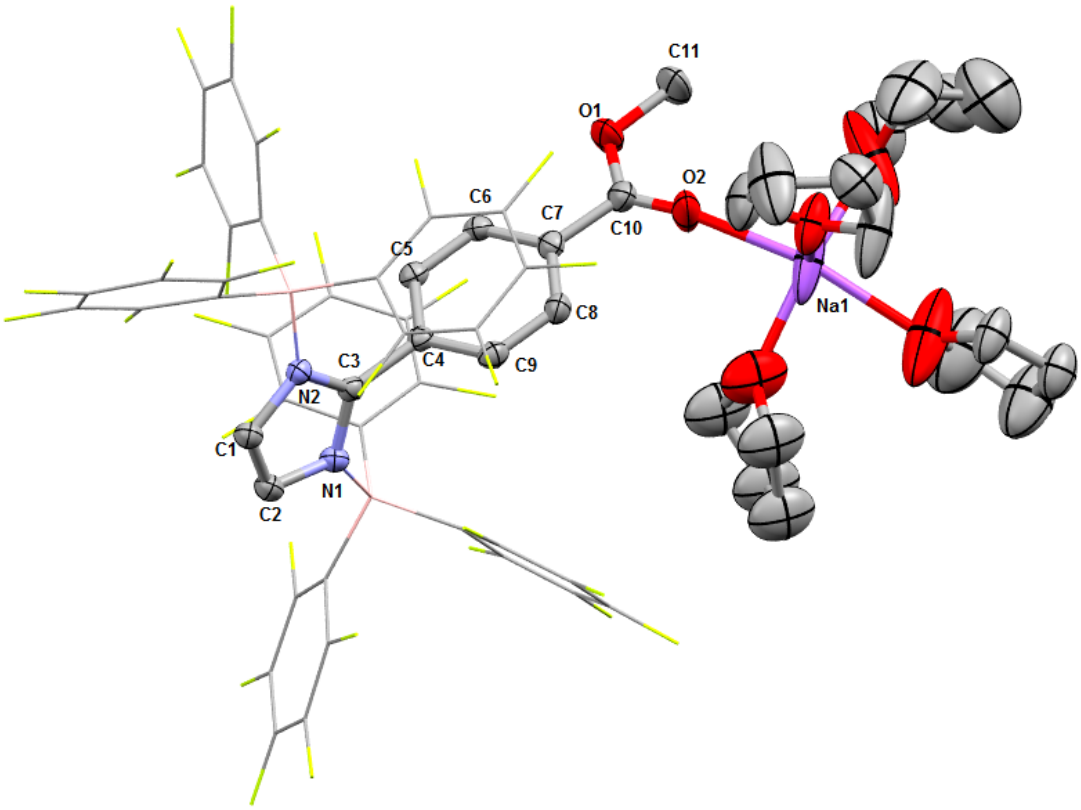
Crystal Structure Report for Na[IMP-CO_2Me]



Thermal ellipsoid plot of 5460. Ellipsoids shown at 50% probability, $B(C_6F_5)_3$ substituents shown in wireframe, DCM solvate and hydrogen atoms hidden for clarity.

A specimen of $C_{66.07}H_{41.08}B_2Cl_2F_{30}N_2NaO_{6.50}$ was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å). The integration of the data using a triclinic unit cell yielded a total of 58618 reflections to a maximum θ angle of 28.00° (0.76 Å resolution), of which 15632 were independent (average redundancy 3.750, completeness = 99.4%, R_{int} = 3.20%, R_{sig} =3.54%) and 10814 (69.18%) were greater than $2\sigma(F^2)$. The final cell constants of a = 12.2126(18) Å, b = 16.759(2) Å, c =17.209(3) Å, α = 90.069(3)°, β = 104.596(3)°, γ = 106.610(3)°, volume = 3256.1(8) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The final anisotropic full-matrix least-squares refinement on F^2 with 1060 variables converged at R1 = 7.37%, for the observed data and wR2 = 24.19% for all data. The goodness-of-fit was 1.065. The largest peak in the final difference electron density synthesis was 1.306 $e^-/Å^3$ and the largest hole was -1.092 $e^-/Å^3$ with an RMS deviation of 0.095 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.685 g/cm^3 and F(000), 1657 e^-.

Table 1. Sample and crystal data for 5460.

Identification code	5460	
Chemical formula	$C_{66.07}H_{41.08}B_2Cl_2F_{30}N_2NaO_{6.50}$	
Formula weight	1652.38 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 12.2126(18) Å	α = 90.069(3)°
	b = 16.759(2) Å	β = 104.596(3)°
	c = 17.209(3) Å	γ = 106.610(3)°
Volume	3256.1(8) $Å^3$	
Z	2	
Density (calculated)	1.685 g/cm^3	
Absorption coefficient	0.250 mm^{-1}	
F(000)	1657	

Table 2. Data collection and structure refinement for 5460.

Theta range for data collection	1.23 to 28.00°	
Index ranges	-11<=h<=16, -22<=k<=16, -22<=l<=22	
Reflections collected	58618	
Independent reflections	15632 [R(int) = 0.0320]	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	15632 / 69 / 1060	
Goodness-of-fit on F^2	1.065	
Final R indices	10814 data; I>2σ(I)	R1 = 0.0737, wR2 = 0.2159
	all data	R1 = 0.1033, wR2 = 0.2419
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.1285P)^2+4.4290P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	1.306 and -1.092 $eÅ^{-3}$	
R.M.S. deviation from mean	0.095 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for 5460.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij}tensor.

	x/a	y/b	z/c	U(eq)
Cl1	0.21284(14)	0.22865(10)	0.12694(8)	0.0574(4)
Cl2	0.98882(15)	0.11888(10)	0.03017(9)	0.0613(4)
F003	0.3702(2)	0.72535(14)	0.90913(13)	0.0275(5)
F004	0.3758(2)	0.45323(14)	0.84252(14)	0.0288(5)
F005	0.2132(2)	0.59379(15)	0.97093(14)	0.0295(5)
F006	0.4144(2)	0.54737(15)	0.71996(14)	0.0295(5)
F007	0.0130(2)	0.72349(15)	0.60554(15)	0.0333(5)
F008	0.0957(2)	0.37116(15)	0.76861(15)	0.0348(5)
F009	0.5983(2)	0.48945(16)	0.93366(15)	0.0343(5)
F00A	0.5875(2)	0.75761(16)	0.00199(15)	0.0361(6)
F00B	0.0035(2)	0.49274(16)	0.69458(15)	0.0358(6)
F00C	0.9276(2)	0.80691(16)	0.70041(16)	0.0358(6)
F00D	0.7057(2)	0.64186(17)	0.01663(15)	0.0379(6)
F00E	0.2436(2)	0.00605(15)	0.66033(17)	0.0368(6)
F00F	0.1179(2)	0.48840(18)	0.06647(15)	0.0391(6)
F00G	0.3883(2)	0.91172(16)	0.65709(19)	0.0408(6)
F00H	0.2663(2)	0.02105(16)	0.84314(17)	0.0397(6)
F00I	0.2928(3)	0.87402(17)	0.90696(16)	0.0428(6)
F00J	0.0044(3)	0.26931(16)	0.86580(19)	0.0453(7)
F00K	0.3662(3)	0.48334(19)	0.57183(16)	0.0465(7)
F00L	0.0104(3)	0.32508(18)	0.01608(18)	0.0473(7)
F00M	0.7914(2)	0.8961(2)	0.7236(2)	0.0529(8)
F00N	0.9576(3)	0.4260(2)	0.54489(17)	0.0540(8)
Na1	0.4057(4)	0.70964(16)	0.33858(14)	0.1028(14)
F00P	0.1275(3)	0.1059(2)	0.8697(2)	0.0560(8)
F00Q	0.1383(3)	0.4225(2)	0.48088(16)	0.0588(9)
F00R	0.1618(3)	0.0329(2)	0.5069(2)	0.0623(9)
F00S	0.5235(3)	0.9192(2)	0.9821(2)	0.0674(11)
F00T	0.6136(2)	0.9615(2)	0.7319(3)	0.0672(11)
F00U	0.8895(3)	0.0472(2)	0.8115(2)	0.0648(10)
N2	0.1733(3)	0.63727(19)	0.79460(18)	0.0213(6)
N1	0.1541(3)	0.7615(2)	0.76329(19)	0.0239(6)
F00X	0.9344(3)	0.7513(2)	0.4543(2)	0.0720(12)
O1	0.6308(3)	0.7427(3)	0.5834(2)	0.0462(9)
F00Z	0.6877(3)	0.9622(2)	0.8964(3)	0.0811(14)
O2	0.4801(3)	0.7056(3)	0.4741(2)	0.0563(11)
F011	0.0031(4)	0.9070(3)	0.4023(2)	0.0987(17)

	x/a	y/b	z/c	U(eq)
O6	0.3311(5)	0.5670(3)	0.3125(2)	0.0681(13)
C3	0.2086(3)	0.7040(2)	0.7535(2)	0.0209(7)
C5	0.4136(3)	0.7372(2)	0.7331(2)	0.0223(7)
C24	0.3632(3)	0.5888(2)	0.8659(2)	0.0221(7)
C25	0.4267(3)	0.5313(2)	0.8787(2)	0.0236(7)
C4	0.2915(3)	0.7107(2)	0.7013(2)	0.0214(7)
C1	0.0909(3)	0.6528(2)	0.8298(2)	0.0246(7)
C29	0.4215(3)	0.6637(2)	0.9113(2)	0.0237(7)
C17	0.1582(3)	0.5140(2)	0.9402(2)	0.0261(8)
C18	0.2104(4)	0.5211(2)	0.7173(2)	0.0259(8)
C7	0.4413(3)	0.7184(2)	0.6016(2)	0.0258(7)
C26	0.5408(3)	0.5474(3)	0.9265(2)	0.0262(8)
C6	0.4886(3)	0.7414(2)	0.6837(2)	0.0239(7)
C2	0.0805(3)	0.7286(3)	0.8118(2)	0.0268(8)
C12	0.1544(3)	0.4913(2)	0.8615(2)	0.0241(7)
C9	0.2446(3)	0.6877(2)	0.6191(2)	0.0263(8)
C23	0.2985(4)	0.5168(2)	0.6810(2)	0.0279(8)
C27	0.5952(3)	0.6239(3)	0.9686(2)	0.0287(8)
C28	0.5350(3)	0.6830(3)	0.9615(2)	0.0269(8)
C13	0.1007(3)	0.4065(3)	0.8403(2)	0.0280(8)
C8	0.3188(4)	0.6918(3)	0.5697(2)	0.0287(8)
C36	0.1404(3)	0.8624(3)	0.6407(3)	0.0283(8)
C10	0.5176(4)	0.7214(3)	0.5459(3)	0.0333(9)
C37	0.0583(3)	0.8010(3)	0.5847(3)	0.0330(9)
C14	0.0513(4)	0.3505(3)	0.8901(3)	0.0332(9)
C19	0.0966(4)	0.4912(3)	0.6665(2)	0.0310(8)
C42	0.3266(3)	0.8929(2)	0.7782(3)	0.0308(9)
C41	0.1702(4)	0.9402(3)	0.6101(3)	0.0336(9)
C30	0.1050(4)	0.9066(3)	0.7712(3)	0.0294(8)
C15	0.0561(4)	0.3782(3)	0.9661(3)	0.0349(9)
C43	0.4147(4)	0.9161(3)	0.7378(3)	0.0359(10)
C31	0.1494(4)	0.9845(3)	0.8134(3)	0.0335(9)
C35	0.9821(4)	0.8805(3)	0.7432(3)	0.0337(9)
C16	0.1102(4)	0.4601(3)	0.9913(2)	0.0300(8)
C22	0.2761(4)	0.4843(3)	0.6028(3)	0.0352(9)
C47	0.3702(4)	0.8951(3)	0.8616(3)	0.0375(10)
C20	0.0713(4)	0.4572(3)	0.5888(3)	0.0399(10)

	x/a	y/b	z/c	U(eq)
C21	0.1617(5)	0.4536(3)	0.5570(3)	0.0424(11)
C33	0.9572(5)	0.0018(3)	0.7978(3)	0.0454(12)
C32	0.0777(5)	0.0311(3)	0.8276(3)	0.0411(11)
C34	0.9093(4)	0.9265(3)	0.7550(3)	0.0406(11)
C40	0.1272(4)	0.9558(3)	0.5318(3)	0.0467(12)
C46	0.4885(5)	0.9183(3)	0.9019(3)	0.0489(14)
C38	0.0130(4)	0.8136(4)	0.5044(3)	0.0514(14)
C44	0.5347(4)	0.9412(3)	0.7756(4)	0.0487(14)
B1	0.1840(4)	0.8556(3)	0.7381(3)	0.0253(8)
C45	0.5712(4)	0.9406(3)	0.8576(4)	0.0555(16)
B2	0.2258(4)	0.5600(3)	0.8081(2)	0.0216(8)
C11	0.7120(5)	0.7479(5)	0.5330(4)	0.0616(17)
C64	0.1388(5)	0.1651(4)	0.0368(3)	0.0529(13)
C39	0.0486(5)	0.8928(4)	0.4789(3)	0.0608(17)
C52	0.2864(7)	0.7061(4)	0.1340(3)	0.0656(17)
C53	0.2889(7)	0.7684(4)	0.0737(4)	0.0663(17)
O3	0.5831(8)	0.7320(3)	0.3122(5)	0.147(3)
C60	0.3164(8)	0.5136(4)	0.3736(4)	0.0733(19)
C62	0.2711(8)	0.4320(5)	0.2494(5)	0.080(2)
C63	0.2762(12)	0.5199(5)	0.2377(4)	0.126(5)
C61	0.2630(13)	0.4266(5)	0.3312(6)	0.127(5)
C58	0.7399(9)	0.8093(6)	0.2673(6)	0.101(3)
O4	0.3294(10)	0.7545(4)	0.2090(3)	0.157(3)
O5	0.2736(6)	0.7576(5)	0.3706(6)	0.095(2)
C51	0.1501(7)	0.7305(6)	0.3284(10)	0.095(2)
C54	0.3192(13)	0.8477(6)	0.1130(6)	0.131(4)
C56	0.6334(12)	0.6773(6)	0.2812(7)	0.132(4)
C59	0.6892(10)	0.8088(7)	0.3327(7)	0.117(3)
C57	0.6803(13)	0.7336(8)	0.2155(8)	0.144(5)
C48	0.2979(10)	0.8376(8)	0.4157(7)	0.095(2)
C49	0.2228(11)	0.8821(5)	0.3560(10)	0.095(2)
C50	0.1136(10)	0.8117(7)	0.3159(10)	0.095(2)
C55	0.3906(15)	0.8426(7)	0.1954(8)	0.168(5)
C51A	0.3349(12)	0.8873(8)	0.4309(9)	0.059(3)
O5A	0.4026(7)	0.8479(5)	0.3951(5)	0.051(2)
C50A	0.4103(13)	0.9734(9)	0.4692(9)	0.064(3)
C49A	0.5389(14)	0.9574(10)	0.4828(10)	0.073(3)

	x/a	y/b	z/c	U(eq)
C48A	0.5262(10)	0.9062(7)	0.4175(8)	0.050(2)
Cl1	0.21284(14)	0.22865(10)	0.12694(8)	0.0574(4)
Cl2	0.98882(15)	0.11888(10)	0.03017(9)	0.0613(4)
F003	0.3702(2)	0.72535(14)	0.90913(13)	0.0275(5)
F004	0.3758(2)	0.45323(14)	0.84252(14)	0.0288(5)
F005	0.2132(2)	0.59379(15)	0.97093(14)	0.0295(5)

Table 4. Bond lengths (Å) for 5460.

Cl1-C64	1.760(6)	Cl2-C64	1.747(6)
F003-C29	1.348(4)	F004-C25	1.351(4)
F005-C17	1.351(5)	F006-C23	1.349(5)
F007-C37	1.346(5)	F008-C13	1.347(5)
F009-C26	1.342(4)	F00A-C28	1.332(5)
F00B-C19	1.349(5)	F00C-C35	1.337(5)
F00D-C27	1.341(4)	F00E-C41	1.347(5)
F00F-C16	1.348(5)	F00G-C43	1.342(6)
F00H-C31	1.345(5)	F00I-C47	1.345(6)
F00J-C14	1.337(5)	F00K-C22	1.342(5)
F00L-C15	1.342(5)	F00M-C34	1.346(6)
F00N-C20	1.352(5)	Na1-O2	2.289(4)
Na1-O6	2.301(5)	Na1-O3	2.252(8)
Na1-O4	2.401(7)	Na1-O5	2.178(7)
Na1-O5A	2.525(9)	F00P-C32	1.343(6)
F00Q-C21	1.340(5)	F00R-C40	1.346(6)
F00S-C46	1.337(7)	F00T-C44	1.337(7)
F00U-C33	1.331(5)	N2-C3	1.348(5)
N2-C1	1.381(5)	N2-B2	1.595(5)
N1-C3	1.350(5)	N1-C2	1.380(5)
N1-B1	1.599(5)	F00X-C38	1.329(6)
O1-C10	1.312(5)	O1-C11	1.459(5)
F00Z-C45	1.351(5)	O2-C10	1.205(6)
F011-C39	1.345(6)	O6-C60	1.395(7)
O6-C63	1.411(8)	C3-C4	1.496(5)
C5-C4	1.389(5)	C5-C6	1.387(5)
C24-C25	1.385(5)	C24-C29	1.379(5)
C24-B2	1.653(5)	C25-C26	1.377(5)

C4-C9	1.394(5)	C1-C2	1.341(5)
C29-C28	1.382(5)	C17-C12	1.392(5)
C17-C16	1.377(6)	C18-C23	1.392(6)
C18-C19	1.391(6)	C18-B2	1.638(5)
C7-C6	1.391(5)	C7-C8	1.394(5)
C7-C10	1.488(6)	C26-C27	1.370(6)
C12-C13	1.389(6)	C12-B2	1.661(6)
C9-C8	1.379(5)	C23-C22	1.382(6)
C27-C28	1.381(6)	C13-C14	1.385(6)
C36-C37	1.383(6)	C36-C41	1.391(6)
C36-B1	1.641(6)	C37-C38	1.393(6)
C14-C15	1.370(7)	C19-C20	1.378(6)
C42-C43	1.389(6)	C42-C47	1.396(7)
C42-B1	1.634(6)	C41-C40	1.371(7)
C30-C31	1.386(6)	C30-C35	1.390(6)
C30-B1	1.654(6)	C15-C16	1.358(7)
C43-C44	1.384(6)	C31-C32	1.391(6)
C35-C34	1.382(6)	C22-C21	1.368(7)
C47-C46	1.376(6)	C20-C21	1.365(7)
C33-C32	1.369(8)	C33-C34	1.355(8)
C40-C39	1.358(8)	C46-C45	1.384(9)
C38-C39	1.382(8)	C44-C45	1.369(9)
C52-C53	1.473(8)	C52-O4	1.418(7)
C53-C54	1.397(10)	O3-C56	1.411(10)
O3-C59	1.509(10)	C60-C61	1.515(11)
C62-C63	1.474(12)	C62-C61	1.436(12)
C58-C59	1.414(11)	C58-C57	1.441(12)
O4-C55	1.501(12)	O5-C51	1.437(8)
O5-C48	1.463(8)	O5-O5A	1.803(12)
C51-C50	1.548(8)	C54-C55	1.483(13)
C56-C57	1.586(13)	C48-C49	1.539(9)
C48-C51A	0.832(15)	C48-O5A	1.375(16)
C49-C50	1.509(8)	C49-C51A	1.608(19)
C51A-O5A	1.439(15)	C51A-C50A	1.515(18)
O5A-C48A	1.498(14)	C50A-C49A	1.63(2)
C49A-C48A	1.36(2)		

Table 5. Bond angles (°) for 5460.

O2-Na1-O6	95.09(19)	O2-Na1-O4	163.1(2)
O2-Na1-O5A	77.3(2)	O6-Na1-O4	100.5(2)
O6-Na1-O5A	152.2(3)	O3-Na1-O2	93.8(3)
O3-Na1-O6	100.5(2)	O3-Na1-O4	89.8(4)
O3-Na1-O5A	106.6(3)	O4-Na1-O5A	85.8(3)
O5-Na1-O2	86.0(3)	O5-Na1-O6	109.2(3)
O5-Na1-O3	150.2(3)	O5-Na1-O4	82.7(4)
O5-Na1-O5A	44.3(3)	C3-N2-C1	106.4(3)
C3-N2-B2	127.1(3)	C1-N2-B2	126.2(3)
C3-N1-C2	106.4(3)	C3-N1-B1	127.5(3)
C2-N1-B1	125.3(3)	C10-O1-C11	116.3(4)
C10-O2-Na1	165.4(4)	C60-O6-Na1	122.0(4)
C60-O6-C63	108.4(5)	C63-O6-Na1	128.8(4)
N2-C3-N1	110.3(3)	N2-C3-C4	124.3(3)
N1-C3-C4	125.3(3)	C6-C5-C4	120.6(3)
C25-C24-B2	119.4(3)	C29-C24-C25	113.4(3)
C29-C24-B2	126.8(3)	F004-C25-C24	119.3(3)
F004-C25-C26	116.0(3)	C26-C25-C24	124.8(4)
C5-C4-C3	121.7(3)	C5-C4-C9	119.4(3)
C9-C4-C3	118.9(3)	C2-C1-N2	108.4(3)
F003-C29-C24	121.3(3)	F003-C29-C28	114.4(3)
C24-C29-C28	124.3(3)	F005-C17-C12	119.6(3)
F005-C17-C16	115.9(3)	C16-C17-C12	124.6(4)
C23-C18-B2	128.3(3)	C19-C18-C23	113.4(4)
C19-C18-B2	118.2(3)	C6-C7-C8	119.7(3)
C6-C7-C10	122.0(4)	C8-C7-C10	118.3(4)
F009-C26-C25	121.4(4)	F009-C26-C27	119.7(3)
C27-C26-C25	118.9(3)	C5-C6-C7	119.8(3)
C1-C2-N1	108.4(3)	C17-C12-B2	120.2(3)
C13-C12-C17	112.7(4)	C13-C12-B2	126.6(3)
C8-C9-C4	120.3(3)	F006-C23-C18	121.5(3)
F006-C23-C22	114.8(4)	C22-C23-C18	123.7(4)
F00D-C27-C26	120.9(4)	F00D-C27-C28	119.8(4)
C26-C27-C28	119.3(3)	F00A-C28-C29	121.3(3)
F00A-C28-C27	119.6(3)	C27-C28-C29	119.1(4)
F008-C13-C12	121.7(4)	F008-C13-C14	114.0(4)
C14-C13-C12	124.2(4)	C9-C8-C7	120.2(4)

C37-C36-C41	113.3(4)	C37-C36-B1	126.6(4)
C41-C36-B1	119.1(4)	O1-C10-C7	112.8(4)
O2-C10-O1	123.3(4)	O2-C10-C7	123.9(4)
F007-C37-C36	121.2(4)	F007-C37-C38	114.7(4)
C36-C37-C38	124.1(4)	F00J-C14-C13	120.4(4)
F00J-C14-C15	120.0(4)	C15-C14-C13	119.5(4)
F00B-C19-C18	119.1(4)	F00B-C19-C20	116.7(4)
C20-C19-C18	124.1(4)	C43-C42-C47	113.7(4)
C43-C42-B1	127.1(4)	C47-C42-B1	118.9(4)
F00E-C41-C36	118.7(4)	F00E-C41-C40	116.6(4)
C40-C41-C36	124.7(4)	C31-C30-C35	113.4(4)
C31-C30-B1	125.5(4)	C35-C30-B1	119.9(4)
F00L-C15-C14	120.8(4)	F00L-C15-C16	120.1(4)
C16-C15-C14	119.1(4)	F00G-C43-C42	121.4(4)
F00G-C43-C44	114.5(4)	C44-C43-C42	124.1(5)
F00H-C31-C30	121.9(4)	F00H-C31-C32	114.9(4)
C30-C31-C32	123.2(4)	F00C-C35-C30	119.7(4)
F00C-C35-C34	115.8(4)	C34-C35-C30	124.5(4)
F00F-C16-C17	120.0(4)	F00F-C16-C15	120.2(4)
C15-C16-C17	119.8(4)	F00K-C22-C23	120.1(4)
F00K-C22-C21	120.2(4)	C21-C22-C23	119.7(4)
F00I-C47-C42	118.9(4)	F00I-C47-C46	116.7(5)
C46-C47-C42	124.5(5)	F00N-C20-C19	120.2(4)
F00N-C20-C21	120.3(4)	C21-C20-C19	119.5(4)
F00Q-C21-C22	120.5(5)	F00Q-C21-C20	120.1(5)
C20-C21-C22	119.4(4)	F00U-C33-C32	119.8(5)
F00U-C33-C34	121.3(5)	C34-C33-C32	118.8(4)
F00P-C32-C31	119.6(5)	F00P-C32-C33	120.0(4)
C33-C32-C31	120.4(5)	F00M-C34-C35	119.6(5)
F00M-C34-C33	120.6(4)	C33-C34-C35	119.7(5)
F00R-C40-C41	120.8(5)	F00R-C40-C39	119.6(5)
C39-C40-C41	119.6(5)	F00S-C46-C47	121.1(6)
F00S-C46-C45	120.3(5)	C47-C46-C45	118.6(5)
F00X-C38-C37	120.4(5)	F00X-C38-C39	120.9(5)
C39-C38-C37	118.7(5)	F00T-C44-C43	120.1(6)
F00T-C44-C45	120.7(5)	C45-C44-C43	119.1(5)
N1-B1-C36	113.3(3)	N1-B1-C42	103.2(3)
N1-B1-C30	110.7(3)	C36-B1-C30	100.8(3)

C42-B1-C36	115.3(3)	C42-B1-C30	113.8(3)
F00Z-C45-C46	119.1(6)	F00Z-C45-C44	120.9(6)
C44-C45-C46	120.0(4)	N2-B2-C24	111.3(3)
N2-B2-C18	104.8(3)	N2-B2-C12	110.8(3)
C24-B2-C12	102.7(3)	C18-B2-C24	114.8(3)
C18-B2-C12	112.7(3)	Cl2-C64-Cl1	112.1(3)
F011-C39-C40	120.7(5)	F011-C39-C38	119.7(5)
C40-C39-C38	119.6(5)	O4-C52-C53	104.3(5)
C54-C53-C52	108.9(6)	C56-O3-Na1	131.3(6)
C56-O3-C59	99.1(8)	C59-O3-Na1	129.2(5)
O6-C60-C61	105.2(6)	C61-C62-C63	101.2(7)
O6-C63-C62	108.5(7)	C62-C61-C60	108.0(7)
C59-C58-C57	110.0(9)	C52-O4-Na1	127.2(5)
C52-O4-C55	108.7(7)	C55-O4-Na1	115.2(6)
C51-O5-Na1	123.3(6)	C51-O5-C48	108.1(6)
C51-O5-O5A	142.8(7)	C48-O5-Na1	125.5(6)
C48-O5-O5A	48.4(6)	O5A-O5-Na1	78.1(4)
O5-C51-C50	105.0(6)	C53-C54-C55	105.8(8)
O3-C56-C57	98.3(7)	C58-C59-O3	103.6(8)
C58-C57-C56	97.2(9)	O5-C48-C49	102.2(6)
C51A-C48-O5	154.9(19)	C51A-C48-C49	79.3(15)
C51A-C48-O5A	77.0(15)	O5A-C48-O5	78.8(7)
O5A-C48-C49	108.2(13)	C48-C49-C51A	30.5(6)
C50-C49-C48	103.0(6)	C50-C49-C51A	132.9(9)
C49-C50-C51	106.0(5)	C54-C55-O4	99.7(9)
C48-C51A-C49	70.1(12)	C48-C51A-O5A	68.7(13)
C48-C51A-C50A	172.(2)	O5A-C51A-C49	101.5(11)
O5A-C51A-C50A	110.3(11)	C50A-C51A-C49	117.4(12)
O5-O5A-Na1	57.6(3)	C48-O5A-Na1	109.4(6)
C48-O5A-O5	52.8(5)	C48-O5A-C51A	34.3(6)
C48-O5A-C48A	138.4(8)	C51A-O5A-Na1	143.6(7)
C51A-O5A-O5	86.9(7)	C51A-O5A-C48A	105.4(9)
C48A-O5A-Na1	108.9(6)	C48A-O5A-O5	165.3(8)
C51A-C50A-C49A	97.5(11)	C48A-C49A-C50A	104.3(12)
C49A-C48A-O5A	108.6(10)		

Table 6. Anisotropic atomic displacement parameters ($Å^2$) for 5460.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	0.0694(9)	0.0599(8)	0.0390(7)	0.0048(6)	0.0173(6)	0.0106(7)
Cl2	0.0695(9)	0.0541(8)	0.0540(8)	0.0127(6)	0.0170(7)	0.0080(7)
F003	0.0296(11)	0.0258(11)	0.0264(11)	-0.0012(9)	0.0023(9)	0.0116(9)
F004	0.0363(12)	0.0260(11)	0.0274(11)	0.0026(9)	0.0088(9)	0.0137(10)
F005	0.0367(12)	0.0301(12)	0.0234(11)	0.0006(9)	0.0089(9)	0.0116(10)
F006	0.0323(12)	0.0326(12)	0.0266(11)	0.0029(9)	0.0110(9)	0.0115(10)
F007	0.0246(11)	0.0340(13)	0.0359(13)	0.0069(10)	0.0032(10)	0.0045(10)
F008	0.0391(13)	0.0255(12)	0.0362(13)	-0.0033(10)	0.0105(11)	0.0036(10)
F009	0.0347(12)	0.0422(14)	0.0352(13)	0.0113(11)	0.0107(10)	0.0242(11)
F00A	0.0311(12)	0.0349(13)	0.0329(13)	-0.0074(10)	-0.0037(10)	0.0060(10)
F00B	0.0275(12)	0.0416(14)	0.0320(13)	-0.0013(11)	-0.0015(10)	0.0085(10)
F00C	0.0229(11)	0.0393(14)	0.0461(15)	0.0088(11)	0.0077(10)	0.0121(10)
F00D	0.0251(11)	0.0500(15)	0.0348(13)	0.0054(11)	-0.0019(10)	0.0136(11)
F00E	0.0396(13)	0.0260(12)	0.0510(16)	0.0094(11)	0.0189(12)	0.0130(10)
F00F	0.0446(14)	0.0568(17)	0.0262(12)	0.0141(11)	0.0158(11)	0.0252(13)
F00G	0.0337(13)	0.0337(13)	0.0654(19)	0.0122(12)	0.0263(13)	0.0145(11)
F00H	0.0415(14)	0.0331(13)	0.0457(15)	-0.0038(11)	0.0105(12)	0.0136(11)
F00I	0.0511(16)	0.0388(14)	0.0345(14)	0.0031(11)	0.0010(12)	0.0161(12)
F00J	0.0447(15)	0.0263(13)	0.0615(18)	0.0094(12)	0.0155(13)	0.0037(11)
F00K	0.0659(19)	0.0518(17)	0.0316(14)	0.0010(12)	0.0252(13)	0.0219(15)
F00L	0.0485(16)	0.0481(16)	0.0540(17)	0.0309(14)	0.0258(14)	0.0169(13)
F00M	0.0335(14)	0.068(2)	0.071(2)	0.0203(16)	0.0204(14)	0.0316(14)
F00N	0.0522(17)	0.0583(19)	0.0285(14)	-0.0065(13)	-0.0115(12)	0.0003(14)
Na1	0.193(4)	0.0489(14)	0.0244(11)	-0.0035(10)	0.0139(16)	-0.0170(18)
F00P	0.082(2)	0.0480(17)	0.0539(18)	-0.0041(14)	0.0309(17)	0.0332(17)
F00Q	0.084(2)	0.061(2)	0.0209(13)	-0.0129(13)	0.0098(14)	0.0088(17)
F00R	0.0598(19)	0.0551(19)	0.067(2)	0.0387(17)	0.0128(16)	0.0132(16)
F00S	0.069(2)	0.0441(17)	0.065(2)	-0.0150(15)	-0.0330(18)	0.0248(16)
F00T	0.0266(14)	0.0413(17)	0.140(4)	0.0064(19)	0.0337(18)	0.0090(12)
F00U	0.072(2)	0.073(2)	0.081(2)	0.0111(19)	0.0390(19)	0.0526(19)
N2	0.0210(14)	0.0238(15)	0.0184(14)	0.0011(11)	0.0035(11)	0.0067(12)
N1	0.0207(14)	0.0263(16)	0.0256(16)	0.0023(12)	0.0057(12)	0.0085(12)
F00X	0.060(2)	0.077(2)	0.0386(17)	0.0167(16)	-0.0169(15)	-0.0163(18)
O1	0.0257(15)	0.080(3)	0.0357(17)	0.0037(17)	0.0133(13)	0.0154(16)
F00Z	0.0263(14)	0.0447(18)	0.145(4)	-0.018(2)	-0.0237(18)	0.0093(13)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O2	0.0392(18)	0.106(3)	0.0271(17)	0.0102(19)	0.0133(14)	0.022(2)
F011	0.087(3)	0.103(3)	0.057(2)	0.048(2)	-0.023(2)	-0.013(2)
O6	0.101(3)	0.049(2)	0.0331(19)	0.0007(17)	0.006(2)	-0.001(2)
C3	0.0170(15)	0.0236(17)	0.0205(16)	0.0007(13)	0.0020(13)	0.0061(13)
C5	0.0218(16)	0.0210(17)	0.0233(17)	0.0026(13)	0.0033(13)	0.0074(14)
C24	0.0262(17)	0.0265(18)	0.0156(16)	0.0036(13)	0.0065(13)	0.0102(15)
C25	0.0296(18)	0.0259(18)	0.0177(16)	0.0041(14)	0.0091(14)	0.0096(15)
C4	0.0215(16)	0.0210(17)	0.0226(17)	0.0043(13)	0.0055(13)	0.0079(13)
C1	0.0218(16)	0.0277(19)	0.0249(18)	0.0027(14)	0.0064(14)	0.0081(14)
C29	0.0274(18)	0.0254(18)	0.0200(17)	0.0037(14)	0.0062(14)	0.0105(15)
C17	0.0270(18)	0.0290(19)	0.0238(18)	0.0023(15)	0.0049(14)	0.0122(15)
C18	0.0331(19)	0.0235(18)	0.0195(17)	0.0028(14)	0.0044(15)	0.0081(15)
C7	0.0284(18)	0.0254(18)	0.0262(19)	0.0072(15)	0.0095(15)	0.0100(15)
C26	0.0287(18)	0.033(2)	0.0237(18)	0.0121(15)	0.0111(15)	0.0163(16)
C6	0.0200(16)	0.0248(18)	0.0276(19)	0.0042(14)	0.0046(14)	0.0090(14)
C2	0.0228(17)	0.032(2)	0.0282(19)	0.0044(15)	0.0086(15)	0.0103(15)
C12	0.0232(16)	0.0277(18)	0.0219(17)	0.0046(14)	0.0039(14)	0.0102(15)
C9	0.0223(17)	0.0286(19)	0.0248(18)	0.0006(15)	0.0009(14)	0.0071(15)
C23	0.036(2)	0.0265(19)	0.0211(18)	0.0018(14)	0.0057(15)	0.0106(16)
C27	0.0210(17)	0.042(2)	0.0235(18)	0.0086(16)	0.0035(14)	0.0113(16)
C28	0.0270(18)	0.030(2)	0.0214(18)	0.0004(15)	0.0033(14)	0.0069(15)
C13	0.0276(18)	0.0292(19)	0.0273(19)	0.0040(15)	0.0057(15)	0.0097(16)
C8	0.0305(19)	0.035(2)	0.0210(18)	0.0050(15)	0.0062(15)	0.0104(17)
C36	0.0241(17)	0.031(2)	0.035(2)	0.0101(16)	0.0110(15)	0.0131(16)
C10	0.032(2)	0.042(2)	0.031(2)	0.0133(18)	0.0116(17)	0.0158(18)
C37	0.0232(18)	0.039(2)	0.035(2)	0.0130(18)	0.0057(16)	0.0078(17)
C14	0.0271(19)	0.029(2)	0.043(2)	0.0123(18)	0.0082(17)	0.0090(16)
C19	0.033(2)	0.033(2)	0.0236(19)	0.0023(16)	0.0043(16)	0.0077(17)
C42	0.0243(18)	0.0201(18)	0.048(2)	0.0020(16)	0.0046(17)	0.0103(15)
C41	0.0260(18)	0.036(2)	0.042(2)	0.0117(18)	0.0100(17)	0.0120(17)
C30	0.0288(19)	0.032(2)	0.034(2)	0.0098(17)	0.0125(16)	0.0154(16)
C15	0.031(2)	0.039(2)	0.044(2)	0.0231(19)	0.0173(18)	0.0171(18)
C43	0.0236(18)	0.0218(19)	0.064(3)	0.0043(19)	0.0119(19)	0.0088(15)
C31	0.039(2)	0.034(2)	0.035(2)	0.0058(17)	0.0158(18)	0.0172(18)
C35	0.031(2)	0.036(2)	0.041(2)	0.0127(18)	0.0153(18)	0.0151(18)
C16	0.0279(18)	0.041(2)	0.0263(19)	0.0105(17)	0.0092(15)	0.0166(17)
C22	0.050(3)	0.033(2)	0.024(2)	0.0003(16)	0.0129(18)	0.0115(19)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C47	0.039(2)	0.024(2)	0.046(3)	0.0003(18)	0.001(2)	0.0119(18)
C20	0.044(2)	0.038(2)	0.026(2)	-0.0023(18)	-0.0041(18)	0.006(2)
C21	0.064(3)	0.039(2)	0.0185(19)	-0.0053(17)	0.0050(19)	0.010(2)
C33	0.053(3)	0.055(3)	0.053(3)	0.019(2)	0.032(2)	0.037(3)
C32	0.060(3)	0.039(2)	0.039(2)	0.0054(19)	0.025(2)	0.025(2)
C34	0.037(2)	0.055(3)	0.046(3)	0.021(2)	0.023(2)	0.028(2)
C40	0.039(2)	0.045(3)	0.056(3)	0.029(2)	0.012(2)	0.013(2)
C46	0.043(3)	0.029(2)	0.062(3)	-0.007(2)	-0.016(2)	0.017(2)
C38	0.035(2)	0.062(3)	0.038(3)	0.017(2)	-0.006(2)	-0.002(2)
C44	0.023(2)	0.023(2)	0.099(5)	0.000(2)	0.012(2)	0.0085(17)
B1	0.0188(18)	0.024(2)	0.035(2)	0.0047(17)	0.0080(16)	0.0089(16)
C45	0.023(2)	0.025(2)	0.103(5)	-0.010(3)	-0.010(3)	0.0066(18)
B2	0.0232(18)	0.0219(19)	0.0210(19)	0.0016(15)	0.0051(15)	0.0094(15)
C11	0.035(3)	0.115(5)	0.046(3)	0.018(3)	0.024(2)	0.028(3)
C64	0.063(3)	0.059(3)	0.041(3)	0.000(2)	0.013(2)	0.025(3)
C39	0.044(3)	0.076(4)	0.043(3)	0.030(3)	-0.005(2)	0.001(3)
C52	0.101(5)	0.047(3)	0.036(3)	0.000(2)	0.002(3)	0.015(3)
C53	0.089(4)	0.055(3)	0.044(3)	0.000(3)	0.008(3)	0.011(3)
O3	0.247(7)	0.052(3)	0.167(5)	-0.025(3)	0.172(5)	-0.018(4)
C60	0.102(6)	0.064(4)	0.051(4)	0.019(3)	0.023(4)	0.016(4)
C62	0.080(5)	0.064(4)	0.087(5)	-0.012(4)	0.023(4)	0.008(4)
C63	0.232(13)	0.056(4)	0.036(3)	-0.003(3)	0.015(5)	-0.022(6)
C61	0.250(14)	0.051(4)	0.107(7)	0.023(4)	0.101(9)	0.040(6)
C58	0.106(6)	0.085(5)	0.109(6)	-0.005(5)	0.032(5)	0.022(5)
O4	0.320(9)	0.059(3)	0.053(3)	0.004(3)	0.012(4)	0.029(5)
O5	0.072(4)	0.071(4)	0.105(5)	-0.028(3)	-0.022(3)	0.007(3)
C51	0.072(4)	0.072(4)	0.105(5)	-0.028(3)	-0.022(3)	0.006(3)
C54	0.209(9)	0.076(5)	0.087(6)	0.010(5)	0.003(6)	0.040(6)
C56	0.212(9)	0.077(5)	0.114(7)	0.002(5)	0.012(6)	0.082(6)
C59	0.131(7)	0.102(6)	0.111(6)	0.001(5)	0.039(6)	0.016(5)
C57	0.156(8)	0.133(8)	0.152(8)	-0.012(7)	0.071(7)	0.028(6)
C48	0.073(4)	0.072(4)	0.105(5)	-0.028(3)	-0.021(3)	0.006(3)
C49	0.072(4)	0.072(4)	0.105(5)	-0.028(3)	-0.021(3)	0.006(3)
C50	0.072(4)	0.072(4)	0.105(5)	-0.028(3)	-0.021(3)	0.006(3)
C55	0.227(10)	0.114(7)	0.132(8)	0.014(7)	0.016(7)	0.030(7)
C51A	0.053(5)	0.053(5)	0.070(6)	-0.005(5)	0.026(5)	0.008(4)
O5A	0.049(4)	0.047(4)	0.058(4)	-0.005(3)	0.019(3)	0.010(3)

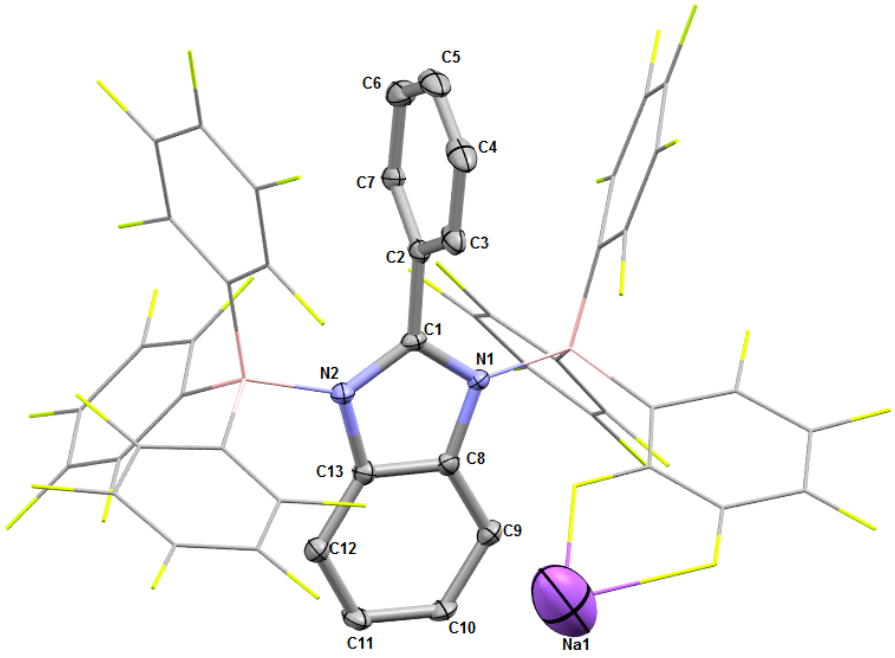
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C50A	0.070(6)	0.051(5)	0.058(6)	0.001(4)	0.021(5)	-0.007(5)
C49A	0.072(6)	0.055(6)	0.072(6)	0.000(5)	0.012(5)	-0.004(5)
C48A	0.050(5)	0.044(5)	0.067(5)	0.024(4)	0.031(4)	0.017(4)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 5460.

	x/a	y/b	z/c	U(eq)
H5	0.4461	0.7525	0.7892	0.027
H1	0.0486	0.6161	0.8614	0.03
H6	0.5721	0.7598	0.7058	0.029
H2	0.0309	0.7551	0.8294	0.032
H9	0.1612	0.6691	0.5971	0.032
H8	0.2862	0.6765	0.5136	0.034
H11A	0.7112	0.7951	0.4996	0.092
H11B	0.6872	0.6961	0.4983	0.092
H11C	0.7923	0.7560	0.5673	0.092
H64A	0.1464	1.1993	0.9905	0.063
H64B	0.1769	1.1208	1.0336	0.063
H52A	0.2047	0.6693	0.1277	0.079
H52B	0.3379	0.6713	0.1291	0.079
H53A	0.3477	0.7663	0.0439	0.08
H53B	0.2102	0.7561	0.0346	0.08
H60A	0.2626	0.5268	0.4028	0.088
H60B	0.3935	0.5185	0.4125	0.088
H62A	0.2007	0.3933	0.2117	0.096
H62B	0.3435	0.4202	0.2431	0.096
H63A	0.3220	0.5414	0.1982	0.151
H63B	0.1952	0.5246	0.2166	0.151
H61A	0.3067	0.3887	0.3586	0.152
H61B	0.1792	0.4044	0.3323	0.152
H58A	0.8251	0.8141	0.2878	0.121
H58B	0.7330	0.8582	0.2363	0.121
H51A	0.1034	0.6933	0.3607	0.114
H51B	0.1377	0.7002	0.2760	0.114
H54A	0.2472	0.8627	0.1150	0.158
H54B	0.3660	0.8903	0.0847	0.158

	x/a	y/b	z/c	U(eq)
H56A	0.5736	0.6240	0.2567	0.158
H56B	0.6987	0.6658	0.3226	0.158
H59A	0.6649	0.8598	0.3369	0.14
H59B	0.7455	0.8047	0.3841	0.14
H57A	0.7355	0.7126	0.1938	0.173
H57B	0.6150	0.7400	0.1708	0.173
H48A	0.3831	0.8691	0.4287	0.114
H48B	0.2725	0.8297	0.4661	0.114
H49A	0.2023	0.9248	0.3845	0.113
H49B	0.2649	0.9089	0.3163	0.113
H50A	0.0871	0.8189	0.2577	0.114
H50B	0.0484	0.8102	0.3408	0.114
H55A	0.3851	0.8835	0.2348	0.201
H55B	0.4748	0.8507	0.1973	0.201
H51C	0.3061	0.8527	0.4724	0.07
H51D	0.2651	0.8921	0.3891	0.07
H50C	0.3943	0.9865	0.5206	0.077
H50D	0.4011	1.0177	0.4323	0.077
H49C	0.6018	1.0106	0.4851	0.087
H49D	0.5589	0.9302	0.5333	0.087
H48C	0.5841	0.8741	0.4304	0.06
H48D	0.5408	0.9398	0.3719	0.06

Crystal Structure Report for Na[BIMP]



Thermal ellipsoid plot of 5534_1. Ellipsoids shown at 50% probability, $B(C_6F_5)_3$ substituents shown in wireframe, solvent molecules and hydrogen atoms hidden for clarity.

A specimen of $C_{60}H_{35}B_2F_{30}N_2NaO_{3.50}$ was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å). The integration of the data using a monoclinic unit cell yielded a total of 56025 reflections to a maximum θ angle of 28.00° (0.76Å resolution), of which 13889 were independent (average redundancy 4.034, completeness = 99.4%, R_{int} = 8.23%, R_{sig} =8.41%) and 7606 (54.76%) were greater than $2\sigma(F^2)$. The final cell constants of a = 15.0906(12) Å, b = 16.8592(13) Å, c =23.0499(18) Å, β = 99.144(2)°, volume = 5789.7(8) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The final anisotropic full-matrix least-squares refinement on F^2 with 885 variables converged at R1 = 9.60%, for the observed data and wR2 = 33.37% for all data. The goodness-of-fit was 1.034. The largest peak in the final difference electron density synthesis was 3.692 $e^-/Å^3$ and the largest hole was -1.069 $e^-/Å^3$ with an RMS deviation of 0.164 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.669 g/cm^3 and F(000), 2912 e^-.

Table 1. Sample and crystal data for 5534_1.

Identification code	5534_1
Chemical formula	$C_{60}H_{35}B_2F_{30}N_2NaO_{3.50}$
Formula weight	1454.51 g/mol
Temperature	100(2) K

Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 15.0906(12) Å	α = 90°
	b = 16.8592(13) Å	β = 99.144(2)°
	c = 23.0499(18) Å	γ = 90°
Volume	5789.7(8) $Å^3$	
Z	4	
Density (calculated)	1.669 g/cm^3	
Absorption coefficient	0.175 mm^{-1}	
F(000)	2912	

Table 2. Data collection and structure refinement for 5534_1.

