5)
F99—C44—F97	106.7 (3)	F71A—C32A—F70A	104.2 (6)
F98—C44—F97	106.9 (3)	F72A—C32A—F70A	104.1 (5)
F99—C44—C41	113.0 (3)	F71A—C32A—C29	110.4 (5)
F98—C44—C41	110.5 (3)	F72A—C32A—C29	124.8 (6)
F97—C44—C41	111.0 (3)	F70A—C32A—C29	107.6 (5)
O12—C45—C46	110.9 (3)	F68A—C31A—F67A	106.8 (5)
O12—C45—C47	110.7 (3)	F68A—C31A—F69A	106.6 (6)
C46—C45—C47	109.1 (3)	F67A—C31A—F69A	105.9 (6)
O12—C45—C48	107.2 (2)	F68A—C31A—C29	106.8 (6)
C46—C45—C48	110.3 (3)	F67A—C31A—C29	118.6 (5)
C47—C45—C48	108.7 (2)	F69A—C31A—C29	111.6 (6)
F106—C48—F107	107.7 (3)	F56—C26—F55	109.0 (3)
F106—C48—F108	109.4 (3)	F56—C26—F57	108.8 (3)
F107—C48—F108	106.4 (3)	F55—C26—F57	107.8 (3)
F106—C48—C45	111.4 (3)	F56—C26—C25	110.2 (3)
F107—C48—C45	113.0 (3)	F55—C26—C25	107.7 (3)
F108—C48—C45	108.8 (3)	F57—C26—C25	113.2 (3)
F104—C47—F105	109.7 (3)	F59—C27—F58	107.6 (3)
F104—C47—F103	104.4 (3)	F59—C27—F60	106.4 (3)
F105—C47—F103	105.1 (3)	F58—C27—F60	107.8 (3)
F104—C47—C45	112.2 (3)	F59—C27—C25	109.6 (3)
F105—C47—C45	113.8 (3)	F58—C27—C25	111.6 (3)
F103—C47—C45	110.9 (3)	F60—C27—C25	113.6 (3)
F89—C40—F88	110.1 (3)	F63—C28—F62	107.0 (3)
F89—C40—F90	105.5 (3)	F63—C28—F61	107.7 (3)
F88—C40—F90	107.0 (3)	F62—C28—F61	105.8 (3)
F89—C40—C37	111.3 (3)	F63—C28—C25	112.5 (3)
F88—C40—C37	113.0 (3)	F62—C28—C25	110.6 (3)
F90—C40—C37	109.6 (3)	F61—C28—C25	112.8 (3)
F100—C46—F102	108.6 (3)	F55A—C26A—F56	110.9 (5)
F100—C46—F101	106.5 (3)	F55A—C26A—F57A	110.7 (6)
F102—C46—F101	105.0 (3)	F56—C26A—F57A	110.2 (5)
F100—C46—C45	112.2 (3)	F55A—C26A—C25	97.7 (6)
F102—C46—C45	114.4 (3)	F56—C26A—C25	110.4 (4)

F101—C46—C45	109.5 (3)	F57A—C26A—C25	116.4 (6)
F95—C43—F94	108.1 (4)	F59A—C27A—F58A	99.0 (6)
F95—C43—F96	108.0 (4)	F59A—C27A—F60A	98.5 (6)
F94—C43—F96	106.6 (3)	F58A—C27A—F60A	98.6 (6)
F95—C43—C41	112.2 (3)	F59A—C27A—C25	118.9 (7)
F94—C43—C41	109.6 (3)	F58A—C27A—C25	118.2 (6)
F96—C43—C41	112.1 (3)	F60A—C27A—C25	119.3 (6)
F85—C39—F87	108.2 (3)	F62A—C28A—F63A	115.6 (7)
F85—C39—F86	107.8 (4)	F62A—C28A—F61A	115.2 (6)
F87—C39—F86	108.0 (3)	F63A—C28A—F61A	115.4 (6)
F85—C39—C37	112.0 (3)	F62A—C28A—C25	101.5 (6)
F87—C39—C37	110.9 (3)	F63A—C28A—C25	99.3 (9)
F86—C39—C37	109.6 (3)	F61A—C28A—C25	106.9 (6)
F91—C42—F92	109.0 (4)		

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+2, −*y*, −*z*+1; (iv) −*x*, −*y*+2, −*z*.

Fig. 1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C12i
C10i
Al1i
C10
C12
Al1
FO1
O3i
C9i
O1i
C4i
C11i
O2
C7
C5
C3i
C1i
C8
C2i
C6