Theta range for data collection	1.51 to 28.00°	
Index ranges	-19<=h<=19, -22<=k<=17, -30<=l<=30	
Reflections collected	56025	
Independent reflections	13889 [R(int) = 0.0823]	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	13889 / 40 / 885	
Goodness-of-fit on F^2	1.034	
Final R indices	7606 data; I>2σ(I)	R1 = 0.0960, wR2 = 0.2815
	all data	R1 = 0.1669, wR2 = 0.3337
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.1879P)^2+13.4093P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	3.692 and -1.069 $eÅ^{-3}$	
R.M.S. deviation from mean	0.164 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for 5534_1.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij}tensor.

	x/a	y/b	z/c	U(eq)
Na1	0.5287(4)	0.4664(3)	0.4287(2)	0.1156(18)
F1	0.49365(19)	0.73806(19)	0.06640(13)	0.0252(7)
F2	0.6494(2)	0.7686(2)	0.03343(14)	0.0307(8)

	x/a	y/b	z/c	U(eq)
F3	0.8065(2)	0.7340(2)	0.10424(15)	0.0333(8)
F4	0.80243(18)	0.67333(19)	0.21427(13)	0.0264(7)
F5	0.64759(18)	0.64182(18)	0.24892(12)	0.0202(6)
F6	0.40547(18)	0.59656(18)	0.07166(13)	0.0225(7)
F7	0.2621(2)	0.6357(2)	0.99412(13)	0.0295(8)
F8	0.1476(2)	0.7514(2)	0.01919(14)	0.0346(8)
F9	0.18134(19)	0.82590(19)	0.12545(14)	0.0279(7)
F10	0.31927(18)	0.78623(17)	0.20451(13)	0.0212(6)
F11	0.4857(2)	0.83243(18)	0.19187(15)	0.0286(7)
F12	0.5325(3)	0.9236(2)	0.28607(19)	0.0481(11)
F13	0.5628(2)	0.8580(3)	0.39619(18)	0.0522(12)
F14	0.5402(2)	0.6987(3)	0.40841(14)	0.0398(9)
F15	0.4979(2)	0.6064(2)	0.31594(13)	0.0279(7)
F16	0.39560(19)	0.41683(18)	0.07297(13)	0.0225(7)
F17	0.2490(2)	0.3875(2)	0.99540(14)	0.0309(8)
F18	0.1275(2)	0.2761(2)	0.01894(15)	0.0344(8)
F19	0.15675(19)	0.1991(2)	0.12417(14)	0.0297(8)
F20	0.29611(19)	0.23234(18)	0.20383(13)	0.0225(7)
F21	0.4573(2)	0.17446(18)	0.19290(14)	0.0257(7)
F22	0.4907(2)	0.0825(2)	0.28796(17)	0.0404(9)
F23	0.5203(2)	0.1490(2)	0.39798(16)	0.0443(10)
F24	0.5182(2)	0.3093(2)	0.40891(13)	0.0339(8)
F25	0.4896(2)	0.40179(19)	0.31662(13)	0.0258(7)
F26	0.63613(18)	0.34982(17)	0.24896(12)	0.0195(6)
F27	0.78537(18)	0.30310(19)	0.21342(13)	0.0250(7)
F28	0.7804(2)	0.2368(2)	0.10416(15)	0.0317(8)
F29	0.6204(2)	0.2179(2)	0.03350(13)	0.0291(8)
F30	0.47043(19)	0.26802(19)	0.06538(13)	0.0249(7)
O1	0.6679(7)	0.4850(5)	0.3909(5)	0.128(4)
O4	0.3922(4)	0.5130(4)	0.3918(3)	0.0655(16)
N1	0.4457(2)	0.4380(2)	0.19858(16)	0.0125(8)
N2	0.4508(2)	0.5709(2)	0.19841(17)	0.0149(8)
C1	0.4911(3)	0.5026(3)	0.1856(2)	0.0134(9)
C2	0.5762(3)	0.4992(3)	0.1608(2)	0.0167(10)
C3	0.6578(3)	0.4953(3)	0.1999(3)	0.0204(11)
C4	0.7388(3)	0.4903(3)	0.1776(3)	0.0285(13)
C5	0.7384(4)	0.4906(3)	0.1178(3)	0.0308(13)

	x/a	y/b	z/c	U(eq)
C6	0.6592(4)	0.4944(3)	0.0790(3)	0.0287(13)
C7	0.5772(3)	0.4987(3)	0.1006(2)	0.0191(10)
C8	0.3709(3)	0.4660(3)	0.2215(2)	0.0152(9)
C9	0.3028(3)	0.4248(3)	0.2438(2)	0.0179(10)
C10	0.2375(3)	0.4694(3)	0.2645(2)	0.0203(11)
C11	0.2411(3)	0.5536(3)	0.2642(2)	0.0199(10)
C12	0.3097(3)	0.5933(3)	0.2435(2)	0.0170(10)
C13	0.3742(3)	0.5483(3)	0.2218(2)	0.0146(9)
C14	0.5604(3)	0.6816(3)	0.1588(2)	0.0165(10)
C15	0.6436(3)	0.6714(3)	0.1940(2)	0.0164(10)
C16	0.7257(3)	0.6876(3)	0.1772(2)	0.0197(10)
C17	0.7277(3)	0.7185(3)	0.1224(2)	0.0224(11)
C18	0.6478(3)	0.7347(3)	0.0864(2)	0.0209(11)
C19	0.5670(3)	0.7166(3)	0.1048(2)	0.0177(10)
C20	0.4842(3)	0.7146(3)	0.2483(2)	0.0178(10)
C21	0.5012(3)	0.6858(3)	0.3052(2)	0.0222(11)
C22	0.5247(3)	0.7324(4)	0.3545(2)	0.0271(13)
C23	0.5357(4)	0.8119(4)	0.3491(3)	0.0336(15)
C24	0.5206(4)	0.8451(4)	0.2936(3)	0.0331(14)
C25	0.4971(3)	0.7965(3)	0.2459(2)	0.0225(11)
C26	0.3742(3)	0.6910(3)	0.1418(2)	0.0156(10)
C27	0.3515(3)	0.6538(3)	0.0872(2)	0.0177(10)
C28	0.2774(3)	0.6735(3)	0.0457(2)	0.0201(10)
C29	0.2199(3)	0.7310(3)	0.0588(2)	0.0234(11)
C30	0.2368(3)	0.7683(3)	0.1122(2)	0.0211(11)
C31	0.3117(3)	0.7473(3)	0.1522(2)	0.0174(10)
C32	0.4656(3)	0.2932(3)	0.2488(2)	0.0178(10)
C33	0.4700(3)	0.2113(3)	0.2461(2)	0.0210(11)
C34	0.4867(4)	0.1620(3)	0.2948(3)	0.0272(12)
C35	0.5025(3)	0.1942(4)	0.3503(3)	0.0302(13)
C36	0.5008(3)	0.2759(4)	0.3550(2)	0.0244(12)
C37	0.4840(3)	0.3232(3)	0.3056(2)	0.0212(11)
C38	0.5433(3)	0.3178(3)	0.1581(2)	0.0154(9)
C39	0.6275(3)	0.3205(3)	0.1935(2)	0.0170(10)
C40	0.7065(3)	0.2949(3)	0.1768(2)	0.0180(10)
C41	0.7049(3)	0.2621(3)	0.1224(2)	0.0210(11)
C42	0.6230(3)	0.2533(3)	0.0859(2)	0.0212(11)

	x/a	y/b	z/c	U(eq)
C43	0.5457(3)	0.2813(3)	0.1043(2)	0.0178(10)
C44	0.3583(3)	0.3237(3)	0.1420(2)	0.0149(9)
C45	0.2920(3)	0.2706(3)	0.1521(2)	0.0179(10)
C46	0.2158(3)	0.2537(3)	0.1116(2)	0.0221(11)
C47	0.2007(3)	0.2921(3)	0.0583(2)	0.0234(11)
C48	0.2626(3)	0.3479(3)	0.0468(2)	0.0207(11)
C49	0.3376(3)	0.3625(3)	0.0885(2)	0.0176(10)
C50	0.7234(11)	0.4188(7)	0.3839(6)	0.122(6)
C51	0.7164(16)	0.5551(8)	0.3832(8)	0.172(10)
C52	0.8055(13)	0.5375(9)	0.3580(9)	0.150(8)
C53	0.8084(11)	0.4445(7)	0.3589(9)	0.147(7)
B1	0.4538(3)	0.3442(3)	0.1863(2)	0.0160(11)
B2	0.4675(3)	0.6638(3)	0.1861(2)	0.0162(11)
O5	0.2266(7)	0.4940(6)	0.4364(5)	0.123(3)
C54	0.1820(13)	0.5637(10)	0.4393(9)	0.164(6)
C55	0.0943(13)	0.5616(10)	0.4346(10)	0.178(7)
C56	0.0766(11)	0.4822(11)	0.4266(12)	0.191(8)
C57	0.1510(10)	0.4381(7)	0.4261(8)	0.128(5)
C58	0.0457(4)	0.5147(4)	0.0130(3)	0.0415(16)
C59	0.0820(5)	0.4852(4)	0.0742(3)	0.0442(17)
C60	0.1695(5)	0.5177(4)	0.1020(3)	0.0467(17)

Table 4. Bond lengths (Å) for 5534_1.

Na1-O4	2.242(8)	Na1-O1	2.419(14)
Na1-F24	2.688(7)	Na1-F25	2.779(5)
Na1-Na1	3.708(10)	F1-C19	1.352(5)
F2-C18	1.352(6)	F3-C17	1.347(5)
F4-C16	1.347(5)	F5-C15	1.353(5)
F6-C27	1.348(5)	F7-C28	1.336(6)
F8-C29	1.352(6)	F9-C30	1.348(6)
F10-C31	1.362(5)	F11-C25	1.372(6)
F12-C24	1.350(7)	F13-C23	1.345(6)
F14-C22	1.353(7)	F15-C21	1.362(6)
F16-C49	1.354(5)	F17-C48	1.347(6)
F18-C47	1.341(6)	F19-C46	1.345(6)
F20-C45	1.348(6)	F21-C33	1.360(6)

F22-C34	1.353(7)	F23-C35	1.330(6)
F24-C36	1.352(6)	F25-C37	1.348(6)
F26-C39	1.358(5)	F27-C40	1.352(5)
F28-C41	1.346(5)	F29-C42	1.343(6)
F30-C43	1.349(5)	O1-C51	1.416(18)
O1-C50	1.420(14)	N1-C1	1.345(6)
N1-C8	1.403(6)	N1-B1	1.614(7)
N2-C1	1.358(6)	N2-C13	1.404(6)
N2-B2	1.619(7)	C1-C2	1.485(6)
C2-C7	1.391(7)	C2-C3	1.407(7)
C3-C4	1.401(7)	C4-C5	1.378(9)
C5-C6	1.375(9)	C6-C7	1.407(7)
C8-C13	1.387(7)	C8-C9	1.404(6)
C9-C10	1.383(7)	C10-C11	1.420(8)
C11-C12	1.380(7)	C12-C13	1.389(6)
C14-C15	1.393(7)	C14-C19	1.397(7)
C14-B2	1.652(7)	C15-C16	1.384(7)
C16-C17	1.371(7)	C17-C18	1.378(7)
C18-C19	1.386(7)	C20-C21	1.384(7)
C20-C25	1.397(7)	C20-B2	1.654(7)
C21-C22	1.382(7)	C22-C23	1.358(9)
C23-C24	1.382(9)	C24-C25	1.370(8)
C26-C31	1.385(7)	C26-C27	1.400(7)
C26-B2	1.666(7)	C27-C28	1.392(7)
C28-C29	1.367(7)	C29-C30	1.368(8)
C30-C31	1.387(7)	C32-C33	1.384(7)
C32-C37	1.390(7)	C32-B1	1.663(7)
C33-C34	1.389(8)	C34-C35	1.374(9)
C35-C36	1.381(9)	C36-C37	1.380(7)
C38-C43	1.391(7)	C38-C39	1.396(7)
C38-B1	1.650(7)	C39-C40	1.378(6)
C40-C41	1.367(7)	C41-C42	1.388(7)
C42-C43	1.385(7)	C44-C49	1.387(7)
C44-C45	1.389(7)	C44-B1	1.664(7)
C45-C46	1.391(7)	C46-C47	1.374(8)
C47-C48	1.382(7)	C48-C49	1.386(7)
C50-C53	1.55(2)	C51-C52	1.57(3)
C52-C53	1.57(2)	O5-C54	1.362(18)

O5-C57	1.470(16)	C54-C55	1.31(2)
C55-C56	1.37(2)	C56-C57	1.348(19)
C58-C58	1.499(13)	C58-C59	1.515(10)
C59-C60	1.479(10)		

Table 5. Bond angles (°) for 5534_1.

O4-Na1-O1	128.0(4)	O4-Na1-F24	104.8(3)
O1-Na1-F24	95.6(3)	O4-Na1-F25	74.8(2)
O1-Na1-F25	77.5(3)	F24-Na1-F25	57.18(14)
O4-Na1-Na1	84.2(3)	O1-Na1-Na1	128.2(4)
F24-Na1-Na1	115.8(3)	F25-Na1-Na1	154.0(3)
C36-F24-Na1	124.3(3)	C37-F25-Na1	123.9(3)
C51-O1-C50	108.4(15)	C51-O1-Na1	130.5(12)
C50-O1-Na1	120.1(10)	C1-N1-C8	106.3(4)
C1-N1-B1	134.3(4)	C8-N1-B1	118.9(4)
C1-N2-C13	106.1(4)	C1-N2-B2	134.1(4)
C13-N2-B2	119.4(4)	N1-C1-N2	112.1(4)
N1-C1-C2	123.8(4)	N2-C1-C2	124.1(4)
C7-C2-C3	119.4(4)	C7-C2-C1	122.0(4)
C3-C2-C1	118.6(4)	C4-C3-C2	119.7(5)
C5-C4-C3	120.1(5)	C6-C5-C4	121.0(5)
C5-C6-C7	119.7(6)	C2-C7-C6	120.2(5)
C13-C8-N1	107.9(4)	C13-C8-C9	121.4(4)
N1-C8-C9	130.6(5)	C10-C9-C8	117.4(5)
C9-C10-C11	120.8(4)	C12-C11-C10	121.2(4)
C11-C12-C13	117.9(5)	C8-C13-C12	121.4(4)
C8-C13-N2	107.5(4)	C12-C13-N2	131.1(4)
C15-C14-C19	112.7(4)	C15-C14-B2	119.8(4)
C19-C14-B2	127.0(4)	F5-C15-C16	115.2(4)
F5-C15-C14	119.5(4)	C16-C15-C14	125.3(5)
F4-C16-C17	120.7(4)	F4-C16-C15	120.3(4)
C17-C16-C15	119.0(4)	F3-C17-C16	120.6(4)
F3-C17-C18	120.4(5)	C16-C17-C18	119.0(4)
F2-C18-C17	119.1(4)	F2-C18-C19	120.8(5)
C17-C18-C19	120.1(5)	F1-C19-C18	114.2(4)
F1-C19-C14	121.9(4)	C18-C19-C14	123.8(5)
C21-C20-C25	112.2(5)	C21-C20-B2	128.3(5)

C25-C20-B2	118.7(4)	F15-C21-C22	114.9(5)
F15-C21-C20	120.7(5)	C22-C21-C20	124.3(5)
F14-C22-C23	119.6(5)	F14-C22-C21	120.0(6)
C23-C22-C21	120.4(5)	F13-C23-C22	121.5(6)
F13-C23-C24	119.8(6)	C22-C23-C24	118.6(5)
F12-C24-C25	120.4(6)	F12-C24-C23	120.6(5)
C25-C24-C23	118.9(6)	C24-C25-F11	116.3(5)
C24-C25-C20	125.4(5)	F11-C25-C20	118.3(4)
C31-C26-C27	112.7(4)	C31-C26-B2	128.0(4)
C27-C26-B2	119.3(4)	F6-C27-C28	116.2(4)
F6-C27-C26	119.3(4)	C28-C27-C26	124.5(4)
F7-C28-C29	120.6(4)	F7-C28-C27	120.3(4)
C29-C28-C27	119.1(5)	F8-C29-C28	120.3(5)
F8-C29-C30	120.3(5)	C28-C29-C30	119.4(5)
F9-C30-C29	120.1(5)	F9-C30-C31	120.2(5)
C29-C30-C31	119.7(5)	F10-C31-C26	121.3(4)
F10-C31-C30	114.3(4)	C26-C31-C30	124.5(5)
C33-C32-C37	113.7(5)	C33-C32-B1	118.4(4)
C37-C32-B1	127.3(5)	F21-C33-C32	119.7(5)
F21-C33-C34	115.9(5)	C32-C33-C34	124.3(5)
F22-C34-C35	119.8(5)	F22-C34-C33	120.3(5)
C35-C34-C33	119.9(5)	F23-C35-C34	121.6(6)
F23-C35-C36	120.7(6)	C34-C35-C36	117.6(5)
F24-C36-C37	120.0(5)	F24-C36-C35	118.9(5)
C37-C36-C35	121.0(5)	F25-C37-C36	114.6(5)
F25-C37-C32	122.1(5)	C36-C37-C32	123.3(5)
C43-C38-C39	112.6(4)	C43-C38-B1	127.5(4)
C39-C38-B1	119.2(4)	F26-C39-C40	114.7(4)
F26-C39-C38	120.2(4)	C40-C39-C38	125.1(5)
F27-C40-C41	120.0(4)	F27-C40-C39	120.6(4)
C41-C40-C39	119.4(4)	F28-C41-C40	121.5(4)
F28-C41-C42	119.6(5)	C40-C41-C42	118.9(4)
F29-C42-C43	121.4(4)	F29-C42-C41	119.2(4)
C43-C42-C41	119.4(5)	F30-C43-C42	113.7(4)
F30-C43-C38	121.9(4)	C42-C43-C38	124.4(5)
C49-C44-C45	112.7(4)	C49-C44-B1	119.8(4)
C45-C44-B1	127.4(4)	F20-C45-C44	121.6(4)
F20-C45-C46	114.4(4)	C44-C45-C46	124.0(5)

F19-C46-C47	119.6(5)	F19-C46-C45	120.0(5)
C47-C46-C45	120.4(5)	F18-C47-C46	120.8(5)
F18-C47-C48	121.1(5)	C46-C47-C48	118.2(5)
F17-C48-C47	119.6(4)	F17-C48-C49	121.0(4)
C47-C48-C49	119.3(5)	F16-C49-C48	115.3(4)
F16-C49-C44	119.4(4)	C48-C49-C44	125.2(4)
O1-C50-C53	111.1(12)	O1-C51-C52	112.2(14)
C53-C52-C51	102.0(14)	C50-C53-C52	105.2(13)
N1-B1-C38	115.0(4)	N1-B1-C32	110.8(4)
C38-B1-C32	102.7(4)	N1-B1-C44	103.3(4)
C38-B1-C44	112.7(4)	C32-B1-C44	112.7(4)
N2-B2-C14	114.0(4)	N2-B2-C20	110.8(4)
C14-B2-C20	102.4(4)	N2-B2-C26	103.5(4)
C14-B2-C26	113.7(4)	C20-B2-C26	112.7(4)
C54-O5-C57	100.6(11)	C55-C54-O5	118.2(15)
C54-C55-C56	102.1(15)	C57-C56-C55	113.2(16)
C56-C57-O5	105.8(12)	C58-C58-C59	115.9(8)
C60-C59-C58	116.6(6)		

Table 6. Anisotropic atomic displacement parameters (Å^2) for 5534_1.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Na1	0.141(4)	0.121(4)	0.074(3)	-0.017(3)	-0.016(3)	0.051(3)
F1	0.0172(14)	0.0358(19)	0.0222(16)	0.0104(14)	0.0019(11)	-0.0005(13)
F2	0.0248(16)	0.045(2)	0.0241(17)	0.0110(15)	0.0082(13)	-0.0068(14)
F3	0.0162(14)	0.049(2)	0.0368(19)	0.0036(16)	0.0114(13)	-0.0090(14)
F4	0.0131(13)	0.0352(19)	0.0302(17)	-0.0017(14)	0.0010(12)	-0.0013(12)
F5	0.0191(14)	0.0230(16)	0.0187(14)	0.0029(12)	0.0037(11)	0.0003(12)
F6	0.0203(14)	0.0231(17)	0.0242(16)	-0.0063(13)	0.0040(12)	0.0072(12)
F7	0.0271(16)	0.038(2)	0.0214(16)	-0.0102(14)	-0.0009(12)	0.0035(14)
F8	0.0225(16)	0.049(2)	0.0300(18)	-0.0012(16)	-0.0037(13)	0.0126(15)
F9	0.0193(14)	0.0291(18)	0.0361(18)	-0.0022(15)	0.0070(13)	0.0117(13)
F10	0.0205(14)	0.0215(16)	0.0222(15)	-0.0082(12)	0.0057(11)	0.0045(12)
F11	0.0281(16)	0.0148(16)	0.044(2)	-0.0001(14)	0.0071(14)	0.0001(13)
F12	0.043(2)	0.0182(19)	0.080(3)	-0.0222(19)	-0.001(2)	-0.0022(15)
F13	0.037(2)	0.063(3)	0.052(2)	-0.042(2)	-0.0077(17)	0.0089(19)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F14	0.0238(16)	0.076(3)	0.0184(17)	-0.0104(17)	-0.0005(13)	0.0000(17)
F15	0.0305(16)	0.0320(19)	0.0208(16)	0.0017(14)	0.0026(13)	-0.0096(14)
F16	0.0208(14)	0.0235(17)	0.0239(16)	0.0054(13)	0.0053(12)	-0.0071(12)
F17	0.0267(16)	0.039(2)	0.0257(17)	0.0138(15)	0.0002(13)	-0.0058(14)
F18	0.0186(15)	0.050(2)	0.0320(18)	0.0040(16)	-0.0037(13)	-0.0100(14)
F19	0.0179(14)	0.0351(19)	0.0371(19)	0.0075(15)	0.0071(13)	-0.0103(13)
F20	0.0224(14)	0.0226(16)	0.0238(16)	0.0058(13)	0.0079(12)	-0.0060(12)
F21	0.0316(16)	0.0160(16)	0.0302(17)	0.0009(13)	0.0070(13)	0.0004(13)
F22	0.044(2)	0.0199(18)	0.055(2)	0.0154(17)	-0.0008(17)	-0.0025(15)
F23	0.041(2)	0.047(2)	0.041(2)	0.0295(18)	-0.0046(16)	-0.0070(17)
F24	0.0325(17)	0.050(2)	0.0185(16)	0.0049(15)	0.0029(13)	0.0039(16)
F25	0.0328(17)	0.0235(17)	0.0203(15)	-0.0034(13)	0.0020(12)	0.0047(13)
F26	0.0183(13)	0.0206(16)	0.0201(15)	-0.0008(12)	0.0047(11)	-0.0003(11)
F27	0.0125(13)	0.0322(18)	0.0297(17)	0.0015(14)	0.0016(12)	0.0026(12)
F28	0.0183(15)	0.043(2)	0.0356(19)	-0.0069(16)	0.0110(13)	0.0109(14)
F29	0.0265(16)	0.040(2)	0.0218(16)	-0.0098(14)	0.0069(13)	0.0073(14)
F30	0.0174(14)	0.0328(18)	0.0238(16)	-0.0101(14)	0.0014(12)	0.0030(12)
O1	0.112(7)	0.086(7)	0.164(9)	-0.019(6)	-0.044(6)	0.000(5)
O4	0.066(4)	0.067(4)	0.068(4)	-0.012(3)	0.027(3)	-0.010(3)
N1	0.0128(17)	0.012(2)	0.0134(19)	0.0021(16)	0.0045(14)	0.0004(15)
N2	0.0135(18)	0.014(2)	0.018(2)	0.0015(16)	0.0063(15)	0.0005(15)
C1	0.011(2)	0.017(3)	0.013(2)	0.0009(19)	0.0035(16)	-0.0008(17)
C2	0.015(2)	0.010(2)	0.028(3)	0.001(2)	0.0095(19)	0.0007(17)
C3	0.016(2)	0.013(3)	0.033(3)	0.000(2)	0.006(2)	-0.0008(18)
C4	0.013(2)	0.019(3)	0.055(4)	0.001(3)	0.010(2)	-0.001(2)
C5	0.022(3)	0.021(3)	0.054(4)	0.001(3)	0.023(3)	0.001(2)
C6	0.031(3)	0.021(3)	0.040(3)	0.002(2)	0.022(3)	-0.002(2)
C7	0.023(2)	0.012(3)	0.024(2)	0.000(2)	0.011(2)	-0.0004(19)
C8	0.016(2)	0.017(2)	0.013(2)	0.0024(19)	0.0042(17)	0.0028(18)
C9	0.019(2)	0.016(3)	0.020(2)	0.002(2)	0.0066(19)	-0.0024(19)
C10	0.018(2)	0.021(3)	0.025(3)	0.003(2)	0.0127(19)	-0.003(2)
C11	0.014(2)	0.020(3)	0.027(3)	-0.002(2)	0.0087(19)	0.0025(19)
C12	0.017(2)	0.016(2)	0.019(2)	0.001(2)	0.0045(18)	-0.0004(19)
C13	0.015(2)	0.013(2)	0.016(2)	-0.0007(19)	0.0033(17)	-0.0011(18)
C14	0.019(2)	0.012(2)	0.019(2)	-0.0024(19)	0.0041(18)	-0.0007(18)
C15	0.018(2)	0.014(2)	0.018(2)	-0.0006(19)	0.0058(18)	-0.0022(19)
C16	0.015(2)	0.023(3)	0.021(3)	-0.005(2)	0.0026(18)	-0.0011(19)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C17	0.014(2)	0.028(3)	0.027(3)	-0.003(2)	0.0089(19)	-0.006(2)
C18	0.024(2)	0.023(3)	0.017(2)	0.001(2)	0.0064(19)	-0.008(2)
C19	0.015(2)	0.019(3)	0.018(2)	0.001(2)	0.0032(18)	-0.0040(19)
C20	0.013(2)	0.020(3)	0.022(3)	-0.003(2)	0.0085(18)	0.0020(19)
C21	0.013(2)	0.030(3)	0.025(3)	-0.005(2)	0.0064(19)	-0.004(2)
C22	0.018(2)	0.045(4)	0.019(3)	-0.010(2)	0.0045(19)	0.001(2)
C23	0.019(3)	0.042(4)	0.038(3)	-0.025(3)	-0.001(2)	0.005(2)
C24	0.020(3)	0.025(3)	0.053(4)	-0.017(3)	0.004(2)	0.004(2)
C25	0.018(2)	0.019(3)	0.031(3)	-0.006(2)	0.005(2)	0.000(2)
C26	0.015(2)	0.014(2)	0.019(2)	0.0026(19)	0.0055(18)	0.0012(18)
C27	0.013(2)	0.021(3)	0.021(2)	-0.003(2)	0.0061(18)	0.0014(19)
C28	0.017(2)	0.025(3)	0.017(2)	-0.001(2)	0.0010(18)	0.001(2)
C29	0.016(2)	0.031(3)	0.023(3)	0.003(2)	0.0015(19)	0.001(2)
C30	0.017(2)	0.020(3)	0.027(3)	0.002(2)	0.006(2)	0.0057(19)
C31	0.017(2)	0.018(3)	0.018(2)	-0.005(2)	0.0046(18)	-0.0034(19)
C32	0.013(2)	0.020(3)	0.021(2)	0.004(2)	0.0044(18)	0.0004(18)
C33	0.019(2)	0.018(3)	0.026(3)	0.001(2)	0.004(2)	-0.001(2)
C34	0.023(3)	0.017(3)	0.041(3)	0.009(2)	0.003(2)	-0.001(2)
C35	0.018(2)	0.038(4)	0.034(3)	0.020(3)	0.001(2)	0.000(2)
C36	0.016(2)	0.037(3)	0.019(3)	0.007(2)	0.0012(19)	0.001(2)
C37	0.014(2)	0.024(3)	0.028(3)	0.003(2)	0.0090(19)	0.004(2)
C38	0.019(2)	0.010(2)	0.019(2)	0.0047(19)	0.0066(18)	0.0002(18)
C39	0.019(2)	0.015(3)	0.018(2)	-0.002(2)	0.0056(18)	0.0003(19)
C40	0.015(2)	0.016(3)	0.022(3)	0.000(2)	0.0022(18)	0.0024(18)
C41	0.014(2)	0.022(3)	0.029(3)	0.001(2)	0.0079(19)	0.0065(19)
C42	0.020(2)	0.021(3)	0.022(3)	-0.001(2)	0.005(2)	0.005(2)
C43	0.015(2)	0.019(3)	0.020(2)	0.001(2)	0.0041(18)	0.0006(19)
C44	0.016(2)	0.014(2)	0.016(2)	-0.0015(19)	0.0082(17)	0.0006(18)
C45	0.018(2)	0.020(3)	0.017(2)	0.002(2)	0.0048(18)	0.0027(19)
C46	0.014(2)	0.022(3)	0.032(3)	-0.001(2)	0.009(2)	-0.006(2)
C47	0.017(2)	0.030(3)	0.023(3)	0.000(2)	0.0009(19)	0.000(2)
C48	0.017(2)	0.025(3)	0.019(3)	0.003(2)	0.0020(19)	0.000(2)
C49	0.014(2)	0.019(3)	0.022(3)	0.001(2)	0.0075(18)	-0.0029(18)
C50	0.177(14)	0.053(7)	0.105(9)	-0.027(6)	-0.078(10)	0.039(8)
C51	0.29(3)	0.050(8)	0.135(14)	0.022(8)	-0.084(16)	-0.018(13)
C52	0.163(16)	0.085(11)	0.172(17)	-0.024(11)	-0.067(13)	0.032(11)
C53	0.125(12)	0.054(8)	0.24(2)	0.013(10)	-0.039(13)	-0.002(8)

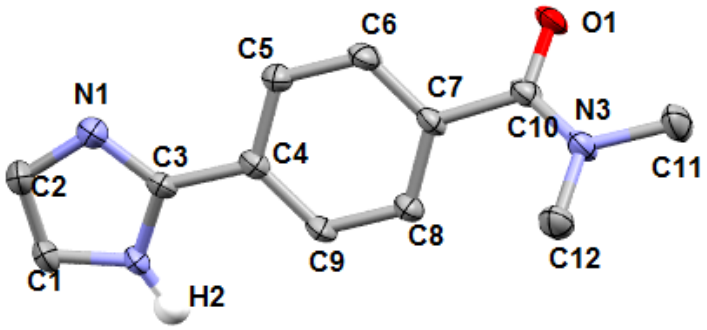
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
B1	0.015(2)	0.013(3)	0.022(3)	0.001(2)	0.008(2)	0.001(2)
B2	0.015(2)	0.014(3)	0.021(3)	-0.001(2)	0.007(2)	-0.001(2)
O5	0.099(6)	0.164(9)	0.105(7)	-0.013(6)	0.012(5)	0.006(5)
C54	0.188(12)	0.100(8)	0.224(16)	-0.103(11)	0.087(13)	-0.045(8)
C55	0.180(12)	0.098(8)	0.248(18)	0.023(12)	0.011(15)	0.072(9)
C56	0.097(8)	0.164(11)	0.32(2)	-0.137(14)	0.045(13)	-0.011(8)
C57	0.149(10)	0.056(6)	0.193(14)	0.029(8)	0.074(10)	0.018(6)
C58	0.038(4)	0.043(4)	0.041(4)	-0.006(3)	-0.001(3)	0.006(3)
C59	0.050(4)	0.043(4)	0.040(4)	-0.009(3)	0.006(3)	0.006(3)
C60	0.047(4)	0.039(4)	0.052(4)	0.002(3)	-0.001(3)	0.005(3)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 5534_1.

	x/a	y/b	z/c	U(eq)
H4A	0.3643	0.4790	0.3661	0.098
H4B	0.3967	0.5562	0.3708	0.098
H3	0.6580	0.4960	0.2411	0.025
H4	0.7940	0.4868	0.2038	0.034
H5	0.7937	0.4882	0.1031	0.037
H6	0.6599	0.4940	0.0379	0.034
H7	0.5224	0.5013	0.0739	0.023
H9	0.3015	0.3685	0.2446	0.021
H10	0.1897	0.4434	0.2791	0.024
H11	0.1954	0.5830	0.2785	0.024
H12	0.3127	0.6496	0.2441	0.02
H50A	0.6892	0.3799	0.3570	0.147
H50B	0.7415	0.3926	0.4224	0.147
H51A	0.7314	0.5826	0.4214	0.207
H51B	0.6780	0.5909	0.3559	0.207
H52A	0.8024	0.5584	0.3176	0.18
H52B	0.8584	0.5605	0.3833	0.18
H53A	0.8072	0.4232	0.3187	0.177
H53B	0.8634	0.4253	0.3842	0.177
H54A	0.2059	0.5893	0.4772	0.197
H54B	0.1972	0.5987	0.4078	0.197
H55A	0.0652	0.5931	0.4006	0.214

	x/a	y/b	z/c	U(eq)
H55B	0.0741	0.5815	0.4708	0.214
H56A	0.0451	0.4630	0.4584	0.229
H56B	0.0358	0.4746	0.3889	0.229
H57A	0.1489	0.4112	0.3878	0.153
H57B	0.1567	0.3975	0.4575	0.153
H58A	0.0440	0.5734	0.0139	0.05
H58B	0.0884	0.4992	-0.0135	0.05
H59A	0.0372	0.4973	0.1000	0.053
H59B	0.0875	0.4268	0.0726	0.053
H60A	0.2142	0.5090	0.0762	0.07
H60B	0.1888	0.4911	0.1397	0.07
H60C	0.1635	0.5748	0.1087	0.07

Crystal Structure Report for 4-(1H-imidazol-2-yl)-N,N-dimethylbenzamide



Thermal ellipsoid plot of 5916. Ellipsoids shown at 50% probability, solvent (DCM) and hydrogens other than imidazole N-H hidden for clarity.

A specimen of $C_{12.50}H_{14}ClN_3O$, approximate dimensions 0.038 mm x 0.310 mm x 0.317 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The integration of the data using an orthorhombic unit cell yielded a total of 22149 reflections to a maximum θ angle of 27.93° (0.76 Å resolution), of which 3076 were independent (average redundancy 7.201, completeness = 99.8%, R_{int} = 5.27%, R_{sig} = 4.20%) and 2354 (76.53%) were greater than $2\sigma(F^2)$. The final cell constants of a = 7.9951(13) Å, b = 14.758(2) Å, c = 21.725(4) Å, volume = 2563.4(7) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9140 and 0.9890. The final anisotropic full-matrix least-squares refinement on F^2 with 165 variables converged at R1 = 6.63%, for the observed data and wR2 = 14.69% for all data. The goodness-of-fit was 1.196. The largest peak in the final difference electron density synthesis was 0.292 $e^-/Å^3$ and the largest hole was -0.328 $e^-/Å^3$ with an RMS deviation of 0.062 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.336 g/cm^3 and F(000), 1080 e^-.

Table 1. Sample and crystal data for 5916.

Identification code	5916	
Chemical formula	$C_{12.50}H_{14}ClN_3O$	
Formula weight	257.72 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.038 x 0.310 x 0.317 mm	
Crystal system	orthorhombic	
Space group	P b c n	
Unit cell dimensions	a = 7.9951(13) Å	α = 90°
	b = 14.758(2) Å	β = 90°
	c = 21.725(4) Å	γ = 90°

Volume	2563.4(7) $Å^3$
Z	8
Density (calculated)	1.336 g/cm^3
Absorption coefficient	0.288 mm^{-1}
F(000)	1080

Table 2. Data collection and structure refinement for 5916.

Theta range for data collection	1.88 to 27.93°	
Index ranges	-10<=h<=9, -16<=k<=19, -27<=l<=28	
Reflections collected	22149	
Independent reflections	3076 [R(int) = 0.0527]	
Max. and min. transmission	0.9890 and 0.9140	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	3076 / 0 / 165	
Goodness-of-fit on F^2	1.196	
Δ/σ_{max}	0.001	
Final R indices	2354 data; I>2σ(I)	R1 = 0.0663, wR2 = 0.1396
	all data	R1 = 0.0884, wR2 = 0.1469
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0226P)^2+4.3563P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.292 and -0.328 $eÅ^{-3}$	
R.M.S. deviation from mean	0.062 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for 5916.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Cl1	0.68259(12)	0.80027(5)	0.74960(5)	0.0489(3)
O1	0.3204(3)	0.97655(11)	0.45502(9)	0.0318(5)
N2	0.3439(3)	0.50928(14)	0.56587(10)	0.0264(5)
N3	0.4439(3)	0.91368(14)	0.37228(10)	0.0262(5)
N1	0.4798(4)	0.58767(15)	0.63759(11)	0.0336(6)
C4	0.4131(3)	0.66978(16)	0.54135(12)	0.0214(5)
C10	0.3894(3)	0.91016(16)	0.43057(12)	0.0232(5)
C3	0.4153(4)	0.59011(16)	0.58155(12)	0.0229(5)
C8	0.3675(4)	0.74007(16)	0.44268(12)	0.0244(6)
C9	0.3714(4)	0.66357(16)	0.47966(12)	0.0255(6)
C7	0.4069(3)	0.82471(16)	0.46688(12)	0.0211(5)

	x/a	y/b	z/c	U(eq)
C6	0.4485(4)	0.83122(17)	0.52879(12)	0.0267(6)
C5	0.4529(4)	0.75487(17)	0.56544(12)	0.0257(6)
C12	0.5535(4)	0.84780(19)	0.34322(13)	0.0311(6)
C1	0.3648(4)	0.45233(18)	0.61494(13)	0.0347(7)
C2	0.4477(5)	0.5008(2)	0.65807(14)	0.0407(8)
C11	0.4058(4)	0.99339(19)	0.33482(14)	0.0369(7)
C13	0.5	0.7322(3)	0.75	0.0395(11)

Table 4. Bond lengths (Å) for 5916.

Cl1-C13	1.772(2)	O1-C10	1.244(3)
N2-C3	1.366(3)	N2-C1	1.368(3)
N3-C10	1.340(3)	N3-C12	1.454(3)
N3-C11	1.462(3)	N1-C3	1.323(3)
N1-C2	1.381(4)	C4-C9	1.384(4)
C4-C5	1.397(3)	C4-C3	1.465(3)
C10-C7	1.494(3)	C8-C9	1.386(3)
C8-C7	1.391(3)	C7-C6	1.389(4)
C6-C5	1.380(4)	C1-C2	1.352(4)
C13-Cl1	1.772(2)		

Table 5. Bond angles (°) for 5916.

C3-N2-C1	106.9(2)	C10-N3-C12	125.5(2)
C10-N3-C11	119.3(2)	C12-N3-C11	115.0(2)
C3-N1-C2	104.4(2)	C9-C4-C5	118.5(2)
C9-C4-C3	121.8(2)	C5-C4-C3	119.7(2)
O1-C10-N3	121.1(2)	O1-C10-C7	118.8(2)
N3-C10-C7	120.1(2)	N1-C3-N2	111.6(2)
N1-C3-C4	125.1(2)	N2-C3-C4	123.2(2)
C9-C8-C7	120.5(2)	C4-C9-C8	120.8(2)
C6-C7-C8	118.8(2)	C6-C7-C10	118.4(2)
C8-C7-C10	122.5(2)	C5-C6-C7	120.5(2)
C6-C5-C4	120.8(2)	C2-C1-N2	105.9(2)
C1-C2-N1	111.1(3)	Cl1-C13-Cl1	110.9(2)

Table 6. Anisotropic atomic displacement parameters (Å^2) for 5916.

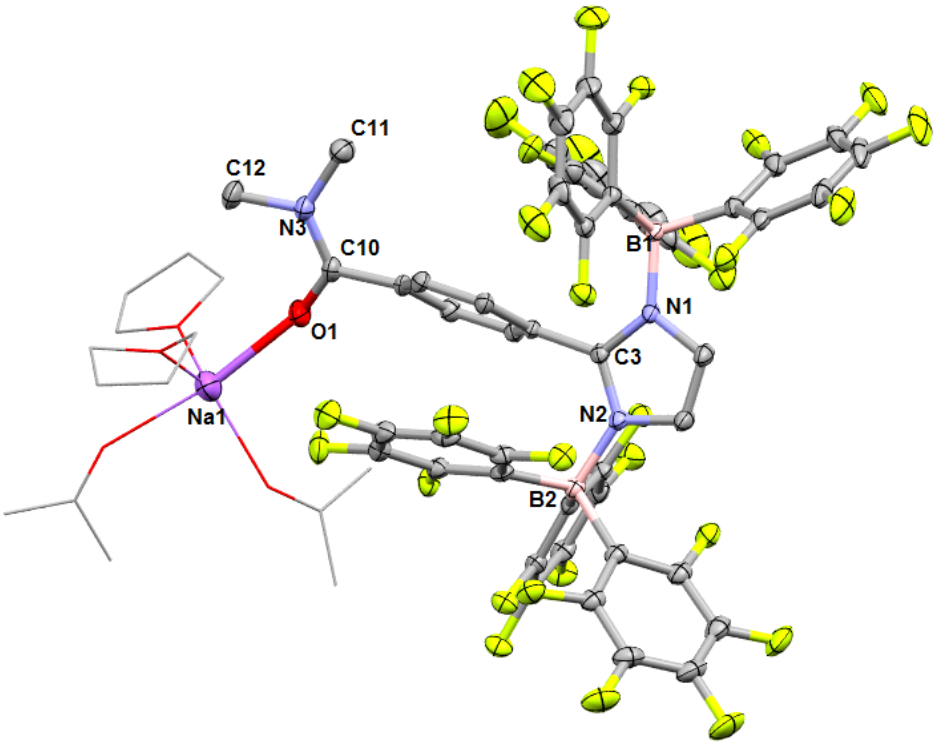
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	0.0587(5)	0.0327(4)	0.0553(5)	0.0045(4)	-0.0074(4)	0.0068(4)
O1	0.0535(14)	0.0123(8)	0.0295(10)	-0.0004(7)	0.0090(10)	0.0058(9)
N2	0.0446(15)	0.0125(9)	0.0221(11)	0.0020(8)	-0.0049(11)	-0.0004(10)
N3	0.0356(14)	0.0163(10)	0.0267(11)	0.0019(9)	0.0072(10)	0.0034(9)
N1	0.0558(17)	0.0209(11)	0.0242(12)	-0.0010(9)	-0.0057(11)	0.0036(12)
C4	0.0235(13)	0.0152(11)	0.0255(13)	-0.0006(10)	0.0009(10)	0.0002(10)
C10	0.0281(14)	0.0143(11)	0.0273(13)	-0.0003(10)	0.0039(11)	-0.0017(10)
C3	0.0318(15)	0.0134(11)	0.0237(13)	-0.0027(10)	-0.0007(11)	0.0021(11)
C8	0.0338(16)	0.0158(11)	0.0235(13)	-0.0004(10)	-0.0018(11)	-0.0031(11)
C9	0.0368(16)	0.0122(11)	0.0274(13)	-0.0013(10)	-0.0038(12)	-0.0030(11)
C7	0.0250(14)	0.0120(10)	0.0263(13)	0.0017(9)	0.0031(10)	0.0000(10)
C6	0.0386(17)	0.0142(11)	0.0274(14)	-0.0033(10)	0.0025(12)	-0.0046(11)
C5	0.0364(16)	0.0193(12)	0.0213(13)	-0.0020(10)	-0.0025(11)	-0.0024(11)
C12	0.0386(17)	0.0257(13)	0.0289(14)	-0.0005(11)	0.0073(13)	0.0066(12)
C1	0.062(2)	0.0160(12)	0.0264(14)	0.0042(10)	-0.0023(14)	0.0046(13)
C2	0.076(3)	0.0219(13)	0.0242(14)	0.0034(12)	-0.0076(15)	0.0071(15)
C11	0.059(2)	0.0222(13)	0.0297(15)	0.0080(12)	0.0105(15)	0.0056(14)
C13	0.075(3)	0.0157(16)	0.027(2)	0	-0.007(2)	0

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 5916.

	x/a	y/b	z/c	U(eq)
H8	0.3378	0.7347	0.4005	0.029
H9	0.3451	0.6061	0.4624	0.031
H6	0.4742	0.8887	0.5461	0.032
H5	0.4833	0.7602	0.6076	0.031
H12A	0.5956	0.8055	0.3744	0.047
H12B	0.6479	0.8793	0.3239	0.047
H12C	0.4911	0.8142	0.3118	0.047
H1	0.3286	0.3912	0.6181	0.042
H2A	0.4795	0.4781	0.6973	0.049
H11A	0.3196	1.0297	0.3553	0.055
H11B	0.3650	0.9740	0.2944	0.055
H11C	0.5072	1.0299	0.3297	0.055
H13A	0.5006	0.6928	0.7869	0.047
H13B	0.4994	0.6928	0.7131	0.047
H2	0.294(4)	0.495(2)	0.5300(15)	0.038(9)

Crystal Structure Report for Na[IMP-DMA]



Thermal ellipsoid plot of 5922. Ellipsoids shown at 50% probability, Na-bound THF and acetone molecules shown in wireframe, hydrogens and DCM molecule hidden for clarity.

A specimen of $C_{62.50}H_{41}B_2ClF_{30}N_3NaO_5$, approximate dimensions 0.124 mm x 0.317 mm x 0.385 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The integration of the data using a monoclinic unit cell yielded a total of 64223 reflections to a maximum θ angle of 27.96° (0.76 Å resolution), of which 15883 were independent (average redundancy 4.044, completeness = 99.7%, R_{int} = 2.99%, R_{sig} = 2.93%) and 12493 (78.66%) were greater than $2\sigma(F^2)$. The final cell constants of a = 13.3526(11) Å, b = 30.789(2) Å, c = 16.1477(13) Å, β = 93.240(2)°, volume = 6627.9(9) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9270 and 0.9760. The final anisotropic full-matrix least-squares refinement on F^2 with 961 variables converged at R1 = 8.15%, for the observed data and wR2 = 22.76% for all data. The goodness-of-fit was 1.114. The largest peak in the final difference electron density synthesis was 1.193 $e^-/Å^3$ and the largest hole was -0.866 $e^-/Å^3$ with an RMS deviation of 0.097 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.567 g/cm^3 and F(000), 3140 e^-.

Table 1. Sample and crystal data for 5922.

Identification code	5922
Chemical formula	$C_{62.50}H_{41}B_2ClF_{30}N_3NaO_5$
Formula weight	1564.04 g/mol
Temperature	100(2) K

Wavelength	0.71073 Å	
Crystal size	0.124 x 0.317 x 0.385 mm	
Crystal system	monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 13.3526(11) Å	α = 90°
	b = 30.789(2) Å	β = 93.240(2)°
	c = 16.1477(13) Å	γ = 90°
Volume	6627.9(9) $Å^3$	
Z	4	
Density (calculated)	1.567 g/cm^3	
Absorption coefficient	0.200 mm^{-1}	
F(000)	3140	

Table 2. Data collection and structure refinement for 5922.

Theta range for data collection	1.43 to 27.96°	
Index ranges	-17<=h<=17, -21<=k<=40, -21<=l<=21	
Reflections collected	64223	
Independent reflections	15883 [R(int) = 0.0299]	
Max. and min. transmission	0.9760 and 0.9270	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	15883 / 37 / 961	
Goodness-of-fit on F^2	1.114	
Final R indices	12493 data; I>2σ(I)	R1 = 0.0815, wR2 = 0.2159
	all data	R1 = 0.0999, wR2 = 0.2276
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0857P)^2+19.8698P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	1.193 and -0.866 $eÅ^{-3}$	
R.M.S. deviation from mean	0.097 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for 5922.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Na1	0.15925(13)	0.09181(5)	0.42573(12)	0.0415(4)
F30	0.47472(15)	0.31678(6)	0.28272(12)	0.0246(4)
F27	0.68753(15)	0.16807(6)	0.32773(12)	0.0259(4)
F26	0.63497(15)	0.21211(6)	0.45977(11)	0.0229(4)
F21	0.42693(15)	0.20212(6)	0.45371(12)	0.0249(4)

	x/a	y/b	z/c	U(eq)
F25	0.48012(16)	0.32603(7)	0.62349(13)	0.0274(4)
F20	0.63857(15)	0.26724(7)	0.63331(13)	0.0291(5)
F1	0.32179(16)	0.46867(7)	0.53215(13)	0.0291(5)
F11	0.04320(15)	0.44136(7)	0.39254(13)	0.0288(4)
F15	0.27875(15)	0.38238(6)	0.59132(13)	0.0267(4)
F29	0.52161(17)	0.27042(8)	0.15296(12)	0.0313(5)
F28	0.63062(16)	0.19642(7)	0.17131(12)	0.0299(5)
F16	0.67646(15)	0.33962(7)	0.37722(13)	0.0284(4)
F22	0.31118(18)	0.16888(7)	0.56413(15)	0.0364(5)
F24	0.36065(17)	0.29212(8)	0.73334(13)	0.0344(5)
F5	0.19081(18)	0.46486(7)	0.25263(14)	0.0353(5)
F10	0.05319(15)	0.35207(7)	0.38018(14)	0.0313(5)
F23	0.27419(17)	0.21316(8)	0.70566(14)	0.0378(5)
F6	0.34182(18)	0.40432(8)	0.25571(14)	0.0365(5)
F19	0.82543(17)	0.28515(9)	0.67748(14)	0.0386(6)
F14	0.1547(2)	0.39920(8)	0.70938(14)	0.0422(6)
F17	0.86150(17)	0.36062(9)	0.42764(17)	0.0437(6)
F4	0.2065(2)	0.54904(8)	0.24559(17)	0.0482(7)
F18	0.94057(17)	0.33343(9)	0.57872(18)	0.0462(6)
F2	0.3286(2)	0.55400(7)	0.52398(18)	0.0454(6)
F12	0.91939(18)	0.45750(9)	0.51246(17)	0.0444(6)
O1	0.1218(2)	0.16384(8)	0.39521(19)	0.0334(6)
F13	0.9731(2)	0.43594(10)	0.67259(17)	0.0543(8)
F3	0.2719(2)	0.59640(7)	0.3810(2)	0.0563(8)
F9	0.9918(2)	0.31527(10)	0.23978(19)	0.0591(8)
N1	0.34644(19)	0.38506(8)	0.43091(17)	0.0182(5)
N2	0.46708(19)	0.33617(8)	0.44959(17)	0.0186(5)
F7	0.2798(3)	0.36521(10)	0.11437(17)	0.0621(9)
O2	0.3304(2)	0.09596(10)	0.42051(19)	0.0395(7)
F8	0.0998(3)	0.32266(10)	0.10321(18)	0.0693(10)
N3	0.9865(2)	0.20459(9)	0.4212(2)	0.0259(6)
C3	0.3675(2)	0.34225(10)	0.43480(18)	0.0164(6)
C37	0.4617(2)	0.26584(10)	0.53281(19)	0.0180(6)
C44	0.6037(2)	0.22771(10)	0.38468(19)	0.0186(6)
C46	0.6037(2)	0.21820(11)	0.2384(2)	0.0219(6)
C4	0.2917(2)	0.30664(10)	0.42604(19)	0.0160(6)
C42	0.4151(2)	0.22599(10)	0.5224(2)	0.0195(6)
C13	0.1660(2)	0.40902(10)	0.4843(2)	0.0196(6)
C43	0.5470(2)	0.26563(10)	0.3795(2)	0.0180(6)
C48	0.5231(2)	0.27900(10)	0.2990(2)	0.0192(6)
C6	0.1579(2)	0.26524(10)	0.4832(2)	0.0186(6)

	x/a	y/b	z/c	U(eq)
C5	0.2274(2)	0.29867(10)	0.48988(19)	0.0178(6)
C7	0.1510(2)	0.23897(10)	0.4133(2)	0.0189(6)
C45	0.6323(2)	0.20417(10)	0.3171(2)	0.0198(6)
C38	0.4398(2)	0.28678(11)	0.6063(2)	0.0208(6)
C14	0.1895(3)	0.39973(10)	0.5667(2)	0.0226(7)
C47	0.5488(2)	0.25573(11)	0.2293(2)	0.0217(6)
C9	0.2831(2)	0.28077(10)	0.3552(2)	0.0191(6)
C10	0.0842(3)	0.19955(11)	0.4084(2)	0.0229(7)
C20	0.2931(2)	0.48670(11)	0.4588(2)	0.0245(7)
C35	0.6884(2)	0.29098(11)	0.5789(2)	0.0230(7)
C8	0.2142(2)	0.24683(10)	0.3491(2)	0.0204(6)
C41	0.3533(3)	0.20799(11)	0.5791(2)	0.0247(7)
C1	0.4362(2)	0.40655(11)	0.4427(2)	0.0233(7)
C31	0.7084(3)	0.32642(11)	0.4540(2)	0.0236(7)
C36	0.6431(2)	0.30395(10)	0.5033(2)	0.0206(6)
C40	0.3335(3)	0.23040(12)	0.6501(2)	0.0269(7)
C39	0.3778(3)	0.26988(12)	0.6637(2)	0.0247(7)
C2	0.5094(2)	0.37705(11)	0.4547(2)	0.0234(7)
C18	0.0726(3)	0.42884(11)	0.4702(2)	0.0242(7)
C15	0.1260(3)	0.40847(12)	0.6302(2)	0.0297(8)
C26	0.1108(3)	0.35813(11)	0.3161(2)	0.0273(7)
O3	0.1725(4)	0.01660(12)	0.4642(3)	0.0705(11)
C25	0.1986(3)	0.38230(10)	0.3244(2)	0.0219(6)
C34	0.7868(3)	0.30006(12)	0.6037(2)	0.0283(8)
C24	0.2302(3)	0.48417(11)	0.3221(2)	0.0269(7)
O5	0.0605(4)	0.06831(13)	0.3120(3)	0.0740(13)
C19	0.2600(2)	0.46064(10)	0.3923(2)	0.0223(6)
C30	0.2540(3)	0.38253(12)	0.2542(2)	0.0288(7)
C32	0.8059(3)	0.33738(12)	0.4780(3)	0.0299(8)
C33	0.8451(3)	0.32405(13)	0.5543(3)	0.0319(8)
C11	0.9347(3)	0.24593(12)	0.4242(3)	0.0313(8)
C22	0.2698(3)	0.55277(11)	0.3844(3)	0.0389(10)
C21	0.2985(3)	0.53158(12)	0.4560(3)	0.0327(9)
C17	0.0080(3)	0.43804(12)	0.5316(3)	0.0318(8)
C23	0.2364(3)	0.52904(12)	0.3166(3)	0.0345(9)
C16	0.0352(3)	0.42750(13)	0.6121(3)	0.0353(9)
C49	0.3957(3)	0.11215(13)	0.3811(3)	0.0342(8)
C27	0.0784(3)	0.33786(13)	0.2434(3)	0.0389(10)
B2	0.5280(3)	0.29201(11)	0.4663(2)	0.0167(6)
C29	0.2233(4)	0.36243(14)	0.1810(3)	0.0413(10)
C12	0.9224(3)	0.16632(13)	0.4265(3)	0.0349(9)

	x/a	y/b	z/c	U(eq)
C50	0.3710(4)	0.14142(13)	0.3099(3)	0.0411(10)
B1	0.2420(3)	0.40778(11)	0.4077(2)	0.0174(6)
C28	0.1336(4)	0.34063(15)	0.1748(3)	0.0461(11)
C51	0.5040(4)	0.10276(17)	0.4024(4)	0.0524(12)
O4	0.0829(6)	0.09872(16)	0.5501(4)	0.129(3)
C55	0.0256(6)	0.0972(2)	0.2465(4)	0.0710(18)
C58	0.0286(6)	0.0255(2)	0.2932(4)	0.0696(17)
C57	0.9841(7)	0.0254(3)	0.2069(5)	0.097(3)
C56	0.9703(7)	0.0719(2)	0.1875(5)	0.094(3)
C62	0.0812(7)	0.1365(3)	0.5991(5)	0.095(2)
C61	0.1290(7)	0.1197(3)	0.6759(6)	0.102(3)
C54	0.1970(10)	0.9508(2)	0.5358(6)	0.135(4)
C52	0.2240(8)	0.9863(2)	0.4795(6)	0.114(3)
Cl1	0.0907(11)	0.5694(4)	0.8723(6)	0.246(5)
C53	0.3268(9)	0.9839(4)	0.4531(7)	0.140(4)
C60	0.0870(8)	0.0791(4)	0.6889(8)	0.152(5)
Cl2	0.1461(10)	0.5131(4)	0.7532(10)	0.341(10)
C59	0.0332(12)	0.0673(4)	0.5967(7)	0.152(5)
C63	0.0908(17)	0.5669(9)	0.7793(14)	0.159(9)

Table 4. Bond lengths (Å) for 5922.

Na1-O2	2.295(4)	Na1-O4	2.313(5)
Na1-O5	2.316(4)	Na1-O1	2.320(3)
Na1-O3	2.402(4)	F30-C48	1.349(4)
F27-C45	1.339(4)	F26-C44	1.348(4)
F21-C42	1.348(4)	F25-C38	1.345(4)
F20-C35	1.347(4)	F1-C20	1.345(4)
F11-C18	1.348(4)	F15-C14	1.345(4)
F29-C47	1.344(4)	F28-C46	1.340(4)
F16-C31	1.351(4)	F22-C41	1.345(4)
F24-C39	1.348(4)	F5-C24	1.350(5)
F10-C26	1.337(4)	F23-C40	1.340(4)
F6-C30	1.350(5)	F19-C34	1.352(4)
F14-C15	1.344(4)	F17-C32	1.339(4)
F4-C23	1.342(5)	F18-C33	1.345(4)
F2-C21	1.339(5)	F12-C17	1.346(4)
O1-C10	1.232(4)	F13-C16	1.342(4)
F3-C22	1.345(4)	F9-C27	1.348(5)
N1-C3	1.348(4)	N1-C1	1.372(4)
N1-B1	1.586(4)	N2-C3	1.351(4)

N2-C2	1.380(4)	N2-B2	1.600(4)
F7-C29	1.350(5)	O2-C49	1.216(5)
F8-C28	1.338(5)	N3-C10	1.341(4)
N3-C11	1.451(5)	N3-C12	1.462(4)
C3-C4	1.493(4)	C37-C42	1.381(4)
C37-C38	1.396(4)	C37-B2	1.642(5)
C44-C45	1.383(4)	C44-C43	1.391(4)
C46-C47	1.372(5)	C46-C45	1.375(5)
C4-C9	1.393(4)	C4-C5	1.399(4)
C42-C41	1.383(5)	C13-C14	1.379(5)
C13-C18	1.396(5)	C13-B1	1.644(5)
C43-C48	1.385(4)	C43-B2	1.651(5)
C48-C47	1.393(5)	C6-C7	1.386(4)
C6-C5	1.387(4)	C7-C8	1.395(5)
C7-C10	1.505(4)	C38-C39	1.379(5)
C14-C15	1.394(5)	C9-C8	1.392(4)
C20-C21	1.384(5)	C20-C19	1.392(5)
C35-C34	1.380(5)	C35-C36	1.390(5)
C41-C40	1.376(5)	C1-C2	1.340(5)
C31-C32	1.380(5)	C31-C36	1.396(5)
C36-B2	1.658(5)	C40-C39	1.364(5)
C18-C17	1.381(5)	C15-C16	1.363(6)
C26-C27	1.379(5)	C26-C25	1.388(5)
O3-C52	1.178(8)	C25-C30	1.388(5)
C25-B1	1.635(5)	C34-C33	1.364(6)
C24-C19	1.384(5)	C24-C23	1.387(5)
O5-C58	1.414(7)	O5-C55	1.439(7)
C19-B1	1.666(5)	C30-C29	1.376(6)
C32-C33	1.372(6)	C22-C21	1.363(6)
C22-C23	1.370(7)	C17-C16	1.368(6)
C49-C50	1.483(6)	C49-C51	1.495(6)
C27-C28	1.367(7)	C29-C28	1.372(7)
O4-C62	1.408(9)	O4-C59	1.413(11)
C55-C56	1.408(9)	C58-C57	1.483(9)
C57-C56	1.475(11)	C62-C61	1.458(11)
C61-C60	1.391(14)	C54-C52	1.480(11)
C52-C53	1.462(12)	Cl1-C63	1.50(2)
C60-C59	1.656(17)	Cl2-C63	1.87(3)

Table 5. Bond angles (°) for 5922.

O2-Na1-O4	121.0(2)	O2-Na1-O5	120.77(17)

O4-Na1-O5	117.3(3)	O2-Na1-O1	98.17(12)
O4-Na1-O1	89.78(17)	O5-Na1-O1	91.37(13)
O2-Na1-O3	90.25(15)	O4-Na1-O3	83.89(18)
O5-Na1-O3	86.24(16)	O1-Na1-O3	171.28(16)
C10-O1-Na1	154.3(3)	C3-N1-C1	106.7(3)
C3-N1-B1	128.3(3)	C1-N1-B1	124.7(3)
C3-N2-C2	106.2(3)	C3-N2-B2	129.3(3)
C2-N2-B2	124.2(3)	C49-O2-Na1	142.0(3)
C10-N3-C11	125.2(3)	C10-N3-C12	119.6(3)
C11-N3-C12	115.0(3)	N1-C3-N2	110.1(3)
N1-C3-C4	125.1(3)	N2-C3-C4	124.8(3)
C42-C37-C38	113.5(3)	C42-C37-B2	127.8(3)
C38-C37-B2	118.4(3)	F26-C44-C45	116.0(3)
F26-C44-C43	119.5(3)	C45-C44-C43	124.5(3)
F28-C46-C47	120.1(3)	F28-C46-C45	121.1(3)
C47-C46-C45	118.8(3)	C9-C4-C5	118.6(3)
C9-C4-C3	121.4(3)	C5-C4-C3	120.0(3)
F21-C42-C37	120.8(3)	F21-C42-C41	115.4(3)
C37-C42-C41	123.9(3)	C14-C13-C18	113.7(3)
C14-C13-B1	127.2(3)	C18-C13-B1	118.1(3)
C48-C43-C44	113.7(3)	C48-C43-B2	127.8(3)
C44-C43-B2	118.1(3)	F30-C48-C43	121.5(3)
F30-C48-C47	115.0(3)	C43-C48-C47	123.5(3)
C7-C6-C5	120.7(3)	C6-C5-C4	120.5(3)
C6-C7-C8	119.2(3)	C6-C7-C10	121.7(3)
C8-C7-C10	118.8(3)	F27-C45-C46	120.1(3)
F27-C45-C44	120.5(3)	C46-C45-C44	119.3(3)
F25-C38-C39	116.7(3)	F25-C38-C37	119.4(3)
C39-C38-C37	124.0(3)	F15-C14-C13	121.1(3)
F15-C14-C15	115.1(3)	C13-C14-C15	123.7(3)
F29-C47-C46	119.7(3)	F29-C47-C48	120.1(3)
C46-C47-C48	120.1(3)	C8-C9-C4	120.7(3)
O1-C10-N3	122.6(3)	O1-C10-C7	118.9(3)
N3-C10-C7	118.5(3)	F1-C20-C21	115.3(3)
F1-C20-C19	120.2(3)	C21-C20-C19	124.4(4)
F20-C35-C34	114.7(3)	F20-C35-C36	121.5(3)
C34-C35-C36	123.8(3)	C9-C8-C7	120.2(3)
F22-C41-C40	120.1(3)	F22-C41-C42	119.9(3)
C40-C41-C42	120.0(3)	C2-C1-N1	108.5(3)
F16-C31-C32	115.3(3)	F16-C31-C36	119.8(3)
C32-C31-C36	124.8(3)	C35-C36-C31	112.9(3)
C35-C36-B2	126.9(3)	C31-C36-B2	120.0(3)

F23-C40-C39	120.8(3)	F23-C40-C41	120.5(3)
C39-C40-C41	118.6(3)	F24-C39-C40	119.6(3)
F24-C39-C38	120.4(3)	C40-C39-C38	120.0(3)
C1-C2-N2	108.5(3)	F11-C18-C17	116.6(3)
F11-C18-C13	119.2(3)	C17-C18-C13	124.1(3)
F14-C15-C16	119.9(3)	F14-C15-C14	120.4(3)
C16-C15-C14	119.7(3)	F10-C26-C27	115.4(3)
F10-C26-C25	121.4(3)	C27-C26-C25	123.2(4)
C52-O3-Na1	148.5(6)	C26-C25-C30	114.2(3)
C26-C25-B1	126.4(3)	C30-C25-B1	119.3(3)
F19-C34-C33	119.8(3)	F19-C34-C35	119.8(4)
C33-C34-C35	120.3(4)	F5-C24-C19	122.0(3)
F5-C24-C23	114.0(3)	C19-C24-C23	124.0(4)
C58-O5-C55	109.7(5)	C58-O5-Na1	127.8(3)
C55-O5-Na1	122.4(4)	C24-C19-C20	113.2(3)
C24-C19-B1	126.6(3)	C20-C19-B1	119.3(3)
F6-C30-C29	117.1(4)	F6-C30-C25	119.3(3)
C29-C30-C25	123.6(4)	F17-C32-C33	120.6(3)
F17-C32-C31	120.5(4)	C33-C32-C31	119.0(3)
F18-C33-C34	120.5(4)	F18-C33-C32	120.4(4)
C34-C33-C32	119.1(3)	F3-C22-C21	120.5(4)
F3-C22-C23	120.4(4)	C21-C22-C23	119.1(3)
F2-C21-C22	120.4(3)	F2-C21-C20	120.1(4)
C22-C21-C20	119.5(4)	F12-C17-C16	120.4(3)
F12-C17-C18	120.2(4)	C16-C17-C18	119.4(3)
F4-C23-C22	120.4(3)	F4-C23-C24	119.7(4)
C22-C23-C24	119.8(4)	F13-C16-C15	120.3(4)
F13-C16-C17	120.3(4)	C15-C16-C17	119.4(3)
O2-C49-C50	121.3(4)	O2-C49-C51	120.9(4)
C50-C49-C51	117.8(4)	F9-C27-C28	119.9(4)
F9-C27-C26	119.9(4)	C28-C27-C26	120.3(4)
N2-B2-C37	103.8(2)	N2-B2-C43	112.1(3)
C37-B2-C43	115.3(3)	N2-B2-C36	108.9(2)
C37-B2-C36	113.4(3)	C43-B2-C36	103.4(2)
F7-C29-C28	119.9(4)	F7-C29-C30	120.2(4)
C28-C29-C30	119.9(4)	N1-B1-C25	104.4(2)
N1-B1-C13	113.9(3)	C25-B1-C13	115.2(3)
N1-B1-C19	109.5(2)	C25-B1-C19	113.1(3)
C13-B1-C19	101.0(2)	F8-C28-C27	120.2(5)
F8-C28-C29	121.0(5)	C27-C28-C29	118.8(4)
C62-O4-C59	104.1(7)	C62-O4-Na1	125.9(5)
C59-O4-Na1	130.0(6)	C56-C55-O5	106.9(5)

O5-C58-C57	107.7(5)	C56-C57-C58	103.7(6)
C55-C56-C57	109.8(6)	O4-C62-C61	99.4(8)
C60-C61-C62	106.7(9)	O3-C52-C53	121.8(9)
O3-C52-C54	123.6(10)	C53-C52-C54	114.0(8)
C61-C60-C59	102.6(8)	O4-C59-C60	97.9(9)
Cl1-C63-Cl2	107.0(14)		

Table 6. Anisotropic atomic displacement parameters (Å^2) for 5922.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Na1	0.0393(9)	0.0259(8)	0.0589(11)	0.0027(7)	0.0004(8)	0.0003(7)
F30	0.0246(10)	0.0230(10)	0.0270(10)	0.0051(8)	0.0077(8)	0.0067(8)
F27	0.0274(10)	0.0226(10)	0.0282(10)	-0.0045(8)	0.0046(8)	0.0075(8)
F26	0.0267(10)	0.0229(9)	0.0190(9)	-0.0013(7)	0.0015(7)	0.0050(8)
F21	0.0301(10)	0.0199(9)	0.0256(10)	-0.0058(8)	0.0083(8)	-0.0047(8)
F25	0.0282(10)	0.0263(10)	0.0282(10)	-0.0109(8)	0.0058(8)	-0.0011(8)
F20	0.0229(10)	0.0387(12)	0.0255(10)	-0.0002(9)	-0.0009(8)	-0.0002(9)
F1	0.0286(11)	0.0238(10)	0.0350(11)	-0.0077(8)	0.0023(9)	-0.0041(8)
F11	0.0233(10)	0.0306(11)	0.0328(11)	0.0071(9)	0.0043(8)	0.0054(8)
F15	0.0285(11)	0.0236(10)	0.0276(10)	-0.0010(8)	-0.0012(8)	0.0020(8)
F29	0.0341(11)	0.0411(12)	0.0190(10)	0.0053(9)	0.0047(8)	0.0075(10)
F28	0.0339(11)	0.0358(12)	0.0208(10)	-0.0077(8)	0.0080(8)	0.0069(9)
F16	0.0224(10)	0.0306(11)	0.0331(11)	0.0028(9)	0.0088(8)	-0.0017(8)
F22	0.0395(13)	0.0248(11)	0.0462(13)	0.0029(10)	0.0142(10)	-0.0111(9)
F24	0.0364(12)	0.0464(13)	0.0215(10)	-0.0080(9)	0.0110(9)	0.0070(10)
F5	0.0464(14)	0.0270(11)	0.0327(12)	0.0074(9)	0.0040(10)	0.0057(10)
F10	0.0229(10)	0.0316(11)	0.0393(12)	0.0015(9)	0.0020(9)	-0.0093(9)
F23	0.0322(12)	0.0464(14)	0.0367(12)	0.0124(10)	0.0196(10)	0.0031(10)
F6	0.0391(13)	0.0348(12)	0.0376(12)	0.0022(10)	0.0194(10)	0.0026(10)
F19	0.0255(11)	0.0543(15)	0.0349(12)	-0.0109(11)	-0.0069(9)	0.0044(10)
F14	0.0639(17)	0.0378(13)	0.0262(11)	0.0066(10)	0.0138(11)	0.0125(12)
F17	0.0224(11)	0.0477(14)	0.0623(16)	0.0015(12)	0.0140(11)	-0.0113(10)
F4	0.0597(17)	0.0281(12)	0.0592(16)	0.0213(11)	0.0245(13)	0.0157(11)
F18	0.0172(11)	0.0570(16)	0.0639(17)	-0.0133(13)	-0.0021(10)	-0.0090(10)
F2	0.0464(14)	0.0221(11)	0.0691(17)	-0.0208(11)	0.0164(12)	-0.0117(10)
F12	0.0282(12)	0.0497(15)	0.0572(16)	0.0120(12)	0.0198(11)	0.0166(11)
O1	0.0292(13)	0.0158(12)	0.0554(17)	-0.0023(11)	0.0053(12)	-0.0020(10)
F13	0.0584(17)	0.0598(17)	0.0489(15)	0.0147(13)	0.0396(13)	0.0222(14)
F3	0.0677(19)	0.0120(10)	0.093(2)	0.0019(12)	0.0346(17)	0.0027(11)
F9	0.0610(18)	0.0508(17)	0.0625(18)	-0.0086(14)	-0.0226(15)	-0.0249(14)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	0.0154(12)	0.0138(12)	0.0260(13)	-0.0024(10)	0.0067(10)	-0.0016(10)
N2	0.0149(12)	0.0155(12)	0.0257(13)	-0.0023(10)	0.0047(10)	-0.0005(10)
F7	0.098(2)	0.0589(18)	0.0325(14)	-0.0084(12)	0.0264(15)	0.0052(17)
O2	0.0429(17)	0.0335(15)	0.0427(16)	-0.0005(12)	0.0080(13)	-0.0007(13)
F8	0.114(3)	0.0555(18)	0.0360(15)	-0.0209(13)	-0.0144(16)	-0.0078(18)
N3	0.0219(14)	0.0192(14)	0.0367(16)	0.0004(12)	0.0031(12)	-0.0053(11)
C3	0.0164(14)	0.0151(14)	0.0182(14)	-0.0005(11)	0.0055(11)	0.0002(11)
C37	0.0141(14)	0.0219(15)	0.0181(14)	-0.0013(12)	0.0026(11)	0.0019(11)
C44	0.0177(14)	0.0191(15)	0.0190(14)	-0.0008(11)	0.0011(11)	-0.0011(11)
C46	0.0199(15)	0.0265(16)	0.0200(15)	-0.0072(12)	0.0074(12)	-0.0013(12)
C4	0.0137(13)	0.0133(13)	0.0211(14)	0.0003(11)	0.0030(11)	-0.0005(11)
C42	0.0180(14)	0.0207(15)	0.0202(15)	-0.0014(12)	0.0034(11)	0.0008(12)
C13	0.0195(15)	0.0145(14)	0.0254(16)	-0.0004(12)	0.0063(12)	-0.0016(11)
C43	0.0143(13)	0.0178(14)	0.0224(15)	-0.0011(11)	0.0053(11)	-0.0029(11)
C48	0.0147(14)	0.0199(15)	0.0237(15)	0.0011(12)	0.0057(11)	0.0008(11)
C6	0.0163(14)	0.0189(14)	0.0209(15)	0.0022(12)	0.0045(11)	-0.0019(11)
C5	0.0171(14)	0.0178(14)	0.0186(14)	0.0007(11)	0.0026(11)	-0.0018(11)
C7	0.0159(14)	0.0145(14)	0.0260(16)	0.0017(12)	-0.0002(12)	-0.0019(11)
C45	0.0168(14)	0.0187(15)	0.0243(15)	-0.0019(12)	0.0037(12)	0.0013(11)
C38	0.0180(15)	0.0239(16)	0.0208(15)	-0.0045(12)	0.0033(12)	0.0033(12)
C14	0.0248(16)	0.0149(14)	0.0286(17)	0.0003(12)	0.0058(13)	-0.0010(12)
C47	0.0185(15)	0.0294(17)	0.0175(14)	0.0029(13)	0.0053(11)	-0.0013(13)
C9	0.0185(14)	0.0181(14)	0.0211(15)	-0.0001(12)	0.0052(11)	0.0003(12)
C10	0.0222(16)	0.0186(15)	0.0279(16)	0.0000(13)	0.0013(13)	-0.0046(12)
C20	0.0168(15)	0.0187(15)	0.0391(19)	-0.0025(14)	0.0112(13)	-0.0013(12)
C35	0.0196(15)	0.0222(16)	0.0275(17)	-0.0075(13)	0.0034(12)	0.0016(12)
C8	0.0212(15)	0.0166(14)	0.0234(15)	-0.0029(12)	0.0019(12)	-0.0009(12)
C41	0.0208(16)	0.0230(16)	0.0305(17)	0.0045(13)	0.0041(13)	-0.0005(13)
C1	0.0181(15)	0.0154(14)	0.0370(18)	-0.0039(13)	0.0067(13)	-0.0026(12)
C31	0.0201(16)	0.0216(16)	0.0296(17)	-0.0062(13)	0.0055(13)	0.0012(12)
C36	0.0161(14)	0.0186(15)	0.0275(16)	-0.0066(12)	0.0045(12)	0.0003(12)
C40	0.0211(16)	0.0344(19)	0.0259(17)	0.0091(14)	0.0080(13)	0.0050(14)
C39	0.0220(16)	0.0339(18)	0.0186(15)	-0.0017(13)	0.0055(12)	0.0082(14)
C2	0.0160(15)	0.0181(15)	0.0366(18)	-0.0042(13)	0.0056(13)	-0.0032(12)
C18	0.0210(16)	0.0232(16)	0.0291(17)	0.0034(13)	0.0075(13)	0.0006(13)
C15	0.041(2)	0.0241(17)	0.0251(17)	0.0061(14)	0.0142(15)	0.0030(15)
C26	0.0289(18)	0.0200(16)	0.0323(18)	-0.0004(14)	-0.0041(14)	-0.0004(13)
O3	0.089(3)	0.041(2)	0.081(3)	0.0151(19)	0.000(2)	0.008(2)
C25	0.0258(16)	0.0160(14)	0.0238(16)	0.0003(12)	0.0003(13)	0.0041(12)
C34	0.0209(16)	0.0306(18)	0.0327(18)	-0.0112(15)	-0.0039(14)	0.0062(14)
C24	0.0243(17)	0.0201(16)	0.0373(19)	0.0040(14)	0.0106(14)	0.0024(13)

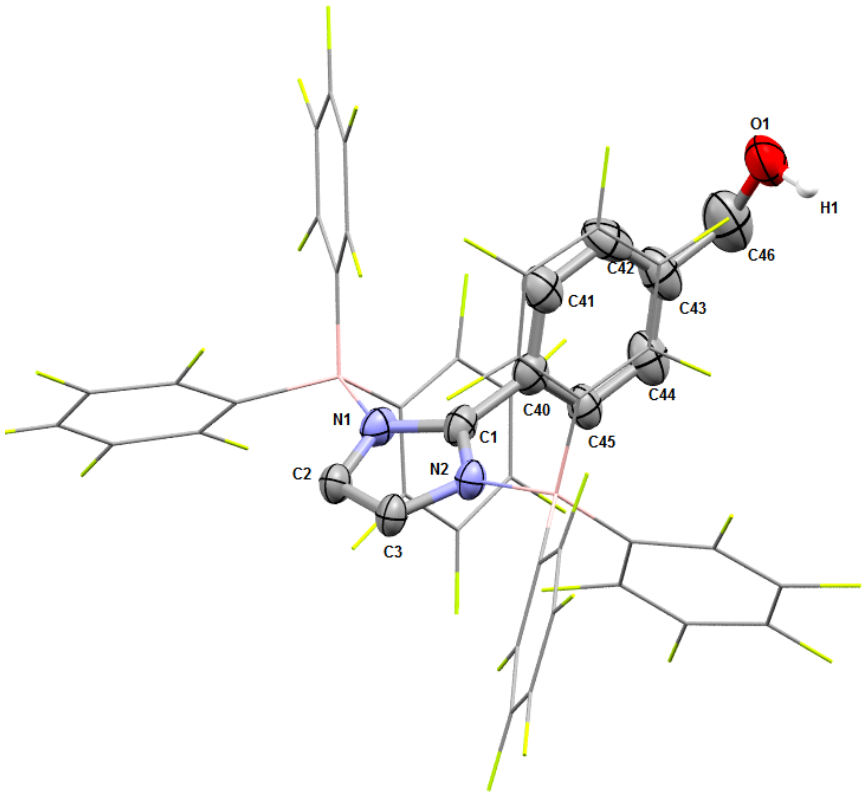
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O5	0.092(3)	0.046(2)	0.079(3)	0.0107(19)	-0.038(2)	-0.008(2)
C19	0.0177(15)	0.0157(14)	0.0343(18)	-0.0002(13)	0.0094(13)	0.0000(12)
C30	0.0352(19)	0.0211(16)	0.0309(18)	0.0008(14)	0.0077(15)	0.0047(14)
C32	0.0190(16)	0.0264(17)	0.045(2)	-0.0076(15)	0.0104(15)	-0.0016(13)
C33	0.0156(16)	0.0332(19)	0.047(2)	-0.0159(17)	0.0007(15)	-0.0002(14)
C11	0.0236(17)	0.0240(17)	0.046(2)	-0.0045(16)	0.0023(15)	0.0000(14)
C22	0.037(2)	0.0126(16)	0.070(3)	0.0027(17)	0.029(2)	0.0025(14)
C21	0.0262(18)	0.0193(17)	0.054(2)	-0.0095(16)	0.0171(17)	-0.0050(14)
C17	0.0241(17)	0.0279(18)	0.045(2)	0.0066(16)	0.0166(16)	0.0072(14)
C23	0.036(2)	0.0197(17)	0.050(2)	0.0112(16)	0.0219(18)	0.0097(15)
C16	0.039(2)	0.034(2)	0.035(2)	0.0078(16)	0.0247(17)	0.0065(17)
C49	0.041(2)	0.0252(18)	0.037(2)	-0.0055(15)	0.0053(17)	0.0007(16)
C27	0.046(2)	0.0254(19)	0.044(2)	-0.0044(16)	-0.0117(19)	-0.0078(17)
B2	0.0166(15)	0.0167(16)	0.0172(15)	-0.0033(12)	0.0035(12)	-0.0002(12)
C29	0.063(3)	0.035(2)	0.0265(19)	-0.0023(16)	0.0105(19)	0.010(2)
C12	0.0250(18)	0.0270(18)	0.053(2)	0.0003(17)	0.0059(16)	-0.0104(15)
C50	0.058(3)	0.0274(19)	0.038(2)	-0.0039(17)	0.0020(19)	-0.0052(18)
B1	0.0140(15)	0.0154(15)	0.0232(17)	0.0004(13)	0.0047(12)	-0.0006(12)
C28	0.073(3)	0.033(2)	0.031(2)	-0.0097(17)	-0.008(2)	0.001(2)
C51	0.040(3)	0.044(3)	0.074(3)	0.010(2)	0.013(2)	0.007(2)
O4	0.238(8)	0.047(3)	0.113(4)	-0.009(3)	0.102(5)	-0.030(4)
C55	0.101(5)	0.057(3)	0.054(3)	0.007(3)	-0.006(3)	0.024(3)
C58	0.087(5)	0.059(3)	0.062(4)	0.008(3)	-0.003(3)	-0.017(3)
C57	0.106(6)	0.093(5)	0.087(5)	0.015(4)	-0.039(5)	-0.035(5)
C56	0.115(6)	0.070(4)	0.091(5)	0.012(4)	-0.049(5)	0.006(4)
C62	0.090(6)	0.095(6)	0.097(6)	-0.019(5)	-0.009(4)	0.003(5)
C61	0.107(7)	0.101(6)	0.100(6)	0.020(5)	0.026(5)	0.019(5)
C54	0.245(12)	0.051(4)	0.108(7)	0.014(4)	-0.004(7)	0.032(6)
C52	0.165(8)	0.045(4)	0.129(7)	-0.002(4)	-0.024(6)	0.037(5)
Cl1	0.343(15)	0.232(10)	0.159(7)	0.015(7)	-0.031(8)	-0.057(10)
C53	0.169(8)	0.147(9)	0.105(7)	-0.018(6)	0.007(6)	0.080(8)
C60	0.091(7)	0.192(12)	0.172(11)	0.125(10)	0.009(7)	-0.007(7)
Cl2	0.279(13)	0.259(12)	0.46(2)	-0.193(14)	-0.215(14)	0.095(10)
C59	0.229(15)	0.100(7)	0.130(9)	0.027(7)	0.031(10)	-0.033(9)
C63	0.139(17)	0.194(18)	0.131(10)	-0.002(13)	-0.100(12)	0.059(15)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 5922.

	x/a	y/b	z/c	U(eq)
H6	0.1145	0.2603	0.5268	0.022

	x/a	y/b	z/c	U(eq)
H5	0.2315	0.3163	0.5382	0.021
H9	0.3248	0.2863	0.3106	0.023
H8	0.2103	0.2290	0.3010	0.024
H1	0.4449	0.4372	0.4425	0.028
H2	0.5787	0.3832	0.4650	0.028
H11A	-0.0881	0.2506	0.4801	0.047
H11B	-0.1233	0.2457	0.3842	0.047
H11C	-0.0195	0.2694	0.4103	0.047
H12A	-0.1164	0.1623	0.3737	0.052
H12B	-0.1236	0.1704	0.4710	0.052
H12C	-0.0359	0.1406	0.4383	0.052
H50A	0.3877	0.1271	0.2583	0.062
H50B	0.4097	0.1683	0.3168	0.062
H50C	0.2991	0.1482	0.3076	0.062
H51A	0.5367	0.1289	0.4257	0.079
H51B	0.5367	0.0940	0.3523	0.079
H51C	0.5095	0.0792	0.4433	0.079
H55A	-0.0173	0.1202	0.2686	0.085
H55B	0.0831	0.1112	0.2209	0.085
H58A	-0.0218	0.0161	0.3321	0.084
H58B	0.0863	0.0053	0.2983	0.084
H57A	0.0300	0.0116	0.1686	0.116
H57B	-0.0808	0.0098	0.2033	0.116
H56A	-0.0069	0.0780	0.1314	0.113
H56B	-0.1018	0.0794	0.1880	0.113
H62A	0.0119	0.1466	0.6067	0.114
H62B	0.1205	0.1604	0.5757	0.114
H61A	0.2023	0.1171	0.6710	0.123
H61B	0.1166	0.1394	0.7227	0.123
H54A	0.1903	-0.0376	0.5917	0.203
H54B	0.2496	-0.0715	0.5375	0.203
H54C	0.1332	-0.0622	0.5155	0.203
H53A	0.3363	0.0056	0.4099	0.21
H53B	0.3392	-0.0452	0.4309	0.21
H53C	0.3739	-0.0105	0.5006	0.21
H60A	0.0369	0.0804	0.7317	0.182
H60B	0.1391	0.0575	0.7057	0.182
H59A	0.0481	0.0373	0.5791	0.183
H59B	-0.0403	0.0720	0.5946	0.183
H63A	0.1315	0.5909	0.7577	0.191
H63B	0.0216	0.5694	0.7545	0.191

Crystal Structure Report for Na[IMP-CH_2OH]



Thermal ellipsoid plot of 5636. Ellipsoids shown at 50% probability, $B(C_6F_5)_3$ substituents shown in wireframe, sodium cation, THF molecules, and hydrogen atoms (except for O*H*) hidden for clarity.

A specimen of $C_{68}H_{53}B_2F_{30}N_2NaO_{6.50}$, approximate dimensions 0.287 mm x 0.296 mm x 0.328 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å). The total exposure time was 24.03 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 32050 reflections to a maximum θ angle of28.06° (0.76 Å resolution), of which 14919 were independent (average redundancy 2.148, completeness = 92.7%, R_{int} =3.55%, R_{sig} = 7.10%) and 7041 (47.19%) were greater than $2\sigma(F^2)$. The final cell constants of a = 12.7032(13) Å, b =13.4507(13) Å, c = 20.407(2) Å, α = 91.293(2)°, β = 91.963(2)°, γ = 107.760(2)°, volume = 3316.8(6) $Å^3$, are based upon the refinement of the XYZ-centroids of 5406 reflections above 20 σ(I) with 5.021° < 2θ < 48.82°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.912. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6799 and 0.7456. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P -1, with Z = 2 for the formula unit, $C_{68}H_{53}B_2F_{30}N_2NaO_{6.50}$. The final anisotropic full-matrix least-squares

refinement on F^2 with 1012 variables converged at R1 = 10.31%, for the observed data and wR2 = 36.39% for all data. The goodness-of-fit was 1.035. The largest peak in the final difference electron density synthesis was 0.823 $e^-/Å^3$ and the largest hole was -1.135 $e^-/Å^3$ with an RMS deviation of 0.100 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.619 g/cm^3 and F(000), 1636 e^-.

Table 1. Sample and crystal data for 5636.

Identification code	5636	
Chemical formula	$C_{68}H_{53}B_2F_{30}N_2NaO_{6.50}$	
Formula weight	1616.73 g/mol	
Wavelength	0.71073 Å	
Crystal size	0.287 x 0.296 x 0.328 mm	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 12.7032(13) Å	α = 91.293(2)°
	b = 13.4507(13) Å	β = 91.963(2)°
	c = 20.407(2) Å	γ = 107.760(2)°
Volume	3316.8(6) $Å^3$	
Z	2	
Density (calculated)	1.619 g/cm^3	
Absorption coefficient	0.165 mm^{-1}	
F(000)	1636	

Table 2. Data collection and structure refinement for 5636.

Theta range for data collection	1.00 to 28.06°
Index ranges	-16<=h<=15, -9<=k<=17, -26<=l<=26
Reflections collected	32050
Independent reflections	14919 [R(int) = 0.0355]
Coverage of independent reflections	92.7%
Absorption correction	Multi-Scan
Max. and min. transmission	0.7456 and 0.6799
Structure solution technique	direct methods
Structure solution program	SHELXT 2014/5 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	XL (Sheldrick, 2008)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	14919 / 176 / 1012

Goodness-of-fit on F^2	1.035	
Final R indices	7041 data; I>2σ(I)	R1 = 0.1031, wR2 = 0.2907
	all data	R1 = 0.1930, wR2 = 0.3639
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.1925P)^2+4.6573P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.823 and -1.135 eÅ^{-3}	
R.M.S. deviation from mean	0.100 eÅ^{-3}	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 5636.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij}tensor.

	x/a	y/b	z/c	U(eq)
F26	0.6053(2)	0.1604(2)	0.47901(13)	0.0421(7)
F20	0.5985(2)	0.3012(2)	0.39208(14)	0.0436(7)
F25	0.7749(3)	0.9638(2)	0.36928(14)	0.0443(7)
F30	0.6451(2)	0.0129(2)	0.27297(13)	0.0423(7)
F16	0.9769(2)	0.3227(3)	0.40447(15)	0.0483(8)
F27	0.3933(2)	0.0493(3)	0.47478(14)	0.0483(8)
F1	0.1108(3)	0.3268(3)	0.17165(15)	0.0538(9)
F21	0.8649(3)	0.2553(3)	0.51845(15)	0.0540(9)
F6	0.7846(3)	0.0346(3)	0.12729(15)	0.0541(9)
F5	0.8535(3)	0.1267(3)	0.00945(14)	0.0589(9)
F15	0.9862(3)	0.4221(3)	0.24638(17)	0.0580(9)
F24	0.8385(3)	0.8557(3)	0.46063(18)	0.0648(10)
F29	0.4365(3)	0.9018(3)	0.27048(16)	0.0640(10)
F19	0.6535(3)	0.5028(3)	0.41970(18)	0.0635(10)
F4	0.0163(3)	0.0952(3)	0.94581(16)	0.0655(10)
F22	0.9301(3)	0.1449(4)	0.60667(16)	0.0731(12)
F28	0.3051(3)	0.9155(3)	0.37096(18)	0.0674(11)
F10	0.6838(3)	0.3398(4)	0.09333(18)	0.0708(11)
F11	0.8627(3)	0.3700(3)	0.02474(17)	0.0685(11)
F23	0.9186(3)	0.9448(4)	0.58073(18)	0.0754(13)
F17	0.0303(3)	0.5271(3)	0.42747(19)	0.0673(11)
F2	0.2723(3)	0.2981(4)	0.1036(2)	0.0780(12)
N2	0.8248(3)	0.1790(3)	0.31274(18)	0.0322(9)
F18	0.8680(4)	0.6206(3)	0.4374(2)	0.0792(12)
F7	0.5791(4)	0.9202(4)	0.0920(2)	0.0847(14)

	x/a	y/b	z/c	U(eq)
F3	0.2287(4)	0.1810(4)	0.99010(19)	0.0822(13)
N1	0.8743(3)	0.2172(3)	0.21184(18)	0.0356(10)
F14	0.0382(4)	0.6262(3)	0.2339(2)	0.0921(15)
F12	0.9105(5)	0.5754(4)	0.0137(2)	0.0961(16)
O1	0.4636(4)	0.4998(4)	0.2621(2)	0.0662(13)
F8	0.4250(4)	0.0123(5)	0.0564(2)	0.1013(18)
F9	0.4835(4)	0.2247(5)	0.05616(19)	0.0916(16)
O6	0.3342(4)	0.4181(5)	0.3594(3)	0.0895(11)
F13	0.9990(6)	0.7067(4)	0.1185(3)	0.120(2)
C1	0.8031(4)	0.2242(4)	0.2576(2)	0.0359(11)
C36	0.7077(4)	0.3509(4)	0.4046(2)	0.0393(12)
C40	0.7133(4)	0.2724(4)	0.2497(2)	0.0390(12)
C3	0.9133(4)	0.1439(4)	0.3007(2)	0.0359(11)
C28	0.8207(4)	0.1177(5)	0.4368(2)	0.0383(12)
C26	0.5656(4)	0.1003(4)	0.4249(2)	0.0360(11)
C27	0.6354(4)	0.1011(4)	0.3740(2)	0.0345(11)
C35	0.7847(4)	0.2992(4)	0.3997(2)	0.0368(12)
C34	0.8933(4)	0.3642(5)	0.4077(2)	0.0422(13)
C2	0.9423(4)	0.1661(4)	0.2390(2)	0.0367(11)
C45	0.6064(4)	0.2141(5)	0.2311(2)	0.0411(12)
C22	0.5866(4)	0.0280(4)	0.3237(2)	0.0400(12)
O5	0.4582(5)	0.7047(5)	0.3329(3)	0.0830(16)
C30	0.8461(4)	0.9543(5)	0.4740(3)	0.0487(15)
C25	0.4559(4)	0.0413(5)	0.4241(3)	0.0426(13)
C33	0.8593(4)	0.1584(5)	0.4998(2)	0.0457(14)
C23	0.4770(5)	0.9674(5)	0.3220(3)	0.0447(13)
C9	0.0823(5)	0.2660(5)	0.1161(3)	0.0466(14)
C29	0.8146(4)	0.0140(5)	0.4279(2)	0.0397(12)
C41	0.7356(5)	0.3792(5)	0.2598(3)	0.0479(14)
C5	0.9547(5)	0.1676(5)	0.0380(2)	0.0447(13)
C37	0.7337(5)	0.4576(5)	0.4168(3)	0.0532(15)
C24	0.4116(4)	0.9743(5)	0.3726(3)	0.0475(14)
C39	0.9232(5)	0.4696(5)	0.4194(3)	0.0486(15)
C4	0.9712(5)	0.2231(5)	0.0966(2)	0.0458(14)
C21	0.7485(5)	0.1935(5)	0.1097(2)	0.0475(14)
C20	0.7129(5)	0.0856(5)	0.1099(3)	0.0510(15)
C38	0.8425(6)	0.5175(5)	0.4253(3)	0.0590(17)

	x/a	y/b	z/c	U(eq)
C32	0.8930(5)	0.1014(6)	0.5469(3)	0.0534(17)
C10	0.9130(5)	0.3842(5)	0.1372(3)	0.0539(16)
C8	0.1689(6)	0.2547(5)	0.0814(3)	0.0557(16)
C31	0.8864(4)	0.0016(7)	0.5346(3)	0.0581(19)
C16	0.6655(6)	0.2358(6)	0.0907(3)	0.0570(17)
C43	0.5459(6)	0.3659(6)	0.2319(3)	0.0576(17)
C44	0.5242(5)	0.2593(6)	0.2226(3)	0.0533(16)
C6	0.0398(6)	0.1527(5)	0.0024(3)	0.0532(16)
C17	0.5591(6)	0.1766(8)	0.0724(3)	0.0638(19)
C19	0.6069(6)	0.0241(6)	0.0919(3)	0.0649(19)
C18	0.5314(6)	0.0723(8)	0.0734(3)	0.072(2)
C15	0.9625(6)	0.4539(5)	0.1878(3)	0.0591(17)
C42	0.6515(6)	0.4251(5)	0.2508(3)	0.0577(17)
C11	0.9016(6)	0.4315(5)	0.0794(3)	0.0608(18)
O7	0.1902(7)	0.0982(6)	0.2073(4)	0.124(3)
O4	0.6853(8)	0.7300(7)	0.2481(4)	0.1400(18)
C7	0.1461(6)	0.1955(6)	0.0240(3)	0.0573(17)
C12	0.9268(7)	0.5375(6)	0.0717(4)	0.072(2)
B1	0.7653(5)	0.1757(5)	0.3805(3)	0.0345(12)
C14	0.9923(7)	0.5641(6)	0.1830(4)	0.071(2)
B2	0.8752(6)	0.2551(5)	0.1384(3)	0.0425(15)
C13	0.9725(8)	0.6025(6)	0.1250(4)	0.083(3)
C46	0.4546(7)	0.4130(7)	0.2189(3)	0.077(2)
O2	0.3774(10)	0.6605(6)	0.1821(4)	0.163(3)
C59	0.3437(7)	0.6671(7)	0.3453(4)	0.078(2)
C63	0.2212(7)	0.3645(7)	0.3383(5)	0.0911(11)
C64	0.3635(7)	0.3557(7)	0.4090(5)	0.0902(11)
C60	0.3330(8)	0.6459(9)	0.4177(4)	0.096(3)
C66	0.3128(7)	0.2523(8)	0.3859(5)	0.0917(12)
C61	0.4514(8)	0.6533(9)	0.4406(4)	0.092(3)
C62	0.5200(8)	0.7319(9)	0.3945(4)	0.097(3)
C70	0.2164(10)	0.0546(9)	0.1475(5)	0.105(3)
C58	0.2787(12)	0.5731(9)	0.1707(6)	0.132(3)
C69	0.2418(12)	0.9572(9)	0.1650(5)	0.124(4)
C67	0.1726(12)	0.0234(9)	0.2559(5)	0.127(4)
C68	0.1691(10)	0.9200(9)	0.2217(5)	0.109(3)
C52	0.8487(12)	0.8481(11)	0.2144(6)	0.1408(18)

	x/a	y/b	z/c	U(eq)
C57	0.2362(14)	0.5790(10)	0.1021(6)	0.147(4)
C56	0.2776(16)	0.6958(10)	0.0960(6)	0.169(4)
C53	0.8803(12)	0.7998(11)	0.2705(7)	0.1408(18)
C51	0.7328(12)	0.8152(10)	0.2052(7)	0.1404(18)
C54	0.7815(11)	0.7262(11)	0.2923(7)	0.1408(18)
C65	0.1995(7)	0.2607(8)	0.3554(5)	0.0924(12)
C55	0.3315(16)	0.7352(11)	0.1555(7)	0.179(4)
Na1	0.5189(4)	0.6665(5)	0.2358(3)	0.1485(19)
O3	0.5677(10)	0.6154(10)	0.1282(4)	0.143(3)
C50	0.6639(9)	0.5946(13)	0.1048(5)	0.143(3)
C48	0.5339(11)	0.5689(12)	0.0150(5)	0.144(3)
C49	0.6275(12)	0.5291(11)	0.0411(6)	0.144(3)
C47	0.5332(12)	0.6508(10)	0.0680(5)	0.143(3)

Table 4. Bond lengths (Å) for 5636.

F26-C26	1.342(6)	F20-C36	1.356(6)
F25-C29	1.362(6)	F30-C22	1.342(6)
F16-C34	1.345(6)	F27-C25	1.348(6)
F1-C9	1.354(6)	F21-C33	1.331(7)
F6-C20	1.340(7)	F5-C5	1.341(7)
F15-C15	1.333(8)	F24-C30	1.321(7)
F29-C23	1.339(6)	F19-C37	1.339(7)
F4-C6	1.348(7)	F22-C32	1.347(7)
F28-C24	1.342(6)	F10-C16	1.346(8)
F11-C11	1.358(8)	F23-C31	1.354(7)
F17-C39	1.347(6)	F2-C8	1.324(8)
N2-C1	1.350(6)	N2-C3	1.374(6)
N2-B1	1.593(6)	F18-C38	1.340(7)
F7-C19	1.333(9)	F3-C7	1.337(7)
N1-C1	1.343(6)	N1-C2	1.368(7)
N1-B2	1.593(7)	F14-C14	1.320(9)
F12-C12	1.334(8)	O1-H1	0.872(9)
O1-C46	1.421(9)	O1-Na1	2.220(7)
F8-C18	1.375(8)	F9-C17	1.348(8)
O6-C63	1.442(10)	O6-C64	1.439(10)
F13-C13	1.348(9)	C1-C40	1.481(8)

C36-C35	1.368(8)	C36-C37	1.386(8)
C40-C45	1.379(8)	C40-C41	1.387(8)
C3-H3	0.95	C3-C2	1.339(7)
C28-C33	1.396(7)	C28-C29	1.381(8)
C28-B1	1.656(8)	C26-C27	1.386(7)
C26-C25	1.377(7)	C27-C22	1.394(7)
C27-B1	1.649(8)	C35-C34	1.391(7)
C35-B1	1.639(8)	C34-C39	1.364(8)
C2-H2	0.95	C45-H45	0.95
C45-C44	1.368(8)	C22-C23	1.381(8)
O5-C59	1.420(10)	O5-C62	1.439(10)
O5-Na1	2.254(8)	C30-C29	1.376(8)
C30-C31	1.386(9)	C25-C24	1.356(8)
C33-C32	1.378(9)	C23-C24	1.366(8)
C9-C4	1.393(8)	C9-C8	1.373(8)
C41-H41	0.95	C41-C42	1.396(9)
C5-C4	1.370(8)	C5-C6	1.384(8)
C37-C38	1.373(9)	C39-C38	1.374(10)
C4-B2	1.665(8)	C21-C20	1.383(9)
C21-C16	1.390(9)	C21-B2	1.650(9)
C20-C19	1.380(9)	C32-C31	1.336(10)
C10-C15	1.376(9)	C10-C11	1.376(9)
C10-B2	1.655(9)	C8-C7	1.373(9)
C16-C17	1.377(10)	C43-C44	1.382(10)
C43-C42	1.372(10)	C43-C46	1.501(10)
C44-H44	0.95	C6-C7	1.350(9)
C17-C18	1.339(12)	C19-C18	1.360(12)
C15-C14	1.420(10)	C42-H42	0.95
C11-C12	1.376(10)	O7-C70	1.434(12)
O7-C67	1.403(12)	O4-C51	1.450(13)
O4-C54	1.509(15)	O4-Na1	2.028(11)
C12-C13	1.374(12)	C14-C13	1.348(11)
C46-H46A	0.99	C46-H46B	0.99
O2-C58	1.442(14)	O2-C55	1.415(17)
O2-Na1	2.052(12)	C59-H59A	0.99
C59-H59B	0.99	C59-C60	1.514(12)
C63-H63A	0.99	C63-H63B	0.99
C63-C65	1.393(12)	C64-H64A	0.99

C64-H64B	0.99	C64-C66	1.406(13)
C60-H60A	0.99	C60-H60B	0.99
C60-C61	1.533(12)	C66-H66A	0.99
C66-H66B	0.99	C66-C65	1.585(12)
C61-H61A	0.99	C61-H61B	0.99
C61-C62	1.516(14)	C62-H62A	0.99
C62-H62B	0.99	C70-H70A	0.99
C70-H70B	0.99	C70-C69	1.491(15)
C58-H58A	0.99	C58-H58B	0.99
C58-C57	1.496(15)	C69-H69A	0.99
C69-H69B	0.99	C69-C68	1.504(14)
C67-H67A	0.99	C67-H67B	0.99
C67-C68	1.529(15)	C68-H68A	0.99
C68-H68B	0.99	C52-H52A	0.99
C52-H52B	0.99	C52-C53	1.434(15)
C52-C51	1.407(16)	C57-H57A	0.99
C57-H57B	0.99	C57-C56	1.506(17)
C56-H56A	0.99	C56-H56B	0.99
C56-C55	1.385(16)	C53-H53A	0.99
C53-H53B	0.99	C53-C54	1.432(16)
C51-H51A	0.99	C51-H51B	0.99
C54-H54A	0.99	C54-H54B	0.99
C65-H65A	0.99	C65-H65B	0.99
C55-H55A	0.99	C55-H55B	0.99
Na1-O3	2.444(10)	O3-C50	1.4294(10)
O3-C47	1.4298(10)	C50-H50A	0.99
C50-H50B	0.99	C50-C49	1.5293(10)
C48-C48	1.87(3)	C48-H48A	0.99
C48-H48B	0.99	C48-C49	1.5293(10)
C48-C47	1.5298(10)	C49-H49A	0.99
C49-H49B	0.99	C47-H47A	0.99
C47-H47B	0.99		

Table 5. Bond angles (°) for 5636.

C1-N2-C3	106.8(4)	C1-N2-B1	126.4(4)
C3-N2-B1	126.6(4)	C1-N1-C2	107.0(4)
C1-N1-B2	126.7(5)	C2-N1-B2	126.2(4)

C46-O1-H1	108.2(16)	C46-O1-Na1	125.9(5)
Na1-O1-H1	125.0(16)	C64-O6-C63	106.5(6)
N2-C1-C40	124.3(4)	N1-C1-N2	109.6(5)
N1-C1-C40	126.1(4)	F20-C36-C35	121.3(5)
F20-C36-C37	114.5(5)	C35-C36-C37	124.0(5)
C45-C40-C1	121.9(5)	C45-C40-C41	118.0(5)
C41-C40-C1	120.1(5)	N2-C3-H3	126.0
C2-C3-N2	108.1(4)	C2-C3-H3	126.0
C33-C28-B1	125.8(5)	C29-C28-C33	113.4(5)
C29-C28-B1	120.0(5)	F26-C26-C27	119.2(4)
F26-C26-C25	116.5(4)	C25-C26-C27	124.3(5)
C26-C27-C22	113.2(5)	C26-C27-B1	119.9(4)
C22-C27-B1	126.7(4)	C36-C35-C34	113.5(5)
C36-C35-B1	128.6(4)	C34-C35-B1	117.7(5)
F16-C34-C35	119.3(5)	F16-C34-C39	115.9(5)
C39-C34-C35	124.8(5)	N1-C2-H2	125.8
C3-C2-N1	108.5(4)	C3-C2-H2	125.8
C40-C45-H45	119.2	C44-C45-C40	121.6(6)
C44-C45-H45	119.2	F30-C22-C27	121.0(5)
F30-C22-C23	115.6(5)	C23-C22-C27	123.3(5)
C59-O5-C62	108.7(6)	C59-O5-Na1	120.0(5)
C62-O5-Na1	127.7(5)	F24-C30-C29	121.1(6)
F24-C30-C31	121.4(6)	C29-C30-C31	117.5(6)
F27-C25-C26	119.9(5)	F27-C25-C24	120.3(5)
C24-C25-C26	119.8(5)	F21-C33-C28	121.8(5)
F21-C33-C32	115.4(5)	C32-C33-C28	122.8(7)
F29-C23-C22	119.1(5)	F29-C23-C24	120.9(5)
C24-C23-C22	120.1(5)	F1-C9-C4	119.8(5)
F1-C9-C8	115.6(5)	C8-C9-C4	124.6(5)
F25-C29-C28	119.3(4)	F25-C29-C30	115.3(6)
C30-C29-C28	125.4(5)	C40-C41-H41	119.9
C40-C41-C42	120.2(6)	C42-C41-H41	119.9
F5-C5-C4	121.8(5)	F5-C5-C6	114.7(5)
C4-C5-C6	123.5(6)	F19-C37-C36	120.4(5)
F19-C37-C38	119.8(6)	C38-C37-C36	119.8(6)
F28-C24-C25	120.8(5)	F28-C24-C23	120.1(5)
C25-C24-C23	119.1(5)	F17-C39-C34	121.2(6)
F17-C39-C38	119.4(5)	C34-C39-C38	119.4(5)

C9-C4-B2	119.5(5)	C5-C4-C9	113.5(5)
C5-C4-B2	126.4(5)	C20-C21-C16	113.2(6)
C20-C21-B2	118.1(5)	C16-C21-B2	128.4(6)
F6-C20-C21	119.5(5)	F6-C20-C19	116.1(6)
C19-C20-C21	124.5(6)	F18-C38-C37	120.0(6)
F18-C38-C39	121.4(6)	C37-C38-C39	118.5(6)
F22-C32-C33	120.2(7)	C31-C32-F22	119.1(6)
C31-C32-C33	120.7(6)	C15-C10-C11	113.5(6)
C15-C10-B2	127.1(5)	C11-C10-B2	119.3(6)
F2-C8-C9	120.6(5)	F2-C8-C7	120.6(6)
C9-C8-C7	118.8(6)	F23-C31-C30	118.7(7)
C32-C31-F23	121.1(6)	C32-C31-C30	120.2(6)
F10-C16-C21	120.7(6)	F10-C16-C17	115.5(6)
C17-C16-C21	123.7(7)	C44-C43-C46	119.1(7)
C42-C43-C44	118.5(6)	C42-C43-C46	122.4(7)
C45-C44-C43	120.8(6)	C45-C44-H44	119.6
C43-C44-H44	119.6	F4-C6-C5	119.8(6)
F4-C6-C7	119.8(5)	C7-C6-C5	120.4(5)
F9-C17-C16	119.4(8)	C18-C17-F9	121.1(7)
C18-C17-C16	119.4(7)	F7-C19-C20	121.2(7)
F7-C19-C18	120.6(7)	C18-C19-C20	118.2(8)
C17-C18-F8	120.1(8)	C17-C18-C19	121.0(7)
C19-C18-F8	119.0(9)	F15-C15-C10	121.9(6)
F15-C15-C14	114.3(6)	C10-C15-C14	123.8(7)
C41-C42-H42	119.5	C43-C42-C41	120.9(6)
C43-C42-H42	119.5	F11-C11-C10	118.4(6)
F11-C11-C12	116.2(6)	C12-C11-C10	125.4(7)
C67-O7-C70	109.4(9)	C51-O4-C54	104.2(10)
C51-O4-Na1	114.2(8)	C54-O4-Na1	141.3(7)
F3-C7-C8	120.0(6)	F3-C7-C6	120.8(6)
C6-C7-C8	119.2(6)	F12-C12-C11	120.8(7)
F12-C12-C13	121.3(7)	C13-C12-C11	117.9(7)
N2-B1-C28	111.0(4)	N2-B1-C27	111.5(4)
N2-B1-C35	103.5(4)	C27-B1-C28	103.1(4)
C35-B1-C28	112.2(4)	C35-B1-C27	115.8(4)
F14-C14-C15	120.5(7)	F14-C14-C13	121.5(7)
C13-C14-C15	118.0(7)	N1-B2-C4	110.9(5)
N1-B2-C21	102.9(4)	N1-B2-C10	110.7(4)

C21-B2-C4	112.5(5)	C21-B2-C10	115.9(5)
C10-B2-C4	104.2(4)	F13-C13-C12	119.0(8)
F13-C13-C14	119.7(8)	C14-C13-C12	121.2(7)
O1-C46-C43	111.9(6)	O1-C46-H46A	109.2
O1-C46-H46B	109.2	C43-C46-H46A	109.2
C43-C46-H46B	109.2	H46A-C46-H46B	107.9
C58-O2-Na1	128.4(7)	C55-O2-C58	95.2(11)
C55-O2-Na1	135.3(8)	O5-C59-H59A	110.1
O5-C59-H59B	110.1	O5-C59-C60	108.0(6)
H59A-C59-H59B	108.4	C60-C59-H59A	110.1
C60-C59-H59B	110.1	O6-C63-H63A	110.3
O6-C63-H63B	110.3	H63A-C63-H63B	108.6
C65-C63-O6	106.9(7)	C65-C63-H63A	110.3
C65-C63-H63B	110.3	O6-C64-H64A	110.9
O6-C64-H64B	110.9	H64A-C64-H64B	108.9
C66-C64-O6	104.2(8)	C66-C64-H64A	110.9
C66-C64-H64B	110.9	C59-C60-H60A	111.2
C59-C60-H60B	111.2	C59-C60-C61	102.9(7)
H60A-C60-H60B	109.1	C61-C60-H60A	111.2
C61-C60-H60B	111.2	C64-C66-H66A	111.6
C64-C66-H66B	111.6	C64-C66-C65	100.8(8)
H66A-C66-H66B	109.4	C65-C66-H66A	111.6
C65-C66-H66B	111.6	C60-C61-H61A	111.3
C60-C61-H61B	111.3	H61A-C61-H61B	109.2
C62-C61-C60	102.2(8)	C62-C61-H61A	111.3
C62-C61-H61B	111.3	O5-C62-C61	103.1(7)
O5-C62-H62A	111.1	O5-C62-H62B	111.1
C61-C62-H62A	111.1	C61-C62-H62B	111.1
H62A-C62-H62B	109.1	O7-C70-H70A	110.4
O7-C70-H70B	110.4	O7-C70-C69	106.5(8)
H70A-C70-H70B	108.6	C69-C70-H70A	110.4
C69-C70-H70B	110.4	O2-C58-H58A	110.2
O2-C58-H58B	110.2	O2-C58-C57	107.4(10)
H58A-C58-H58B	108.5	C57-C58-H58A	110.2
C57-C58-H58B	110.2	C70-C69-H69A	111.3
C70-C69-H69B	111.3	C70-C69-C68	102.6(10)
H69A-C69-H69B	109.2	C68-C69-H69A	111.3
C68-C69-H69B	111.3	O7-C67-H67A	110.4

O7-C67-H67B	110.4	O7-C67-C68	106.8(8)
H67A-C67-H67B	108.6	C68-C67-H67A	110.4
C68-C67-H67B	110.4	C69-C68-C67	101.5(8)
C69-C68-H68A	111.5	C69-C68-H68B	111.5
C67-C68-H68A	111.5	C67-C68-H68B	111.5
H68A-C68-H68B	109.3	H52A-C52-H52B	108.2
C53-C52-H52A	109.7	C53-C52-H52B	109.7
C51-C52-H52A	109.7	C51-C52-H52B	109.7
C51-C52-C53	109.9(11)	C58-C57-H57A	112.1
C58-C57-H57B	112.1	C58-C57-C56	98.5(10)
H57A-C57-H57B	109.7	C56-C57-H57A	112.1
C56-C57-H57B	112.1	C57-C56-H56A	110.6
C57-C56-H56B	110.6	H56A-C56-H56B	108.7
C55-C56-C57	105.7(11)	C55-C56-H56A	110.6
C55-C56-H56B	110.6	C52-C53-H53A	110.3
C52-C53-H53B	110.3	H53A-C53-H53B	108.6
C54-C53-C52	106.9(12)	C54-C53-H53A	110.3
C54-C53-H53B	110.3	O4-C51-H51A	109.8
O4-C51-H51B	109.8	C52-C51-O4	109.4(10)
C52-C51-H51A	109.8	C52-C51-H51B	109.8
H51A-C51-H51B	108.2	O4-C54-H54A	110.0
O4-C54-H54B	110.0	C53-C54-O4	108.7(10)
C53-C54-H54A	110.0	C53-C54-H54B	110.0
H54A-C54-H54B	108.3	C63-C65-C66	105.5(7)
C63-C65-H65A	110.6	C63-C65-H65B	110.6
C66-C65-H65A	110.6	C66-C65-H65B	110.6
H65A-C65-H65B	108.8	O2-C55-H55A	110.0
O2-C55-H55B	110.0	C56-C55-O2	108.6(13)
C56-C55-H55A	110.0	C56-C55-H55B	110.0
H55A-C55-H55B	108.3	O1-Na1-O5	87.8(3)
O1-Na1-O3	89.6(4)	O5-Na1-O3	174.8(4)
O4-Na1-O1	111.7(3)	O4-Na1-O5	102.7(4)
O4-Na1-O2	147.4(4)	O4-Na1-O3	82.4(4)
O2-Na1-O1	95.5(3)	O2-Na1-O5	95.7(4)
O2-Na1-O3	80.1(5)	C50-O3-Na1	133.2(7)
C50-O3-C47	97.21(19)	C47-O3-Na1	123.2(7)
O3-C50-H50A	110.4	O3-C50-H50B	110.4
O3-C50-C49	106.44(10)	H50A-C50-H50B	108.6

C49-C50-H50A	110.4	C49-C50-H50B	110.4
C48-C48-H48A	36.3	C48-C48-H48B	97.8
H48A-C48-H48B	109.3	C49-C48-C48	85.4(11)
C49-C48-H48A	111.5	C49-C48-H48B	111.5
C49-C48-C47	101.58(9)	C47-C48-C48	144.3(12)
C47-C48-H48A	111.5	C47-C48-H48B	111.5
C50-C49-C48	101.63(9)	C50-C49-H49A	111.4
C50-C49-H49B	111.4	C48-C49-H49A	111.4
C48-C49-H49B	111.4	H49A-C49-H49B	109.3
O3-C47-C48	106.34(10)	O3-C47-H47A	110.5
O3-C47-H47B	110.5	C48-C47-H47A	110.5
C48-C47-H47B	110.5	H47A-C47-H47B	108.7

Table 6. Anisotropic atomic displacement parameters (Å^2) for 5636.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F26	0.0382(16)	0.0575(19)	0.0291(15)	-0.0015(13)	0.0077(12)	0.0118(14)
F20	0.0394(17)	0.0508(19)	0.0413(17)	-0.0023(13)	0.0075(13)	0.0145(14)
F25	0.0493(18)	0.0490(18)	0.0374(16)	0.0044(13)	0.0095(13)	0.0182(15)
F30	0.0462(18)	0.0477(18)	0.0304(15)	-0.0034(12)	0.0071(12)	0.0102(14)
F16	0.0307(16)	0.066(2)	0.0420(17)	-0.0051(15)	0.0066(13)	0.0050(15)
F27	0.0343(16)	0.071(2)	0.0384(16)	0.0118(15)	0.0145(13)	0.0129(15)
F1	0.060(2)	0.057(2)	0.0401(18)	-0.0015(15)	0.0183(15)	0.0105(17)
F21	0.0460(19)	0.073(2)	0.0339(16)	-0.0102(15)	0.0009(13)	0.0059(17)
F6	0.065(2)	0.053(2)	0.0396(17)	0.0024(14)	0.0042(15)	0.0107(17)
F5	0.070(2)	0.080(3)	0.0273(16)	-0.0008(15)	0.0089(15)	0.024(2)
F15	0.071(2)	0.050(2)	0.050(2)	0.0024(16)	0.0183(17)	0.0119(17)
F24	0.065(2)	0.077(3)	0.063(2)	0.0327(19)	0.0227(18)	0.032(2)
F29	0.056(2)	0.070(2)	0.046(2)	-0.0128(17)	-0.0013(16)	-0.0091(18)
F19	0.070(2)	0.057(2)	0.068(2)	-0.0120(17)	0.0109(18)	0.0252(19)
F4	0.092(3)	0.078(3)	0.0337(17)	-0.0035(16)	0.0180(17)	0.035(2)
F22	0.045(2)	0.132(4)	0.0295(17)	0.0124(19)	-0.0006(14)	0.009(2)
F28	0.0372(19)	0.092(3)	0.055(2)	0.0022(19)	0.0025(15)	-0.0062(18)
F10	0.079(3)	0.102(3)	0.049(2)	0.027(2)	0.0150(18)	0.051(2)
F11	0.096(3)	0.080(3)	0.043(2)	0.0302(19)	0.0265(19)	0.042(2)
F23	0.052(2)	0.126(4)	0.056(2)	0.052(2)	0.0142(17)	0.034(2)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F17	0.052(2)	0.062(2)	0.070(2)	-0.0158(18)	0.0020(18)	-0.0079(18)
F2	0.055(2)	0.104(3)	0.068(3)	-0.014(2)	0.0221(19)	0.014(2)
N2	0.031(2)	0.040(2)	0.0249(19)	0.0031(16)	0.0056(16)	0.0101(18)
F18	0.087(3)	0.051(2)	0.087(3)	-0.026(2)	0.006(2)	0.006(2)
F7	0.079(3)	0.082(3)	0.073(3)	-0.027(2)	0.003(2)	-0.003(2)
F3	0.079(3)	0.120(4)	0.058(2)	-0.007(2)	0.025(2)	0.043(3)
N1	0.044(2)	0.039(2)	0.0235(19)	0.0028(16)	0.0090(17)	0.0099(19)
F14	0.121(4)	0.056(3)	0.089(3)	-0.006(2)	0.036(3)	0.009(3)
F12	0.149(4)	0.091(3)	0.074(3)	0.052(3)	0.055(3)	0.067(3)
O1	0.077(3)	0.077(3)	0.062(3)	0.012(2)	0.024(2)	0.046(3)
F8	0.060(3)	0.176(5)	0.055(2)	-0.029(3)	-0.006(2)	0.020(3)
F9	0.075(3)	0.171(5)	0.046(2)	0.015(3)	0.0033(19)	0.063(3)
O6	0.068(2)	0.101(3)	0.103(3)	0.034(2)	0.0064(19)	0.0297(19)
F13	0.192(6)	0.050(3)	0.124(4)	0.033(3)	0.069(4)	0.040(3)
C1	0.036(3)	0.040(3)	0.027(2)	-0.002(2)	0.008(2)	0.005(2)
C36	0.036(3)	0.045(3)	0.034(3)	-0.002(2)	0.009(2)	0.007(2)
C40	0.048(3)	0.048(3)	0.025(2)	0.004(2)	0.008(2)	0.018(3)
C3	0.033(3)	0.045(3)	0.030(2)	0.004(2)	0.009(2)	0.011(2)
C28	0.027(2)	0.057(4)	0.029(2)	0.004(2)	0.0103(19)	0.008(2)
C26	0.036(3)	0.047(3)	0.024(2)	0.006(2)	0.0037(19)	0.012(2)
C27	0.036(3)	0.043(3)	0.025(2)	0.005(2)	0.0007(19)	0.013(2)
C35	0.035(3)	0.049(3)	0.022(2)	-0.005(2)	0.0032(19)	0.006(2)
C34	0.037(3)	0.056(4)	0.031(3)	-0.002(2)	0.009(2)	0.010(3)
C2	0.041(3)	0.041(3)	0.030(2)	0.003(2)	0.012(2)	0.015(2)
C45	0.046(3)	0.054(3)	0.029(3)	0.000(2)	0.007(2)	0.024(3)
C22	0.042(3)	0.043(3)	0.035(3)	0.002(2)	0.008(2)	0.012(2)
O5	0.078(4)	0.104(4)	0.074(3)	0.000(3)	-0.004(3)	0.041(3)
C30	0.038(3)	0.062(4)	0.051(3)	0.025(3)	0.024(3)	0.018(3)
C25	0.031(3)	0.061(4)	0.036(3)	0.012(3)	0.012(2)	0.014(3)
C33	0.025(3)	0.073(4)	0.032(3)	0.008(3)	0.007(2)	0.003(3)
C23	0.043(3)	0.047(3)	0.037(3)	-0.001(2)	-0.005(2)	0.005(3)
C9	0.052(4)	0.057(4)	0.031(3)	0.007(2)	0.014(2)	0.014(3)
C29	0.034(3)	0.056(4)	0.029(3)	0.011(2)	0.009(2)	0.012(2)
C41	0.061(4)	0.058(4)	0.030(3)	-0.003(2)	0.006(2)	0.027(3)
C5	0.051(3)	0.055(4)	0.028(3)	0.008(2)	0.003(2)	0.016(3)
C37	0.056(4)	0.057(4)	0.047(3)	-0.012(3)	0.014(3)	0.018(3)
C24	0.032(3)	0.060(4)	0.040(3)	0.011(3)	0.000(2)	-0.001(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C39	0.041(3)	0.050(4)	0.042(3)	-0.013(3)	0.005(2)	-0.004(3)
C4	0.065(4)	0.047(3)	0.028(3)	0.012(2)	0.018(2)	0.019(3)
C21	0.057(4)	0.069(4)	0.022(2)	0.012(2)	0.010(2)	0.027(3)
C20	0.054(4)	0.069(4)	0.026(3)	0.000(3)	0.007(2)	0.011(3)
C38	0.066(4)	0.048(4)	0.055(4)	-0.015(3)	0.008(3)	0.006(3)
C32	0.034(3)	0.089(5)	0.031(3)	0.019(3)	0.008(2)	0.009(3)
C10	0.069(4)	0.060(4)	0.042(3)	0.016(3)	0.021(3)	0.029(3)
C8	0.057(4)	0.062(4)	0.047(3)	0.002(3)	0.020(3)	0.016(3)
C31	0.028(3)	0.104(6)	0.042(3)	0.037(4)	0.011(2)	0.015(3)
C16	0.068(4)	0.078(5)	0.030(3)	0.007(3)	0.008(3)	0.030(4)
C43	0.069(4)	0.079(5)	0.039(3)	-0.004(3)	0.002(3)	0.045(4)
C44	0.060(4)	0.077(5)	0.032(3)	-0.006(3)	0.000(3)	0.035(3)
C6	0.083(5)	0.055(4)	0.026(3)	0.003(2)	0.020(3)	0.026(3)
C17	0.061(4)	0.110(7)	0.031(3)	0.005(3)	0.004(3)	0.040(4)
C19	0.072(5)	0.082(5)	0.035(3)	-0.011(3)	0.002(3)	0.015(4)
C18	0.052(4)	0.130(8)	0.026(3)	-0.019(4)	-0.005(3)	0.018(5)
C15	0.080(5)	0.045(4)	0.057(4)	0.007(3)	0.030(3)	0.023(3)
C42	0.088(5)	0.054(4)	0.043(3)	-0.005(3)	0.004(3)	0.039(4)
C11	0.087(5)	0.061(4)	0.044(3)	0.014(3)	0.034(3)	0.033(4)
O7	0.181(8)	0.106(5)	0.101(5)	0.020(4)	0.032(5)	0.064(5)
O4	0.174(5)	0.132(4)	0.134(4)	0.055(3)	0.030(3)	0.070(3)
C7	0.063(4)	0.068(4)	0.044(3)	0.003(3)	0.024(3)	0.024(3)
C12	0.099(6)	0.070(5)	0.059(4)	0.037(4)	0.044(4)	0.038(4)
B1	0.031(3)	0.048(3)	0.022(2)	0.003(2)	0.009(2)	0.009(2)
C14	0.083(5)	0.067(5)	0.058(4)	0.006(4)	0.036(4)	0.013(4)
B2	0.057(4)	0.049(4)	0.024(3)	0.011(2)	0.015(3)	0.018(3)
C13	0.123(7)	0.056(4)	0.081(6)	0.012(4)	0.049(5)	0.039(5)
C46	0.093(6)	0.109(7)	0.050(4)	0.011(4)	0.010(4)	0.058(5)
O2	0.265(8)	0.090(4)	0.100(5)	0.006(4)	-0.046(5)	0.009(5)
C59	0.079(5)	0.086(6)	0.078(5)	-0.021(4)	-0.010(4)	0.040(4)
C63	0.070(2)	0.102(3)	0.104(3)	0.034(2)	0.0049(19)	0.029(2)
C64	0.069(2)	0.102(3)	0.104(3)	0.034(2)	0.0056(19)	0.029(2)
C60	0.099(7)	0.130(8)	0.068(5)	-0.041(5)	-0.002(4)	0.053(6)
C66	0.071(2)	0.102(3)	0.105(3)	0.034(2)	0.005(2)	0.028(2)
C61	0.117(7)	0.127(8)	0.053(4)	-0.022(5)	-0.009(5)	0.070(6)
C62	0.080(6)	0.145(9)	0.079(6)	-0.010(6)	-0.003(5)	0.054(6)
C70	0.130(9)	0.107(8)	0.070(6)	0.008(5)	-0.003(5)	0.027(7)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C58	0.198(8)	0.093(5)	0.105(5)	0.004(5)	-0.038(6)	0.048(6)
C69	0.197(13)	0.108(8)	0.064(6)	0.011(5)	0.007(7)	0.044(8)
C67	0.217(14)	0.105(8)	0.075(6)	0.024(6)	0.039(7)	0.067(9)
C68	0.122(8)	0.107(8)	0.091(7)	0.015(6)	0.016(6)	0.020(6)
C52	0.174(5)	0.133(4)	0.135(4)	0.053(3)	0.030(3)	0.069(4)
C57	0.231(9)	0.116(6)	0.084(5)	-0.009(5)	-0.015(6)	0.040(7)
C56	0.274(10)	0.117(6)	0.096(6)	0.001(5)	-0.041(6)	0.034(7)
C53	0.174(5)	0.133(4)	0.134(4)	0.053(3)	0.030(3)	0.070(4)
C51	0.174(5)	0.133(4)	0.134(4)	0.054(3)	0.030(3)	0.070(4)
C54	0.174(5)	0.133(4)	0.134(4)	0.054(3)	0.029(3)	0.069(3)
C65	0.071(2)	0.103(3)	0.106(3)	0.033(2)	0.004(2)	0.028(2)
C55	0.282(10)	0.110(6)	0.116(6)	0.004(5)	-0.059(7)	0.026(7)
Na1	0.128(4)	0.148(4)	0.179(5)	0.042(4)	0.015(3)	0.051(3)
O3	0.192(7)	0.181(7)	0.099(5)	0.040(5)	0.058(5)	0.113(6)
C50	0.193(7)	0.181(7)	0.100(5)	0.040(5)	0.058(5)	0.113(6)
C48	0.193(7)	0.181(7)	0.100(5)	0.040(5)	0.058(5)	0.113(6)
C49	0.193(7)	0.181(7)	0.100(5)	0.040(5)	0.058(5)	0.113(6)
C47	0.193(7)	0.181(7)	0.100(5)	0.040(5)	0.058(5)	0.113(6)

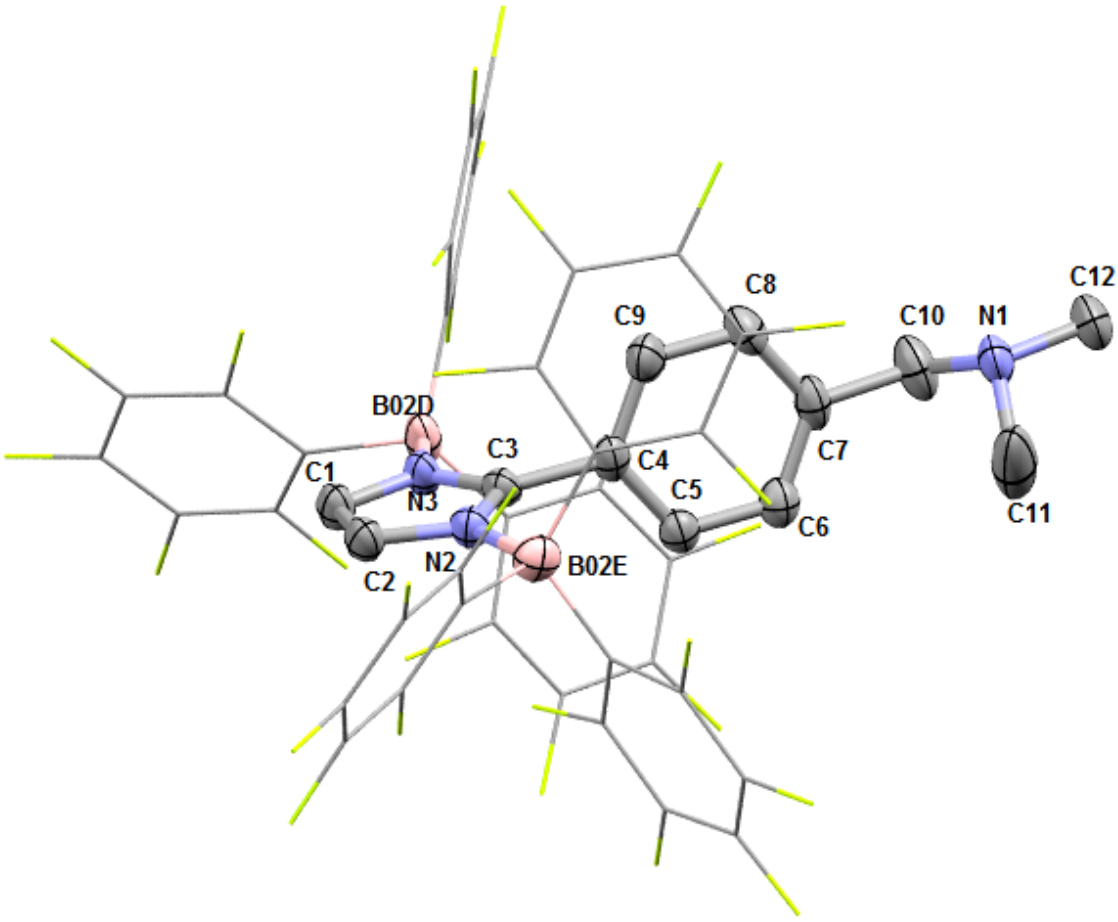
Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for 5636.

	x/a	y/b	z/c	U(eq)
H1	0.432(6)	0.4763(16)	0.2983(17)	0.099
H3	0.9480	0.1097	0.3309	0.043
H2	1.0002	0.1493	0.2176	0.044
H45	0.5895	0.1407	0.2241	0.049
H41	0.8083	0.4214	0.2729	0.057
H44	0.4512	0.2170	0.2102	0.064
H42	0.6676	0.4984	0.2579	0.069
H46A	0.4569	0.4358	0.1731	0.093
H46B	0.3824	0.3593	0.2242	0.093
H59A	0.3080	0.6022	0.3189	0.094
H59B	0.3071	0.7198	0.3333	0.094
H63A	0.1703	0.3963	0.3601	0.109
H63B	0.2112	0.3689	0.2902	0.109
H64A	0.4448	0.3712	0.4138	0.108

	x/a	y/b	z/c	U(eq)
H64B	0.3350	0.3686	0.4519	0.108
H60A	0.2812	0.5756	0.4248	0.115
H60B	0.3070	0.6989	0.4409	0.115
H66A	0.3006	0.2027	0.4221	0.11
H66B	0.3567	0.2310	0.3523	0.11
H61A	0.4669	0.6787	0.4869	0.111
H61B	0.4650	0.5849	0.4356	0.111
H62A	0.5266	0.8042	0.4092	0.117
H62B	0.5950	0.7248	0.3914	0.117
H70A	0.2810	0.1045	0.1280	0.126
H70B	0.1528	0.0386	0.1153	0.126
H58A	0.2224	0.5765	0.2023	0.159
H58B	0.2957	0.5066	0.1762	0.159
H69A	0.3210	-0.0281	0.1782	0.148
H69B	0.2227	-0.0948	0.1279	0.148
H67A	0.1019	0.0167	0.2770	0.153
H67B	0.2333	0.0439	0.2899	0.153
H68A	0.1994	-0.1234	0.2509	0.131
H68B	0.0928	-0.1204	0.2065	0.131
H52A	0.8761	0.9250	0.2209	0.169
H52B	0.8824	0.8289	0.1749	0.169
H57A	0.1545	0.5515	0.0977	0.177
H57B	0.2691	0.5423	0.0699	0.177
H56A	0.3292	0.7147	0.0598	0.203
H56B	0.2151	0.7239	0.0872	0.203
H53A	0.9346	0.7638	0.2586	0.169
H53B	0.9142	0.8530	0.3057	0.169
H51A	0.7118	0.7917	0.1589	0.169
H51B	0.7039	0.8741	0.2151	0.169
H54A	0.7691	0.7439	0.3382	0.169
H54B	0.7889	0.6550	0.2907	0.169
H65A	0.1749	0.2133	0.3163	0.111
H65B	0.1411	0.2422	0.3879	0.111
H55A	0.2786	0.7496	0.1861	0.215
H55B	0.3908	0.8013	0.1491	0.215
H50A	0.6937	0.5557	0.1374	0.172
H50B	0.7221	0.6607	0.0965	0.172

	x/a	y/b	z/c	U(eq)
H48A	0.4625	0.5122	0.0114	0.172
H48B	0.5504	0.6005	-0.0283	0.172
H49A	0.6004	0.4535	0.0496	0.172
H49B	0.6884	0.5423	0.0102	0.172
H47A	0.5847	0.7198	0.0577	0.172
H47B	0.4580	0.6574	0.0712	0.172

Crystal Structure Report for Na[IMP-$CH_2N(Me)_2$]



Thermal ellipsoid plot of 5999. Ellipsoids shown at 50% probability, solvent, cation, and hydrogen atoms hidden for clarity, C_6F_5 rings shown in wireframe.

A specimen of $C_{64}H_{46}B_2F_{30}N_3NaO_4$ was used for the X-ray crystallographic analysis. The X-ray intensity data were measured(λ = 0.71073 Å). The integration of the data using a monoclinic unit cell yielded a total of 30324 reflections to a maximum θ angle of 27.91° (0.76Å resolution), of which 12545 were independent (average redundancy 2.417, completeness = 99.5%, R_{int} = 3.29%, R_{sig} =4.89%) and 8360 (66.64%) were greater than $2\sigma(F^2)$. The final cell constants of a = 12.1872(17) Å, b = 19.000(3) Å, c =14.971(2) Å, β = 111.618(3)°, volume = 3222.8(8) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21 1, with Z = 2for the formula unit, $C_{64}H_{46}B_2F_{30}N_3NaO_4$. The final anisotropic full-matrix least-squares refinement on F^2 with 939 variables converged at R1 = 7.53%, for the observed data and wR2 = 23.99% for all data. The goodness-of-fit was 1.034. The largest peak in the final difference electron density synthesis was 0.854 $e^-/Å^3$ and the largest

hole was -0.465 $e^-/Å^3$ with an RMS deviation of 0.077 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.582 g/cm^3 and F(000), 1548 e^-.

Table 1. Sample and crystal data for 5999.

Identification code	5999	
Chemical formula	$C_{64}H_{46}B_2F_{30}N_3NaO_4$	
Formula weight	1535.65 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 12.1872(17) Å	α = 90°
	b = 19.000(3) Å	β = 111.618(3)°
	c = 14.971(2) Å	γ = 90°
Volume	3222.8(8) $Å^3$	
Z	2	
Density (calculated)	1.582 g/cm^3	
Absorption coefficient	0.163 mm^{-1}	
F(000)	1548	

Table 2. Data collection and structure refinement for 5999.

Theta range for data collection	1.80 to 27.91°	
Index ranges	-16<=h<=16, -14<=k<=25, -19<=l<=19	
Reflections collected	30324	
Independent reflections	12545 [R(int) = 0.0329]	
Structure solution technique	direct methods	
Structure solution program	SHELXT 2014/4 (Sheldrick, 2014)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	12545 / 122 / 939	
Goodness-of-fit on F^2	1.034	
Final R indices	8360 data; I>2σ(I)	R1 = 0.0753, wR2 = 0.2094
	all data	R1 = 0.1100, wR2 = 0.2399
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.1566P)^2+0.6005P]$ where $P=(F_o^2+2F_c^2)/3$	

Absolute structure parameter	0.2(2)
Largest diff. peak and hole	0.854 and -0.465 eÅ^{-3}
R.M.S. deviation from mean	0.077 eÅ^{-3}

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 5999.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij}tensor.

	x/a	y/b	z/c	U(eq)
F11	0.6425(4)	0.2717(8)	0.4023(3)	0.0473(9)
F10	0.6158(3)	0.3889(8)	0.5084(2)	0.0412(8)
F20	0.8588(3)	0.4449(8)	0.6258(3)	0.0476(9)
F16	0.7373(3)	0.6807(8)	0.5412(3)	0.0468(9)
F6	0.2827(3)	0.3458(8)	0.2265(3)	0.0611(12)
F30	0.0157(3)	0.5240(8)	0.3874(4)	0.0568(11)
F1	0.3034(3)	0.4867(8)	0.2475(3)	0.0573(10)
F21	0.7877(4)	0.5812(8)	0.2793(3)	0.0576(11)
F9	0.4914(4)	0.3600(8)	0.6135(3)	0.0620(12)
F19	0.7492(4)	0.4464(8)	0.7497(3)	0.0653(12)
F25	0.9752(3)	0.6827(8)	0.5862(5)	0.0782(16)
F5	0.6151(4)	0.4272(8)	0.1450(3)	0.0697(13)
F17	0.6368(4)	0.6821(8)	0.6687(3)	0.0625(11)
N2	0.6502(4)	0.4229(8)	0.3444(3)	0.0320(10)
F26	0.0371(3)	0.5407(8)	0.7113(3)	0.0703(14)
F29	0.2435(4)	0.4910(8)	0.4522(5)	0.0785(15)
F12	0.6498(5)	0.1405(8)	0.3492(4)	0.0740(14)
F8	0.2614(5)	0.3244(8)	0.5320(5)	0.0850(17)
N1	0.2380(4)	0.7096(8)	0.3273(4)	0.0457(13)
F15	0.4192(4)	0.3326(8)	0.0804(3)	0.0775(15)
F7	0.1587(4)	0.3144(8)	0.3373(5)	0.0822(16)
N3	0.7960(4)	0.4924(8)	0.4301(4)	0.0339(10)
F18	0.6365(5)	0.5651(8)	0.7726(4)	0.0836(16)
F24	0.9914(5)	0.8040(8)	0.5029(7)	0.118(3)
F2	0.2256(5)	0.5779(9)	0.1059(5)	0.0954(19)
C3	0.6779(4)	0.4857(8)	0.3870(4)	0.0298(10)
F22	0.7969(6)	0.7027(9)	0.1965(5)	0.108(3)
F28	0.3707(4)	0.4829(8)	0.6425(6)	0.100(2)
C2	0.7568(5)	0.3885(8)	0.3606(4)	0.0361(12)

	x/a	y/b	z/c	U(eq)
F27	0.2606(4)	0.5064(9)	0.7718(5)	0.109(2)
F14	0.4264(5)	0.2008(9)	0.0311(4)	0.108(2)
C7	0.4343(5)	0.6495(8)	0.3878(5)	0.0382(13)
C23	0.7489(6)	0.5046(9)	0.7000(5)	0.0484(16)
C5	0.5373(4)	0.5423(9)	0.4540(4)	0.0323(11)
C24	0.8053(5)	0.5059(9)	0.6344(5)	0.0436(14)
C42	0.5024(6)	0.3737(8)	0.4599(5)	0.0425(14)
C6	0.4610(5)	0.5963(8)	0.4540(4)	0.0360(12)
C4	0.5906(4)	0.5419(8)	0.3851(4)	0.0326(12)
C19	0.8094(4)	0.5634(8)	0.5798(4)	0.0378(13)
C14	0.8335(6)	0.6356(9)	0.3399(7)	0.057(2)
C29	0.1910(6)	0.5026(9)	0.5149(8)	0.069(3)
F13	0.5415(7)	0.1021(8)	0.1630(6)	0.110(2)
C1	0.8436(5)	0.4307(8)	0.4118(4)	0.0373(13)
C32	0.5899(6)	0.2578(9)	0.3077(5)	0.0441(15)
C44	0.5180(7)	0.4630(9)	0.1385(5)	0.061(2)
C38	0.3368(6)	0.3523(9)	0.3232(5)	0.0479(16)
C40	0.3239(7)	0.3383(9)	0.4768(6)	0.0554(19)
C17	0.9390(8)	0.7487(9)	0.4485(13)	0.088(4)
F23	0.8996(6)	0.8174(8)	0.3108(8)	0.148(4)
C13	0.8730(5)	0.6264(8)	0.4390(6)	0.0473(17)
O3	0.0335(7)	0.3065(10)	0.9338(6)	0.107(3)
C43	0.4618(5)	0.4484(9)	0.2015(4)	0.0463(15)
C9	0.5617(5)	0.5948(9)	0.3164(5)	0.0418(14)
C30	0.0723(6)	0.5194(9)	0.4839(7)	0.058(2)
C18	0.9275(5)	0.6858(9)	0.4867(8)	0.064(2)
F4	0.5433(7)	0.5247(9)	0.0101(5)	0.127(3)
C41	0.4400(7)	0.3570(9)	0.5187(5)	0.0483(16)
C20	0.7501(5)	0.6216(9)	0.5942(5)	0.0422(14)
C8	0.4842(5)	0.6481(9)	0.3170(4)	0.0400(13)
C39	0.2725(6)	0.3349(9)	0.3796(7)	0.058(2)
C33	0.5947(7)	0.1881(9)	0.2836(6)	0.0535(18)
C22	0.6933(6)	0.5653(9)	0.7126(5)	0.0538(17)
C10	0.3612(6)	0.7113(9)	0.3933(5)	0.0524(17)
C37	0.4522(5)	0.3740(8)	0.3599(5)	0.0379(13)
F3	0.3414(8)	0.6005(9)	0.9852(5)	0.133(3)
C48	0.3640(6)	0.4910(9)	0.1881(5)	0.0517(16)

	x/a	y/b	z/c	U(eq)
C12	0.1787(6)	0.7745(9)	0.3386(6)	0.0558(18)
C34	0.5430(8)	0.1673(9)	0.1896(7)	0.068(2)
C28	0.2556(6)	0.4966(9)	0.6127(9)	0.077(3)
C21	0.6950(6)	0.6231(9)	0.6602(5)	0.0496(16)
C15	0.8413(7)	0.6997(9)	0.2966(9)	0.080(3)
C35	0.4819(8)	0.2194(10)	0.1223(7)	0.073(3)
C26	0.0820(6)	0.5266(9)	0.6412(7)	0.062(2)
C25	0.0111(5)	0.5308(9)	0.5453(6)	0.0478(16)
C31	0.5337(5)	0.3112(9)	0.2447(4)	0.0420(14)
C16	0.8938(9)	0.7565(9)	0.3543(14)	0.103(5)
C36	0.4796(7)	0.2880(9)	0.1509(6)	0.060(2)
C27	0.1988(6)	0.5100(9)	0.6739(7)	0.072(3)
O4	0.9568(11)	0.2303(11)	0.0894(8)	0.1413(9)
C11	0.1777(8)	0.6485(9)	0.3489(11)	0.099(4)
O2	0.9521(14)	0.6340(14)	0.0465(13)	0.2026(11)
C47	0.3235(7)	0.5407(10)	0.1143(7)	0.074(3)
Na1	0.2029(10)	0.7314(10)	0.1370(6)	0.189(4)
C45	0.4824(9)	0.5133(10)	0.0673(6)	0.085(3)
B02D	0.8701(5)	0.5546(9)	0.4979(6)	0.0412(16)
B02E	0.5229(5)	0.3903(9)	0.2865(5)	0.0355(14)
C46	0.3835(10)	0.5524(10)	0.0552(7)	0.092(4)
C59	0.1546(10)	0.3168(11)	0.9709(9)	0.100(4)
C63	0.8412(18)	0.2012(13)	0.1767(13)	0.1414(9)
C61	0.9166(18)	0.2925(13)	0.1097(13)	0.1414(9)
C58	0.1808(14)	0.3921(14)	0.9439(16)	0.158(8)
C64	0.9335(18)	0.1769(14)	0.1459(13)	0.1414(9)
C60	0.9803(11)	0.3722(11)	0.8983(12)	0.119(5)
C62	0.8673(18)	0.2805(14)	0.1884(13)	0.1414(9)
C53	0.978(2)	0.5843(14)	0.1267(18)	0.2026(11)
C54	0.852(2)	0.6186(19)	0.9726(17)	0.2026(11)
C57	0.0646(17)	0.4291(15)	0.919(2)	0.190(11)
C55	0.816(2)	0.5355(19)	0.9969(17)	0.2026(11)
C56	0.8923(19)	0.5226(13)	0.0912(17)	0.2026(11)
O1	0.3989(14)	0.7896(13)	0.1093(13)	0.2090(10)
C52	0.3746(18)	0.8595(15)	0.0995(19)	0.2090(10)
C49	0.5289(12)	0.78347(11)	0.1591(19)	0.2090(10)
C50	0.5792(15)	0.8495(10)	0.1725(19)	0.2090(10)

	x/a	y/b	z/c	U(eq)
C51	0.4817(12)	0.90120(10)	0.144(2)	0.2090(10)

Table 4. Bond lengths (Å) for 5999.

F11-C32	1.349(7)	F10-C42	1.335(8)
F20-C24	1.360(8)	F16-C20	1.352(8)
F6-C38	1.356(9)	F30-C30	1.356(10)
F1-C48	1.353(9)	F21-C14	1.353(10)
F9-C41	1.325(9)	F19-C23	1.333(9)
F25-C18	1.386(11)	F5-C44	1.337(10)
F17-C21	1.356(8)	N2-C3	1.335(8)
N2-C2	1.393(7)	N2-B02E	1.598(8)
F26-C26	1.377(10)	F29-C29	1.335(11)
F12-C33	1.321(10)	F8-C40	1.340(8)
N1-C10	1.462(8)	N1-C12	1.471(9)
N1-C11	1.473(11)	N1-Na1	2.753(10)
F15-C36	1.342(11)	F7-C39	1.353(8)
N3-C3	1.350(7)	N3-C1	1.379(8)
N3-B02D	1.602(9)	F18-C22	1.321(9)
F24-C17	1.339(13)	F2-C47	1.352(11)
F2-Na1	2.982(13)	C3-C4	1.500(8)
F22-C15	1.394(13)	F28-C28	1.331(8)
C2-C1	1.323(9)	C2-H2	0.95
F27-C27	1.381(12)	F14-C35	1.328(10)
C7-C6	1.369(9)	C7-C8	1.403(9)
C7-C10	1.496(9)	C23-C22	1.386(11)
C23-C24	1.391(10)	C5-C6	1.384(8)
C5-C4	1.407(7)	C5-H5	0.95
C24-C19	1.375(10)	C42-C37	1.392(9)
C42-C41	1.395(8)	C6-H6	0.95
C4-C9	1.387(9)	C19-C20	1.381(9)
C19-B02D	1.657(10)	C14-C13	1.392(12)
C14-C15	1.399(11)	C29-C30	1.383(9)
C29-C28	1.388(15)	F13-C34	1.300(10)
C1-H1	0.95	C32-C33	1.379(10)
C32-C31	1.384(11)	C44-C45	1.377(13)
C44-C43	1.382(11)	C38-C37	1.371(9)

C38-C39	1.388(10)	C40-C39	1.357(12)
C40-C41	1.366(11)	C17-C16	1.320(18)
C17-C18	1.353(14)	F23-C16	1.344(12)
C13-C18	1.370(11)	C13-B02D	1.633(11)
O3-C59	1.385(14)	O3-C60	1.417(18)
C43-C48	1.392(10)	C43-B02E	1.642(10)
C9-C8	1.387(9)	C9-H9	0.95
C30-C25	1.397(11)	F4-C45	1.342(12)
C20-C21	1.385(10)	C8-H8	0.95
C33-C34	1.372(12)	C22-C21	1.354(12)
C10-H10A	0.99	C10-H10B	0.99
C37-B02E	1.657(8)	F3-C46	1.341(12)
C48-C47	1.397(13)	C12-H12A	0.98
C12-H12B	0.98	C12-H12C	0.98
C34-C35	1.413(16)	C28-C27	1.361(14)
C15-C16	1.382(19)	C35-C36	1.376(13)
C26-C27	1.360(10)	C26-C25	1.379(12)
C25-B02D	1.662(8)	C31-C36	1.384(10)
C31-B02E	1.651(10)	O4-C61	1.36(2)
O4-C64	1.42(2)	C11-H11A	0.98
C11-H11B	0.98	C11-H11C	0.98
O2-C54	1.34(2)	O2-C53	1.47(3)
C47-C46	1.359(15)	Na1-O1	2.80(2)
C45-C46	1.370(16)	C59-C58	1.55(2)
C59-H59A	0.99	C59-H59B	0.99
C63-C64	1.44(2)	C63-C62	1.54(3)
C63-H63A	0.99	C63-H63B	0.99
C61-C62	1.52(2)	C61-H61A	0.99
C61-H61B	0.99	C58-C57	1.50(3)
C58-H58A	0.99	C58-H58B	0.99
C64-H64A	0.99	C64-H64B	0.99
C60-C57	1.44(3)	C60-H60A	0.99
C60-H60B	0.99	C62-H62A	0.99
C62-H62B	0.99	C53-C56	1.5298(14)
C53-H53A	0.99	C53-H53B	0.99
C54-C55	1.71(4)	C54-H54A	0.99
C54-H54B	0.99	C57-H57A	0.99
C57-H57B	0.99	C55-C56	1.39(3)

C55-H55A	0.99	C55-H55B	0.99
C56-H56A	0.99	C56-H56B	0.99
O1-C52	1.36(2)	O1-C49	1.487(16)
C52-C51	1.460(19)	C52-H52A	0.99
C52-H52B	0.99	C49-C50	1.379(19)
C49-H49A	0.99	C49-H49B	0.99
C50-C51	1.477(16)	C50-H50A	0.99
C50-H50B	0.99	C51-H51A	0.99
C51-H51B	0.99		

Table 5. Bond angles (°) for 5999.

C3-N2-C2	106.3(4)	C3-N2-B02E	129.0(5)
C2-N2-B02E	124.6(5)	C10-N1-C12	109.2(6)
C10-N1-C11	109.9(7)	C12-N1-C11	109.2(6)
C10-N1-Na1	115.2(5)	C12-N1-Na1	95.6(5)
C11-N1-Na1	116.5(7)	C3-N3-C1	106.1(5)
C3-N3-B02D	128.7(5)	C1-N3-B02D	125.0(4)
C47-F2-Na1	128.8(6)	N2-C3-N3	110.5(5)
N2-C3-C4	125.0(5)	N3-C3-C4	124.5(5)
C1-C2-N2	108.1(5)	C1-C2-H2	125.9
N2-C2-H2	125.9	C6-C7-C8	118.7(5)
C6-C7-C10	121.8(6)	C8-C7-C10	119.4(6)
F19-C23-C22	121.1(6)	F19-C23-C24	120.6(6)
C22-C23-C24	118.4(7)	C6-C5-C4	119.8(6)
C6-C5-H5	120.1	C4-C5-H5	120.1
F20-C24-C19	119.8(6)	F20-C24-C23	115.5(6)
C19-C24-C23	124.7(6)	F10-C42-C37	122.7(5)
F10-C42-C41	113.7(6)	C37-C42-C41	123.6(6)
C7-C6-C5	121.8(5)	C7-C6-H6	119.1
C5-C6-H6	119.1	C9-C4-C5	118.6(5)
C9-C4-C3	121.0(5)	C5-C4-C3	120.4(5)
C24-C19-C20	114.0(6)	C24-C19-B02D	118.9(5)
C20-C19-B02D	126.8(6)	F21-C14-C13	120.8(6)
F21-C14-C15	115.9(9)	C13-C14-C15	123.2(9)
F29-C29-C30	121.0(9)	F29-C29-C28	119.6(6)
C30-C29-C28	119.4(8)	C2-C1-N3	109.0(5)
C2-C1-H1	125.5	N3-C1-H1	125.5

F11-C32-C33	114.4(7)	F11-C32-C31	119.8(6)
C33-C32-C31	125.8(6)	F5-C44-C45	115.2(7)
F5-C44-C43	119.8(7)	C45-C44-C43	125.0(8)
F6-C38-C37	118.7(6)	F6-C38-C39	117.7(6)
C37-C38-C39	123.5(7)	F8-C40-C39	120.6(7)
F8-C40-C41	119.7(7)	C39-C40-C41	119.6(6)
C16-C17-F24	118.6(12)	C16-C17-C18	118.9(10)
F24-C17-C18	122.5(14)	C18-C13-C14	111.3(7)
C18-C13-B02D	120.7(7)	C14-C13-B02D	127.9(6)
C59-O3-C60	107.4(11)	C44-C43-C48	113.5(7)
C44-C43-B02E	117.8(6)	C48-C43-B02E	128.5(6)
C4-C9-C8	120.8(5)	C4-C9-H9	119.6
C8-C9-H9	119.6	F30-C30-C29	115.6(7)
F30-C30-C25	120.4(6)	C29-C30-C25	124.1(9)
C17-C18-C13	127.8(11)	C17-C18-F25	115.0(9)
C13-C18-F25	117.2(7)	F9-C41-C40	120.2(6)
F9-C41-C42	120.9(7)	C40-C41-C42	118.9(7)
F16-C20-C19	121.8(6)	F16-C20-C21	114.9(6)
C19-C20-C21	123.3(7)	C9-C8-C7	120.3(6)
C9-C8-H8	119.9	C7-C8-H8	119.9
F7-C39-C40	120.3(7)	F7-C39-C38	119.7(8)
C40-C39-C38	120.0(6)	F12-C33-C34	118.8(7)
F12-C33-C32	121.4(7)	C34-C33-C32	119.8(8)
F18-C22-C21	121.4(7)	F18-C22-C23	119.7(7)
C21-C22-C23	118.9(6)	N1-C10-C7	115.4(6)
N1-C10-H10A	108.4	C7-C10-H10A	108.4
N1-C10-H10B	108.4	C7-C10-H10B	108.4
H10A-C10-H10B	107.5	C38-C37-C42	114.2(5)
C38-C37-B02E	119.8(6)	C42-C37-B02E	125.7(5)
F1-C48-C43	121.0(7)	F1-C48-C47	116.2(7)
C43-C48-C47	122.8(8)	N1-C12-H12A	109.5
N1-C12-H12B	109.5	H12A-C12-H12B	109.5
N1-C12-H12C	109.5	H12A-C12-H12C	109.5
H12B-C12-H12C	109.5	F13-C34-C33	122.5(10)
F13-C34-C35	120.4(9)	C33-C34-C35	116.9(7)
F28-C28-C27	123.0(10)	F28-C28-C29	119.3(9)
C27-C28-C29	117.5(6)	C22-C21-F17	119.7(6)
C22-C21-C20	120.8(7)	F17-C21-C20	119.5(7)

C16-C15-F22	123.2(10)	C16-C15-C14	119.0(11)
F22-C15-C14	117.8(10)	F14-C35-C36	120.8(11)
F14-C35-C34	118.8(9)	C36-C35-C34	120.5(7)
C27-C26-F26	115.4(8)	C27-C26-C25	124.0(9)
F26-C26-C25	120.6(6)	C26-C25-C30	113.2(6)
C26-C25-B02D	127.8(6)	C30-C25-B02D	118.7(7)
C32-C31-C36	112.9(7)	C32-C31-B02E	119.8(5)
C36-C31-B02E	126.8(7)	C17-C16-F23	122.7(14)
C17-C16-C15	119.7(9)	F23-C16-C15	117.6(16)
F15-C36-C35	114.9(7)	F15-C36-C31	121.0(8)
C35-C36-C31	124.2(9)	C26-C27-C28	121.7(9)
C26-C27-F27	118.8(9)	C28-C27-F27	119.4(7)
C61-O4-C64	108.8(13)	N1-C11-H11A	109.5
N1-C11-H11B	109.5	H11A-C11-H11B	109.5
N1-C11-H11C	109.5	H11A-C11-H11C	109.5
H11B-C11-H11C	109.5	C54-O2-C53	113.(2)
F2-C47-C46	121.5(9)	F2-C47-C48	118.0(9)
C46-C47-C48	120.5(8)	N1-Na1-O1	113.4(5)
N1-Na1-F2	91.5(3)	O1-Na1-F2	103.3(6)
F4-C45-C46	119.6(8)	F4-C45-C44	121.1(9)
C46-C45-C44	119.3(9)	N3-B02D-C13	113.2(6)
N3-B02D-C19	104.0(4)	C13-B02D-C19	114.8(5)
N3-B02D-C25	108.8(5)	C13-B02D-C25	103.5(5)
C19-B02D-C25	112.7(6)	N2-B02E-C43	103.4(5)
N2-B02E-C31	111.2(5)	C43-B02E-C31	113.3(5)
N2-B02E-C37	110.5(5)	C43-B02E-C37	116.2(5)
C31-B02E-C37	102.5(5)	F3-C46-C47	118.5(10)
F3-C46-C45	122.6(10)	C47-C46-C45	118.9(8)
O3-C59-C58	108.4(11)	O3-C59-H59A	110.0
C58-C59-H59A	110.0	O3-C59-H59B	110.0
C58-C59-H59B	110.0	H59A-C59-H59B	108.4
C64-C63-C62	101.4(17)	C64-C63-H63A	111.5
C62-C63-H63A	111.5	C64-C63-H63B	111.5
C62-C63-H63B	111.5	H63A-C63-H63B	109.3
O4-C61-C62	108.7(16)	O4-C61-H61A	110.0
C62-C61-H61A	110.0	O4-C61-H61B	110.0
C62-C61-H61B	110.0	H61A-C61-H61B	108.3
C57-C58-C59	103.3(14)	C57-C58-H58A	111.1

C59-C58-H58A	111.1	C57-C58-H58B	111.1
C59-C58-H58B	111.1	H58A-C58-H58B	109.1
O4-C64-C63	108.3(16)	O4-C64-H64A	110.0
C63-C64-H64A	110.0	O4-C64-H64B	110.0
C63-C64-H64B	110.0	H64A-C64-H64B	108.4
O3-C60-C57	112.8(12)	O3-C60-H60A	109.0
C57-C60-H60A	109.0	O3-C60-H60B	109.0
C57-C60-H60B	109.0	H60A-C60-H60B	107.8
C61-C62-C63	100.5(15)	C61-C62-H62A	111.7
C63-C62-H62A	111.7	C61-C62-H62B	111.7
C63-C62-H62B	111.7	H62A-C62-H62B	109.4
O2-C53-C56	107.1(18)	O2-C53-H53A	110.3
C56-C53-H53A	110.3	O2-C53-H53B	110.3
C56-C53-H53B	110.3	H53A-C53-H53B	108.5
O2-C54-C55	104.(2)	O2-C54-H54A	110.9
C55-C54-H54A	110.9	O2-C54-H54B	110.9
C55-C54-H54B	110.9	H54A-C54-H54B	108.9
C60-C57-C58	103.6(18)	C60-C57-H57A	111.0
C58-C57-H57A	111.0	C60-C57-H57B	111.0
C58-C57-H57B	111.0	H57A-C57-H57B	109.0
C56-C55-C54	104.6(19)	C56-C55-H55A	110.8
C54-C55-H55A	110.8	C56-C55-H55B	110.8
C54-C55-H55B	110.8	H55A-C55-H55B	108.9
C55-C56-C53	109.(2)	C55-C56-H56A	109.8
C53-C56-H56A	109.8	C55-C56-H56B	109.8
C53-C56-H56B	109.8	H56A-C56-H56B	108.3
C52-O1-C49	106.3(16)	C52-O1-Na1	103.8(16)
C49-O1-Na1	134.8(14)	O1-C52-C51	111.0(17)
O1-C52-H52A	109.4	C51-C52-H52A	109.4
O1-C52-H52B	109.4	C51-C52-H52B	109.4
H52A-C52-H52B	108.0	C50-C49-O1	109.6(12)
C50-C49-H49A	109.8	O1-C49-H49A	109.8
C50-C49-H49B	109.8	O1-C49-H49B	109.8
H49A-C49-H49B	108.2	C49-C50-C51	107.2(12)
C49-C50-H50A	110.3	C51-C50-H50A	110.3
C49-C50-H50B	110.3	C51-C50-H50B	110.3
H50A-C50-H50B	108.5	C52-C51-C50	105.1(14)
C52-C51-H51A	110.7	C50-C51-H51A	110.7

C52-C51-H51B	110.7	C50-C51-H51B	110.7		
H51A-C51-H51B	108.8				

Table 6. Anisotropic atomic displacement parameters (Å^2) for 5999.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F11	0.073(2)	0.027(2)	0.0491(19)	-0.0001(16)	0.0309(18)	0.0051(18)
F10	0.0466(18)	0.031(2)	0.0486(18)	-0.0004(16)	0.0206(15)	0.0022(16)
F20	0.0443(18)	0.030(2)	0.062(2)	-0.0019(17)	0.0126(16)	0.0043(16)
F16	0.0361(16)	0.026(2)	0.076(2)	-0.0059(18)	0.0184(16)	0.0020(15)
F6	0.0404(18)	0.053(3)	0.082(3)	-0.021(2)	0.0127(19)	-0.0122(19)
F30	0.0412(18)	0.035(2)	0.104(3)	0.005(2)	0.038(2)	0.0092(16)
F1	0.0381(17)	0.046(3)	0.079(3)	-0.008(2)	0.0114(17)	0.0029(18)
F21	0.053(2)	0.047(3)	0.086(3)	0.022(2)	0.042(2)	0.014(2)
F9	0.094(3)	0.043(3)	0.070(3)	0.004(2)	0.055(2)	0.009(2)
F19	0.080(3)	0.055(3)	0.064(2)	0.010(2)	0.029(2)	0.010(2)
F25	0.0343(19)	0.033(2)	0.155(5)	-0.033(3)	0.020(3)	-0.0063(17)
F5	0.076(3)	0.082(4)	0.061(2)	0.026(2)	0.037(2)	0.019(3)
F17	0.059(2)	0.050(3)	0.082(3)	-0.018(2)	0.030(2)	0.011(2)
N2	0.030(2)	0.024(3)	0.044(2)	-0.002(2)	0.0154(18)	-0.0016(19)
F26	0.0358(18)	0.069(3)	0.086(3)	-0.020(3)	-0.0019(19)	0.011(2)
F29	0.050(2)	0.040(3)	0.163(5)	0.009(3)	0.060(3)	0.010(2)
F12	0.124(4)	0.028(2)	0.097(3)	0.000(2)	0.072(3)	0.008(3)
F8	0.094(3)	0.055(3)	0.145(4)	-0.013(3)	0.091(4)	-0.016(3)
N1	0.032(2)	0.038(3)	0.070(3)	0.011(3)	0.021(2)	0.013(2)
F15	0.073(3)	0.093(4)	0.050(2)	-0.019(3)	0.003(2)	0.017(3)
F7	0.051(2)	0.063(3)	0.139(4)	-0.021(3)	0.043(3)	-0.026(2)
N3	0.030(2)	0.018(2)	0.055(3)	0.001(2)	0.0179(19)	0.0013(19)
F18	0.099(4)	0.083(4)	0.083(3)	-0.001(3)	0.050(3)	0.013(3)
F24	0.052(2)	0.025(3)	0.280(9)	-0.018(4)	0.066(4)	-0.011(2)
F2	0.067(3)	0.076(4)	0.113(4)	0.017(3)	-0.003(3)	0.032(3)
C3	0.029(2)	0.022(3)	0.039(2)	0.002(2)	0.013(2)	0.000(2)
F22	0.111(4)	0.089(5)	0.163(6)	0.082(5)	0.098(4)	0.055(4)
F28	0.034(2)	0.062(4)	0.185(6)	-0.023(4)	0.017(3)	0.013(2)
C2	0.035(3)	0.025(3)	0.052(3)	0.000(3)	0.020(2)	0.004(2)
F27	0.041(2)	0.105(5)	0.137(5)	-0.041(4)	-0.018(3)	0.025(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F14	0.091(4)	0.131(6)	0.082(3)	-0.071(4)	0.009(3)	0.004(4)
C7	0.027(2)	0.026(3)	0.057(3)	-0.009(3)	0.011(2)	0.003(2)
C23	0.042(3)	0.043(4)	0.055(4)	-0.004(3)	0.010(3)	0.001(3)
C5	0.027(2)	0.028(3)	0.040(3)	-0.002(2)	0.010(2)	-0.002(2)
C24	0.034(3)	0.038(4)	0.052(3)	-0.003(3)	0.008(2)	0.008(3)
C42	0.061(4)	0.018(3)	0.061(4)	0.000(3)	0.038(3)	0.001(3)
C6	0.033(2)	0.034(3)	0.041(3)	-0.004(3)	0.013(2)	0.002(2)
C4	0.024(2)	0.023(3)	0.050(3)	-0.005(2)	0.014(2)	-0.003(2)
C19	0.024(2)	0.026(3)	0.051(3)	-0.004(3)	0.000(2)	-0.002(2)
C14	0.038(3)	0.034(4)	0.115(6)	0.027(4)	0.045(4)	0.015(3)
C29	0.029(3)	0.024(4)	0.160(9)	-0.005(4)	0.042(4)	0.003(3)
F13	0.132(5)	0.071(4)	0.150(6)	-0.059(4)	0.078(5)	-0.017(4)
C1	0.032(2)	0.026(3)	0.056(3)	-0.002(3)	0.019(2)	0.002(2)
C32	0.054(3)	0.036(4)	0.051(3)	-0.016(3)	0.030(3)	-0.010(3)
C44	0.057(4)	0.067(6)	0.048(4)	0.011(4)	0.007(3)	0.006(4)
C38	0.044(3)	0.032(4)	0.066(4)	-0.014(3)	0.019(3)	-0.011(3)
C40	0.070(4)	0.035(4)	0.083(5)	-0.001(4)	0.054(4)	-0.001(3)
C17	0.041(4)	0.023(4)	0.213(13)	-0.005(6)	0.061(6)	-0.004(3)
F23	0.102(4)	0.053(4)	0.342(12)	0.088(6)	0.143(7)	0.035(3)
C13	0.028(3)	0.023(3)	0.098(5)	0.001(3)	0.032(3)	0.005(2)
O3	0.080(5)	0.107(7)	0.116(6)	-0.003(5)	0.013(4)	0.005(5)
C43	0.039(3)	0.046(4)	0.045(3)	-0.001(3)	0.004(2)	-0.004(3)
C9	0.028(2)	0.042(4)	0.058(3)	0.004(3)	0.018(2)	0.001(3)
C30	0.033(3)	0.023(3)	0.119(7)	-0.005(4)	0.030(4)	-0.002(3)
C18	0.024(3)	0.029(4)	0.137(8)	-0.004(5)	0.027(4)	-0.002(3)
F4	0.148(6)	0.154(8)	0.096(4)	0.077(5)	0.065(4)	0.045(6)
C41	0.070(4)	0.029(3)	0.061(4)	0.000(3)	0.041(3)	0.003(3)
C20	0.030(3)	0.033(4)	0.054(3)	-0.013(3)	0.004(2)	-0.003(2)
C8	0.035(3)	0.032(3)	0.047(3)	0.005(3)	0.008(2)	0.008(3)
C39	0.040(3)	0.027(4)	0.113(6)	-0.004(4)	0.034(4)	-0.014(3)
C33	0.071(4)	0.032(4)	0.075(5)	-0.010(4)	0.047(4)	-0.006(3)
C22	0.052(4)	0.053(5)	0.057(4)	-0.005(4)	0.021(3)	0.003(3)
C10	0.040(3)	0.041(4)	0.065(4)	-0.012(3)	0.007(3)	0.009(3)
C37	0.037(3)	0.024(3)	0.060(3)	-0.008(3)	0.026(3)	-0.003(2)
F3	0.145(6)	0.132(8)	0.100(4)	0.058(5)	0.020(4)	0.042(6)
C48	0.040(3)	0.045(4)	0.058(4)	-0.004(3)	0.004(3)	-0.003(3)
C12	0.050(4)	0.046(4)	0.077(5)	0.014(4)	0.030(3)	0.022(3)

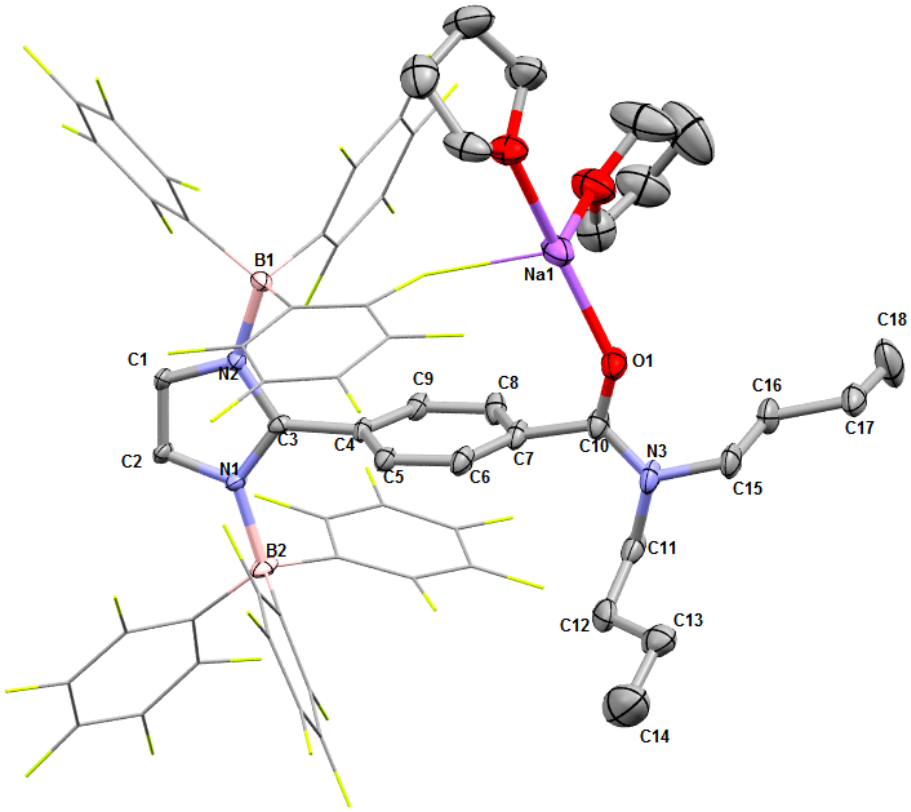
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C34	0.075(5)	0.047(5)	0.099(6)	-0.037(5)	0.052(5)	-0.016(4)
C28	0.027(3)	0.041(5)	0.152(9)	-0.021(5)	0.021(4)	0.007(3)
C21	0.043(3)	0.045(4)	0.057(4)	-0.014(3)	0.014(3)	0.007(3)
C15	0.057(4)	0.059(6)	0.156(9)	0.047(6)	0.076(5)	0.030(4)
C35	0.059(4)	0.085(7)	0.074(5)	-0.051(5)	0.024(4)	-0.014(5)
C26	0.035(3)	0.037(4)	0.101(6)	-0.016(4)	0.008(4)	0.001(3)
C25	0.029(3)	0.022(3)	0.094(5)	-0.007(3)	0.024(3)	0.000(2)
C31	0.045(3)	0.038(4)	0.046(3)	-0.012(3)	0.020(3)	-0.010(3)
C16	0.056(5)	0.031(5)	0.256(17)	0.045(8)	0.097(8)	0.017(4)
C36	0.051(4)	0.064(6)	0.062(4)	-0.019(4)	0.016(3)	-0.005(4)
C27	0.038(3)	0.040(5)	0.112(7)	-0.023(5)	-0.001(4)	0.003(3)
O4	0.1662(14)	0.1377(14)	0.1339(14)	0.0132(15)	0.0714(11)	0.0185(14)
C11	0.057(5)	0.042(5)	0.219(14)	0.008(7)	0.075(7)	0.002(4)
O2	0.1615(17)	0.2260(16)	0.1843(16)	-0.0626(15)	0.0216(16)	-0.0262(15)
C47	0.057(4)	0.057(6)	0.080(5)	0.004(5)	-0.008(4)	0.010(4)
Na1	0.254(10)	0.170(9)	0.156(6)	0.019(5)	0.092(6)	0.052(7)
C45	0.090(6)	0.096(8)	0.062(5)	0.040(5)	0.019(4)	0.024(6)
B02D	0.024(3)	0.023(4)	0.073(5)	-0.005(3)	0.014(3)	0.001(3)
B02E	0.033(3)	0.032(4)	0.041(3)	-0.005(3)	0.014(2)	-0.009(3)
C46	0.097(7)	0.101(9)	0.060(5)	0.046(6)	0.007(5)	0.019(7)
C59	0.076(6)	0.104(10)	0.103(7)	0.001(7)	0.014(6)	0.019(6)
C63	0.1662(14)	0.1377(14)	0.1339(14)	0.0132(15)	0.0714(11)	0.0185(14)
C61	0.1662(14)	0.1377(14)	0.1339(14)	0.0132(15)	0.0714(11)	0.0185(14)
C58	0.098(9)	0.147(18)	0.189(17)	0.048(14)	0.005(10)	-0.022(11)
C64	0.1662(14)	0.1377(14)	0.1339(14)	0.0132(15)	0.0714(11)	0.0185(14)
C60	0.067(6)	0.102(11)	0.156(12)	-0.033(10)	0.004(7)	0.013(7)
C62	0.1662(14)	0.1377(14)	0.1339(14)	0.0132(15)	0.0714(11)	0.0185(14)
C53	0.1615(17)	0.2260(16)	0.1843(16)	-0.0626(15)	0.0216(16)	-0.0262(15)
C54	0.1615(17)	0.2260(16)	0.1843(16)	-0.0626(15)	0.0216(16)	-0.0262(15)
C57	0.128(14)	0.135(18)	0.31(3)	0.08(2)	0.091(18)	0.033(14)
C55	0.1615(17)	0.2260(16)	0.1843(16)	-0.0626(15)	0.0216(16)	-0.0262(15)
C56	0.1615(17)	0.2260(16)	0.1843(16)	-0.0626(15)	0.0216(16)	-0.0262(15)
O1	0.1812(14)	0.2140(14)	0.1849(16)	0.0155(16)	0.0125(15)	-0.0106(13)
C52	0.1812(14)	0.2140(14)	0.1849(16)	0.0155(16)	0.0125(15)	-0.0106(13)
C49	0.1812(14)	0.2140(14)	0.1849(16)	0.0155(16)	0.0125(15)	-0.0106(13)
C50	0.1812(14)	0.2140(14)	0.1849(16)	0.0155(16)	0.0125(15)	-0.0106(13)
C51	0.1812(14)	0.2140(14)	0.1849(16)	0.0155(16)	0.0125(15)	-0.0106(13)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 5999.

	x/a	y/b	z/c	U(eq)
H2	0.7656	0.3427	0.3386	0.043
H5	0.5537	0.5058	0.5004	0.039
H6	0.4262	0.5964	0.5013	0.043
H1	0.9254	0.4201	0.4326	0.045
H9	0.5954	0.5945	0.2684	0.05
H8	0.4648	0.6838	0.2692	0.048
H10A	0.3627	0.7148	0.4598	0.063
H10B	0.3983	0.7546	0.3804	0.063
H12A	0.1922	0.7816	0.4067	0.084
H12B	0.0938	0.7706	0.3018	0.084
H12C	0.2106	0.8147	0.3149	0.084
H11A	0.2265	0.6063	0.3555	0.149
H11B	0.1014	0.6416	0.2966	0.149
H11C	0.1652	0.6568	0.4091	0.149
H59A	0.1936	0.2815	-0.0560	0.12
H59B	0.1854	0.3113	0.0417	0.12
H63A	-0.1530	0.1793	0.2382	0.17
H63B	-0.2379	0.1918	0.1275	0.17
H61A	-0.1459	0.3113	0.0514	0.17
H61B	-0.0182	0.3271	0.1316	0.17
H58A	0.2427	0.4152	-0.0012	0.19
H58B	0.2063	0.3911	-0.1116	0.19
H64A	0.0057	0.1666	0.2025	0.17
H64B	-0.0916	0.1332	0.1077	0.17
H60A	-0.0789	0.3831	-0.0729	0.142
H60B	-0.0616	0.3687	-0.1721	0.142
H62A	-0.2052	0.3083	0.1771	0.17
H62B	-0.0738	0.2917	0.2528	0.17
H53A	-0.0327	0.6073	0.1823	0.243
H53B	0.0606	0.5675	0.1470	0.243
H54A	-0.1349	0.6196	-0.0889	0.243
H54B	-0.2111	0.6524	-0.0310	0.243
H57A	0.0628	0.4578	-0.0264	0.227

	x/a	y/b	z/c	U(eq)
H57B	0.0487	0.4599	-0.1377	0.227
H55A	-0.2670	0.5333	-0.0086	0.243
H55B	-0.1711	0.5008	-0.0477	0.243
H56A	-0.0631	0.4786	0.0938	0.243
H56B	-0.1539	0.5168	0.1330	0.243
H52A	0.3173	0.8712	0.1300	0.251
H52B	0.3382	0.8715	0.0304	0.251
H49A	0.5472	0.7601	0.2221	0.251
H49B	0.5620	0.7544	0.1202	0.251
H50A	0.6278	0.8554	0.1326	0.251
H50B	0.6305	0.8564	0.2407	0.251
H51A	0.4794	0.9269	0.2006	0.251
H51B	0.4911	0.9356	0.0976	0.251

Crystal Structure Report for Na[IMP-DBA]



Thermal ellipsoid plot of 5991. Ellipsoids shown at 50% probability, C_6F_5 rings shown in wireframe, DCM solvate and hydrogen atoms hidden for clarity.

A specimen of $C_{126}H_{84}B_4Cl_4F_{60}N_6Na_2O_6$, approximate dimensions 0.108 mm x 0.266 mm x 0.467 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å). The integration of the data using a monoclinic unit cell yielded a total of 118693 reflections to a maximum θ angle of 27.93° (0.76Å resolution), of which 30809 were independent (average redundancy 3.853, completeness = 99.4%, R_{int} = 4.44%, R_{sig} =5.80%) and 18582 (60.31%) were greater than $2\sigma(F^2)$. The final cell constants of a = 33.184(3) Å, b = 15.7566(14) Å, c =26.172(2) Å, β = 109.217(2)°, volume = 12922.(2) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8950 and 0.9740. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/c 1, with Z =4 for the formula unit, $C_{126}H_{84}B_4Cl_4F_{60}N_6Na_2O_6$. The final anisotropic full-matrix least-squares refinement on F^2 with 1925variables converged at R1 = 9.33%, for the observed data and wR2 = 28.26% for all data. The goodness-of-fit was 1.040. The largest peak in the final difference electron density

synthesis was 1.105 $e^-/Å^3$ and the largest hole was -1.557 $e^-/Å^3$ with an RMS deviation of 0.109 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.619 g/cm^3 and F(000), 6320 e^-.

Table 1. Sample and crystal data for 5991.

Identification code	5991	
Chemical formula	$C_{126}H_{84}B_4Cl_4F_{60}N_6Na_2O_6$	
Formula weight	3149.01 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.108 x 0.266 x 0.467 mm	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 33.184(3) Å	α = 90°
	b = 15.7566(14) Å	β = 109.217(2)°
	c = 26.172(2) Å	γ = 90°
Volume	12922.(2) $Å^3$	
Z	4	
Density (calculated)	1.619 g/cm^3	
Absorption coefficient	0.244 mm^{-1}	
F(000)	6320	

Table 2. Data collection and structure refinement for 5991.

Theta range for data collection	1.30 to 27.93°	
Index ranges	-43<=h<=43, -20<=k<=17, -34<=l<=16	
Reflections collected	118693	
Independent reflections	30809 [R(int) = 0.0444]	
Max. and min. transmission	0.9740 and 0.8950	
Structure solution technique	direct methods	
Structure solution program	SHELXT 2014/4 (Sheldrick, 2014)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	30809 / 149 / 1925	
Goodness-of-fit on F^2	1.040	
Final R indices	18582 data; I>2σ(I)	R1 = 0.0933, wR2 = 0.2463
	all data	R1 = 0.1486, wR2 = 0.2826

Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.1259P)^2+40.0219P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	1.105 and -1.557 eÅ^{-3}
R.M.S. deviation from mean	0.109 eÅ^{-3}

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 5991.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij}tensor.

	x/a	y/b	z/c	U(eq)
Cl3	0.75893(5)	0.51350(11)	0.22575(8)	0.0622(4)
Cl4	0.76923(6)	0.35215(12)	0.17844(10)	0.0788(6)
Na1	0.95906(6)	0.05658(12)	0.80076(7)	0.0377(5)
Cl2	0.73839(6)	0.48985(13)	0.75402(11)	0.0915(7)
Cl1	0.73336(7)	0.64531(13)	0.81096(12)	0.1003(8)
F30	0.92126(7)	0.70225(15)	0.59600(9)	0.0219(5)
F40	0.58263(7)	0.29092(14)	0.39585(9)	0.0214(5)
F50	0.53408(8)	0.36560(15)	0.28215(9)	0.0249(5)
F31	0.64183(8)	0.41540(15)	0.45650(9)	0.0254(5)
F10	0.85888(8)	0.60202(15)	0.79040(9)	0.0255(5)
Na2	0.53809(7)	0.94286(13)	0.19189(8)	0.0487(6)
F45	0.64282(7)	0.39546(15)	0.20005(10)	0.0258(5)
F12	0.97166(8)	0.63613(15)	0.71696(9)	0.0257(5)
F16	0.86427(7)	0.57441(15)	0.53725(9)	0.0255(5)
F56	0.68228(8)	0.06644(15)	0.45346(10)	0.0286(6)
F26	0.80123(8)	0.80739(16)	0.45495(9)	0.0285(6)
F21	0.75747(8)	0.69533(16)	0.60298(10)	0.0311(6)
F36	0.70191(8)	0.17886(16)	0.53507(9)	0.0292(6)
F25	0.81982(7)	0.92139(15)	0.53584(10)	0.0275(6)
F32	0.67755(9)	0.53152(17)	0.53090(10)	0.0357(6)
F60	0.74522(8)	0.29044(16)	0.38544(11)	0.0331(6)
F41	0.49495(8)	0.35528(19)	0.16740(10)	0.0361(7)
F46	0.55090(9)	0.09657(16)	0.21085(10)	0.0351(6)
F20	0.72934(8)	0.71087(17)	0.48760(10)	0.0341(6)
F35	0.77498(8)	0.27298(17)	0.50070(11)	0.0371(7)
F39	0.53223(8)	0.24091(18)	0.44945(11)	0.0351(6)
F44	0.62530(9)	0.52677(17)	0.13295(11)	0.0349(6)
F17	0.83093(9)	0.45455(16)	0.46496(10)	0.0361(6)

	x/a	y/b	z/c	U(eq)
F57	0.73879(9)	0.96048(16)	0.43860(11)	0.0379(7)
F24	0.76255(8)	0.02616(16)	0.54989(11)	0.0371(7)
F33	0.76103(10)	0.51563(19)	0.59448(10)	0.0438(8)
F29	0.97122(8)	0.7489(2)	0.54110(11)	0.0391(7)
F11	0.94715(9)	0.90729(17)	0.77825(10)	0.0363(6)
F18	0.74772(10)	0.46501(19)	0.39950(10)	0.0442(8)
F37	0.65012(9)	0.13266(19)	0.58951(10)	0.0404(7)
F19	0.69765(9)	0.5921(2)	0.41534(11)	0.0459(8)
F34	0.80890(9)	0.3876(2)	0.57450(11)	0.0475(8)
F49	0.48070(9)	0.2979(2)	0.32673(11)	0.0404(7)
F27	0.85294(9)	0.85285(19)	0.39991(10)	0.0402(7)
F9	0.87779(10)	0.47644(18)	0.86167(11)	0.0424(7)
F22	0.70185(9)	0.8046(2)	0.62062(13)	0.0488(8)
F1	0.82112(9)	0.74954(19)	0.74138(13)	0.0442(7)
F55	0.67728(9)	0.24143(18)	0.23891(14)	0.0450(8)
F43	0.54266(10)	0.5725(2)	0.08038(12)	0.0455(8)
F6	0.00630(8)	0.6625(2)	0.83410(10)	0.0451(8)
F13	0.02781(9)	0.7038(2)	0.67654(12)	0.0425(7)
F38	0.56448(9)	0.1605(2)	0.54697(12)	0.0453(8)
F51	0.53342(10)	0.20716(19)	0.12720(11)	0.0440(7)
F47	0.49408(10)	0.03293(18)	0.25005(13)	0.0485(8)
F59	0.79932(10)	0.1795(2)	0.36609(15)	0.0514(8)
F15	0.00635(10)	0.97094(18)	0.74353(12)	0.0460(8)
F42	0.47906(9)	0.4833(2)	0.09824(12)	0.0521(9)
F23	0.70258(9)	0.9706(2)	0.59188(14)	0.0495(8)
F58	0.79814(10)	0.0140(2)	0.39479(14)	0.0510(8)
F28	0.93876(10)	0.8246(2)	0.44268(12)	0.0486(8)
F48	0.45759(9)	0.1314(2)	0.30925(13)	0.0526(9)
F5	0.95973(12)	0.8059(2)	0.86406(11)	0.0518(9)
F14	0.04747(9)	0.8719(2)	0.69029(13)	0.0513(9)
N2	0.88584(10)	0.69256(19)	0.70653(12)	0.0158(6)
N5	0.61744(10)	0.30427(19)	0.28478(12)	0.0160(6)
N1	0.84734(10)	0.69456(19)	0.61964(12)	0.0156(6)
O1	0.92426(10)	0.12172(19)	0.72167(13)	0.0314(7)
F7	0.02342(10)	0.5432(3)	0.90851(12)	0.0656(12)
N4	0.65649(10)	0.29674(19)	0.37163(12)	0.0172(7)
F8	0.96061(12)	0.4446(2)	0.92238(13)	0.0631(11)

	x/a	y/b	z/c	U(eq)
O3	0.01278(11)	0.0051(2)	0.87333(13)	0.0387(8)
O4	0.57661(12)	0.8721(2)	0.26755(16)	0.0490(10)
O6	0.48140(12)	0.9939(2)	0.12195(14)	0.0451(9)
N3	0.87961(12)	0.1620(2)	0.64069(15)	0.0269(8)
F54	0.70249(15)	0.1648(2)	0.1650(2)	0.0907(16)
C67	0.63412(11)	0.2515(2)	0.32767(14)	0.0152(7)
C3	0.86886(11)	0.7424(2)	0.66255(14)	0.0147(7)
F52	0.55955(16)	0.1290(2)	0.05340(14)	0.0814(14)
N6	0.62225(12)	0.8320(2)	0.34740(16)	0.0314(9)
C2	0.85099(12)	0.6117(2)	0.63700(15)	0.0172(8)
O2	0.90718(14)	0.0785(3)	0.84161(16)	0.0566(11)
C1	0.87462(12)	0.6102(2)	0.68977(15)	0.0174(8)
C66	0.62997(12)	0.3852(2)	0.30330(15)	0.0180(8)
C65	0.65415(12)	0.3804(2)	0.35585(15)	0.0190(8)
C62	0.90068(14)	0.5864(3)	0.81638(15)	0.0221(9)
C4	0.87345(12)	0.8361(2)	0.66218(15)	0.0168(8)
C110	0.60150(13)	0.4166(2)	0.17730(15)	0.0201(8)
C109	0.57068(13)	0.3692(2)	0.18951(14)	0.0179(8)
C97	0.64515(13)	0.2307(2)	0.46022(15)	0.0206(8)
C38	0.90203(13)	0.7430(3)	0.54839(15)	0.0222(8)
C68	0.62847(12)	0.1576(2)	0.32627(15)	0.0172(8)
C40	0.82221(13)	0.5805(3)	0.50945(15)	0.0222(9)
C39	0.79900(13)	0.6481(3)	0.51892(15)	0.0210(8)
C116	0.52508(13)	0.2831(3)	0.27202(16)	0.0234(9)
F2	0.78766(15)	0.8298(3)	0.8060(2)	0.0946(16)
C73	0.59711(13)	0.1215(2)	0.34426(16)	0.0202(8)
C41	0.80598(15)	0.5174(3)	0.47108(16)	0.0251(9)
C32	0.79009(13)	0.8869(3)	0.55442(16)	0.0237(9)
C102	0.60172(13)	0.2479(3)	0.44272(15)	0.0215(8)
C57	0.93119(13)	0.6364(3)	0.80567(14)	0.0209(8)
C9	0.84652(13)	0.8893(2)	0.67794(16)	0.0214(8)
C72	0.59050(13)	0.0344(2)	0.34138(17)	0.0245(9)
C92	0.68397(13)	0.4059(3)	0.48368(15)	0.0232(9)
C34	0.84370(13)	0.7950(3)	0.47841(16)	0.0242(9)
C33	0.85855(13)	0.7585(3)	0.53038(15)	0.0199(8)
C5	0.90570(12)	0.8720(2)	0.64564(15)	0.0200(8)
C7	0.88640(13)	0.0116(2)	0.66564(17)	0.0231(9)

	x/a	y/b	z/c	U(eq)
C93	0.70136(15)	0.4672(3)	0.52331(16)	0.0271(10)
C27	0.79073(12)	0.8011(3)	0.56617(16)	0.0221(8)
F4	0.92509(19)	0.8882(3)	0.92836(16)	0.0989(17)
C51	0.95704(13)	0.7659(3)	0.75172(15)	0.0216(8)
C98	0.65973(13)	0.1927(3)	0.51159(17)	0.0255(9)
C28	0.76013(13)	0.7775(3)	0.58958(17)	0.0259(9)
C111	0.59348(15)	0.4848(3)	0.14181(17)	0.0253(9)
C113	0.52005(14)	0.4620(3)	0.12467(17)	0.0303(10)
C91	0.70607(13)	0.3378(3)	0.47221(15)	0.0223(9)
C71	0.61549(13)	0.9825(2)	0.32176(18)	0.0276(10)
C115	0.54449(13)	0.2367(3)	0.24164(15)	0.0221(9)
C35	0.86940(15)	0.8176(3)	0.44892(17)	0.0297(10)
C96	0.74867(14)	0.3350(3)	0.50487(16)	0.0278(10)
C108	0.71167(13)	0.0999(3)	0.43423(16)	0.0243(9)
C112	0.55182(16)	0.5071(3)	0.11515(16)	0.0292(10)
C6	0.91227(13)	0.9591(2)	0.64797(16)	0.0226(8)
C99	0.63378(15)	0.1692(3)	0.54076(17)	0.0300(10)
C42	0.76422(16)	0.5223(3)	0.43830(16)	0.0324(11)
C101	0.57445(13)	0.2239(3)	0.47008(17)	0.0271(9)
C8	0.85306(13)	0.9771(3)	0.67989(17)	0.0247(9)
C52	0.97922(13)	0.7197(3)	0.72507(16)	0.0251(9)
C44	0.75666(14)	0.6483(3)	0.48521(16)	0.0279(10)
C31	0.76144(14)	0.9437(3)	0.56226(18)	0.0295(10)
C53	0.00946(14)	0.7535(3)	0.70425(17)	0.0304(10)
C103	0.71169(13)	0.1865(3)	0.42270(16)	0.0244(9)
C43	0.73954(14)	0.5868(3)	0.44604(17)	0.0324(11)
C69	0.65408(13)	0.1051(2)	0.30756(18)	0.0250(9)
C70	0.64749(14)	0.0171(3)	0.3053(2)	0.0307(10)
C114	0.52916(14)	0.3952(3)	0.16092(16)	0.0246(9)
C95	0.76715(15)	0.3941(3)	0.54505(17)	0.0334(11)
C55	0.99906(15)	0.8865(3)	0.73860(19)	0.0348(11)
C119	0.50255(15)	0.1177(3)	0.25596(18)	0.0315(11)
C37	0.92917(13)	0.7650(3)	0.52060(18)	0.0280(10)
C104	0.74184(14)	0.2086(3)	0.39872(18)	0.0288(10)
F53	0.6440(2)	0.1075(3)	0.0705(2)	0.1082(19)
C61	0.90933(16)	0.5214(3)	0.85446(17)	0.0310(10)
C10	0.89812(13)	0.1038(3)	0.67732(17)	0.0236(9)

	x/a	y/b	z/c	U(eq)
C45	0.89280(16)	0.7784(3)	0.79812(18)	0.0306(9)
C29	0.73117(14)	0.8326(3)	0.59868(19)	0.0336(11)
C121	0.60374(16)	0.2235(3)	0.18843(18)	0.0302(10)
C56	0.96827(14)	0.8511(3)	0.75694(17)	0.0290(10)
C30	0.73125(14)	0.9160(3)	0.5847(2)	0.0334(11)
C94	0.74368(16)	0.4594(3)	0.55483(16)	0.0336(12)
C15	0.88809(15)	0.2523(3)	0.65554(19)	0.0294(10)
C107	0.74041(14)	0.0428(3)	0.42602(19)	0.0328(11)
C120	0.53214(14)	0.1523(3)	0.23520(17)	0.0288(10)
C117	0.49629(14)	0.2493(3)	0.29536(18)	0.0309(10)
C105	0.77057(14)	0.1520(3)	0.3888(2)	0.0353(11)
C60	0.95108(18)	0.5063(3)	0.88487(18)	0.0415(14)
C58	0.97281(15)	0.6186(3)	0.83822(16)	0.0328(11)
C100	0.59050(16)	0.1839(3)	0.51956(19)	0.0332(10)
C106	0.77021(14)	0.0690(3)	0.4029(2)	0.0351(11)
O5	0.58309(19)	0.9142(4)	0.1419(3)	0.0992(13)
C54	0.01914(15)	0.8380(3)	0.71097(19)	0.0358(12)
C118	0.48482(14)	0.1657(3)	0.28661(19)	0.0355(11)
C16	0.85825(17)	0.2828(3)	0.6852(2)	0.0345(11)
C126	0.57506(18)	0.1951(3)	0.1386(2)	0.0379(12)
C36	0.91281(16)	0.8033(3)	0.47036(18)	0.0333(11)
C59	0.98242(17)	0.5556(4)	0.87714(18)	0.0414(14)
F3	0.8391(2)	0.9009(3)	0.9011(2)	0.135(3)
C46	0.84859(19)	0.7847(3)	0.7863(2)	0.0411(11)
C17	0.86278(16)	0.3773(3)	0.69994(19)	0.0343(11)
C74	0.60366(14)	0.8902(3)	0.3112(2)	0.0318(11)
C122	0.64601(16)	0.2124(3)	0.1946(2)	0.0365(11)
C11	0.84721(15)	0.1426(3)	0.58799(19)	0.0320(11)
C79	0.61414(17)	0.7412(3)	0.3338(2)	0.0383(12)
B4	0.58413(14)	0.2815(3)	0.22634(17)	0.0177(9)
C50	0.9170(2)	0.8137(3)	0.8474(2)	0.0446(12)
B2	0.82366(13)	0.7280(3)	0.55937(17)	0.0189(9)
B1	0.91681(15)	0.7201(3)	0.76498(17)	0.0195(9)
C75	0.6550(2)	0.8514(4)	0.4003(2)	0.0534(11)
C81	0.64125(18)	0.6166(3)	0.2912(2)	0.0428(13)
B3	0.67989(14)	0.2609(3)	0.43130(17)	0.0198(9)
C80	0.64562(19)	0.7091(3)	0.3064(2)	0.0455(13)

	x/a	y/b	z/c	U(eq)
C25	0.0642(2)	0.9118(4)	0.9252(3)	0.0549(16)
C123	0.6606(2)	0.1729(4)	0.1562(3)	0.0600(19)
C125	0.5885(2)	0.1547(4)	0.0999(2)	0.0541(17)
C26	0.05332(17)	0.9688(4)	0.8778(2)	0.0488(15)
C124	0.6310(3)	0.1449(4)	0.1089(3)	0.064(2)
C18	0.8292(3)	0.4054(4)	0.7237(3)	0.0648(19)
C64	0.73558(17)	0.4149(4)	0.2007(3)	0.0544(16)
C49	0.8999(3)	0.8554(4)	0.8819(3)	0.0645(15)
C23	0.0124(2)	0.0169(4)	0.9267(2)	0.0561(16)
C48	0.8560(3)	0.8607(4)	0.8670(3)	0.0735(16)
C82	0.6764(2)	0.5870(4)	0.2705(3)	0.0648(19)
C47	0.8305(2)	0.8263(4)	0.8201(3)	0.0595(14)
C19	0.86407(19)	0.0752(4)	0.8080(3)	0.0530(15)
C88	0.4286(2)	0.0849(4)	0.0699(3)	0.067(2)
C87	0.4422(2)	0.0337(5)	0.1199(2)	0.068(2)
C24	0.0452(2)	0.9565(5)	0.9628(2)	0.0636(19)
C90	0.4786(3)	0.9770(5)	0.0678(2)	0.070(2)
C63	0.7633(2)	0.5859(5)	0.7808(4)	0.081(2)
C22	0.9094(2)	0.1286(7)	0.8885(3)	0.089(3)
C89	0.4476(3)	0.0401(6)	0.0330(3)	0.078(2)
C12	0.8648(3)	0.1210(6)	0.5424(3)	0.036(2)
C83	0.5812(3)	0.8374(6)	0.1081(4)	0.0995(13)
C14	0.9071(3)	0.1630(5)	0.4847(3)	0.079(2)
C76	0.6453(3)	0.8255(7)	0.4488(4)	0.0561(11)
C13	0.8909(3)	0.1896(7)	0.5292(3)	0.040(3)
C20	0.8380(2)	0.1170(6)	0.8378(3)	0.072(2)
C21	0.8701(3)	0.1693(6)	0.8786(4)	0.100(3)
C78	0.5955(2)	0.8446(4)	0.5038(3)	0.0615(12)
C77	0.6069(4)	0.8710(7)	0.4502(4)	0.0591(12)
C86	0.6274(3)	0.9317(6)	0.1671(4)	0.1011(13)
C85	0.6529(3)	0.8704(6)	0.1555(4)	0.1022(13)
C84	0.6229(4)	0.8442(11)	0.1000(7)	0.1006(13)
C84A	0.6147(5)	0.7824(10)	0.1412(6)	0.050(5)
C76A	0.6378(10)	0.875(2)	0.4469(14)	0.104(13)
C77A	0.6085(10)	0.8116(18)	0.4611(10)	0.078(9)
C12A	0.8583(6)	0.1757(14)	0.5391(7)	0.052(7)
C13A	0.8974(9)	0.133(2)	0.5356(15)	0.106(13)

Table 4. Bond lengths (Å) for 5991.

Cl3-C64	1.763(6)	Cl4-C64	1.731(7)
Na1-O1	2.258(4)	Na1-O3	2.283(4)
Na1-O2	2.332(5)	Na1-F13	2.398(4)
Na1-F11	2.426(3)	Na1-F12	2.788(3)
Na1-F15	2.842(4)	Cl2-C63	1.755(8)
Cl1-C63	1.734(9)	F30-C38	1.360(4)
F40-C102	1.361(4)	F50-C116	1.341(5)
F50-Na2	2.958(3)	F31-C92	1.353(5)
F10-C62	1.351(5)	Na2-O4	2.266(4)
Na2-O6	2.296(4)	Na2-O5	2.331(7)
Na2-F49	2.376(4)	Na2-F46	2.481(3)
Na2-F47	2.816(4)	F45-C110	1.345(5)
F12-C52	1.345(5)	F16-C40	1.348(5)
F56-C108	1.343(5)	F26-C34	1.353(5)
F21-C28	1.351(5)	F36-C98	1.348(5)
F25-C32	1.349(5)	F32-C93	1.340(6)
F60-C104	1.350(5)	F41-C114	1.357(5)
F46-C120	1.352(5)	F20-C44	1.355(6)
F35-C96	1.338(6)	F39-C101	1.352(5)
F44-C111	1.329(5)	F17-C41	1.334(5)
F57-C107	1.344(5)	F24-C31	1.342(5)
F33-C94	1.342(5)	F29-C37	1.344(5)
F11-C56	1.358(5)	F18-C42	1.334(5)
F37-C99	1.341(5)	F19-C43	1.360(5)
F34-C95	1.350(5)	F49-C117	1.345(5)
F27-C35	1.338(5)	F9-C61	1.328(6)
F22-C29	1.356(5)	F1-C46	1.347(7)
F55-C122	1.356(6)	F43-C112	1.342(5)
F6-C58	1.343(6)	F13-C53	1.342(6)
F38-C100	1.343(5)	F51-C126	1.328(6)
F47-C119	1.363(5)	F59-C105	1.352(6)
F15-C55	1.351(5)	F42-C113	1.350(5)
F23-C30	1.340(5)	F58-C106	1.335(6)
F28-C36	1.338(5)	F48-C118	1.346(5)
F5-C50	1.346(7)	F14-C54	1.341(5)

N2-C3	1.354(5)	N2-C1	1.381(5)
N2-B1	1.597(5)	N5-C67	1.360(5)
N5-C66	1.378(5)	N5-B4	1.605(5)
N1-C3	1.346(5)	N1-C2	1.374(5)
N1-B2	1.602(5)	O1-C10	1.231(5)
F7-C59	1.352(6)	N4-C67	1.349(5)
N4-C65	1.376(5)	N4-B3	1.601(5)
F8-C60	1.343(5)	O3-C23	1.412(6)
O3-C26	1.431(6)	O4-C74	1.231(5)
O6-C90	1.413(7)	O6-C87	1.428(7)
N3-C10	1.323(5)	N3-C11	1.475(6)
N3-C15	1.476(5)	F54-C123	1.337(8)
C67-C68	1.490(5)	C3-C4	1.484(5)
F52-C125	1.341(7)	N6-C74	1.318(6)
N6-C79	1.477(5)	N6-C75	1.484(7)
C2-C1	1.346(5)	C2-H2	0.95
O2-C19	1.412(7)	O2-C22	1.439(8)
C1-H1	0.95	C66-C65	1.347(5)
C66-H66	0.95	C65-H65	0.95
C62-C57	1.382(6)	C62-C61	1.391(6)
C4-C9	1.383(6)	C4-C5	1.400(6)
C110-C109	1.386(6)	C110-C111	1.388(6)
C109-C114	1.395(6)	C109-B4	1.659(6)
C97-C102	1.388(6)	C97-C98	1.404(5)
C97-B3	1.644(6)	C38-C37	1.376(6)
C38-C33	1.384(6)	C68-C69	1.385(6)
C68-C73	1.396(6)	C40-C39	1.384(6)
C40-C41	1.389(6)	C39-C44	1.391(5)
C39-B2	1.674(6)	C116-C115	1.385(6)
C116-C117	1.398(6)	F2-C47	1.347(8)
C73-C72	1.388(5)	C73-H73	0.95
C41-C42	1.371(6)	C32-C31	1.370(6)
C32-C27	1.386(6)	C102-C101	1.379(6)
C57-C58	1.392(6)	C57-B1	1.664(6)
C9-C8	1.399(6)	C9-H9	0.95
C72-C71	1.379(6)	C72-H72	0.95
C92-C91	1.388(6)	C92-C93	1.395(6)
C34-C35	1.372(6)	C34-C33	1.408(5)

C33-B2	1.651(6)	C5-C6	1.388(5)
C5-H5	0.95	C7-C6	1.376(6)
C7-C8	1.389(6)	C7-C10	1.510(5)
C93-C94	1.380(7)	C27-C28	1.398(6)
C27-B2	1.638(6)	F4-C49	1.333(8)
C51-C52	1.377(6)	C51-C56	1.388(6)
C51-B1	1.652(6)	C98-C99	1.377(6)
C28-C29	1.373(7)	C111-C112	1.373(6)
C113-C112	1.361(7)	C113-C114	1.382(6)
C91-C96	1.391(5)	C91-B3	1.660(6)
C71-C70	1.383(7)	C71-C74	1.507(6)
C115-C120	1.384(6)	C115-B4	1.655(6)
C35-C36	1.381(7)	C96-C95	1.388(6)
C108-C107	1.378(6)	C108-C103	1.398(6)
C6-H6	0.95	C99-C100	1.378(7)
C42-C43	1.362(7)	C101-C100	1.380(6)
C8-H8	0.95	C52-C53	1.395(6)
C44-C43	1.389(6)	C31-C30	1.388(7)
C53-C54	1.368(7)	C103-C104	1.389(6)
C103-B3	1.642(6)	C69-C70	1.402(6)
C69-H69	0.95	C70-H70	0.95
C95-C94	1.365(8)	C55-C54	1.367(8)
C55-C56	1.381(7)	C119-C118	1.369(7)
C119-C120	1.382(7)	C37-C36	1.385(6)
C104-C105	1.391(7)	F53-C124	1.352(7)
C61-C60	1.372(7)	C45-C50	1.391(7)
C45-C46	1.400(8)	C45-B1	1.639(6)
C29-C30	1.365(7)	C121-C122	1.370(7)
C121-C126	1.411(7)	C121-B4	1.633(6)
C15-C16	1.524(7)	C15-H15A	0.99
C15-H15B	0.99	C107-C106	1.381(7)
C117-C118	1.369(7)	C105-C106	1.360(7)
C60-C59	1.366(8)	C58-C59	1.382(6)
O5-C86	1.427(10)	O5-C83	1.486(10)
C16-C17	1.533(6)	C16-H16A	0.99
C16-H16B	0.99	C126-C125	1.389(7)
F3-C48	1.357(7)	C46-C47	1.386(7)
C17-C18	1.512(8)	C17-H17A	0.99

C17-H17B	0.99	C122-C123	1.397(8)
C11-C12	1.530(10)	C11-C12A	1.53(2)
C11-H11A	0.99	C11-H11B	0.99
C11-H11C	0.99	C11-H11D	0.99
C79-C80	1.535(8)	C79-H79A	0.99
C79-H79B	0.99	C50-C49	1.380(8)
C75-C76	1.466(13)	C75-C76A	1.55(4)
C75-H75A	0.99	C75-H75B	0.99
C75-H75C	0.99	C75-H75D	0.99
C81-C80	1.504(7)	C81-C82	1.512(9)
C81-H81A	0.99	C81-H81B	0.99
C80-H80A	0.99	C80-H80B	0.99
C25-C26	1.479(8)	C25-C24	1.506(9)
C25-H25A	0.99	C25-H25B	0.99
C123-C124	1.376(10)	C125-C124	1.360(10)
C26-H26A	0.99	C26-H26B	0.99
C18-H18A	0.98	C18-H18B	0.98
C18-H18C	0.98	C64-H64A	0.99
C64-H64B	0.99	C49-C48	1.380(11)
C23-C24	1.518(8)	C23-H23A	0.99
C23-H23B	0.99	C48-C47	1.354(11)
C82-H82A	0.98	C82-H82B	0.98
C82-H82C	0.98	C19-C20	1.492(9)
C19-H19A	0.99	C19-H19B	0.99
C88-C87	1.474(10)	C88-C89	1.494(10)
C88-H88A	0.99	C88-H88B	0.99
C87-H87A	0.99	C87-H87B	0.99
C24-H24A	0.99	C24-H24B	0.99
C90-C89	1.502(9)	C90-H90A	0.99
C90-H90B	0.99	C63-H63A	0.99
C63-H63B	0.99	C22-C21	1.401(10)
C22-H22A	0.99	C22-H22B	0.99
C89-H89A	0.99	C89-H89B	0.99
C12-C13	1.495(14)	C12-H12A	0.99
C12-H12B	0.99	C83-C84A	1.452(16)
C83-C84	1.474(16)	C83-H83A	0.99
C83-H83B	0.99	C83-H83C	0.99
C83-H83D	0.99	C14-C13	1.495(11)

C14-C13A	1.55(4)	C14-H14A	0.98
C14-H14B	0.98	C14-H14C	0.98
C14-H14D	0.98	C14-H14E	0.98
C14-H14F	0.98	C76-C77	1.473(15)
C76-H76A	0.99	C76-H76B	0.99
C13-H13A	0.99	C13-H13B	0.99
C20-C21	1.485(11)	C20-H20A	0.99
C20-H20B	0.99	C21-H21A	0.99
C21-H21B	0.99	C78-C77A	1.42(2)
C78-C77	1.622(13)	C78-H78A	0.98
C78-H78B	0.98	C78-H78C	0.98
C78-H78D	0.98	C78-H78E	0.98
C78-H78F	0.98	C77-H77A	0.99
C77-H77B	0.99	C86-C85	1.382(12)
C86-H86A	0.99	C86-H86B	0.99
C85-C84	1.524(17)	C85-C84A	1.832(18)
C85-H85A	0.99	C85-H85B	0.99
C85-H85C	0.99	C85-H85D	0.99
C84-H84A	0.99	C84-H84B	0.99
C84A-H84C	0.99	C84A-H84D	0.99
C76A-C77A	1.53(4)	C76A-H76C	0.99
C76A-H76D	0.99	C77A-H77C	0.99
C77A-H77D	0.99	C12A-C13A	1.49(4)
C12A-H12C	0.99	C12A-H12D	0.99
C13A-H13C	0.99	C13A-H13D	0.99

Table 5. Bond angles (°) for 5991.

O1-Na1-O3	161.37(17)	O1-Na1-O2	96.95(15)
O3-Na1-O2	99.41(15)	O1-Na1-F13	77.52(12)
O3-Na1-F13	96.26(14)	O2-Na1-F13	81.05(15)
O1-Na1-F11	102.99(12)	O3-Na1-F11	82.98(13)
O2-Na1-F11	99.74(16)	F13-Na1-F11	178.97(13)
O1-Na1-F12	81.03(12)	O3-Na1-F12	80.63(12)
O2-Na1-F12	141.56(15)	F13-Na1-F12	60.92(10)
F11-Na1-F12	118.22(11)	O1-Na1-F15	86.39(12)
O3-Na1-F15	81.62(12)	O2-Na1-F15	158.62(16)
F13-Na1-F15	120.20(12)	F11-Na1-F15	59.03(10)

F12-Na1-F15	59.81(8)	C116-F50-Na2	107.5(2)
O4-Na2-O6	161.44(19)	O4-Na2-O5	96.5(2)
O6-Na2-O5	97.4(2)	O4-Na2-F49	74.96(13)
O6-Na2-F49	94.73(14)	O5-Na2-F49	82.64(18)
O4-Na2-F46	107.19(13)	O6-Na2-F46	81.88(13)
O5-Na2-F46	101.7(2)	F49-Na2-F46	174.78(15)
O4-Na2-F47	91.11(15)	O6-Na2-F47	79.61(13)
O5-Na2-F47	160.6(2)	F49-Na2-F47	116.59(13)
F46-Na2-F47	59.00(10)	O4-Na2-F50	82.13(14)
O6-Na2-F50	79.31(13)	O5-Na2-F50	139.98(18)
F49-Na2-F50	58.24(10)	F46-Na2-F50	117.01(12)
F47-Na2-F50	58.67(9)	C52-F12-Na1	110.2(2)
C120-F46-Na2	130.8(3)	C56-F11-Na1	131.9(3)
C117-F49-Na2	123.4(3)	C53-F13-Na1	120.6(3)
C119-F47-Na2	115.5(3)	C55-F15-Na1	113.9(3)
C3-N2-C1	106.4(3)	C3-N2-B1	127.8(3)
C1-N2-B1	125.5(3)	C67-N5-C66	106.3(3)
C67-N5-B4	128.0(3)	C66-N5-B4	125.1(3)
C3-N1-C2	106.9(3)	C3-N1-B2	126.2(3)
C2-N1-B2	126.8(3)	C10-O1-Na1	138.5(3)
C67-N4-C65	106.8(3)	C67-N4-B3	126.8(3)
C65-N4-B3	126.3(3)	C23-O3-C26	106.6(4)
C23-O3-Na1	121.1(3)	C26-O3-Na1	131.7(3)
C74-O4-Na2	136.5(3)	C90-O6-C87	106.6(4)
C90-O6-Na2	120.0(4)	C87-O6-Na2	132.9(3)
C10-N3-C11	123.7(3)	C10-N3-C15	118.3(4)
C11-N3-C15	117.6(3)	N4-C67-N5	109.9(3)
N4-C67-C68	125.1(3)	N5-C67-C68	125.0(3)
N1-C3-N2	110.0(3)	N1-C3-C4	125.4(3)
N2-C3-C4	124.6(3)	C74-N6-C79	119.7(4)
C74-N6-C75	123.7(4)	C79-N6-C75	116.3(4)
C1-C2-N1	108.3(3)	C1-C2-H2	125.8
N1-C2-H2	125.8	C19-O2-C22	107.9(5)
C19-O2-Na1	117.3(3)	C22-O2-Na1	129.2(4)
C2-C1-N2	108.3(3)	C2-C1-H1	125.8
N2-C1-H1	125.8	C65-C66-N5	108.5(3)
C65-C66-H66	125.8	N5-C66-H66	125.8
C66-C65-N4	108.4(3)	C66-C65-H65	125.8

N4-C65-H65	125.8	F10-C62-C57	119.6(3)
F10-C62-C61	115.5(4)	C57-C62-C61	124.9(4)
C9-C4-C5	118.8(3)	C9-C4-C3	121.5(4)
C5-C4-C3	119.7(4)	F45-C110-C109	119.1(3)
F45-C110-C111	115.5(4)	C109-C110-C111	125.3(4)
C110-C109-C114	113.0(3)	C110-C109-B4	120.3(3)
C114-C109-B4	125.8(4)	C102-C97-C98	113.1(4)
C102-C97-B3	126.9(3)	C98-C97-B3	119.4(3)
F30-C38-C37	114.4(4)	F30-C38-C33	121.2(3)
C37-C38-C33	124.5(4)	C69-C68-C73	119.2(4)
C69-C68-C67	120.9(4)	C73-C68-C67	119.8(3)
F16-C40-C39	119.8(3)	F16-C40-C41	115.2(4)
C39-C40-C41	125.0(4)	C40-C39-C44	113.2(4)
C40-C39-B2	120.4(3)	C44-C39-B2	125.5(4)
F50-C116-C115	120.7(4)	F50-C116-C117	115.0(4)
C115-C116-C117	124.3(4)	C72-C73-C68	120.4(4)
C72-C73-H73	119.8	C68-C73-H73	119.8
F17-C41-C42	120.4(4)	F17-C41-C40	120.7(4)
C42-C41-C40	118.9(4)	F25-C32-C31	114.7(4)
F25-C32-C27	120.9(4)	C31-C32-C27	124.4(4)
F40-C102-C101	114.5(4)	F40-C102-C97	121.3(4)
C101-C102-C97	124.2(4)	C62-C57-C58	114.0(4)
C62-C57-B1	120.4(4)	C58-C57-B1	124.7(4)
C4-C9-C8	120.2(4)	C4-C9-H9	119.9
C8-C9-H9	119.9	C71-C72-C73	120.2(4)
C71-C72-H72	119.9	C73-C72-H72	119.9
F31-C92-C91	120.0(3)	F31-C92-C93	114.7(4)
C91-C92-C93	125.3(4)	F26-C34-C35	117.1(3)
F26-C34-C33	118.6(4)	C35-C34-C33	124.4(4)
C38-C33-C34	113.3(4)	C38-C33-B2	127.0(3)
C34-C33-B2	119.2(3)	C6-C5-C4	120.8(4)
C6-C5-H5	119.6	C4-C5-H5	119.6
C6-C7-C8	119.7(4)	C6-C7-C10	119.9(4)
C8-C7-C10	119.8(4)	F32-C93-C94	120.8(4)
F32-C93-C92	120.9(4)	C94-C93-C92	118.2(4)
C32-C27-C28	113.4(4)	C32-C27-B2	128.7(4)
C28-C27-B2	117.8(4)	C52-C51-C56	113.0(4)
C52-C51-B1	118.6(4)	C56-C51-B1	127.7(4)

F36-C98-C99	116.7(4)	F36-C98-C97	119.0(4)
C99-C98-C97	124.4(4)	F21-C28-C29	116.8(4)
F21-C28-C27	119.2(4)	C29-C28-C27	123.9(4)
F44-C111-C112	120.6(4)	F44-C111-C110	120.9(4)
C112-C111-C110	118.5(4)	F42-C113-C112	119.1(4)
F42-C113-C114	119.8(4)	C112-C113-C114	121.1(4)
C92-C91-C96	113.2(4)	C92-C91-B3	120.2(3)
C96-C91-B3	125.7(4)	C72-C71-C70	119.9(4)
C72-C71-C74	119.3(4)	C70-C71-C74	120.2(4)
C120-C115-C116	113.7(4)	C120-C115-B4	127.4(4)
C116-C115-B4	118.1(3)	F27-C35-C34	120.9(4)
F27-C35-C36	119.9(4)	C34-C35-C36	119.2(4)
F35-C96-C95	114.5(4)	F35-C96-C91	122.1(4)
C95-C96-C91	123.4(5)	F56-C108-C107	115.3(4)
F56-C108-C103	121.0(4)	C107-C108-C103	123.6(4)
F43-C112-C113	120.6(4)	F43-C112-C111	120.4(4)
C113-C112-C111	119.0(4)	C7-C6-C5	120.1(4)
C7-C6-H6	119.9	C5-C6-H6	119.9
F37-C99-C98	120.8(4)	F37-C99-C100	119.8(4)
C98-C99-C100	119.4(4)	F18-C42-C43	120.1(4)
F18-C42-C41	121.1(5)	C43-C42-C41	118.8(4)
F39-C101-C102	120.6(4)	F39-C101-C100	119.6(4)
C102-C101-C100	119.8(4)	C7-C8-C9	120.3(4)
C7-C8-H8	119.9	C9-C8-H8	119.9
F12-C52-C51	119.7(4)	F12-C52-C53	115.6(4)
C51-C52-C53	124.7(4)	F20-C44-C43	115.1(4)
F20-C44-C39	121.6(4)	C43-C44-C39	123.3(5)
F24-C31-C32	121.4(4)	F24-C31-C30	119.2(4)
C32-C31-C30	119.4(4)	F13-C53-C54	120.6(4)
F13-C53-C52	120.1(4)	C54-C53-C52	119.3(5)
C104-C103-C108	113.2(4)	C104-C103-B3	118.3(4)
C108-C103-B3	128.4(4)	F19-C43-C42	120.4(4)
F19-C43-C44	118.9(5)	C42-C43-C44	120.7(4)
C68-C69-C70	120.0(4)	C68-C69-H69	120.0
C70-C69-H69	120.0	C71-C70-C69	120.2(4)
C71-C70-H70	119.9	C69-C70-H70	119.9
F41-C114-C113	115.8(4)	F41-C114-C109	121.1(4)
C113-C114-C109	123.1(4)	F34-C95-C94	119.5(4)

F34-C95-C96	119.8(5)	C94-C95-C96	120.7(4)
F15-C55-C54	119.8(4)	F15-C55-C56	119.6(5)
C54-C55-C56	120.3(4)	F47-C119-C118	119.7(4)
F47-C119-C120	119.3(5)	C118-C119-C120	120.7(4)
F29-C37-C38	121.0(4)	F29-C37-C36	119.5(4)
C38-C37-C36	119.5(4)	F60-C104-C103	119.3(4)
F60-C104-C105	116.4(4)	C103-C104-C105	124.2(4)
F9-C61-C60	121.2(4)	F9-C61-C62	120.5(4)
C60-C61-C62	118.3(5)	O1-C10-N3	122.6(4)
O1-C10-C7	117.8(4)	N3-C10-C7	119.6(4)
C50-C45-C46	114.7(5)	C50-C45-B1	118.9(4)
C46-C45-B1	125.5(4)	F22-C29-C30	119.4(4)
F22-C29-C28	120.6(4)	C30-C29-C28	120.0(4)
C122-C121-C126	114.9(4)	C122-C121-B4	126.7(4)
C126-C121-B4	117.2(4)	F11-C56-C55	114.9(4)
F11-C56-C51	120.9(4)	C55-C56-C51	124.2(5)
F23-C30-C29	121.1(5)	F23-C30-C31	120.1(4)
C29-C30-C31	118.8(4)	F33-C94-C95	121.1(4)
F33-C94-C93	119.8(5)	C95-C94-C93	119.1(4)
N3-C15-C16	109.8(4)	N3-C15-H15A	109.7
C16-C15-H15A	109.7	N3-C15-H15B	109.7
C16-C15-H15B	109.7	H15A-C15-H15B	108.2
F57-C107-C108	120.4(5)	F57-C107-C106	119.2(4)
C108-C107-C106	120.4(4)	F46-C120-C119	115.2(4)
F46-C120-C115	121.2(4)	C119-C120-C115	123.5(5)
F49-C117-C118	120.6(4)	F49-C117-C116	120.4(4)
C118-C117-C116	119.1(4)	F59-C105-C106	119.9(4)
F59-C105-C104	120.1(4)	C106-C105-C104	119.9(5)
F8-C60-C59	120.8(5)	F8-C60-C61	119.9(5)
C59-C60-C61	119.2(4)	F6-C58-C59	115.6(4)
F6-C58-C57	121.9(4)	C59-C58-C57	122.5(5)
F38-C100-C99	120.5(4)	F38-C100-C101	120.6(4)
C99-C100-C101	118.9(4)	F58-C106-C105	120.8(5)
F58-C106-C107	120.7(4)	C105-C106-C107	118.5(4)
C86-O5-C83	105.6(6)	C86-O5-Na2	117.1(6)
C83-O5-Na2	125.5(5)	F14-C54-C55	121.3(5)
F14-C54-C53	120.2(5)	C55-C54-C53	118.5(4)
F48-C118-C117	120.2(5)	F48-C118-C119	121.0(5)

C117-C118-C119	118.7(4)	C15-C16-C17	114.1(4)
C15-C16-H16A	108.7	C17-C16-H16A	108.7
C15-C16-H16B	108.7	C17-C16-H16B	108.7
H16A-C16-H16B	107.6	F51-C126-C125	117.5(5)
F51-C126-C121	119.9(4)	C125-C126-C121	122.6(6)
F28-C36-C35	120.7(4)	F28-C36-C37	120.2(4)
C35-C36-C37	119.2(4)	F7-C59-C60	119.4(4)
F7-C59-C58	119.6(5)	C60-C59-C58	121.0(5)
F1-C46-C47	116.1(6)	F1-C46-C45	121.5(4)
C47-C46-C45	122.4(6)	C18-C17-C16	111.3(4)
C18-C17-H17A	109.4	C16-C17-H17A	109.4
C18-C17-H17B	109.4	C16-C17-H17B	109.4
H17A-C17-H17B	108.0	O4-C74-N6	122.1(4)
O4-C74-C71	117.4(4)	N6-C74-C71	120.4(4)
F55-C122-C121	121.5(4)	F55-C122-C123	114.6(5)
C121-C122-C123	123.9(6)	N3-C11-C12	115.3(5)
N3-C11-C12A	114.1(7)	N3-C11-H11A	108.5
C12-C11-H11A	108.5	N3-C11-H11B	108.5
C12-C11-H11B	108.5	H11A-C11-H11B	107.5
N3-C11-H11C	108.7	C12A-C11-H11C	108.7
N3-C11-H11D	108.7	C12A-C11-H11D	108.7
H11C-C11-H11D	107.6	N6-C79-C80	109.5(4)
N6-C79-H79A	109.8	C80-C79-H79A	109.8
N6-C79-H79B	109.8	C80-C79-H79B	109.8
H79A-C79-H79B	108.2	N5-B4-C121	114.6(3)
N5-B4-C115	102.6(3)	C121-B4-C115	114.6(3)
N5-B4-C109	109.7(3)	C121-B4-C109	101.4(3)
C115-B4-C109	114.4(3)	F5-C50-C49	116.6(6)
F5-C50-C45	119.2(4)	C49-C50-C45	124.2(7)
N1-B2-C27	104.6(3)	N1-B2-C33	110.9(3)
C27-B2-C33	116.0(3)	N1-B2-C39	110.8(3)
C27-B2-C39	113.1(3)	C33-B2-C39	101.5(3)
N2-B1-C45	112.8(3)	N2-B1-C51	103.1(3)
C45-B1-C51	115.7(3)	N2-B1-C57	110.9(3)
C45-B1-C57	101.1(3)	C51-B1-C57	113.6(3)
C76-C75-N6	116.6(6)	N6-C75-C76A	115.9(11)
C76-C75-H75A	108.2	N6-C75-H75A	108.2
C76-C75-H75B	108.2	N6-C75-H75B	108.2

H75A-C75-H75B	107.3	N6-C75-H75C	108.3
C76A-C75-H75C	108.3	N6-C75-H75D	108.3
C76A-C75-H75D	108.3	H75C-C75-H75D	107.4
C80-C81-C82	112.0(5)	C80-C81-H81A	109.2
C82-C81-H81A	109.2	C80-C81-H81B	109.2
C82-C81-H81B	109.2	H81A-C81-H81B	107.9
N4-B3-C103	104.2(3)	N4-B3-C97	111.3(3)
C103-B3-C97	115.8(3)	N4-B3-C91	110.8(3)
C103-B3-C91	112.7(3)	C97-B3-C91	102.2(3)
C81-C80-C79	114.9(5)	C81-C80-H80A	108.5
C79-C80-H80A	108.5	C81-C80-H80B	108.5
C79-C80-H80B	108.5	H80A-C80-H80B	107.5
C26-C25-C24	103.1(5)	C26-C25-H25A	111.1
C24-C25-H25A	111.1	C26-C25-H25B	111.1
C24-C25-H25B	111.1	H25A-C25-H25B	109.1
F54-C123-C124	121.2(6)	F54-C123-C122	120.4(7)
C124-C123-C122	118.4(6)	F52-C125-C124	121.1(5)
F52-C125-C126	119.6(6)	C124-C125-C126	119.3(6)
O3-C26-C25	105.8(5)	O3-C26-H26A	110.6
C25-C26-H26A	110.6	O3-C26-H26B	110.6
C25-C26-H26B	110.6	H26A-C26-H26B	108.7
F53-C124-C125	119.1(7)	F53-C124-C123	120.1(7)
C125-C124-C123	120.8(5)	C17-C18-H18A	109.5
C17-C18-H18B	109.5	H18A-C18-H18B	109.5
C17-C18-H18C	109.5	H18A-C18-H18C	109.5
H18B-C18-H18C	109.5	Cl4-C64-Cl3	112.0(3)
Cl4-C64-H64A	109.2	Cl3-C64-H64A	109.2
Cl4-C64-H64B	109.2	Cl3-C64-H64B	109.2
H64A-C64-H64B	107.9	F4-C49-C48	121.4(6)
F4-C49-C50	120.8(8)	C48-C49-C50	117.8(6)
O3-C23-C24	107.3(5)	O3-C23-H23A	110.3
C24-C23-H23A	110.3	O3-C23-H23B	110.3
C24-C23-H23B	110.3	H23A-C23-H23B	108.5
C47-C48-F3	120.8(8)	C47-C48-C49	121.2(5)
F3-C48-C49	117.9(8)	C81-C82-H82A	109.5
C81-C82-H82B	109.5	H82A-C82-H82B	109.5
C81-C82-H82C	109.5	H82A-C82-H82C	109.5
H82B-C82-H82C	109.5	F2-C47-C48	121.3(6)

F2-C47-C46	119.0(7)	C48-C47-C46	119.7(7)
O2-C19-C20	107.5(5)	O2-C19-H19A	110.2
C20-C19-H19A	110.2	O2-C19-H19B	110.2
C20-C19-H19B	110.2	H19A-C19-H19B	108.5
C87-C88-C89	104.2(5)	C87-C88-H88A	110.9
C89-C88-H88A	110.9	C87-C88-H88B	110.9
C89-C88-H88B	110.9	H88A-C88-H88B	108.9
O6-C87-C88	106.4(6)	O6-C87-H87A	110.4
C88-C87-H87A	110.4	O6-C87-H87B	110.4
C88-C87-H87B	110.4	H87A-C87-H87B	108.6
C25-C24-C23	104.6(5)	C25-C24-H24A	110.8
C23-C24-H24A	110.8	C25-C24-H24B	110.8
C23-C24-H24B	110.8	H24A-C24-H24B	108.9
O6-C90-C89	106.9(5)	O6-C90-H90A	110.3
C89-C90-H90A	110.3	O6-C90-H90B	110.3
C89-C90-H90B	110.3	H90A-C90-H90B	108.6
Cl1-C63-Cl2	112.4(4)	Cl1-C63-H63A	109.1
Cl2-C63-H63A	109.1	Cl1-C63-H63B	109.1
Cl2-C63-H63B	109.1	H63A-C63-H63B	107.8
C21-C22-O2	108.1(6)	C21-C22-H22A	110.1
O2-C22-H22A	110.1	C21-C22-H22B	110.1
O2-C22-H22B	110.1	H22A-C22-H22B	108.4
C88-C89-C90	105.6(5)	C88-C89-H89A	110.6
C90-C89-H89A	110.6	C88-C89-H89B	110.6
C90-C89-H89B	110.6	H89A-C89-H89B	108.8
C13-C12-C11	114.8(7)	C13-C12-H12A	108.6
C11-C12-H12A	108.6	C13-C12-H12B	108.6
C11-C12-H12B	108.6	H12A-C12-H12B	107.5
C84A-C83-O5	104.9(10)	C84-C83-O5	99.7(9)
C84-C83-H83A	111.8	O5-C83-H83A	111.8
C84-C83-H83B	111.8	O5-C83-H83B	111.8
H83A-C83-H83B	109.6	C84A-C83-H83C	110.8
O5-C83-H83C	110.8	C84A-C83-H83D	110.8
O5-C83-H83D	110.8	H83C-C83-H83D	108.8
C13-C14-H14A	109.5	C13-C14-H14B	109.5
H14A-C14-H14B	109.5	C13-C14-H14C	109.5
H14A-C14-H14C	109.5	H14B-C14-H14C	109.5
C13A-C14-H14D	109.5	C13A-C14-H14E	109.5

H14D-C14-H14E	109.5	C13A-C14-H14F	109.5
H14D-C14-H14F	109.5	H14E-C14-H14F	109.5
C75-C76-C77	109.0(8)	C75-C76-H76A	109.9
C77-C76-H76A	109.9	C75-C76-H76B	109.9
C77-C76-H76B	109.9	H76A-C76-H76B	108.3
C14-C13-C12	111.2(8)	C14-C13-H13A	109.4
C12-C13-H13A	109.4	C14-C13-H13B	109.4
C12-C13-H13B	109.4	H13A-C13-H13B	108.0
C21-C20-C19	102.7(6)	C21-C20-H20A	111.2
C19-C20-H20A	111.2	C21-C20-H20B	111.2
C19-C20-H20B	111.2	H20A-C20-H20B	109.1
C22-C21-C20	106.3(7)	C22-C21-H21A	110.5
C20-C21-H21A	110.5	C22-C21-H21B	110.5
C20-C21-H21B	110.5	H21A-C21-H21B	108.7
C77-C78-H78A	109.5	C77-C78-H78B	109.5
H78A-C78-H78B	109.5	C77-C78-H78C	109.5
H78A-C78-H78C	109.5	H78B-C78-H78C	109.5
C77A-C78-H78D	109.5	C77A-C78-H78E	109.5
H78D-C78-H78E	109.5	C77A-C78-H78F	109.5
H78D-C78-H78F	109.5	H78E-C78-H78F	109.5
C76-C77-C78	110.3(8)	C76-C77-H77A	109.6
C78-C77-H77A	109.6	C76-C77-H77B	109.6
C78-C77-H77B	109.6	H77A-C77-H77B	108.1
C85-C86-O5	112.1(8)	C85-C86-H86A	109.2
O5-C86-H86A	109.2	C85-C86-H86B	109.2
O5-C86-H86B	109.2	H86A-C86-H86B	107.9
C86-C85-C84	98.3(9)	C86-C85-C84A	98.1(8)
C86-C85-H85A	112.1	C84-C85-H85A	112.1
C86-C85-H85B	112.1	C84-C85-H85B	112.1
H85A-C85-H85B	109.8	C86-C85-H85C	112.1
C84A-C85-H85C	112.1	C86-C85-H85D	112.1
C84A-C85-H85D	112.1	H85C-C85-H85D	109.8
C83-C84-C85	103.4(12)	C83-C84-H84A	111.1
C85-C84-H84A	111.1	C83-C84-H84B	111.1
C85-C84-H84B	111.1	H84A-C84-H84B	109.0
C83-C84A-C85	90.8(10)	C83-C84A-H84C	113.5
C85-C84A-H84C	113.5	C83-C84A-H84D	113.5
C85-C84A-H84D	113.5	H84C-C84A-H84D	110.8

C77A-C76A-C75	117.(2)	C77A-C76A-H76C	108.0
C75-C76A-H76C	108.0	C77A-C76A-H76D	108.0
C75-C76A-H76D	108.0	H76C-C76A-H76D	107.2
C78-C77A-C76A	109.(3)	C78-C77A-H77C	109.8
C76A-C77A-H77C	109.8	C78-C77A-H77D	109.8
C76A-C77A-H77D	109.8	H77C-C77A-H77D	108.3
C13A-C12A-C11	110.(2)	C13A-C12A-H12C	109.6
C11-C12A-H12C	109.6	C13A-C12A-H12D	109.6
C11-C12A-H12D	109.6	H12C-C12A-H12D	108.1
C12A-C13A-C14	110.(2)	C12A-C13A-H13C	109.6
C14-C13A-H13C	109.6	C12A-C13A-H13D	109.6
C14-C13A-H13D	109.6	H13C-C13A-H13D	108.1

Table 6. Anisotropic atomic displacement parameters (Å^2) for 5991.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl3	0.0452(8)	0.0598(10)	0.0844(12)	-0.0196(9)	0.0249(8)	-0.0006(7)
Cl4	0.0491(9)	0.0619(11)	0.1249(17)	-0.0394(11)	0.0280(10)	-0.0110(8)
Na1	0.0385(11)	0.0375(11)	0.0289(9)	-0.0069(8)	-0.0001(8)	0.0086(9)
Cl2	0.0610(11)	0.0664(12)	0.161(2)	-0.0226(13)	0.0556(13)	-0.0020(9)
Cl1	0.0634(12)	0.0612(12)	0.169(2)	-0.0324(13)	0.0284(14)	-0.0163(10)
F30	0.0208(12)	0.0240(12)	0.0172(11)	0.0083(9)	0.0011(9)	0.0019(9)
F40	0.0216(12)	0.0207(12)	0.0174(11)	0.0066(9)	0.0004(9)	0.0026(9)
F50	0.0317(13)	0.0250(13)	0.0206(11)	0.0048(10)	0.0121(10)	0.0060(10)
F31	0.0280(13)	0.0224(12)	0.0207(11)	-0.0004(9)	0.0011(10)	-0.0010(10)
F10	0.0296(13)	0.0248(12)	0.0220(12)	0.0060(10)	0.0085(10)	0.0016(10)
Na2	0.0544(13)	0.0348(11)	0.0424(12)	-0.0072(9)	-0.0038(10)	0.0127(10)
F45	0.0233(12)	0.0256(13)	0.0288(13)	0.0034(10)	0.0090(10)	0.0021(10)
F12	0.0294(13)	0.0267(13)	0.0224(12)	0.0077(10)	0.0107(10)	0.0056(10)
F16	0.0260(12)	0.0271(13)	0.0191(11)	-0.0008(10)	0.0018(9)	-0.0020(10)
F56	0.0252(13)	0.0180(12)	0.0363(14)	0.0103(10)	0.0014(10)	-0.0014(10)
F26	0.0243(12)	0.0359(14)	0.0169(11)	0.0120(10)	-0.0046(9)	-0.0029(11)
F21	0.0287(13)	0.0285(14)	0.0356(14)	0.0109(11)	0.0100(11)	-0.0043(11)
F36	0.0260(13)	0.0313(14)	0.0210(12)	0.0120(10)	-0.0049(10)	0.0004(11)
F25	0.0242(12)	0.0210(12)	0.0324(13)	0.0108(10)	0.0029(10)	-0.0022(10)
F32	0.0527(17)	0.0275(14)	0.0269(13)	-0.0068(11)	0.0129(12)	-0.0143(13)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F60	0.0278(13)	0.0279(14)	0.0419(15)	0.0113(12)	0.0090(11)	-0.0035(11)
F41	0.0234(13)	0.0539(18)	0.0273(13)	0.0201(12)	0.0034(10)	0.0009(12)
F46	0.0450(16)	0.0219(13)	0.0317(14)	-0.0069(11)	0.0037(12)	-0.0066(11)
F20	0.0238(13)	0.0386(15)	0.0293(13)	0.0062(12)	-0.0056(10)	-0.0039(11)
F35	0.0230(13)	0.0339(15)	0.0386(15)	0.0080(12)	-0.0112(11)	-0.0013(11)
F39	0.0235(13)	0.0454(16)	0.0351(14)	0.0087(12)	0.0079(11)	-0.0002(12)
F44	0.0443(16)	0.0311(14)	0.0370(15)	0.0097(12)	0.0236(13)	-0.0015(12)
F17	0.0573(18)	0.0235(13)	0.0276(13)	-0.0045(11)	0.0140(12)	-0.0105(13)
F57	0.0369(15)	0.0186(13)	0.0465(16)	0.0069(12)	-0.0019(12)	0.0067(11)
F24	0.0312(14)	0.0240(13)	0.0464(16)	0.0119(12)	-0.0006(12)	0.0086(11)
F33	0.0553(18)	0.0449(17)	0.0230(13)	-0.0070(12)	0.0018(12)	-0.0329(15)
F29	0.0230(13)	0.0555(18)	0.0386(15)	0.0118(13)	0.0096(11)	-0.0030(12)
F11	0.0470(17)	0.0267(14)	0.0296(14)	-0.0076(11)	0.0051(12)	-0.0083(12)
F18	0.0601(19)	0.0421(17)	0.0235(13)	-0.0088(12)	0.0043(13)	-0.0324(15)
F37	0.0466(17)	0.0449(17)	0.0258(13)	0.0212(12)	0.0066(12)	-0.0019(13)
F19	0.0319(15)	0.059(2)	0.0291(14)	0.0032(13)	-0.0135(12)	-0.0224(14)
F34	0.0318(15)	0.062(2)	0.0306(15)	0.0074(14)	-0.0143(12)	-0.0178(14)
F49	0.0385(16)	0.0539(18)	0.0354(15)	0.0203(13)	0.0210(13)	0.0154(14)
F27	0.0456(17)	0.0502(18)	0.0222(13)	0.0194(12)	0.0077(12)	-0.0055(14)
F9	0.065(2)	0.0343(15)	0.0373(15)	0.0150(13)	0.0299(15)	0.0059(14)
F22	0.0314(16)	0.060(2)	0.064(2)	0.0083(16)	0.0272(15)	0.0003(14)
F1	0.0303(15)	0.0384(16)	0.070(2)	0.0253(15)	0.0253(14)	0.0136(13)
F55	0.0278(15)	0.0321(15)	0.081(2)	0.0162(15)	0.0260(15)	0.0119(12)
F43	0.0562(19)	0.0479(18)	0.0402(16)	0.0315(14)	0.0266(14)	0.0202(15)
F6	0.0244(14)	0.083(2)	0.0236(13)	0.0180(14)	0.0022(11)	0.0078(14)
F13	0.0392(16)	0.0533(19)	0.0417(16)	0.0235(14)	0.0223(13)	0.0160(14)
F38	0.0412(17)	0.061(2)	0.0380(16)	0.0188(14)	0.0182(13)	-0.0070(14)
F51	0.058(2)	0.0431(17)	0.0232(13)	-0.0097(12)	0.0027(13)	-0.0146(15)
F47	0.0465(18)	0.0327(16)	0.0521(18)	0.0100(14)	-0.0032(14)	-0.0202(14)
F59	0.0349(17)	0.0489(19)	0.076(2)	0.0061(17)	0.0258(16)	0.0029(14)
F15	0.0485(18)	0.0337(15)	0.0423(16)	0.0051(13)	-0.0032(13)	-0.0231(14)
F42	0.0314(15)	0.085(2)	0.0388(16)	0.0396(17)	0.0102(13)	0.0206(15)
F23	0.0309(16)	0.0494(19)	0.067(2)	0.0010(16)	0.0143(15)	0.0164(14)
F58	0.0356(16)	0.0400(17)	0.074(2)	0.0025(16)	0.0138(15)	0.0154(14)
F28	0.0432(17)	0.070(2)	0.0394(16)	0.0219(15)	0.0222(14)	-0.0107(15)
F48	0.0306(16)	0.067(2)	0.057(2)	0.0302(17)	0.0112(14)	-0.0076(15)
F5	0.077(2)	0.0491(19)	0.0202(13)	-0.0112(13)	0.0043(14)	-0.0208(17)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F14	0.0309(15)	0.063(2)	0.0565(19)	0.0273(17)	0.0098(14)	-0.0094(14)
N2	0.0180(16)	0.0122(15)	0.0142(14)	0.0013(12)	0.0012(12)	0.0000(12)
N5	0.0183(16)	0.0108(15)	0.0158(15)	0.0010(12)	0.0014(12)	-0.0006(12)
N1	0.0174(15)	0.0145(15)	0.0120(14)	0.0031(12)	0.0007(12)	-0.0034(12)
O1	0.0317(17)	0.0205(15)	0.0337(17)	-0.0009(13)	-0.0004(14)	-0.0013(13)
F7	0.0489(19)	0.121(3)	0.0308(16)	0.0396(19)	0.0178(14)	0.051(2)
N4	0.0184(16)	0.0120(15)	0.0171(15)	0.0026(12)	0.0003(12)	-0.0026(12)
F8	0.084(3)	0.076(2)	0.0428(18)	0.0445(17)	0.0387(18)	0.051(2)
O3	0.0331(18)	0.049(2)	0.0297(17)	-0.0001(15)	0.0037(14)	0.0015(16)
O4	0.046(2)	0.0215(17)	0.056(2)	-0.0054(16)	-0.0152(18)	-0.0017(15)
O6	0.046(2)	0.045(2)	0.0351(19)	-0.0032(16)	0.0018(16)	0.0004(17)
N3	0.0273(19)	0.0119(16)	0.037(2)	0.0031(14)	0.0040(16)	-0.0021(14)
F54	0.097(3)	0.053(2)	0.166(5)	0.018(3)	0.102(3)	0.031(2)
C67	0.0144(17)	0.0102(17)	0.0179(17)	0.0003(14)	0.0013(14)	0.0001(13)
C3	0.0124(17)	0.0168(18)	0.0136(16)	0.0017(14)	0.0025(13)	-0.0002(14)
F52	0.149(4)	0.061(2)	0.0419(19)	-0.0329(18)	0.042(2)	-0.027(3)
N6	0.032(2)	0.0128(17)	0.041(2)	0.0010(15)	0.0012(17)	-0.0042(15)
C2	0.0230(19)	0.0124(17)	0.0148(17)	0.0039(14)	0.0044(15)	-0.0035(15)
O2	0.057(3)	0.070(3)	0.042(2)	-0.008(2)	0.0147(19)	0.014(2)
C1	0.026(2)	0.0100(17)	0.0157(17)	0.0024(14)	0.0067(15)	-0.0023(15)
C66	0.0225(19)	0.0115(17)	0.0170(18)	0.0000(14)	0.0023(15)	-0.0030(15)
C65	0.0220(19)	0.0132(18)	0.0179(18)	0.0038(14)	0.0013(15)	-0.0032(15)
C62	0.035(2)	0.020(2)	0.0118(17)	-0.0012(15)	0.0085(16)	0.0093(17)
C4	0.0158(18)	0.0101(17)	0.0186(18)	0.0015(14)	-0.0023(14)	-0.0018(14)
C110	0.025(2)	0.0188(19)	0.0175(18)	-0.0015(15)	0.0085(15)	0.0031(16)
C109	0.027(2)	0.0170(18)	0.0085(16)	-0.0008(14)	0.0044(14)	0.0026(15)
C97	0.023(2)	0.0151(18)	0.0184(18)	0.0036(15)	-0.0009(15)	-0.0015(15)
C38	0.027(2)	0.022(2)	0.0139(17)	0.0072(15)	0.0019(15)	-0.0040(17)
C68	0.0189(19)	0.0111(17)	0.0170(17)	0.0017(14)	-0.0002(14)	0.0005(14)
C40	0.026(2)	0.023(2)	0.0131(17)	0.0054(15)	0.0011(15)	-0.0090(17)
C39	0.023(2)	0.024(2)	0.0124(17)	0.0079(15)	0.0012(15)	-0.0078(16)
C116	0.022(2)	0.027(2)	0.0166(18)	0.0093(16)	0.0002(15)	0.0027(17)
F2	0.104(3)	0.063(3)	0.167(4)	0.052(3)	0.114(3)	0.048(2)
C73	0.022(2)	0.0123(18)	0.0218(19)	0.0037(15)	0.0014(15)	0.0001(15)
C41	0.038(2)	0.020(2)	0.0167(18)	0.0028(16)	0.0085(17)	-0.0121(18)
C32	0.0170(19)	0.027(2)	0.0214(19)	0.0092(17)	-0.0014(15)	-0.0006(16)
C102	0.028(2)	0.0182(19)	0.0136(17)	0.0064(15)	-0.0001(15)	-0.0006(16)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C57	0.031(2)	0.023(2)	0.0076(16)	0.0012(14)	0.0049(15)	0.0064(17)
C9	0.0178(19)	0.0171(19)	0.025(2)	0.0049(16)	0.0017(15)	-0.0008(15)
C72	0.023(2)	0.0139(18)	0.029(2)	0.0062(16)	-0.0018(17)	-0.0043(16)
C92	0.026(2)	0.022(2)	0.0154(18)	0.0060(15)	-0.0012(15)	-0.0072(17)
C34	0.024(2)	0.026(2)	0.0179(19)	0.0062(16)	0.0012(16)	-0.0037(17)
C33	0.024(2)	0.0205(19)	0.0125(17)	0.0043(15)	0.0016(15)	-0.0008(16)
C5	0.0204(19)	0.0162(18)	0.0202(18)	0.0030(15)	0.0025(15)	-0.0002(15)
C7	0.020(2)	0.0138(18)	0.028(2)	0.0036(16)	-0.0020(16)	-0.0024(15)
C93	0.041(3)	0.020(2)	0.0194(19)	0.0030(16)	0.0086(18)	-0.0162(19)
C27	0.0165(19)	0.024(2)	0.0187(18)	0.0060(16)	-0.0038(15)	-0.0012(16)
F4	0.211(5)	0.052(2)	0.051(2)	-0.0315(19)	0.067(3)	-0.028(3)
C51	0.022(2)	0.021(2)	0.0138(17)	0.0041(15)	-0.0050(15)	-0.0015(16)
C98	0.023(2)	0.019(2)	0.025(2)	0.0082(16)	-0.0036(17)	-0.0028(16)
C28	0.018(2)	0.028(2)	0.027(2)	0.0089(18)	0.0014(16)	-0.0009(17)
C111	0.038(2)	0.022(2)	0.022(2)	0.0028(16)	0.0170(18)	0.0047(18)
C113	0.028(2)	0.042(3)	0.021(2)	0.0149(19)	0.0081(17)	0.015(2)
C91	0.025(2)	0.0183(19)	0.0172(18)	0.0062(15)	-0.0024(15)	-0.0068(16)
C71	0.024(2)	0.0101(18)	0.038(2)	0.0029(17)	-0.0042(18)	0.0000(16)
C115	0.024(2)	0.020(2)	0.0143(17)	0.0036(15)	-0.0048(15)	-0.0018(16)
C35	0.035(2)	0.033(2)	0.0173(19)	0.0118(18)	0.0036(17)	-0.007(2)
C96	0.025(2)	0.031(2)	0.020(2)	0.0094(17)	-0.0036(16)	-0.0084(18)
C108	0.019(2)	0.023(2)	0.022(2)	0.0078(16)	-0.0054(16)	-0.0009(16)
C112	0.047(3)	0.028(2)	0.0183(19)	0.0129(17)	0.0182(19)	0.010(2)
C6	0.021(2)	0.0168(19)	0.027(2)	0.0046(16)	0.0027(16)	-0.0049(16)
C99	0.038(3)	0.027(2)	0.021(2)	0.0102(17)	0.0045(18)	-0.0029(19)
C42	0.049(3)	0.030(2)	0.0143(19)	0.0013(17)	0.0047(19)	-0.022(2)
C101	0.022(2)	0.028(2)	0.027(2)	0.0036(18)	0.0027(17)	-0.0011(17)
C8	0.019(2)	0.0160(19)	0.033(2)	0.0005(17)	0.0011(17)	0.0029(16)
C52	0.023(2)	0.029(2)	0.0176(19)	0.0097(17)	-0.0006(16)	0.0037(17)
C44	0.025(2)	0.033(2)	0.0190(19)	0.0093(17)	-0.0023(16)	-0.0082(18)
C31	0.022(2)	0.024(2)	0.034(2)	0.0081(18)	-0.0039(18)	0.0047(17)
C53	0.029(2)	0.038(3)	0.023(2)	0.0130(19)	0.0060(18)	0.009(2)
C103	0.019(2)	0.025(2)	0.0208(19)	0.0091(16)	-0.0047(15)	-0.0010(16)
C43	0.028(2)	0.043(3)	0.0166(19)	0.0082(19)	-0.0051(17)	-0.022(2)
C69	0.018(2)	0.0122(18)	0.040(2)	-0.0005(17)	0.0035(17)	-0.0024(15)
C70	0.021(2)	0.014(2)	0.050(3)	-0.0054(19)	0.0031(19)	0.0039(16)
C114	0.027(2)	0.033(2)	0.0154(18)	0.0068(17)	0.0092(16)	0.0005(18)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C95	0.028(2)	0.039(3)	0.021(2)	0.0097(19)	-0.0084(18)	-0.017(2)
C55	0.031(2)	0.032(2)	0.029(2)	0.0069(19)	-0.0065(19)	-0.014(2)
C119	0.031(2)	0.024(2)	0.028(2)	0.0087(18)	-0.0054(18)	-0.0131(19)
C37	0.022(2)	0.033(2)	0.029(2)	0.0069(19)	0.0071(17)	-0.0067(18)
C104	0.025(2)	0.025(2)	0.031(2)	0.0090(18)	0.0019(18)	0.0001(18)
F53	0.202(6)	0.060(3)	0.114(4)	-0.025(3)	0.122(4)	0.013(3)
C61	0.052(3)	0.028(2)	0.023(2)	0.0087(18)	0.027(2)	0.012(2)
C10	0.020(2)	0.0158(19)	0.031(2)	0.0012(16)	0.0032(17)	-0.0037(16)
C45	0.053(3)	0.0171(19)	0.028(2)	-0.0008(16)	0.0217(19)	0.0057(19)
C29	0.022(2)	0.043(3)	0.035(2)	0.006(2)	0.0076(19)	-0.001(2)
C121	0.047(3)	0.019(2)	0.026(2)	-0.0028(17)	0.014(2)	0.0041(19)
C56	0.028(2)	0.030(2)	0.021(2)	-0.0014(18)	-0.0022(17)	-0.0038(18)
C30	0.021(2)	0.036(3)	0.038(3)	0.000(2)	0.0028(19)	0.0092(19)
C94	0.043(3)	0.035(3)	0.0146(19)	0.0039(18)	-0.0009(18)	-0.025(2)
C15	0.034(2)	0.0125(19)	0.039(2)	0.0016(17)	0.008(2)	-0.0048(17)
C107	0.028(2)	0.018(2)	0.038(3)	0.0057(18)	-0.0091(19)	0.0061(18)
C120	0.029(2)	0.026(2)	0.024(2)	-0.0018(17)	-0.0026(17)	-0.0058(18)
C117	0.028(2)	0.037(3)	0.026(2)	0.0117(19)	0.0067(18)	0.011(2)
C105	0.022(2)	0.038(3)	0.043(3)	0.007(2)	0.007(2)	0.001(2)
C60	0.062(3)	0.051(3)	0.020(2)	0.022(2)	0.024(2)	0.035(3)
C58	0.036(3)	0.050(3)	0.0139(19)	0.0085(19)	0.0093(18)	0.021(2)
C100	0.037(3)	0.035(3)	0.029(2)	0.009(2)	0.013(2)	-0.006(2)
C106	0.023(2)	0.032(3)	0.045(3)	0.001(2)	0.004(2)	0.0077(19)
O5	0.074(2)	0.091(3)	0.132(3)	-0.022(2)	0.033(2)	0.008(2)
C54	0.025(2)	0.046(3)	0.030(2)	0.019(2)	-0.0002(19)	-0.006(2)
C118	0.021(2)	0.047(3)	0.034(2)	0.019(2)	0.0037(19)	-0.004(2)
C16	0.046(3)	0.016(2)	0.040(3)	0.0008(19)	0.013(2)	-0.0031(19)
C126	0.059(3)	0.025(2)	0.034(3)	-0.011(2)	0.021(2)	-0.004(2)
C36	0.037(3)	0.040(3)	0.026(2)	0.008(2)	0.0147(19)	-0.009(2)
C59	0.048(3)	0.064(4)	0.018(2)	0.020(2)	0.020(2)	0.034(3)
F3	0.269(7)	0.059(3)	0.157(5)	-0.002(3)	0.179(5)	0.041(4)
C46	0.065(3)	0.022(2)	0.054(3)	0.014(2)	0.045(2)	0.014(2)
C17	0.041(3)	0.019(2)	0.034(2)	-0.0011(18)	0.000(2)	-0.0035(19)
C74	0.026(2)	0.0126(19)	0.047(3)	-0.0004(18)	-0.001(2)	0.0000(17)
C122	0.038(3)	0.024(2)	0.053(3)	0.002(2)	0.024(2)	0.003(2)
C11	0.032(2)	0.017(2)	0.037(2)	0.0075(18)	-0.0025(19)	-0.0029(18)
C79	0.046(3)	0.011(2)	0.046(3)	0.0017(19)	0.000(2)	-0.0061(19)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
B4	0.023(2)	0.013(2)	0.0147(19)	-0.0008(16)	0.0025(16)	0.0011(17)
C50	0.083(3)	0.024(2)	0.036(2)	-0.0097(19)	0.032(2)	-0.007(2)
B2	0.015(2)	0.022(2)	0.0142(19)	0.0055(17)	-0.0037(16)	-0.0024(17)
B1	0.025(2)	0.016(2)	0.0130(19)	-0.0036(16)	0.0003(17)	0.0028(17)
C75	0.062(3)	0.038(2)	0.051(2)	0.0043(18)	0.0061(19)	0.007(2)
C81	0.048(3)	0.025(2)	0.043(3)	-0.001(2)	-0.002(2)	-0.006(2)
B3	0.019(2)	0.017(2)	0.0147(19)	0.0062(16)	-0.0056(16)	-0.0019(17)
C80	0.057(3)	0.023(2)	0.051(3)	-0.006(2)	0.011(3)	0.005(2)
C25	0.045(3)	0.048(3)	0.062(4)	-0.001(3)	0.003(3)	0.004(3)
C123	0.076(5)	0.029(3)	0.102(6)	0.009(3)	0.065(4)	0.016(3)
C125	0.099(5)	0.032(3)	0.042(3)	-0.016(2)	0.039(3)	-0.006(3)
C26	0.035(3)	0.078(4)	0.029(3)	-0.011(3)	0.005(2)	0.005(3)
C124	0.113(6)	0.037(3)	0.065(4)	-0.010(3)	0.061(4)	0.009(4)
C18	0.106(6)	0.027(3)	0.080(5)	-0.017(3)	0.056(4)	-0.013(3)
C64	0.029(3)	0.059(4)	0.075(4)	0.002(3)	0.016(3)	-0.011(3)
C49	0.135(4)	0.024(2)	0.053(3)	-0.014(2)	0.056(3)	-0.004(3)
C23	0.071(4)	0.062(4)	0.040(3)	0.005(3)	0.025(3)	0.022(3)
C48	0.142(4)	0.036(3)	0.082(4)	-0.002(3)	0.090(3)	0.015(3)
C82	0.082(5)	0.039(3)	0.088(5)	-0.021(3)	0.047(4)	-0.013(3)
C47	0.094(4)	0.029(3)	0.089(4)	0.019(2)	0.075(3)	0.027(3)
C19	0.050(4)	0.049(3)	0.062(4)	-0.003(3)	0.023(3)	-0.002(3)
C88	0.064(4)	0.042(3)	0.078(5)	-0.007(3)	0.000(4)	0.007(3)
C87	0.048(4)	0.106(6)	0.039(3)	-0.018(4)	0.000(3)	0.013(4)
C24	0.071(4)	0.087(5)	0.038(3)	0.017(3)	0.024(3)	0.020(4)
C90	0.101(6)	0.069(5)	0.043(3)	0.007(3)	0.027(4)	0.033(4)
C63	0.039(4)	0.070(5)	0.129(7)	0.017(5)	0.019(4)	-0.015(3)
C22	0.054(4)	0.159(9)	0.049(4)	-0.027(5)	0.007(3)	0.039(5)
C89	0.094(6)	0.094(6)	0.043(4)	0.014(4)	0.016(4)	0.031(5)
C12	0.044(5)	0.022(5)	0.035(4)	0.001(3)	0.006(3)	0.012(3)
C83	0.075(2)	0.092(3)	0.131(3)	-0.023(2)	0.033(2)	0.009(2)
C14	0.101(6)	0.081(5)	0.064(5)	0.011(4)	0.041(4)	0.033(5)
C76	0.064(3)	0.041(2)	0.053(2)	0.0034(18)	0.0061(19)	0.0088(19)
C13	0.041(5)	0.043(6)	0.033(4)	0.006(3)	0.009(3)	0.011(4)
C20	0.063(4)	0.096(6)	0.060(4)	-0.014(4)	0.025(4)	-0.008(4)
C21	0.074(6)	0.106(7)	0.125(8)	-0.055(6)	0.039(5)	0.012(5)
C78	0.068(3)	0.050(2)	0.058(2)	0.0021(19)	0.0096(19)	0.011(2)
C77	0.066(3)	0.046(2)	0.056(2)	0.0025(18)	0.0073(19)	0.0104(19)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C86	0.076(2)	0.093(3)	0.133(3)	-0.023(2)	0.032(2)	0.008(2)
C85	0.076(2)	0.094(3)	0.134(3)	-0.023(2)	0.031(2)	0.009(2)
C84	0.075(2)	0.093(3)	0.132(3)	-0.023(2)	0.032(2)	0.009(2)
C84A	0.044(9)	0.050(9)	0.048(9)	0.010(7)	0.006(7)	0.006(7)
C76A	0.056(18)	0.064(19)	0.14(3)	-0.010(19)	-0.035(17)	-0.030(15)
C77A	0.13(3)	0.072(19)	0.051(13)	0.024(12)	0.055(15)	0.008(16)
C12A	0.044(11)	0.038(13)	0.052(11)	-0.017(8)	-0.014(8)	0.019(8)
C13A	0.054(16)	0.07(2)	0.18(3)	-0.012(19)	0.008(17)	0.028(14)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 5991.

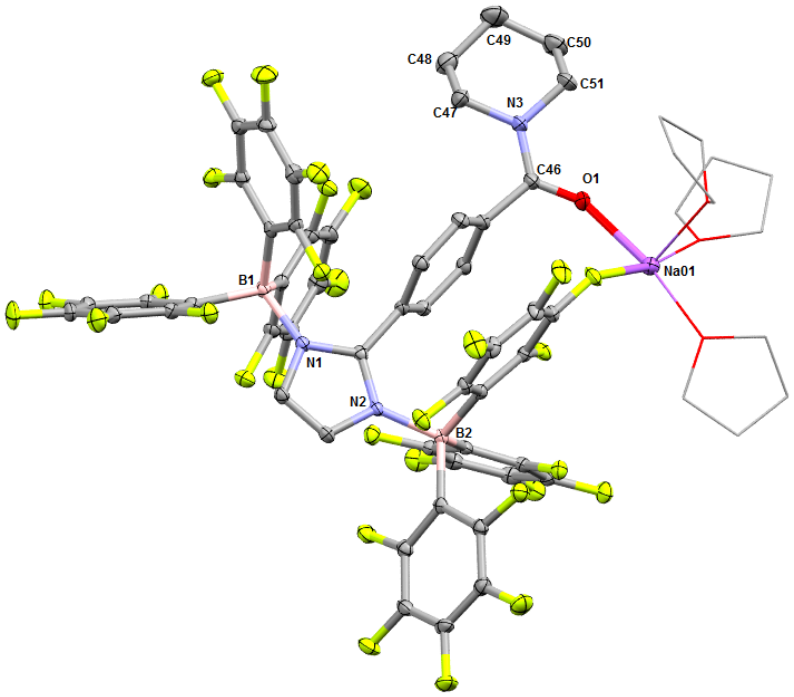
	x/a	y/b	z/c	U(eq)
H2	0.8389	0.5637	0.6154	0.021
H1	0.8823	0.5609	0.7117	0.021
H66	0.6228	0.4357	0.2825	0.022
H65	0.6673	0.4269	0.3782	0.023
H73	0.5802	0.1568	0.3586	0.024
H9	0.8235	0.8661	0.6875	0.026
H72	0.5687	0.0105	0.3530	0.029
H5	0.9233	0.8364	0.6327	0.024
H6	0.9347	0.9826	0.6373	0.027
H8	0.8346	1.0133	0.6910	0.03
H69	0.6761	0.1288	0.2963	0.03
H70	0.6651	-0.0188	0.2925	0.037
H15A	0.8836	1.2867	0.6225	0.035
H15B	0.9181	1.2593	0.6791	0.035
H16A	0.8639	1.2492	0.7188	0.041
H16B	0.8284	1.2716	0.6622	0.041
H17A	0.8915	1.3879	0.7265	0.041
H17B	0.8601	1.4111	0.6671	0.041
H11A	0.8280	1.1921	0.5767	0.038
H11B	0.8298	1.0941	0.5928	0.038
H11C	0.8196	1.1676	0.5872	0.038
H11D	0.8434	1.0803	0.5846	0.038
H79A	0.5845	-0.2665	0.3092	0.046
H79B	0.6176	-0.2919	0.3672	0.046

	x/a	y/b	z/c	U(eq)
H75A	0.6820	-0.1764	0.4013	0.064
H75B	0.6601	-0.0866	0.4023	0.064
H75C	0.6729	-0.1012	0.3951	0.064
H75D	0.6738	-0.1988	0.4118	0.064
H81A	0.6133	-0.3928	0.2629	0.051
H81B	0.6420	-0.4175	0.3232	0.051
H80A	0.6417	-0.2570	0.2733	0.055
H80B	0.6750	-0.2807	0.3311	0.055
H25A	1.0955	0.9057	0.9420	0.066
H25B	1.0513	0.8550	0.9151	0.066
H26A	1.0752	1.0138	0.8831	0.059
H26B	1.0516	0.9365	0.8446	0.059
H18A	0.8008	1.3925	0.6983	0.097
H18B	0.8317	1.4667	0.7305	0.097
H18C	0.8333	1.3753	0.7578	0.097
H64A	0.7283	0.3846	0.2297	0.065
H64B	0.7088	0.4247	0.1704	0.065
H23A	0.9837	1.0045	0.9286	0.067
H23B	1.0199	1.0763	0.9383	0.067
H82A	0.6762	-0.3786	0.2393	0.097
H82B	0.6718	-0.4727	0.2598	0.097
H82C	0.7040	-0.4069	0.2992	0.097
H19A	0.8549	1.0155	0.7997	0.064
H19B	0.8604	1.1053	0.7736	0.064
H88A	0.4396	0.1436	0.0771	0.081
H88B	0.3971	0.0867	0.0542	0.081
H87A	0.4465	0.0704	0.1519	0.081
H87B	0.4204	-0.0095	0.1190	0.081
H24A	1.0674	0.9880	0.9912	0.076
H24B	1.0314	0.9154	0.9804	0.076
H90A	0.4683	-0.0816	0.0577	0.084
H90B	0.5069	-0.0167	0.0633	0.084
H63A	0.7915	0.5736	0.8079	0.098
H63B	0.7681	0.6196	0.7514	0.098
H22A	0.9156	1.0917	0.9208	0.107
H22B	0.9326	1.1712	0.8952	0.107
H89A	0.4625	0.0807	0.0166	0.094

	x/a	y/b	z/c	U(eq)
H89B	0.4252	0.0108	0.0037	0.094
H12A	0.8827	1.0693	0.5527	0.043
H12B	0.8406	1.1075	0.5094	0.043
H83A	0.5788	-0.2153	0.1276	0.119
H83B	0.5573	-0.1597	0.0735	0.119
H83C	0.5530	-0.1906	0.0993	0.119
H83D	0.5862	-0.1476	0.0740	0.119
H14A	0.8840	1.1668	0.4499	0.118
H14B	0.9174	1.1043	0.4908	0.118
H14C	0.9306	1.2003	0.4842	0.118
H14D	0.8869	1.1367	0.4525	0.118
H14E	0.9363	1.1464	0.4875	0.118
H14F	0.9044	1.2249	0.4818	0.118
H76A	0.6696	-0.1610	0.4816	0.067
H76B	0.6402	-0.2365	0.4480	0.067
H13A	0.8733	1.2414	0.5181	0.048
H13B	0.9154	1.2035	0.5618	0.048
H20A	0.8153	1.1528	0.8133	0.087
H20B	0.8249	1.0745	0.8553	0.087
H21A	0.8710	1.2274	0.8646	0.121
H21B	0.8628	1.1732	0.9123	0.121
H78A	0.5874	-0.2154	0.5016	0.092
H78B	0.5718	-0.1205	0.5063	0.092
H78C	0.6206	-0.1461	0.5360	0.092
H78D	0.6165	-0.1711	0.5387	0.092
H78E	0.5676	-0.1789	0.5013	0.092
H78F	0.5935	-0.0934	0.5009	0.092
H77A	0.5825	-0.1431	0.4175	0.071
H77B	0.6119	-0.0671	0.4503	0.071
H86A	0.6341	-0.0124	0.1547	0.121
H86B	0.6338	-0.0653	0.2068	0.121
H85A	0.6590	-0.1771	0.1817	0.123
H85B	0.6800	-0.1057	0.1537	0.123
H85C	0.6788	-0.1416	0.1869	0.123
H85D	0.6613	-0.1144	0.1237	0.123
H84A	0.6223	-0.1124	0.0724	0.121
H84B	0.6316	-0.2109	0.0887	0.121

	x/a	y/b	z/c	U(eq)
H84C	0.6221	-0.2645	0.1206	0.059
H84D	0.6093	-0.2396	0.1737	0.059
H76C	0.6626	-0.1142	0.4798	0.125
H76D	0.6221	-0.0702	0.4372	0.125
H77C	0.5831	-0.1993	0.4289	0.094
H77D	0.6238	-0.2428	0.4724	0.094
H12C	0.8341	1.1648	0.5055	0.062
H12D	0.8631	1.2378	0.5425	0.062
H13C	0.8932	1.0706	0.5340	0.127
H13D	0.9219	1.1461	0.5683	0.127

Crystal Structure Report for Na[IMP-pipA]



Thermal ellipsoid plot of 6003. Ellipsoids shown at 50% probability. THF molecules shown in wireframe, hydrogen atoms hidden for clarity.

A specimen of $C_{63}H_{40}B_2F_{30}N_3NaO_4$ was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The integration of the data using a triclinic unit cell yielded a total of 54105 reflections to a maximum θ angle of 28.02° (0.76 Å resolution), of which 14728 were independent (average redundancy 3.674, completeness = 98.2%, R_{int} = 2.56%, R_{sig} = 2.58%) and 11865 (80.56%) were greater than 2σ(F^2). The final cell constants of a = 14.2164(17) Å, b = 14.4515(17) Å, c = 17.120(2) Å, α = 81.955(2)°, β = 72.302(2)°, γ = 67.813(2)°, volume = 3101.4(6) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The final anisotropic full-matrix least-squares refinement on F^2 with 928 variables converged at R1 = 3.50%, for the observed data and wR2 = 9.00% for all data. The goodness-of-fit was 1.013. The largest peak in the final difference electron density synthesis was 0.448 $e^-/Å^3$ and the largest hole was -0.244 $e^-/Å^3$ with an RMS deviation of 0.049 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.625 g/cm^3 and F(000), 1524 e^-.

Table 1. Sample and crystal data for 6003.

Identification code	6003
Chemical formula	$C_{63}H_{40}B_2F_{30}N_3NaO_4$
Formula weight	1517.59 g/mol
Temperature	100(2) K

Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 14.2164(17) Å	α = 81.955(2)°
	b = 14.4515(17) Å	β = 72.302(2)°
	c = 17.120(2) Å	γ = 67.813(2)°
Volume	3101.4(6) $Å^3$	
Z	2	
Density (calculated)	1.625 g/cm^3	
Absorption coefficient	0.168 mm^{-1}	
F(000)	1524	

Table 2. Data collection and structure refinement for 6003.

Theta range for data collection	1.52 to 28.02°	
Index ranges	-18<=h<=18, -19<=k<=19, -22<=l<=22	
Reflections collected	54105	
Independent reflections	14728 [R(int) = 0.0256]	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	14728 / 0 / 928	
Goodness-of-fit on F^2	1.013	
Δ/σ_{max}	0.001	
Final R indices	11865 data; I>2σ(I)	R1 = 0.0350, wR2 = 0.0828
	all data	R1 = 0.0484, wR2 = 0.0900
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0391P)^2+1.7005P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.448 and -0.244 $eÅ^{-3}$	
R.M.S. deviation from mean	0.049 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for 6003.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Na01	0.53274(5)	0.70729(4)	0.67479(4)	0.01940(12)
F26	0.30604(7)	0.49632(6)	0.69870(5)	0.01765(17)
F6	0.65848(6)	0.19584(6)	0.96827(5)	0.01757(17)
F16	0.48238(7)	0.50733(6)	0.72116(5)	0.01671(17)
F30	0.58014(7)	0.18080(6)	0.63511(5)	0.01895(17)
F20	0.35546(7)	0.31724(6)	0.95002(5)	0.02024(18)

	x/a	y/b	z/c	U(eq)
F1	0.70139(7)	0.99515(6)	0.97885(5)	0.01966(18)
F10	0.00390(7)	0.01546(6)	0.80993(5)	0.02068(18)
F11	0.75690(7)	0.98961(6)	0.68316(5)	0.02072(18)
F15	0.92664(7)	0.19377(6)	0.73229(5)	0.02092(18)
F25	0.38799(7)	0.15500(6)	0.71713(5)	0.02105(18)
F5	0.93962(7)	0.87550(6)	0.72032(5)	0.02130(18)
F21	0.20106(7)	0.45021(6)	0.87236(5)	0.02139(18)
F17	0.48023(7)	0.63080(6)	0.82160(5)	0.02223(19)
F28	0.47667(8)	0.40395(7)	0.42530(5)	0.0264(2)
F9	0.08450(7)	0.06086(7)	0.91506(6)	0.0258(2)
F27	0.33074(7)	0.54038(6)	0.53819(5)	0.02329(19)
F18	0.41269(8)	0.60409(6)	0.98791(6)	0.0272(2)
F7	0.74107(7)	0.23610(7)	0.07419(5)	0.0252(2)
F24	0.20619(8)	0.12837(7)	0.73906(6)	0.0290(2)
F29	0.60036(7)	0.22526(7)	0.47731(5)	0.0267(2)
F22	0.02293(7)	0.42196(7)	0.89114(6)	0.0280(2)
F19	0.35074(8)	0.44572(7)	0.05013(5)	0.0289(2)
F23	0.02082(7)	0.26154(7)	0.82677(6)	0.0303(2)
F4	0.99780(8)	0.69406(6)	0.78603(6)	0.0279(2)
F2	0.76075(8)	0.81275(7)	0.04175(6)	0.0266(2)
F14	0.99446(8)	0.22359(7)	0.57303(6)	0.0282(2)
F8	0.95385(8)	0.17059(7)	0.04932(6)	0.0303(2)
F12	0.82876(8)	0.01934(7)	0.52231(6)	0.0295(2)
F13	0.94786(8)	0.13796(8)	0.46442(5)	0.0317(2)
F3	0.91001(9)	0.65708(7)	0.94726(7)	0.0341(2)
O1	0.70518(9)	0.60961(8)	0.65803(7)	0.0248(2)
O4	0.35134(8)	0.78112(8)	0.71277(7)	0.0231(2)
O3	0.60281(9)	0.77846(8)	0.54833(7)	0.0268(2)
O2	0.52448(9)	0.83467(9)	0.74941(7)	0.0281(3)
N2	0.51073(9)	0.22130(8)	0.80042(7)	0.0128(2)
N1	0.66260(9)	0.11946(8)	0.82371(7)	0.0131(2)
N3	0.86646(10)	0.52908(9)	0.67889(8)	0.0216(3)
C10	0.82761(11)	0.10872(10)	0.87981(8)	0.0143(3)
C1	0.61219(11)	0.20974(10)	0.79247(8)	0.0129(3)
C2	0.49643(11)	0.13520(10)	0.83946(8)	0.0149(3)
C28	0.41556(11)	0.40634(10)	0.82968(8)	0.0130(3)
C29	0.44548(11)	0.48856(10)	0.80216(8)	0.0140(3)
C34	0.44612(11)	0.33944(10)	0.67590(8)	0.0140(3)
C11	0.76515(11)	0.16298(10)	0.95003(9)	0.0154(3)
C22	0.30705(11)	0.30081(10)	0.79748(8)	0.0143(3)
C15	0.93523(11)	0.07423(10)	0.87304(9)	0.0167(3)

	x/a	y/b	z/c	U(eq)
C5	0.77467(11)	0.92321(10)	0.92703(9)	0.0162(3)
C39	0.51649(11)	0.27247(10)	0.61560(9)	0.0157(3)
C35	0.38282(11)	0.42815(10)	0.64564(8)	0.0148(3)
C3	0.58863(11)	0.07330(10)	0.85308(8)	0.0153(3)
C43	0.74084(11)	0.44193(10)	0.70607(9)	0.0156(3)
C16	0.84175(11)	0.08533(10)	0.71750(8)	0.0146(3)
C30	0.44498(11)	0.55502(10)	0.85352(9)	0.0164(3)
C27	0.29943(12)	0.22199(10)	0.76371(9)	0.0167(3)
C4	0.81509(11)	0.94803(10)	0.84520(9)	0.0147(3)
C33	0.38513(11)	0.39546(10)	0.91513(9)	0.0160(3)
C32	0.38193(12)	0.46084(11)	0.96821(9)	0.0194(3)
C17	0.90331(11)	0.14409(10)	0.68397(9)	0.0166(3)
C21	0.81819(11)	0.04648(10)	0.65856(9)	0.0167(3)
C36	0.39261(12)	0.45163(10)	0.56324(9)	0.0175(3)
C46	0.77100(11)	0.53307(10)	0.67850(9)	0.0168(3)
C45	0.67128(11)	0.34185(10)	0.81607(9)	0.0154(3)
C9	0.89081(11)	0.86572(10)	0.80023(9)	0.0165(3)
C41	0.69132(11)	0.31115(10)	0.67644(8)	0.0145(3)
C23	0.20927(12)	0.36737(10)	0.83934(9)	0.0166(3)
C40	0.65962(11)	0.28828(10)	0.76005(8)	0.0133(3)
C42	0.73029(11)	0.38851(10)	0.64961(9)	0.0158(3)
C14	0.97915(12)	0.09426(11)	0.92740(9)	0.0191(3)
C38	0.52869(12)	0.29292(11)	0.53231(9)	0.0188(3)
C6	0.80440(12)	0.82783(11)	0.96201(9)	0.0192(3)
C12	0.80572(12)	0.18434(11)	0.00664(9)	0.0186(3)
C44	0.71262(11)	0.41762(10)	0.78925(9)	0.0170(3)
C26	0.20612(13)	0.20673(11)	0.77343(9)	0.0206(3)
C25	0.11268(12)	0.27368(11)	0.81733(10)	0.0213(3)
C13	0.91326(13)	0.15048(11)	0.99509(9)	0.0205(3)
C31	0.41229(12)	0.54161(10)	0.93701(9)	0.0194(3)
C24	0.11398(12)	0.35509(11)	0.84973(9)	0.0200(3)
C18	0.93921(12)	0.16178(11)	0.60039(9)	0.0203(3)
C37	0.46642(12)	0.38319(11)	0.50608(9)	0.0194(3)
C19	0.91425(12)	0.12052(11)	0.54534(9)	0.0216(3)
C20	0.85311(12)	0.06166(11)	0.57497(9)	0.0209(3)
C8	0.92338(12)	0.76912(10)	0.83335(10)	0.0198(3)
C7	0.87961(13)	0.74974(11)	0.91464(10)	0.0219(3)
C47	0.94663(12)	0.44051(12)	0.70335(10)	0.0237(3)
C59	0.46289(13)	0.85968(13)	0.83337(10)	0.0272(3)
C63	0.28052(13)	0.73000(12)	0.71564(11)	0.0271(3)
C51	0.89415(14)	0.61977(12)	0.66088(11)	0.0282(4)

	x/a	y/b	z/c	U(eq)
C48	0.05225(13)	0.41883(13)	0.63885(11)	0.0292(4)
C60	0.29256(14)	0.88715(12)	0.71260(12)	0.0314(4)
C58	0.54093(14)	0.81443(14)	0.88558(11)	0.0316(4)
C52	0.70368(14)	0.73794(14)	0.48922(11)	0.0310(4)
B2	0.42118(12)	0.31816(11)	0.77569(9)	0.0127(3)
B1	0.78683(12)	0.06774(11)	0.81544(9)	0.0136(3)
C61	0.20986(14)	0.90015(14)	0.67045(11)	0.0357(4)
C56	0.62326(14)	0.84319(14)	0.74399(11)	0.0339(4)
C50	0.99976(15)	0.60023(14)	0.59652(12)	0.0368(4)
C55	0.56555(15)	0.88405(13)	0.53110(13)	0.0348(4)
C49	0.08575(15)	0.51022(15)	0.62132(13)	0.0370(4)
C57	0.65017(15)	0.79132(16)	0.82244(12)	0.0371(4)
C53	0.75548(15)	0.81445(15)	0.48055(13)	0.0387(4)
C62	0.17871(16)	0.80976(16)	0.70531(15)	0.0454(5)
C54	0.66267(18)	0.91208(16)	0.49215(19)	0.0608(7)

Table 4. Bond lengths (Å) for 6003.

Na01-O1	2.2709(13)	Na01-O4	2.3039(13)
Na01-O2	2.3319(12)	Na01-O3	2.3616(12)
Na01-F28	2.5714(11)	Na01-F17	2.6079(11)
F26-C35	1.3501(16)	F6-C11	1.3536(16)
F16-C29	1.3535(15)	F30-C39	1.3564(16)
F20-C33	1.3530(15)	F1-C5	1.3532(16)
F10-C15	1.3531(16)	F11-C21	1.3539(16)
F15-C17	1.3502(16)	F25-C27	1.3577(16)
F5-C9	1.3475(16)	F21-C23	1.3454(16)
F17-C30	1.3525(15)	F28-C37	1.3483(16)
F28-Na01	2.5714(11)	F9-C14	1.3457(17)
F27-C36	1.3513(16)	F18-C31	1.3423(16)
F7-C12	1.3484(17)	F24-C26	1.3469(17)
F29-C38	1.3427(16)	F22-C24	1.3421(17)
F19-C32	1.3493(16)	F23-C25	1.3413(17)
F4-C8	1.3454(17)	F2-C6	1.3416(17)
F14-C18	1.3503(17)	F8-C13	1.3444(17)
F12-C20	1.3457(17)	F13-C19	1.3424(17)
F3-C7	1.3387(16)	O1-C46	1.2373(17)
O4-C60	1.4420(19)	O4-C63	1.4434(19)
O3-C55	1.433(2)	O3-C52	1.440(2)
O2-C56	1.430(2)	O2-C59	1.4506(19)
N2-C1	1.3534(18)	N2-C2	1.3827(17)

N2-B2	1.6048(19)	N1-C1	1.3540(17)
N1-C3	1.3850(17)	N1-B1	1.6057(19)
N3-C46	1.3384(19)	N3-C47	1.4666(19)
N3-C51	1.4733(18)	C10-C15	1.391(2)
C10-C11	1.3920(19)	C10-B1	1.653(2)
C1-C40	1.4918(18)	C2-C3	1.347(2)
C2-H2	0.95	C28-C29	1.3848(18)
C28-C33	1.3979(19)	C28-B2	1.6410(19)
C29-C30	1.3868(19)	C34-C39	1.3871(19)
C34-C35	1.3957(19)	C34-B2	1.645(2)
C11-C12	1.388(2)	C22-C23	1.396(2)
C22-C27	1.3997(19)	C22-B2	1.658(2)
C15-C14	1.380(2)	C5-C6	1.3855(19)
C5-C4	1.395(2)	C39-C38	1.386(2)
C35-C36	1.381(2)	C3-H3	0.95
C43-C44	1.390(2)	C43-C42	1.392(2)
C43-C46	1.5070(18)	C16-C17	1.3914(19)
C16-C21	1.397(2)	C16-B1	1.649(2)
C30-C31	1.372(2)	C27-C26	1.383(2)
C4-C9	1.3970(19)	C4-B1	1.663(2)
C33-C32	1.379(2)	C32-C31	1.378(2)
C17-C18	1.388(2)	C21-C20	1.380(2)
C36-C37	1.378(2)	C45-C44	1.3915(19)
C45-C40	1.3957(19)	C45-H45	0.95
C9-C8	1.391(2)	C41-C42	1.3918(19)
C41-C40	1.3961(19)	C41-H41	0.95
C23-C24	1.387(2)	C42-H42	0.95
C14-C13	1.382(2)	C38-C37	1.376(2)
C6-C7	1.376(2)	C12-C13	1.376(2)
C44-H44	0.95	C26-C25	1.375(2)
C25-C24	1.378(2)	C18-C19	1.375(2)
C19-C20	1.381(2)	C8-C7	1.378(2)
C47-C48	1.518(2)	C47-H47A	0.99
C47-H47B	0.99	C59-C58	1.533(3)
C59-H59A	0.99	C59-H59B	0.99
C63-C62	1.514(3)	C63-H63A	0.99
C63-H63B	0.99	C51-C50	1.520(3)
C51-H51A	0.99	C51-H51B	0.99
C48-C49	1.529(2)	C48-H48A	0.99
C48-H48B	0.99	C60-C61	1.500(3)
C60-H60A	0.99	C60-H60B	0.99
C58-C57	1.543(3)	C58-H58A	0.99

C58-H58B	0.99	C52-C53	1.513(3)
C52-H52A	0.99	C52-H52B	0.99
C61-C62	1.522(3)	C61-H61A	0.99
C61-H61B	0.99	C56-C57	1.525(3)
C56-H56A	0.99	C56-H56B	0.99
C50-C49	1.525(3)	C50-H50A	0.99
C50-H50B	0.99	C55-C54	1.517(3)
C55-H55A	0.99	C55-H55B	0.99
C49-H49A	0.99	C49-H49B	0.99
C57-H57A	0.99	C57-H57B	0.99
C53-C54	1.511(3)	C53-H53A	0.99
C53-H53B	0.99	C62-H62A	0.99
C62-H62B	0.99	C54-H54A	0.99
C54-H54B	0.99		

Table 5. Bond angles (°) for 6003.

O1-Na01-O4	167.82(5)	O1-Na01-O2	99.24(5)
O4-Na01-O2	83.69(4)	O1-Na01-O3	82.30(4)
O4-Na01-O3	109.49(5)	O2-Na01-O3	92.63(5)
O1-Na01-F28	88.49(4)	O4-Na01-F28	90.56(4)
O2-Na01-F28	168.42(5)	O3-Na01-F28	79.79(4)
O1-Na01-F17	91.26(4)	O4-Na01-F17	77.39(4)
O2-Na01-F17	81.83(4)	O3-Na01-F17	170.76(4)
F28-Na01-F17	106.77(3)	C30-F17-Na01	135.12(8)
C37-F28-Na01	124.90(8)	C46-O1-Na01	148.14(10)
C60-O4-C63	107.94(12)	C60-O4-Na01	125.62(10)
C63-O4-Na01	123.93(9)	C55-O3-C52	106.00(13)
C55-O3-Na01	122.19(10)	C52-O3-Na01	128.91(10)
C56-O2-C59	104.21(12)	C56-O2-Na01	115.99(10)
C59-O2-Na01	126.73(9)	C1-N2-C2	106.50(11)
C1-N2-B2	127.41(11)	C2-N2-B2	125.96(11)
C1-N1-C3	106.09(11)	C1-N1-B1	127.35(11)
C3-N1-B1	125.84(11)	C46-N3-C47	124.54(12)
C46-N3-C51	120.37(12)	C47-N3-C51	114.87(12)
C15-C10-C11	113.59(13)	C15-C10-B1	118.66(12)
C11-C10-B1	126.93(12)	N2-C1-N1	110.45(11)
N2-C1-C40	124.87(12)	N1-C1-C40	124.51(12)
C3-C2-N2	108.24(12)	C3-C2-H2	125.9
N2-C2-H2	125.9	C29-C28-C33	113.59(12)
C29-C28-B2	128.49(12)	C33-C28-B2	117.70(11)
F16-C29-C28	121.33(12)	F16-C29-C30	114.65(12)

C28-C29-C30	123.95(13)	C39-C34-C35	113.86(12)
C39-C34-B2	126.70(12)	C35-C34-B2	118.92(12)
F6-C11-C12	115.65(12)	F6-C11-C10	120.69(12)
C12-C11-C10	123.63(13)	C23-C22-C27	113.29(13)
C23-C22-B2	125.32(12)	C27-C22-B2	120.79(12)
F10-C15-C14	115.99(13)	F10-C15-C10	119.27(12)
C14-C15-C10	124.74(13)	F1-C5-C6	115.04(12)
F1-C5-C4	120.02(12)	C6-C5-C4	124.94(13)
F30-C39-C38	114.96(12)	F30-C39-C34	121.21(12)
C38-C39-C34	123.83(13)	F26-C35-C36	116.51(12)
F26-C35-C34	119.44(12)	C36-C35-C34	124.05(13)
C2-C3-N1	108.70(12)	C2-C3-H3	125.6
N1-C3-H3	125.6	C44-C43-C42	119.81(12)
C44-C43-C46	119.60(12)	C42-C43-C46	120.23(12)
C17-C16-C21	113.28(12)	C17-C16-B1	127.41(12)
C21-C16-B1	119.00(12)	F17-C30-C31	119.93(12)
F17-C30-C29	120.18(13)	C31-C30-C29	119.84(13)
F25-C27-C26	115.96(12)	F25-C27-C22	119.51(12)
C26-C27-C22	124.53(14)	C5-C4-C9	112.94(12)
C5-C4-B1	119.47(12)	C9-C4-B1	126.69(12)
F20-C33-C32	116.29(12)	F20-C33-C28	119.56(12)
C32-C33-C28	124.15(13)	F19-C32-C31	119.82(13)
F19-C32-C33	120.68(13)	C31-C32-C33	119.50(13)
F15-C17-C18	114.96(12)	F15-C17-C16	121.14(12)
C18-C17-C16	123.76(13)	F11-C21-C20	116.09(13)
F11-C21-C16	119.25(12)	C20-C21-C16	124.66(13)
F27-C36-C37	119.83(13)	F27-C36-C35	120.89(13)
C37-C36-C35	119.28(13)	O1-C46-N3	122.56(13)
O1-C46-C43	118.36(13)	N3-C46-C43	119.05(12)
C44-C45-C40	120.66(13)	C44-C45-H45	119.7
C40-C45-H45	119.7	F5-C9-C8	114.83(12)
F5-C9-C4	121.38(12)	C8-C9-C4	123.77(13)
C42-C41-C40	120.52(13)	C42-C41-H41	119.7
C40-C41-H41	119.7	F21-C23-C24	114.76(13)
F21-C23-C22	121.45(12)	C24-C23-C22	123.78(13)
C45-C40-C41	118.89(12)	C45-C40-C1	118.30(12)
C41-C40-C1	122.80(12)	C41-C42-C43	120.07(13)
C41-C42-H42	120.0	C43-C42-H42	120.0
F9-C14-C15	121.16(13)	F9-C14-C13	119.81(13)
C15-C14-C13	119.03(14)	F29-C38-C37	119.95(13)
F29-C38-C39	120.51(13)	C37-C38-C39	119.54(13)
F2-C6-C7	120.70(13)	F2-C6-C5	119.83(13)

C7-C6-C5	119.47(14)	F7-C12-C13	119.21(13)
F7-C12-C11	120.89(13)	C13-C12-C11	119.88(13)
C43-C44-C45	120.01(13)	C43-C44-H44	120.0
C45-C44-H44	120.0	F24-C26-C25	120.20(13)
F24-C26-C27	120.55(14)	C25-C26-C27	119.24(13)
F23-C25-C26	120.53(14)	F23-C25-C24	120.18(14)
C26-C25-C24	119.27(13)	F8-C13-C12	120.62(14)
F8-C13-C14	120.30(14)	C12-C13-C14	119.07(13)
F18-C31-C30	120.88(13)	F18-C31-C32	120.14(13)
C30-C31-C32	118.95(13)	F22-C24-C25	119.67(13)
F22-C24-C23	120.51(13)	C25-C24-C23	119.82(14)
F14-C18-C19	119.70(13)	F14-C18-C17	120.02(14)
C19-C18-C17	120.20(13)	F28-C37-C38	120.30(13)
F28-C37-C36	120.38(13)	C38-C37-C36	119.32(13)
F13-C19-C18	120.59(14)	F13-C19-C20	120.70(14)
C18-C19-C20	118.70(13)	F12-C20-C21	120.77(14)
F12-C20-C19	119.85(13)	C21-C20-C19	119.38(14)
F4-C8-C7	119.66(13)	F4-C8-C9	120.09(14)
C7-C8-C9	120.25(14)	F3-C7-C6	120.49(14)
F3-C7-C8	120.89(14)	C6-C7-C8	118.62(13)
N3-C47-C48	110.43(13)	N3-C47-H47A	109.6
C48-C47-H47A	109.6	N3-C47-H47B	109.6
C48-C47-H47B	109.6	H47A-C47-H47B	108.1
O2-C59-C58	105.80(13)	O2-C59-H59A	110.6
C58-C59-H59A	110.6	O2-C59-H59B	110.6
C58-C59-H59B	110.6	H59A-C59-H59B	108.7
O4-C63-C62	106.51(14)	O4-C63-H63A	110.4
C62-C63-H63A	110.4	O4-C63-H63B	110.4
C62-C63-H63B	110.4	H63A-C63-H63B	108.6
N3-C51-C50	110.91(14)	N3-C51-H51A	109.5
C50-C51-H51A	109.5	N3-C51-H51B	109.5
C50-C51-H51B	109.5	H51A-C51-H51B	108.0
C47-C48-C49	111.14(15)	C47-C48-H48A	109.4
C49-C48-H48A	109.4	C47-C48-H48B	109.4
C49-C48-H48B	109.4	H48A-C48-H48B	108.0
O4-C60-C61	105.07(14)	O4-C60-H60A	110.7
C61-C60-H60A	110.7	O4-C60-H60B	110.7
C61-C60-H60B	110.7	H60A-C60-H60B	108.8
C59-C58-C57	103.85(14)	C59-C58-H58A	111.0
C57-C58-H58A	111.0	C59-C58-H58B	111.0
C57-C58-H58B	111.0	H58A-C58-H58B	109.0
O3-C52-C53	104.87(14)	O3-C52-H52A	110.8

C53-C52-H52A	110.8	O3-C52-H52B	110.8
C53-C52-H52B	110.8	H52A-C52-H52B	108.8
N2-B2-C28	103.11(10)	N2-B2-C34	112.36(11)
C28-B2-C34	115.87(11)	N2-B2-C22	111.43(10)
C28-B2-C22	112.70(11)	C34-B2-C22	101.70(11)
N1-B1-C16	103.36(11)	N1-B1-C10	114.40(11)
C16-B1-C10	114.91(11)	N1-B1-C4	109.70(11)
C16-B1-C4	113.90(11)	C10-B1-C4	100.89(10)
C60-C61-C62	100.72(14)	C60-C61-H61A	111.6
C62-C61-H61A	111.6	C60-C61-H61B	111.6
C62-C61-H61B	111.6	H61A-C61-H61B	109.4
O2-C56-C57	104.23(14)	O2-C56-H56A	110.9
C57-C56-H56A	110.9	O2-C56-H56B	110.9
C57-C56-H56B	110.9	H56A-C56-H56B	108.9
C51-C50-C49	111.12(15)	C51-C50-H50A	109.4
C49-C50-H50A	109.4	C51-C50-H50B	109.4
C49-C50-H50B	109.4	H50A-C50-H50B	108.0
O3-C55-C54	106.63(15)	O3-C55-H55A	110.4
C54-C55-H55A	110.4	O3-C55-H55B	110.4
C54-C55-H55B	110.4	H55A-C55-H55B	108.6
C50-C49-C48	110.17(15)	C50-C49-H49A	109.6
C48-C49-H49A	109.6	C50-C49-H49B	109.6
C48-C49-H49B	109.6	H49A-C49-H49B	108.1
C56-C57-C58	103.17(15)	C56-C57-H57A	111.1
C58-C57-H57A	111.1	C56-C57-H57B	111.1
C58-C57-H57B	111.1	H57A-C57-H57B	109.1
C54-C53-C52	102.78(16)	C54-C53-H53A	111.2
C52-C53-H53A	111.2	C54-C53-H53B	111.2
C52-C53-H53B	111.2	H53A-C53-H53B	109.1
C63-C62-C61	104.04(15)	C63-C62-H62A	110.9
C61-C62-H62A	110.9	C63-C62-H62B	110.9
C61-C62-H62B	110.9	H62A-C62-H62B	109.0
C53-C54-C55	105.64(16)	C53-C54-H54A	110.6
C55-C54-H54A	110.6	C53-C54-H54B	110.6
C55-C54-H54B	110.6	H54A-C54-H54B	108.7

Table 6. Anisotropic atomic displacement parameters (Å^2) for 6003.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Na01	0.0183(3)	0.0188(3)	0.0220(3)	0.0000(2)	-0.0059(2)	-0.0074(2)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F26	0.0189(4)	0.0141(4)	0.0184(4)	-0.0005(3)	-0.0057(3)	-0.0037(3)
F6	0.0159(4)	0.0170(4)	0.0181(4)	-0.0015(3)	-0.0024(3)	-0.0054(3)
F16	0.0213(4)	0.0159(4)	0.0144(4)	0.0018(3)	-0.0037(3)	-0.0099(3)
F30	0.0197(4)	0.0149(4)	0.0203(4)	-0.0032(3)	-0.0057(3)	-0.0030(3)
F20	0.0296(5)	0.0179(4)	0.0154(4)	0.0035(3)	-0.0046(3)	-0.0135(4)
F1	0.0217(5)	0.0178(4)	0.0171(4)	0.0011(3)	-0.0025(3)	-0.0071(3)
F10	0.0157(4)	0.0212(4)	0.0217(4)	-0.0027(3)	-0.0025(3)	-0.0041(3)
F11	0.0229(5)	0.0216(4)	0.0225(4)	-0.0004(3)	-0.0066(4)	-0.0131(4)
F15	0.0254(5)	0.0210(4)	0.0221(4)	0.0016(3)	-0.0069(4)	-0.0149(4)
F25	0.0239(5)	0.0180(4)	0.0236(4)	-0.0047(3)	-0.0061(4)	-0.0089(4)
F5	0.0204(4)	0.0186(4)	0.0202(4)	-0.0017(3)	-0.0026(3)	-0.0037(3)
F21	0.0178(4)	0.0182(4)	0.0271(5)	-0.0054(3)	-0.0041(3)	-0.0052(3)
F17	0.0321(5)	0.0143(4)	0.0270(5)	0.0024(3)	-0.0118(4)	-0.0137(4)
F28	0.0385(6)	0.0336(5)	0.0121(4)	0.0047(4)	-0.0071(4)	-0.0199(4)
F9	0.0171(5)	0.0304(5)	0.0324(5)	0.0036(4)	-0.0110(4)	-0.0093(4)
F27	0.0300(5)	0.0204(4)	0.0225(4)	0.0088(3)	-0.0139(4)	-0.0104(4)
F18	0.0448(6)	0.0182(4)	0.0244(5)	-0.0052(4)	-0.0168(4)	-0.0101(4)
F7	0.0288(5)	0.0268(5)	0.0198(4)	-0.0072(4)	-0.0059(4)	-0.0079(4)
F24	0.0366(6)	0.0239(5)	0.0394(6)	0.0015(4)	-0.0183(4)	-0.0195(4)
F29	0.0267(5)	0.0318(5)	0.0173(4)	-0.0085(4)	0.0011(4)	-0.0088(4)
F22	0.0148(4)	0.0295(5)	0.0349(5)	0.0005(4)	-0.0042(4)	-0.0054(4)
F19	0.0481(6)	0.0267(5)	0.0121(4)	-0.0014(3)	-0.0069(4)	-0.0141(4)
F23	0.0217(5)	0.0315(5)	0.0467(6)	0.0128(4)	-0.0175(4)	-0.0179(4)
F4	0.0271(5)	0.0144(4)	0.0382(5)	-0.0058(4)	-0.0101(4)	-0.0004(4)
F2	0.0330(5)	0.0251(5)	0.0223(5)	0.0119(4)	-0.0092(4)	-0.0143(4)
F14	0.0277(5)	0.0316(5)	0.0272(5)	0.0086(4)	-0.0026(4)	-0.0196(4)
F8	0.0328(5)	0.0381(5)	0.0300(5)	-0.0031(4)	-0.0176(4)	-0.0158(5)
F12	0.0367(6)	0.0376(5)	0.0194(5)	-0.0040(4)	-0.0101(4)	-0.0161(5)
F13	0.0355(6)	0.0400(6)	0.0149(4)	0.0046(4)	-0.0013(4)	-0.0144(5)
F3	0.0435(6)	0.0135(4)	0.0431(6)	0.0111(4)	-0.0184(5)	-0.0067(4)
O1	0.0218(6)	0.0157(5)	0.0390(7)	0.0085(4)	-0.0136(5)	-0.0082(4)
O4	0.0197(6)	0.0185(5)	0.0299(6)	-0.0001(4)	-0.0084(4)	-0.0046(4)
O3	0.0221(6)	0.0243(6)	0.0289(6)	0.0061(5)	-0.0035(5)	-0.0080(5)
O2	0.0289(6)	0.0318(6)	0.0276(6)	-0.0062(5)	-0.0021(5)	-0.0177(5)
N2	0.0157(6)	0.0106(5)	0.0134(5)	0.0007(4)	-0.0046(4)	-0.0060(4)
N1	0.0148(6)	0.0111(5)	0.0145(5)	0.0010(4)	-0.0044(4)	-0.0059(4)
N3	0.0214(7)	0.0159(6)	0.0326(7)	0.0075(5)	-0.0125(5)	-0.0111(5)
C10	0.0166(7)	0.0110(6)	0.0164(7)	0.0029(5)	-0.0052(5)	-0.0067(5)
C1	0.0165(7)	0.0119(6)	0.0115(6)	-0.0002(5)	-0.0043(5)	-0.0060(5)
C2	0.0168(7)	0.0132(6)	0.0162(7)	0.0012(5)	-0.0037(5)	-0.0080(5)
C28	0.0122(6)	0.0120(6)	0.0145(6)	-0.0006(5)	-0.0046(5)	-0.0030(5)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C29	0.0144(7)	0.0138(6)	0.0133(6)	0.0009(5)	-0.0047(5)	-0.0042(5)
C34	0.0161(7)	0.0148(6)	0.0145(6)	0.0002(5)	-0.0046(5)	-0.0092(5)
C11	0.0145(7)	0.0130(6)	0.0182(7)	0.0029(5)	-0.0046(5)	-0.0054(5)
C22	0.0173(7)	0.0145(6)	0.0134(6)	0.0044(5)	-0.0066(5)	-0.0079(5)
C15	0.0181(7)	0.0137(6)	0.0170(7)	0.0019(5)	-0.0031(5)	-0.0063(5)
C5	0.0158(7)	0.0149(6)	0.0195(7)	0.0009(5)	-0.0063(5)	-0.0066(5)
C39	0.0165(7)	0.0156(6)	0.0181(7)	-0.0002(5)	-0.0067(5)	-0.0077(5)
C35	0.0164(7)	0.0149(6)	0.0160(7)	-0.0007(5)	-0.0046(5)	-0.0085(5)
C3	0.0171(7)	0.0129(6)	0.0163(7)	0.0023(5)	-0.0033(5)	-0.0078(5)
C43	0.0142(7)	0.0121(6)	0.0214(7)	0.0030(5)	-0.0065(5)	-0.0058(5)
C16	0.0135(7)	0.0121(6)	0.0163(7)	0.0012(5)	-0.0037(5)	-0.0033(5)
C30	0.0192(7)	0.0104(6)	0.0225(7)	0.0025(5)	-0.0096(6)	-0.0065(5)
C27	0.0199(7)	0.0155(6)	0.0159(7)	0.0023(5)	-0.0065(5)	-0.0072(6)
C4	0.0150(7)	0.0137(6)	0.0186(7)	0.0015(5)	-0.0069(5)	-0.0073(5)
C33	0.0183(7)	0.0132(6)	0.0175(7)	0.0020(5)	-0.0055(5)	-0.0070(5)
C32	0.0252(8)	0.0194(7)	0.0122(6)	0.0000(5)	-0.0062(6)	-0.0060(6)
C17	0.0156(7)	0.0157(6)	0.0181(7)	0.0002(5)	-0.0048(5)	-0.0053(5)
C21	0.0144(7)	0.0153(6)	0.0200(7)	0.0008(5)	-0.0037(5)	-0.0060(5)
C36	0.0201(7)	0.0172(6)	0.0199(7)	0.0061(5)	-0.0094(6)	-0.0111(6)
C46	0.0187(7)	0.0145(6)	0.0200(7)	0.0015(5)	-0.0071(6)	-0.0083(6)
C45	0.0163(7)	0.0153(6)	0.0149(6)	0.0007(5)	-0.0039(5)	-0.0067(5)
C9	0.0151(7)	0.0173(6)	0.0197(7)	-0.0001(5)	-0.0060(5)	-0.0076(6)
C41	0.0150(7)	0.0142(6)	0.0161(7)	0.0008(5)	-0.0055(5)	-0.0065(5)
C23	0.0198(7)	0.0150(6)	0.0167(7)	0.0029(5)	-0.0070(5)	-0.0079(6)
C40	0.0119(6)	0.0107(6)	0.0173(7)	0.0016(5)	-0.0045(5)	-0.0042(5)
C42	0.0162(7)	0.0158(6)	0.0152(7)	0.0034(5)	-0.0042(5)	-0.0069(5)
C14	0.0165(7)	0.0181(7)	0.0244(8)	0.0055(6)	-0.0081(6)	-0.0083(6)
C38	0.0188(7)	0.0241(7)	0.0154(7)	-0.0049(5)	-0.0005(5)	-0.0114(6)
C6	0.0218(8)	0.0203(7)	0.0199(7)	0.0071(6)	-0.0096(6)	-0.0120(6)
C12	0.0230(8)	0.0173(6)	0.0153(7)	-0.0007(5)	-0.0039(6)	-0.0081(6)
C44	0.0192(7)	0.0151(6)	0.0197(7)	-0.0013(5)	-0.0065(6)	-0.0081(6)
C26	0.0286(8)	0.0174(7)	0.0247(8)	0.0062(6)	-0.0149(6)	-0.0144(6)
C25	0.0192(8)	0.0244(7)	0.0268(8)	0.0125(6)	-0.0130(6)	-0.0142(6)
C13	0.0273(8)	0.0210(7)	0.0209(7)	0.0036(6)	-0.0133(6)	-0.0132(6)
C31	0.0264(8)	0.0138(6)	0.0204(7)	-0.0047(5)	-0.0114(6)	-0.0045(6)
C24	0.0159(7)	0.0200(7)	0.0223(7)	0.0059(6)	-0.0063(6)	-0.0057(6)
C18	0.0159(7)	0.0191(7)	0.0236(8)	0.0050(6)	-0.0020(6)	-0.0083(6)
C37	0.0250(8)	0.0271(7)	0.0120(6)	0.0032(5)	-0.0056(6)	-0.0167(6)
C19	0.0202(8)	0.0248(7)	0.0143(7)	0.0029(6)	-0.0014(6)	-0.0056(6)
C20	0.0219(8)	0.0223(7)	0.0180(7)	-0.0027(6)	-0.0068(6)	-0.0055(6)
C8	0.0178(7)	0.0139(6)	0.0295(8)	-0.0035(6)	-0.0104(6)	-0.0035(6)

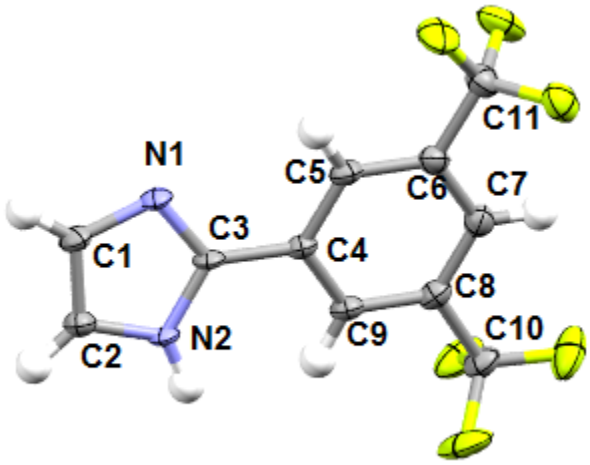
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C7	0.0252(8)	0.0133(6)	0.0318(8)	0.0069(6)	-0.0158(7)	-0.0083(6)
C47	0.0195(8)	0.0222(7)	0.0313(8)	0.0080(6)	-0.0124(6)	-0.0082(6)
C59	0.0262(9)	0.0287(8)	0.0269(8)	-0.0031(6)	-0.0014(7)	-0.0138(7)
C63	0.0222(8)	0.0275(8)	0.0323(9)	-0.0003(7)	-0.0061(7)	-0.0107(7)
C51	0.0285(9)	0.0204(7)	0.0448(10)	0.0069(7)	-0.0161(7)	-0.0167(7)
C48	0.0225(8)	0.0325(9)	0.0310(9)	0.0045(7)	-0.0088(7)	-0.0087(7)
C60	0.0288(9)	0.0186(7)	0.0385(10)	0.0032(7)	-0.0057(7)	-0.0036(7)
C58	0.0325(10)	0.0377(9)	0.0290(9)	-0.0062(7)	-0.0055(7)	-0.0179(8)
C52	0.0246(9)	0.0346(9)	0.0265(9)	0.0031(7)	-0.0010(7)	-0.0085(7)
B2	0.0143(7)	0.0104(6)	0.0134(7)	0.0006(5)	-0.0039(6)	-0.0046(6)
B1	0.0145(7)	0.0121(6)	0.0143(7)	0.0008(5)	-0.0034(6)	-0.0057(6)
C61	0.0273(9)	0.0355(9)	0.0248(9)	0.0006(7)	-0.0045(7)	0.0074(8)
C56	0.0318(10)	0.0400(10)	0.0358(10)	-0.0105(8)	0.0010(8)	-0.0239(8)
C50	0.0368(10)	0.0371(10)	0.0441(11)	0.0123(8)	-0.0117(8)	-0.0257(9)
C55	0.0293(10)	0.0260(8)	0.0458(11)	0.0091(7)	-0.0110(8)	-0.0093(7)
C49	0.0250(9)	0.0439(11)	0.0440(11)	0.0057(8)	-0.0056(8)	-0.0196(8)
C57	0.0279(9)	0.0503(11)	0.0396(10)	-0.0120(9)	-0.0069(8)	-0.0192(9)
C53	0.0272(10)	0.0470(11)	0.0410(11)	0.0059(9)	-0.0062(8)	-0.0172(9)
C62	0.0278(10)	0.0452(11)	0.0657(14)	-0.0101(10)	-0.0197(10)	-0.0074(9)
C54	0.0382(12)	0.0343(11)	0.103(2)	0.0129(12)	-0.0069(12)	-0.0204(10)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 6003.

	x/a	y/b	z/c	U(eq)
H2	0.4326	0.1220	0.8542	0.018
H3	0.6009	0.0087	0.8786	0.018
H45	0.6508	0.3264	0.8731	0.018
H41	0.6863	0.2736	0.6375	0.017
H42	0.7497	0.4049	0.5927	0.019
H44	0.7215	0.4527	0.8278	0.02
H47A	0.9241	0.3822	0.7104	0.028
H47B	0.9540	0.4519	0.7565	0.028
H59A	0.4063	0.8310	0.8505	0.033
H59B	0.4302	0.9331	0.8390	0.033
H63A	0.2674	0.6934	0.7688	0.033
H63B	0.3112	0.6816	0.6710	0.033
H51A	0.8978	0.6417	0.7118	0.034
H51B	0.8385	0.6741	0.6409	0.034
H48A	1.0469	0.3994	0.5876	0.035
H48B	1.1066	0.3621	0.6582	0.035

	x/a	y/b	z/c	U(eq)
H60A	0.3392	0.9244	0.6824	0.038
H60B	0.2595	0.9114	0.7693	0.038
H58A	0.5329	0.7527	0.9151	0.038
H58B	0.5304	0.8626	0.9260	0.038
H52A	0.6946	0.7289	0.4361	0.037
H52B	0.7467	0.6726	0.5090	0.037
H61A	0.2392	0.8978	0.6101	0.043
H61B	0.1494	0.9636	0.6851	0.043
H56A	0.6165	0.9142	0.7413	0.041
H56B	0.6782	0.8096	0.6949	0.041
H50A	1.0199	0.6600	0.5894	0.044
H50B	0.9931	0.5879	0.5433	0.044
H55A	0.5233	0.9207	0.5823	0.042
H55B	0.5207	0.9007	0.4931	0.042
H49A	1.0986	0.5255	0.6709	0.044
H49B	1.1523	0.4957	0.5766	0.044
H57A	0.6949	0.8190	0.8392	0.045
H57B	0.6872	0.7184	0.8154	0.045
H53A	0.7930	0.8034	0.5231	0.046
H53B	0.8059	0.8126	0.4257	0.046
H62A	0.1242	0.8248	0.7587	0.054
H62B	0.1513	0.7885	0.6670	0.054
H54A	0.6588	0.9476	0.4387	0.073
H54B	0.6690	0.9559	0.5284	0.073

Crystal Structure Report for 2-(3,5-bis(trifluoromethyl)phenyl)-1H-imidazole



Thermal ellipsoid plot of 5937. Ellipsoids shown at 50% probability, hydrogen atoms shown in ball and stick.

A specimen of $C_{11}H_6F_6N_2$, approximate dimensions 0.072 mm x 0.202 mm x 0.248 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The integration of the data using a monoclinic unit cell yielded a total of 6794 reflections to a maximum θ angle of 27.99° (0.76 Å resolution), of which 2627 were independent (average redundancy 2.586, completeness = 96.6%, R_{int} = 5.49%, R_{sig} = 6.34%) and 1729 (65.82%) were greater than $2\sigma(F^2)$. The final cell constants of a = 8.061(6) Å, b = 14.293(9) Å, c = 9.908(7) Å, β = 99.483(12)°, volume = 1126.0(13) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.9590 and 0.9880. The final anisotropic full-matrix least-squares refinement on F^2 with 172 variables converged at R1 = 6.43%, for the observed data and wR2 = 17.81% for all data. The goodness-of-fit was 1.048. The largest peak in the final difference electron density synthesis was 0.482 $e^-/Å^3$ and the largest hole was -0.399 $e^-/Å^3$ with an RMS deviation of 0.081 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.653 g/cm^3 and F(000), 560 e^-.

Table 1. Sample and crystal data for 5937.

Identification code	5937
Chemical formula	$C_{11}H_6F_6N_2$
Formula weight	280.18 g/mol
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal size	0.072 x 0.202 x 0.248 mm
Crystal system	monoclinic

Space group	P 1 21/c 1	
Unit cell dimensions	a = 8.061(6) Å	α = 90°
	b = 14.293(9) Å	β = 99.483(12)°
	c = 9.908(7) Å	γ = 90°
Volume	1126.0(13) $Å^3$	
Z	4	
Density (calculated)	1.653 g/cm^3	
Absorption coefficient	0.170 mm^{-1}	
F(000)	560	

Table 2. Data collection and structure refinement for 5937.

Theta range for data collection	2.52 to 27.99°	
Index ranges	-10<=h<=10, -15<=k<=18, -13<=l<=11	
Reflections collected	6794	
Independent reflections	2627 [R(int) = 0.0549]	
Max. and min. transmission	0.9880 and 0.9590	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	2627 / 0 / 172	
Goodness-of-fit on F^2	1.048	
Final R indices	1729 data; I>2σ(I)	R1 = 0.0643, wR2 = 0.1583
	all data	R1 = 0.1025, wR2 = 0.1781
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0769P)^2+1.3124P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.482 and -0.399 $eÅ^{-3}$	
R.M.S. deviation from mean	0.081 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for 5937.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
F2	0.9716(2)	0.60480(14)	0.4094(2)	0.0373(5)
F1	0.7792(3)	0.64833(17)	0.2447(2)	0.0459(6)
F5	0.5655(3)	0.46986(15)	0.8348(2)	0.0452(6)
F3	0.8003(3)	0.50407(14)	0.3071(2)	0.0448(6)
F4	0.8231(3)	0.50955(17)	0.8486(2)	0.0506(6)
F6	0.6502(4)	0.60306(15)	0.91749(19)	0.0555(7)
N1	0.2314(3)	0.76578(18)	0.3558(2)	0.0224(5)
N2	0.2027(3)	0.77039(17)	0.5737(2)	0.0209(5)

	x/a	y/b	z/c	U(eq)
C4	0.4460(4)	0.68002(19)	0.5177(3)	0.0194(6)
C3	0.2961(4)	0.7382(2)	0.4817(3)	0.0198(6)
C9	0.4855(4)	0.6396(2)	0.6472(3)	0.0220(6)
C5	0.5527(4)	0.6648(2)	0.4221(3)	0.0233(6)
C2	0.0725(4)	0.8213(2)	0.5037(3)	0.0246(6)
C8	0.6287(4)	0.5840(2)	0.6789(3)	0.0244(6)
C6	0.6941(4)	0.6096(2)	0.4551(3)	0.0243(6)
C1	0.0915(4)	0.8178(2)	0.3695(3)	0.0256(7)
C7	0.7332(4)	0.5682(2)	0.5845(3)	0.0261(7)
C10	0.6666(4)	0.5413(2)	0.8199(3)	0.0292(7)
C11	0.8102(4)	0.5923(2)	0.3540(3)	0.0305(7)

Table 4. Bond lengths (Å) for 5937.

F2-C11	1.338(4)	F1-C11	1.337(4)
F5-C10	1.330(4)	F3-C11	1.341(4)
F4-C10	1.327(4)	F6-C10	1.331(4)
N1-C3	1.331(3)	N1-C1	1.376(4)
N2-C3	1.355(4)	N2-C2	1.368(4)
N2-H2	0.88	C4-C9	1.395(4)
C4-C5	1.398(4)	C4-C3	1.461(4)
C9-C8	1.394(4)	C9-H9	0.95
C5-C6	1.381(4)	C5-H5	0.95
C2-C1	1.364(4)	C2-H2A	0.95
C8-C7	1.377(4)	C8-C10	1.509(4)
C6-C7	1.399(4)	C6-C11	1.500(4)
C1-H1	0.95	C7-H7	0.95

Table 5. Bond angles (°) for 5937.

C3-N1-C1	105.6(2)	C3-N2-C2	107.7(2)
C3-N2-H2	126.1	C2-N2-H2	126.1
C9-C4-C5	119.1(3)	C9-C4-C3	120.9(3)
C5-C4-C3	120.0(3)	N1-C3-N2	110.7(3)
N1-C3-C4	125.3(3)	N2-C3-C4	123.9(2)
C8-C9-C4	119.9(3)	C8-C9-H9	120.1
C4-C9-H9	120.1	C6-C5-C4	120.3(3)
C6-C5-H5	119.9	C4-C5-H5	119.9
C1-C2-N2	106.0(3)	C1-C2-H2A	127.0
N2-C2-H2A	127.0	C7-C8-C9	121.1(3)
C7-C8-C10	120.6(3)	C9-C8-C10	118.2(3)

C5-C6-C7	120.8(3)	C5-C6-C11	121.1(3)
C7-C6-C11	118.1(3)	C2-C1-N1	110.0(3)
C2-C1-H1	125.0	N1-C1-H1	125.0
C8-C7-C6	118.8(3)	C8-C7-H7	120.6
C6-C7-H7	120.6	F4-C10-F5	107.0(3)
F4-C10-F6	106.0(3)	F5-C10-F6	107.0(3)
F4-C10-C8	112.2(3)	F5-C10-C8	112.2(2)
F6-C10-C8	112.0(3)	F1-C11-F2	106.9(3)
F1-C11-F3	106.9(3)	F2-C11-F3	105.5(3)
F1-C11-C6	112.8(3)	F2-C11-C6	112.0(3)
F3-C11-C6	112.2(3)		

Table 6. Anisotropic atomic displacement parameters (Å^2) for 5937.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

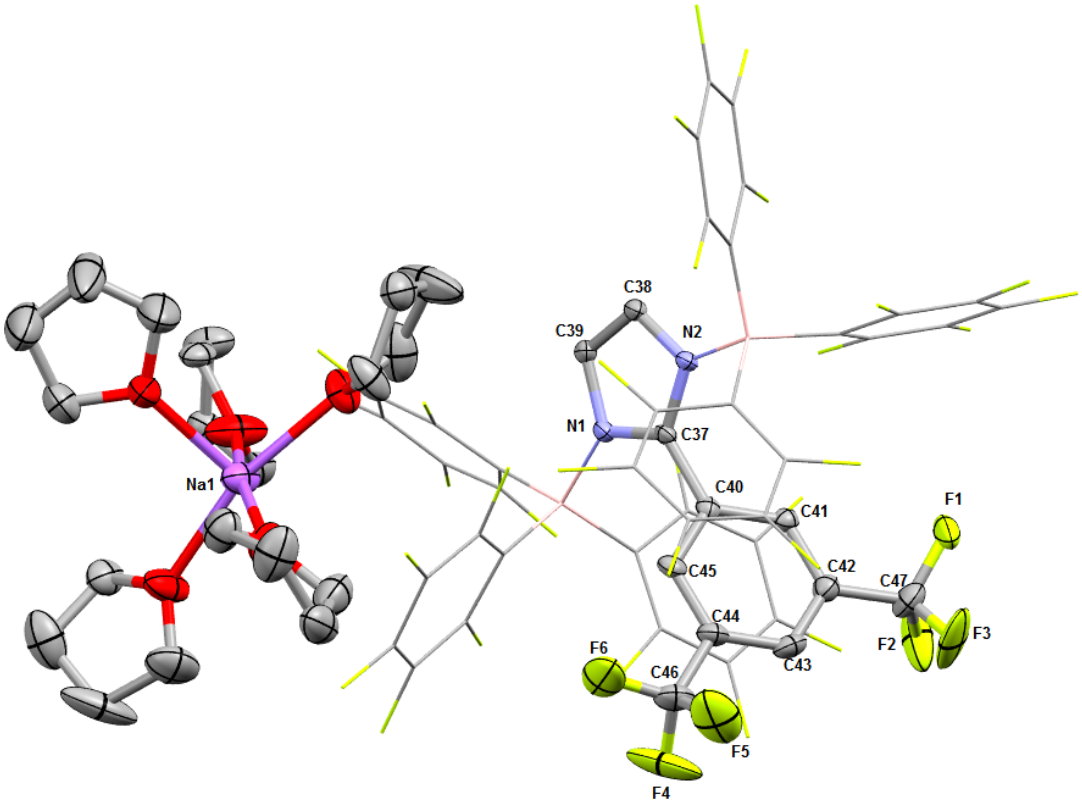
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F2	0.0278(10)	0.0400(12)	0.0459(12)	-0.0058(9)	0.0109(9)	-0.0007(8)
F1	0.0458(13)	0.0674(15)	0.0297(11)	0.0091(10)	0.0215(9)	0.0124(11)
F5	0.0532(13)	0.0540(13)	0.0256(10)	0.0131(9)	-0.0016(9)	-0.0190(10)
F3	0.0454(12)	0.0424(12)	0.0520(13)	-0.0246(10)	0.0238(10)	-0.0092(9)
F4	0.0356(12)	0.0673(16)	0.0457(13)	0.0300(11)	-0.0031(10)	0.0050(10)
F6	0.101(2)	0.0442(13)	0.0150(9)	-0.0012(8)	-0.0079(10)	0.0152(12)
N1	0.0273(13)	0.0308(13)	0.0095(11)	0.0022(9)	0.0039(9)	0.0012(10)
N2	0.0236(13)	0.0314(14)	0.0075(10)	-0.0003(9)	0.0019(9)	0.0006(10)
C4	0.0231(14)	0.0217(14)	0.0132(13)	-0.0009(10)	0.0028(10)	-0.0009(11)
C3	0.0260(15)	0.0253(15)	0.0087(12)	0.0000(10)	0.0045(10)	-0.0002(11)
C9	0.0271(15)	0.0251(15)	0.0137(13)	-0.0013(11)	0.0033(11)	-0.0011(12)
C5	0.0279(16)	0.0282(15)	0.0140(13)	-0.0011(11)	0.0039(11)	-0.0016(12)
C2	0.0257(15)	0.0316(16)	0.0165(14)	-0.0025(11)	0.0036(11)	0.0011(12)
C8	0.0271(16)	0.0262(15)	0.0185(14)	0.0011(11)	-0.0006(12)	-0.0011(12)
C6	0.0240(15)	0.0277(15)	0.0217(14)	-0.0046(12)	0.0048(11)	-0.0020(12)
C1	0.0318(17)	0.0310(16)	0.0135(13)	0.0021(11)	0.0025(12)	0.0041(12)
C7	0.0254(15)	0.0255(16)	0.0260(15)	-0.0011(12)	0.0004(12)	0.0022(12)
C10	0.0359(18)	0.0301(16)	0.0197(14)	0.0042(12)	-0.0014(12)	0.0014(13)
C11	0.0285(17)	0.0348(18)	0.0301(17)	-0.0024(13)	0.0106(13)	0.0015(13)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for 5937.

	x/a	y/b	z/c	U(eq)
H2	0.2222	0.7604	0.6625	0.025

	x/a	y/b	z/c	U(eq)
H9	0.4150	0.6500	0.7137	0.026
H5	0.5279	0.6927	0.3340	0.028
H2A	-0.0136	0.8526	0.5409	0.03
H1	0.0189	0.8471	0.2964	0.031
H7	0.8303	0.5300	0.6068	0.031

Crystal Structure Report for Na[IMP-$(CF_3)_2$]



Thermal ellipsoid plot of 6004. Ellipsoids shown at 50% probability, $B(C_6F_5)_3$ substituents shown in wireframe, hydrogen atoms hidden for clarity.

A specimen of $C_{67}H_{46}B_2F_{36}N_2NaO_6$ was used for the X-ray crystallographic analysis. The X-ray intensity data were measured(λ = 0.71073 Å). The integration of the data using a monoclinic unit cell yielded a total of 62821 reflections to a maximum θ angle of 27.90° (0.76Å resolution), of which 16890 were independent (average redundancy 3.719, completeness = 98.6%, R_{int} = 7.09%, R_{sig} =7.71%) and 9872 (58.45%) were greater than $2\sigma(F^2)$. The final cell constants of a = 15.937(3) Å, b = 25.254(4) Å, c =18.608(3) Å, β = 106.941(3)°, volume = 7164.(2) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The final anisotropic full-matrix least-squares refinement on F^2 with 1030 variables converged at R1 = 7.11%, for the observed data and wR2 = 17.64% for all data. The goodness-of-fit was 1.693. The largest peak in the final difference electron density synthesis was 11.027 $e^-/Å^3$ and the largest hole was -0.682 $e^-/Å^3$ with an RMS deviation of 0.210 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.579 g/cm^3 and F(000), 3420 e^-.

Table 1. Sample and crystal data for 6004.

Identification code	6004
Chemical formula	$C_{67}H_{46}B_2F_{36}N_2NaO_6$

Formula weight	1703.67 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 15.937(3) Å	α = 90°
	b = 25.254(4) Å	β = 106.941(3)°
	c = 18.608(3) Å	γ = 90°
Volume	7164.(2) $Å^3$	
Z	4	
Density (calculated)	1.579 g/cm^3	
Absorption coefficient	0.168 mm^{-1}	
F(000)	3420	

Table 2. Data collection and structure refinement for 6004.

Theta range for data collection	1.40 to 27.90°	
Index ranges	-20<=h<=18, -33<=k<=33, -24<=l<=24	
Reflections collected	62821	
Independent reflections	16890 [R(int) = 0.0709]	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	16890 / 0 / 1030	
Goodness-of-fit on F^2	1.693	
Δ/σ_{max}	2.860	
Final R indices	9872 data; I>2σ(I)	R1 = 0.1336, wR2 = 0.4334
	all data	R1 = 0.0711, wR2 = 0.1765
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.2000P)^2]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	11.027 and -0.682 $eÅ^{-3}$	
R.M.S. deviation from mean	0.210 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for 6004.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij}tensor.

	x/a	y/b	z/c	U(eq)
Na1	0.2315(2)	0.58853(14)	0.7150(2)	0.0385(8)
F26	0.4132(3)	0.75538(16)	0.2166(2)	0.0211(9)
F31	0.5796(3)	0.74118(16)	0.3343(2)	0.0232(9)
F7	0.0293(3)	0.71880(17)	0.2548(2)	0.0238(9)
F17	0.0180(3)	0.78265(17)	0.3672(2)	0.0257(9)
F22	0.5379(3)	0.58354(16)	0.2445(2)	0.0250(9)
F21	0.2608(3)	0.66848(17)	0.4607(2)	0.0230(9)
F27	0.5543(3)	0.56753(16)	0.4244(2)	0.0257(9)
F36	0.4154(3)	0.61731(16)	0.4482(2)	0.0226(9)
F16	0.2807(3)	0.77741(18)	0.5277(2)	0.0280(10)
F11	0.2655(3)	0.83893(17)	0.2798(2)	0.0252(9)
F28	0.7180(3)	0.57276(18)	0.5082(2)	0.0315(10)
F32	0.3585(3)	0.57943(17)	0.1888(2)	0.0270(10)
F30	0.7432(3)	0.74525(18)	0.4196(2)	0.0285(10)
F18	0.9237(3)	0.7227(2)	0.4326(2)	0.0317(11)
F12	0.1171(3)	0.87945(18)	0.3189(2)	0.0296(10)
F20	0.1673(3)	0.61116(18)	0.5297(3)	0.0322(11)
F29	0.8154(3)	0.66152(19)	0.5114(2)	0.0314(10)
F25	0.4596(3)	0.76852(18)	0.0927(2)	0.0318(11)
F19	0.9978(3)	0.6355(2)	0.5160(2)	0.0331(11)
F8	0.9758(3)	0.73810(19)	0.1095(2)	0.0319(11)
F23	0.5850(3)	0.59812(19)	0.1195(3)	0.0345(11)
F10	0.2114(3)	0.85625(19)	0.1323(2)	0.0355(11)
F9	0.0639(3)	0.8077(2)	0.0452(2)	0.0366(12)
F15	0.2913(4)	0.8624(2)	0.6146(2)	0.0409(13)
F13	0.1270(4)	0.96156(19)	0.4074(3)	0.0425(13)
F24	0.5475(3)	0.6908(2)	0.0417(3)	0.0401(13)
F33	0.2632(3)	0.49700(19)	0.2047(3)	0.0398(12)
F14	0.2130(4)	0.9555(2)	0.5576(3)	0.0436(13)
F35	0.3143(4)	0.5361(2)	0.4613(3)	0.0430(13)
F34	0.2373(4)	0.4740(2)	0.3396(3)	0.0468(14)
N2	0.3998(4)	0.7018(2)	0.3444(3)	0.0160(11)
N1	0.2902(4)	0.7472(2)	0.3694(3)	0.0155(11)
F6	0.0792(5)	0.5702(3)	0.3167(4)	0.072(2)
F3	0.1738(5)	0.6233(3)	0.0162(3)	0.069(2)
O4	0.3507(4)	0.5765(2)	0.6696(3)	0.0406(15)
O2	0.1934(5)	0.5007(3)	0.6912(4)	0.0471(17)

	x/a	y/b	z/c	U(eq)
F5	0.0673(5)	0.5296(2)	0.2132(4)	0.074(2)
F4	0.9832(4)	0.5937(3)	0.2168(5)	0.091(3)
O3	0.3158(5)	0.5809(3)	0.8396(4)	0.056(2)
O1	0.0916(5)	0.6064(3)	0.7244(5)	0.063(2)
O5	0.2518(5)	0.6773(3)	0.7117(5)	0.061(2)
C37	0.3123(4)	0.7086(3)	0.3278(4)	0.0156(13)
C38	0.4346(4)	0.7389(3)	0.4006(4)	0.0161(13)
F1	0.2556(5)	0.6893(4)	0.0485(3)	0.092(3)
C40	0.2474(4)	0.6783(3)	0.2668(4)	0.0174(14)
C30	0.5961(5)	0.6136(3)	0.4207(4)	0.0201(14)
F2	0.1181(7)	0.6985(4)	0.0200(3)	0.112(4)
C25	0.5551(5)	0.6550(3)	0.3760(4)	0.0204(15)
C24	0.4519(5)	0.7139(3)	0.1937(4)	0.0211(15)
C27	0.6968(5)	0.7012(3)	0.4222(4)	0.0212(15)
C1	0.2027(4)	0.8230(3)	0.4172(4)	0.0210(15)
C39	0.3695(4)	0.7662(3)	0.4157(3)	0.0161(13)
C8	0.1924(5)	0.8128(3)	0.2389(4)	0.0195(14)
C19	0.4687(4)	0.6677(3)	0.2363(4)	0.0181(14)
C29	0.6824(5)	0.6147(3)	0.4651(4)	0.0205(14)
C26	0.6102(5)	0.6982(3)	0.3777(4)	0.0192(14)
C28	0.7330(5)	0.6596(3)	0.4661(4)	0.0241(16)
C14	0.0558(5)	0.7388(3)	0.4049(4)	0.0211(15)
C18	0.1769(5)	0.6838(3)	0.4518(4)	0.0212(15)
C41	0.2441(5)	0.6864(3)	0.1923(4)	0.0194(14)
C7	0.1489(5)	0.7784(3)	0.2763(4)	0.0205(15)
C13	0.1423(4)	0.7274(3)	0.4068(4)	0.0182(14)
C20	0.5156(5)	0.6299(3)	0.2077(4)	0.0221(15)
C6	0.2433(5)	0.8226(3)	0.4935(4)	0.0233(16)
C2	0.1633(5)	0.8722(3)	0.3915(4)	0.0212(15)
C31	0.3953(5)	0.6023(3)	0.3192(4)	0.0189(14)
C45	0.1879(5)	0.6426(3)	0.2839(4)	0.0215(15)
C5	0.2495(5)	0.8660(3)	0.5418(4)	0.0261(16)
C9	0.1666(5)	0.8218(3)	0.1637(4)	0.0249(16)
C23	0.4765(5)	0.7220(3)	0.1293(4)	0.0229(15)
C21	0.5396(5)	0.6371(3)	0.1430(4)	0.0250(16)
C32	0.3543(5)	0.5696(3)	0.2594(4)	0.0221(15)
C17	0.1303(5)	0.6534(3)	0.4876(4)	0.0224(15)

	x/a	y/b	z/c	U(eq)
C36	0.3797(5)	0.5875(3)	0.3870(4)	0.0198(14)
C12	0.0769(5)	0.7550(3)	0.2287(4)	0.0205(14)
C11	0.0466(5)	0.7635(3)	0.1520(4)	0.0231(15)
C15	0.0072(5)	0.7091(3)	0.4395(4)	0.0226(15)
C42	0.1831(5)	0.6588(3)	0.1348(4)	0.0252(16)
C3	0.1653(5)	0.9160(3)	0.4362(4)	0.0287(17)
C44	0.1291(5)	0.6154(3)	0.2277(4)	0.0275(17)
C16	0.0434(5)	0.6651(3)	0.4811(4)	0.0254(17)
C4	0.2093(6)	0.9127(3)	0.5118(5)	0.035(2)
C10	0.0925(5)	0.7974(3)	0.1190(4)	0.0279(17)
C43	0.1249(5)	0.6232(3)	0.1511(4)	0.0281(17)
C35	0.3270(5)	0.5458(3)	0.3940(4)	0.0290(17)
C22	0.5206(5)	0.6828(3)	0.1037(4)	0.0280(17)
C33	0.3009(5)	0.5262(3)	0.2659(4)	0.0287(17)
C46	0.0634(6)	0.5784(4)	0.2446(5)	0.036(2)
C34	0.2896(6)	0.5149(3)	0.3330(5)	0.0327(18)
C50	0.2193(6)	0.7679(3)	0.7087(5)	0.0348(19)
C47	0.1817(6)	0.6669(4)	0.0565(5)	0.037(2)
B1	0.4526(5)	0.6560(3)	0.3171(4)	0.0152(15)
B2	0.1957(5)	0.7684(3)	0.3668(4)	0.0185(16)
C49	0.3170(7)	0.7605(4)	0.7462(6)	0.048(2)
C58	0.4863(7)	0.5374(4)	0.6789(6)	0.047(2)
C51	0.2016(7)	0.7178(4)	0.6638(6)	0.052(3)
C66	0.2171(9)	0.4095(4)	0.7085(6)	0.063(3)
C55	0.2854(7)	0.5892(4)	0.9044(6)	0.049(2)
C67	0.2157(8)	0.4608(4)	0.7488(6)	0.051(3)
C59	0.3879(7)	0.5257(4)	0.6683(7)	0.051(3)
C61	0.0041(9)	0.6298(4)	0.7954(8)	0.067(4)
C65	0.1424(8)	0.4182(5)	0.6359(6)	0.058(3)
C63	0.0143(8)	0.5765(5)	0.6959(7)	0.061(3)
C62	0.9476(9)	0.6021(5)	0.7306(11)	0.090(5)
C64	0.1564(8)	0.4746(5)	0.6197(6)	0.059(3)
C56	0.3907(9)	0.6112(4)	0.6299(7)	0.063(3)
C60	0.0755(8)	0.6507(5)	0.7668(7)	0.062(3)
C48	0.3248(8)	0.7049(5)	0.7681(7)	0.066(3)
C54	0.3614(9)	0.5860(7)	0.9707(6)	0.082(5)
C57	0.4817(9)	0.5887(8)	0.6390(9)	0.118(8)

	x/a	y/b	z/c	U(eq)
C52	0.4111(8)	0.5707(8)	0.8660(7)	0.088(5)
C53	0.4370(9)	0.5698(9)	0.9428(8)	0.114(7)
O6	0.1388(4)	0.5035(2)	0.0274(3)	0.0300(13)

Table 4. Bond lengths (Å) for 6004.

Na1-O5	2.269(8)	Na1-O2	2.308(7)
Na1-O4	2.313(7)	Na1-O3	2.324(8)
Na1-O1	2.331(8)	F26-C24	1.345(8)
F31-C26	1.355(8)	F7-C12	1.366(8)
F17-C14	1.354(8)	F22-C20	1.350(8)
F21-C18	1.354(8)	F27-C30	1.353(8)
F36-C36	1.345(8)	F16-C6	1.356(9)
F11-C8	1.362(8)	F28-C29	1.350(8)
F32-C32	1.358(8)	F30-C27	1.344(8)
F18-C15	1.343(8)	F12-C2	1.350(8)
F20-C17	1.351(9)	F29-C28	1.339(8)
F25-C23	1.346(9)	F19-C16	1.335(8)
F8-C11	1.338(9)	F23-C21	1.366(8)
F10-C9	1.362(8)	F9-C10	1.339(8)
F15-C5	1.328(9)	F13-C3	1.339(9)
F24-C22	1.357(8)	F33-C33	1.343(9)
F14-C4	1.368(9)	F35-C35	1.347(9)
F34-C34	1.356(9)	N2-C37	1.347(9)
N2-C38	1.392(9)	N2-B1	1.599(9)
N1-C37	1.353(9)	N1-C39	1.391(9)
N1-B2	1.587(9)	F6-C46	1.308(11)
F3-C47	1.318(11)	O4-C56	1.414(12)
O4-C59	1.416(11)	O2-C67	1.438(12)
O2-C64	1.448(12)	F5-C46	1.374(11)
F4-C46	1.290(11)	O3-C55	1.439(11)
O3-C52	1.477(14)	O1-C63	1.410(13)
O1-C60	1.435(13)	O5-C51	1.437(13)
O5-C48	1.492(13)	C37-C40	1.503(9)
C38-C39	1.343(9)	C38-H38	0.95
F1-C47	1.352(11)	C40-C41	1.388(9)
C40-C45	1.411(10)	C30-C25	1.377(10)

C30-C29	1.382(10)	F2-C47	1.314(11)
C25-C26	1.396(10)	C25-B1	1.682(11)
C24-C23	1.382(9)	C24-C19	1.392(10)
C27-C28	1.353(11)	C27-C26	1.390(10)
C1-C6	1.378(10)	C1-C2	1.412(10)
C1-B2	1.651(11)	C39-H39	0.95
C8-C9	1.357(10)	C8-C7	1.416(10)
C19-C20	1.410(9)	C19-B1	1.624(9)
C29-C28	1.389(11)	C14-C15	1.366(10)
C14-C13	1.400(9)	C18-C17	1.370(10)
C18-C13	1.396(10)	C41-C42	1.403(10)
C41-H41	0.95	C7-C12	1.362(10)
C7-B2	1.651(10)	C13-B2	1.649(10)
C20-C21	1.378(10)	C6-C5	1.402(11)
C2-C3	1.380(11)	C31-C32	1.387(10)
C31-C36	1.406(9)	C31-B1	1.642(10)
C45-C44	1.369(10)	C45-H45	0.95
C5-C4	1.379(12)	C9-C10	1.375(11)
C23-C22	1.376(11)	C21-C22	1.354(11)
C32-C33	1.413(11)	C17-C16	1.388(10)
C36-C35	1.377(10)	C12-C11	1.384(10)
C11-C10	1.383(11)	C15-C16	1.382(11)
C42-C43	1.387(11)	C42-C47	1.465(11)
C3-C4	1.379(12)	C44-C43	1.422(11)
C44-C46	1.502(11)	C43-H43	0.95
C35-C34	1.363(12)	C33-C34	1.343(12)
C50-C51	1.498(14)	C50-C49	1.521(13)
C50-H50A	0.99	C50-H50B	0.99
C49-C48	1.457(16)	C49-H49A	0.99
C49-H49B	0.99	C58-C57	1.485(19)
C58-C59	1.550(14)	C58-H58A	0.99
C58-H58B	0.99	C51-H51A	0.99
C51-H51B	0.99	C66-C67	1.500(15)
C66-C65	1.534(17)	C66-H66A	0.99
C66-H66B	0.99	C55-C54	1.457(17)
C55-H55A	0.99	C55-H55B	0.99
C67-H67A	0.99	C67-H67B	0.99
C59-H59A	0.99	C59-H59B	0.99

C61-C62	1.46(2)	C61-C60	1.487(17)
C61-H61A	0.99	C61-H61B	0.99
C65-C64	1.485(17)	C65-H65A	0.99
C65-H65B	0.99	C63-C62	1.538(18)
C63-H63A	0.99	C63-H63B	0.99
C62-H62A	0.99	C62-H62B	0.99
C64-H64A	0.99	C64-H64B	0.99
C56-C57	1.52(2)	C56-H56A	0.99
C56-H56B	0.99	C60-H60A	0.99
C60-H60B	0.99	C48-H48A	0.99
C48-H48B	0.99	C54-C53	1.503(18)
C54-H54A	0.99	C54-H54B	0.99
C57-H57A	0.99	C57-H57B	0.99
C52-C53	1.366(18)	C52-H52A	0.99
C52-H52B	0.99	C53-H53	0.95
O6-H6A	0.8701	O6-H6B	0.8703

Table 5. Bond angles (°) for 6004.

O5-Na1-O2	167.4(3)	O5-Na1-O4	88.9(3)
O2-Na1-O4	90.1(3)	O5-Na1-O3	93.7(3)
O2-Na1-O3	98.9(3)	O4-Na1-O3	93.2(3)
O5-Na1-O1	87.6(3)	O2-Na1-O1	89.8(3)
O4-Na1-O1	163.4(3)	O3-Na1-O1	103.2(3)
C37-N2-C38	104.3(5)	C37-N2-B1	128.7(6)
C38-N2-B1	126.4(5)	C37-N1-C39	105.2(5)
C37-N1-B2	129.0(6)	C39-N1-B2	125.8(5)
C56-O4-C59	107.3(7)	C56-O4-Na1	130.8(6)
C59-O4-Na1	121.3(5)	C67-O2-C64	108.2(8)
C67-O2-Na1	122.4(6)	C64-O2-Na1	128.9(6)
C55-O3-C52	108.1(8)	C55-O3-Na1	125.8(6)
C52-O3-Na1	125.9(6)	C63-O1-C60	110.4(9)
C63-O1-Na1	128.1(7)	C60-O1-Na1	121.4(7)
C51-O5-C48	106.5(8)	C51-O5-Na1	131.4(6)
C48-O5-Na1	122.0(7)	N2-C37-N1	112.7(6)
N2-C37-C40	123.1(6)	N1-C37-C40	124.1(6)
C39-C38-N2	109.8(6)	C39-C38-H38	125.1
N2-C38-H38	125.1	C41-C40-C45	119.1(6)

C41-C40-C37	119.8(6)	C45-C40-C37	121.0(6)
F27-C30-C25	121.9(6)	F27-C30-C29	113.9(6)
C25-C30-C29	124.1(7)	C30-C25-C26	113.3(6)
C30-C25-B1	127.3(6)	C26-C25-B1	119.2(6)
F26-C24-C23	115.6(6)	F26-C24-C19	120.2(6)
C23-C24-C19	124.1(6)	F30-C27-C28	121.5(6)
F30-C27-C26	119.0(6)	C28-C27-C26	119.5(7)
C6-C1-C2	112.6(7)	C6-C1-B2	120.9(7)
C2-C1-B2	126.3(6)	C38-C39-N1	108.1(6)
C38-C39-H39	125.9	N1-C39-H39	125.9
C9-C8-F11	116.7(6)	C9-C8-C7	124.4(7)
F11-C8-C7	119.0(6)	C24-C19-C20	112.8(6)
C24-C19-B1	128.6(6)	C20-C19-B1	118.1(6)
F28-C29-C30	120.8(6)	F28-C29-C28	119.4(6)
C30-C29-C28	119.8(7)	F31-C26-C27	115.7(6)
F31-C26-C25	119.9(6)	C27-C26-C25	124.4(7)
F29-C28-C27	121.3(7)	F29-C28-C29	119.8(7)
C27-C28-C29	118.9(7)	F17-C14-C15	117.7(6)
F17-C14-C13	117.9(6)	C15-C14-C13	124.4(7)
F21-C18-C17	115.8(6)	F21-C18-C13	120.2(6)
C17-C18-C13	124.0(6)	C40-C41-C42	120.3(7)
C40-C41-H41	119.8	C42-C41-H41	119.8
C12-C7-C8	112.7(6)	C12-C7-B2	130.0(6)
C8-C7-B2	117.1(6)	C18-C13-C14	113.1(6)
C18-C13-B2	126.9(6)	C14-C13-B2	119.6(6)
F22-C20-C21	117.3(6)	F22-C20-C19	119.1(6)
C21-C20-C19	123.7(7)	F16-C6-C1	119.9(7)
F16-C6-C5	114.7(6)	C1-C6-C5	125.4(7)
F12-C2-C3	113.9(6)	F12-C2-C1	121.2(6)
C3-C2-C1	124.9(7)	C32-C31-C36	113.4(6)
C32-C31-B1	127.5(6)	C36-C31-B1	119.0(6)
C44-C45-C40	120.3(7)	C44-C45-H45	119.8
C40-C45-H45	119.9	F15-C5-C4	120.4(7)
F15-C5-C6	121.4(7)	C4-C5-C6	118.1(7)
C8-C9-F10	120.6(7)	C8-C9-C10	119.9(7)
F10-C9-C10	119.5(6)	F25-C23-C22	120.0(6)
F25-C23-C24	120.1(7)	C22-C23-C24	119.9(7)
C22-C21-F23	119.9(6)	C22-C21-C20	120.6(7)

F23-C21-C20	119.5(7)	F32-C32-C31	121.5(6)
F32-C32-C33	115.2(6)	C31-C32-C33	123.2(7)
F20-C17-C18	121.2(6)	F20-C17-C16	118.4(6)
C18-C17-C16	120.5(7)	F36-C36-C35	117.8(6)
F36-C36-C31	118.1(6)	C35-C36-C31	124.1(7)
C7-C12-F7	120.6(6)	C7-C12-C11	125.4(7)
F7-C12-C11	114.0(6)	F8-C11-C10	120.0(6)
F8-C11-C12	121.1(6)	C10-C11-C12	118.8(7)
F18-C15-C14	119.8(7)	F18-C15-C16	119.9(6)
C14-C15-C16	120.3(6)	C43-C42-C41	121.0(7)
C43-C42-C47	119.4(7)	C41-C42-C47	119.6(7)
F13-C3-C4	119.9(7)	F13-C3-C2	121.3(7)
C4-C3-C2	118.8(7)	C45-C44-C43	121.2(7)
C45-C44-C46	121.1(7)	C43-C44-C46	117.7(7)
F19-C16-C15	121.7(6)	F19-C16-C17	120.6(7)
C15-C16-C17	117.7(6)	F14-C4-C5	119.6(8)
F14-C4-C3	120.1(8)	C5-C4-C3	120.2(7)
F9-C10-C9	120.6(7)	F9-C10-C11	120.6(7)
C9-C10-C11	118.8(7)	C42-C43-C44	118.0(7)
C42-C43-H43	121.0	C44-C43-H43	121.0
F35-C35-C34	121.5(7)	F35-C35-C36	119.2(7)
C34-C35-C36	119.3(7)	C21-C22-F24	120.6(7)
C21-C22-C23	118.9(6)	F24-C22-C23	120.4(7)
C34-C33-F33	121.6(7)	C34-C33-C32	119.5(7)
F33-C33-C32	119.0(7)	F4-C46-F6	109.3(8)
F4-C46-F5	105.0(8)	F6-C46-F5	106.0(8)
F4-C46-C44	113.5(8)	F6-C46-C44	112.1(7)
F5-C46-C44	110.3(7)	C33-C34-F34	119.9(8)
C33-C34-C35	120.6(7)	F34-C34-C35	119.4(7)
C51-C50-C49	98.8(8)	C51-C50-H50A	112.0
C49-C50-H50A	112.0	C51-C50-H50B	112.0
C49-C50-H50B	112.0	H50A-C50-H50B	109.7
F2-C47-F3	106.4(8)	F2-C47-F1	104.7(9)
F3-C47-F1	103.2(8)	F2-C47-C42	112.6(7)
F3-C47-C42	114.9(8)	F1-C47-C42	114.0(7)
N2-B1-C19	113.7(5)	N2-B1-C31	104.0(5)
C19-B1-C31	114.3(6)	N2-B1-C25	107.8(5)
C19-B1-C25	102.7(5)	C31-B1-C25	114.4(6)

N1-B2-C13	112.6(6)	N1-B2-C1	111.0(6)
C13-B2-C1	103.1(5)	N1-B2-C7	103.0(5)
C13-B2-C7	114.6(6)	C1-B2-C7	112.8(6)
C48-C49-C50	103.9(8)	C48-C49-H49A	111.0
C50-C49-H49A	111.0	C48-C49-H49B	111.0
C50-C49-H49B	111.0	H49A-C49-H49B	109.0
C57-C58-C59	101.6(9)	C57-C58-H58A	111.4
C59-C58-H58A	111.5	C57-C58-H58B	111.5
C59-C58-H58B	111.4	H58A-C58-H58B	109.3
O5-C51-C50	105.9(8)	O5-C51-H51A	110.6
C50-C51-H51A	110.6	O5-C51-H51B	110.5
C50-C51-H51B	110.5	H51A-C51-H51B	108.7
C67-C66-C65	101.3(9)	C67-C66-H66A	111.5
C65-C66-H66A	111.5	C67-C66-H66B	111.5
C65-C66-H66B	111.5	H66A-C66-H66B	109.3
O3-C55-C54	107.6(8)	O3-C55-H55A	110.2
C54-C55-H55A	110.1	O3-C55-H55B	110.2
C54-C55-H55B	110.3	H55A-C55-H55B	108.5
O2-C67-C66	105.5(8)	O2-C67-H67A	110.6
C66-C67-H67A	110.7	O2-C67-H67B	110.6
C66-C67-H67B	110.6	H67A-C67-H67B	108.8
O4-C59-C58	103.8(8)	O4-C59-H59A	111.0
C58-C59-H59A	111.0	O4-C59-H59B	111.0
C58-C59-H59B	111.0	H59A-C59-H59B	109.0
C62-C61-C60	103.1(11)	C62-C61-H61A	111.1
C60-C61-H61A	111.1	C62-C61-H61B	111.2
C60-C61-H61B	111.2	H61A-C61-H61B	109.1
C64-C65-C66	101.1(9)	C64-C65-H65A	111.6
C66-C65-H65A	111.5	C64-C65-H65B	111.5
C66-C65-H65B	111.6	H65A-C65-H65B	109.4
O1-C63-C62	104.6(10)	O1-C63-H63A	110.9
C62-C63-H63A	110.8	O1-C63-H63B	110.8
C62-C63-H63B	110.8	H63A-C63-H63B	108.9
C61-C62-C63	102.3(10)	C61-C62-H62A	111.3
C63-C62-H62A	111.3	C61-C62-H62B	111.3
C63-C62-H62B	111.3	H62A-C62-H62B	109.2
O2-C64-C65	107.2(9)	O2-C64-H64A	110.3
C65-C64-H64A	110.3	O2-C64-H64B	110.3

C65-C64-H64B	110.3	H64A-C64-H64B	108.5
O4-C56-C57	105.7(9)	O4-C56-H56A	110.6
C57-C56-H56A	110.6	O4-C56-H56B	110.6
C57-C56-H56B	110.6	H56A-C56-H56B	108.7
O1-C60-C61	101.4(10)	O1-C60-H60A	111.5
C61-C60-H60A	111.5	O1-C60-H60B	111.5
C61-C60-H60B	111.5	H60A-C60-H60B	109.3
C49-C48-O5	105.5(9)	C49-C48-H48A	110.7
O5-C48-H48A	110.7	C49-C48-H48B	110.6
O5-C48-H48B	110.6	H48A-C48-H48B	108.8
C55-C54-C53	105.9(9)	C55-C54-H54A	110.6
C53-C54-H54A	110.6	C55-C54-H54B	110.5
C53-C54-H54B	110.5	H54A-C54-H54B	108.7
C58-C57-C56	106.8(9)	C58-C57-H57A	110.3
C56-C57-H57A	110.3	C58-C57-H57B	110.4
C56-C57-H57B	110.4	H57A-C57-H57B	108.6
C53-C52-O3	108.6(10)	C53-C52-H52A	110.0
O3-C52-H52A	110.0	C53-C52-H52B	109.9
O3-C52-H52B	110.0	H52A-C52-H52B	108.4
C52-C53-C54	109.2(11)	C52-C53-H53	125.4
C54-C53-H53	125.4	H6A-O6-H6B	109.5

Table 6. Anisotropic atomic displacement parameters (Å^2) for 6004.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Na1	0.0277(19)	0.0366(19)	0.051(2)	-0.0137(15)	0.0116(15)	0.0032(14)
F26	0.020(2)	0.021(2)	0.024(2)	0.0051(16)	0.0086(16)	0.0061(16)
F31	0.018(2)	0.024(2)	0.028(2)	0.0024(17)	0.0092(17)	-0.0020(17)
F7	0.016(2)	0.035(2)	0.021(2)	0.0025(17)	0.0079(16)	-0.0057(17)
F17	0.020(2)	0.032(2)	0.027(2)	0.0045(18)	0.0091(17)	0.0085(18)
F22	0.028(2)	0.022(2)	0.028(2)	0.0022(17)	0.0135(18)	0.0020(17)
F21	0.013(2)	0.032(2)	0.025(2)	0.0049(17)	0.0074(16)	0.0026(17)
F27	0.028(2)	0.017(2)	0.033(2)	0.0011(17)	0.0102(18)	-0.0024(17)
F36	0.025(2)	0.027(2)	0.018(2)	0.0011(16)	0.0094(16)	-0.0029(17)
F16	0.025(2)	0.038(3)	0.022(2)	0.0011(18)	0.0084(17)	0.0000(19)
F11	0.025(2)	0.031(2)	0.020(2)	-0.0004(17)	0.0065(17)	-0.0081(18)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F28	0.028(3)	0.033(3)	0.030(2)	0.0051(19)	0.0031(18)	0.010(2)
F32	0.029(3)	0.033(2)	0.019(2)	-0.0085(18)	0.0074(17)	-0.0055(19)
F30	0.019(2)	0.034(3)	0.034(2)	-0.0030(19)	0.0100(18)	-0.0057(18)
F18	0.015(2)	0.054(3)	0.030(2)	0.000(2)	0.0136(18)	0.001(2)
F12	0.029(3)	0.031(2)	0.027(2)	-0.0006(18)	0.0051(18)	0.0114(19)
F20	0.031(3)	0.033(3)	0.036(3)	0.013(2)	0.016(2)	0.002(2)
F29	0.012(2)	0.047(3)	0.030(2)	0.003(2)	-0.0006(17)	-0.0005(19)
F25	0.036(3)	0.033(3)	0.029(2)	0.0120(19)	0.014(2)	0.002(2)
F19	0.028(3)	0.047(3)	0.030(2)	0.009(2)	0.0171(19)	-0.006(2)
F8	0.020(2)	0.047(3)	0.024(2)	-0.003(2)	-0.0014(17)	-0.008(2)
F23	0.043(3)	0.037(3)	0.033(2)	-0.002(2)	0.026(2)	0.012(2)
F10	0.040(3)	0.042(3)	0.027(2)	0.008(2)	0.015(2)	-0.010(2)
F9	0.042(3)	0.052(3)	0.012(2)	0.0021(19)	0.0007(19)	-0.008(2)
F15	0.049(3)	0.056(3)	0.018(2)	-0.010(2)	0.011(2)	-0.014(3)
F13	0.050(3)	0.028(3)	0.057(3)	-0.004(2)	0.027(3)	0.008(2)
F24	0.051(3)	0.054(3)	0.027(2)	0.011(2)	0.030(2)	0.010(2)
F33	0.039(3)	0.033(3)	0.044(3)	-0.013(2)	0.006(2)	-0.014(2)
F14	0.056(4)	0.040(3)	0.043(3)	-0.018(2)	0.028(3)	-0.013(2)
F35	0.055(4)	0.045(3)	0.037(3)	0.011(2)	0.025(2)	-0.020(2)
F34	0.045(3)	0.037(3)	0.058(3)	0.007(2)	0.013(3)	-0.018(2)
N2	0.012(3)	0.017(3)	0.017(3)	-0.003(2)	0.002(2)	-0.001(2)
N1	0.010(3)	0.024(3)	0.014(3)	-0.003(2)	0.006(2)	-0.005(2)
F6	0.063(4)	0.101(5)	0.057(4)	-0.003(4)	0.027(3)	-0.049(4)
F3	0.115(6)	0.064(4)	0.034(3)	-0.011(3)	0.032(3)	0.006(4)
O4	0.048(4)	0.034(3)	0.047(4)	0.009(3)	0.025(3)	0.012(3)
O2	0.057(5)	0.039(4)	0.047(4)	-0.011(3)	0.019(3)	0.000(3)
F5	0.095(6)	0.048(4)	0.100(5)	-0.016(4)	0.060(4)	-0.039(4)
F4	0.021(4)	0.089(5)	0.153(8)	0.037(5)	0.012(4)	-0.013(3)
O3	0.035(4)	0.095(6)	0.038(4)	-0.021(4)	0.012(3)	-0.004(4)
O1	0.038(4)	0.059(5)	0.099(6)	-0.042(4)	0.032(4)	-0.008(3)
O5	0.031(4)	0.037(4)	0.100(6)	-0.026(4)	-0.004(4)	0.006(3)
C37	0.008(3)	0.020(3)	0.020(3)	0.001(3)	0.008(2)	-0.003(2)
C38	0.012(3)	0.021(3)	0.015(3)	0.002(3)	0.003(2)	0.001(3)
F1	0.094(6)	0.159(8)	0.025(3)	-0.003(4)	0.020(3)	-0.069(5)
C40	0.016(3)	0.019(3)	0.016(3)	0.000(3)	0.002(3)	0.005(3)
C30	0.019(4)	0.020(3)	0.023(4)	-0.003(3)	0.009(3)	0.000(3)
F2	0.159(8)	0.150(8)	0.029(3)	0.035(4)	0.032(4)	0.119(7)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C25	0.017(4)	0.024(4)	0.026(4)	-0.001(3)	0.015(3)	-0.002(3)
C24	0.012(3)	0.030(4)	0.022(3)	0.001(3)	0.006(3)	0.002(3)
C27	0.014(4)	0.030(4)	0.022(4)	-0.005(3)	0.008(3)	-0.004(3)
C1	0.011(3)	0.031(4)	0.025(4)	-0.002(3)	0.012(3)	-0.003(3)
C39	0.016(3)	0.021(3)	0.013(3)	-0.002(3)	0.007(2)	-0.004(3)
C8	0.017(4)	0.021(4)	0.020(3)	-0.001(3)	0.004(3)	-0.001(3)
C19	0.014(3)	0.027(4)	0.017(3)	-0.003(3)	0.009(3)	0.001(3)
C29	0.017(4)	0.025(4)	0.019(3)	0.002(3)	0.006(3)	0.005(3)
C26	0.016(4)	0.019(3)	0.026(4)	0.000(3)	0.010(3)	0.005(3)
C28	0.014(4)	0.039(4)	0.019(3)	-0.003(3)	0.003(3)	0.001(3)
C14	0.013(4)	0.031(4)	0.021(3)	0.000(3)	0.009(3)	0.004(3)
C18	0.019(4)	0.029(4)	0.018(3)	-0.001(3)	0.008(3)	0.006(3)
C41	0.015(4)	0.019(3)	0.021(3)	-0.002(3)	0.000(3)	0.002(3)
C7	0.015(4)	0.030(4)	0.019(3)	-0.001(3)	0.007(3)	0.005(3)
C13	0.016(4)	0.025(4)	0.017(3)	-0.005(3)	0.008(3)	0.002(3)
C20	0.018(4)	0.027(4)	0.022(4)	-0.002(3)	0.007(3)	0.003(3)
C6	0.020(4)	0.034(4)	0.021(4)	0.002(3)	0.015(3)	-0.005(3)
C2	0.022(4)	0.023(4)	0.022(4)	0.001(3)	0.011(3)	0.001(3)
C31	0.017(4)	0.020(3)	0.020(3)	-0.002(3)	0.005(3)	0.001(3)
C45	0.012(3)	0.024(4)	0.027(4)	-0.002(3)	0.003(3)	0.002(3)
C5	0.025(4)	0.036(4)	0.022(4)	-0.002(3)	0.014(3)	-0.004(3)
C9	0.025(4)	0.028(4)	0.025(4)	0.005(3)	0.013(3)	0.000(3)
C23	0.018(4)	0.031(4)	0.017(3)	0.005(3)	0.002(3)	-0.002(3)
C21	0.021(4)	0.035(4)	0.021(4)	0.000(3)	0.009(3)	0.003(3)
C32	0.019(4)	0.023(4)	0.025(4)	-0.001(3)	0.009(3)	-0.003(3)
C17	0.019(4)	0.030(4)	0.019(3)	0.001(3)	0.006(3)	0.000(3)
C36	0.018(4)	0.023(4)	0.022(3)	0.003(3)	0.011(3)	0.004(3)
C12	0.014(4)	0.023(4)	0.023(4)	0.002(3)	0.005(3)	0.001(3)
C11	0.019(4)	0.030(4)	0.018(3)	-0.001(3)	0.003(3)	0.000(3)
C15	0.014(4)	0.035(4)	0.021(3)	-0.002(3)	0.010(3)	0.003(3)
C42	0.027(4)	0.024(4)	0.024(4)	-0.001(3)	0.006(3)	0.006(3)
C3	0.027(4)	0.030(4)	0.032(4)	0.001(3)	0.014(3)	0.006(3)
C44	0.021(4)	0.030(4)	0.035(4)	-0.009(3)	0.013(3)	-0.008(3)
C16	0.018(4)	0.040(5)	0.025(4)	-0.006(3)	0.016(3)	-0.011(3)
C4	0.040(5)	0.039(5)	0.038(5)	-0.015(4)	0.030(4)	-0.018(4)
C10	0.031(4)	0.034(4)	0.018(4)	0.004(3)	0.006(3)	0.006(3)
C43	0.021(4)	0.028(4)	0.029(4)	-0.005(3)	-0.002(3)	-0.003(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C35	0.030(5)	0.024(4)	0.034(4)	0.006(3)	0.010(3)	-0.002(3)
C22	0.027(4)	0.038(5)	0.023(4)	0.006(3)	0.014(3)	-0.004(3)
C33	0.027(4)	0.027(4)	0.029(4)	-0.004(3)	0.003(3)	0.000(3)
C46	0.027(5)	0.034(5)	0.045(5)	-0.006(4)	0.007(4)	-0.013(4)
C34	0.031(5)	0.020(4)	0.048(5)	0.004(4)	0.012(4)	-0.007(3)
C50	0.036(5)	0.027(4)	0.039(5)	0.000(4)	0.008(4)	0.000(4)
C47	0.034(5)	0.046(5)	0.027(4)	-0.006(4)	0.001(3)	-0.001(4)
B1	0.014(4)	0.020(4)	0.014(3)	0.002(3)	0.007(3)	0.000(3)
B2	0.016(4)	0.027(4)	0.014(4)	0.001(3)	0.007(3)	0.000(3)
C49	0.037(6)	0.043(6)	0.059(6)	0.006(5)	0.006(4)	-0.003(4)
C58	0.040(6)	0.057(6)	0.044(5)	-0.006(5)	0.013(4)	0.005(5)
C51	0.044(6)	0.063(7)	0.042(5)	0.001(5)	0.005(4)	0.001(5)
C66	0.085(9)	0.041(6)	0.058(7)	0.003(5)	0.014(6)	0.000(6)
C55	0.042(6)	0.059(6)	0.055(6)	-0.003(5)	0.029(5)	0.000(5)
C67	0.062(7)	0.040(5)	0.055(6)	0.007(5)	0.024(5)	0.001(5)
C59	0.054(7)	0.033(5)	0.079(7)	-0.005(5)	0.040(6)	-0.004(4)
C61	0.091(10)	0.035(6)	0.097(9)	0.011(6)	0.062(8)	0.018(6)
C65	0.060(7)	0.061(7)	0.060(7)	-0.028(6)	0.030(6)	-0.015(6)
C63	0.048(7)	0.052(7)	0.080(8)	0.002(6)	0.015(6)	-0.016(5)
C62	0.040(7)	0.041(7)	0.205(18)	-0.013(9)	0.060(9)	0.003(5)
C64	0.062(8)	0.067(8)	0.041(6)	-0.012(5)	0.004(5)	0.006(6)
C56	0.094(10)	0.042(6)	0.069(8)	0.003(5)	0.047(7)	-0.002(6)
C60	0.055(7)	0.070(8)	0.063(7)	-0.010(6)	0.020(6)	0.018(6)
C48	0.046(7)	0.054(7)	0.079(8)	-0.017(6)	-0.008(6)	0.003(5)
C54	0.063(9)	0.145(14)	0.039(6)	-0.012(7)	0.018(6)	0.014(8)
C57	0.043(8)	0.20(2)	0.100(11)	0.092(12)	0.002(7)	-0.038(10)
C52	0.035(7)	0.169(16)	0.061(8)	-0.020(9)	0.015(5)	0.011(8)
C53	0.037(7)	0.24(2)	0.054(8)	-0.037(11)	-0.002(6)	0.029(10)
O6	0.027(3)	0.023(3)	0.048(3)	-0.002(2)	0.023(3)	0.000(2)

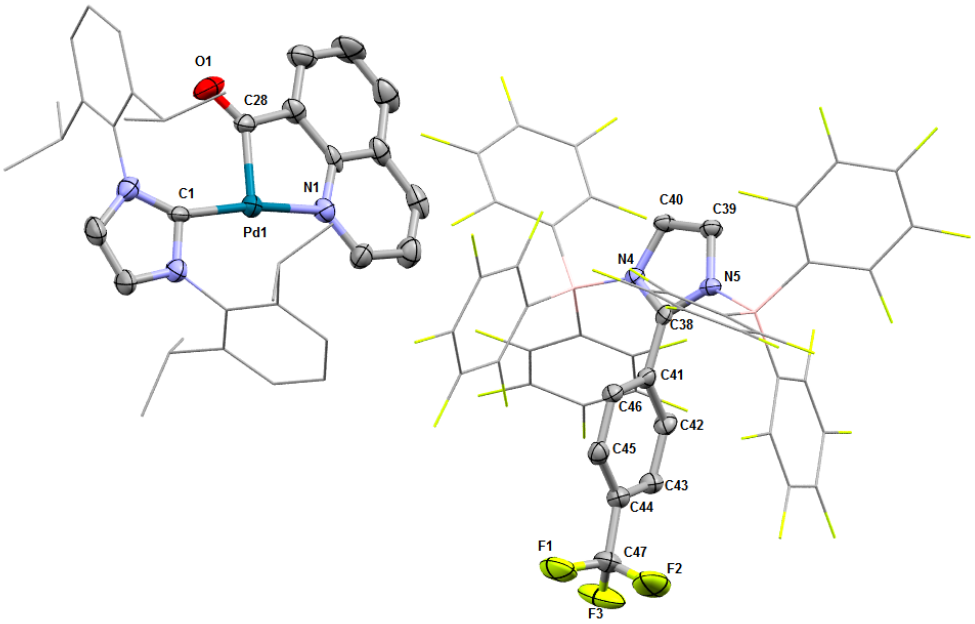
Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 6004.

	x/a	y/b	z/c	U(eq)
H38	0.4954	0.7441	0.4246	0.019
H39	0.3763	0.7938	0.4517	0.019
H41	0.2833	0.7107	0.1801	0.023

	x/a	y/b	z/c	U(eq)
H45	0.1887	0.6374	0.3347	0.026
H43	0.0834	0.6047	0.1122	0.034
H50A	0.1857	0.7696	0.7458	0.042
H50B	0.2070	0.7998	0.6763	0.042
H49A	0.3511	0.7682	0.7108	0.058
H49B	0.3377	0.7837	0.7907	0.058
H58A	0.5193	0.5407	0.7327	0.056
H58B	0.5136	0.5095	0.6557	0.056
H51A	0.1383	0.7091	0.6492	0.062
H51B	0.2201	0.7214	0.6176	0.062
H66A	0.2051	0.3790	0.7374	0.075
H66B	0.2740	0.4041	0.6980	0.075
H55A	0.2418	0.5619	0.9067	0.059
H55B	0.2574	0.6245	0.9016	0.059
H67A	0.1713	0.4596	0.7766	0.061
H67B	0.2738	0.4681	0.7849	0.061
H59A	0.3609	0.5077	0.6197	0.061
H59B	0.3803	0.5032	0.7095	0.061
H61A	0.0275	0.6052	0.8380	0.08
H61B	-0.0279	0.6588	0.8116	0.08
H65A	0.1482	0.3947	0.5951	0.069
H65B	0.0843	0.4127	0.6439	0.069
H63A	0.0243	0.5389	0.7111	0.073
H63B	-0.0064	0.5784	0.6403	0.073
H62A	-0.0914	0.6270	0.6951	0.108
H62B	-0.0885	0.5749	0.7460	0.108
H64A	0.1971	0.4773	0.5885	0.071
H64B	0.1000	0.4913	0.5922	0.071
H56A	0.3948	0.6474	0.6511	0.076
H56B	0.3566	0.6127	0.5762	0.076
H60A	0.0560	0.6822	0.7344	0.075
H60B	0.1281	0.6599	0.8084	0.075
H48A	0.3190	0.7005	0.8193	0.079
H48B	0.3823	0.6905	0.7672	0.079
H54A	0.3514	0.5595	1.0065	0.099
H54B	0.3730	0.6208	0.9963	0.099
H57A	0.4911	0.5833	0.5893	0.142

	x/a	y/b	z/c	U(eq)
H57B	0.5272	0.6133	0.6685	0.142
H52A	0.4246	0.5364	0.8462	0.106
H52B	0.4430	0.5990	0.8478	0.106
H53	0.4938	0.5603	0.9736	0.137
H6A	0.1144	0.4806	0.0499	0.045
H6B	0.1094	0.5050	-0.0200	0.045

Crystal Structure Report for 1[IMP-CF_3]



Thermal ellipsoid plot of 5359. Ellipsoids shown at 50% probability, $B(C_6F_5)_3$ and diisopropylphenyl substituents shown in wireframe. Hydrogen atoms and DCM solvate hidden for clarity.

A specimen of $C_{84}H_{50}B_2Cl_2F_{33}N_5OPd$ was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å). The total exposure time was 12.52 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 110269 reflections to a maximum θ angle of28.33° (0.75 Å resolution), of which 20355 were independent (average redundancy 5.417, completeness = 98.3%, R_{int} =28.13%, R_{sig} = 26.27%) and 7934 (38.98%) were greater than $2\sigma(F^2)$. The final cell constants of a = 14.1686(15) Å, b =18.684(2) Å, c = 19.045(2) Å, α = 114.321(4)°, β = 98.469(4)°, γ = 107.830(4)°, volume = 4150.7(8) $Å^3$, are based upon the refinement of the XYZ-centroids of 4920 reflections above 20 σ(I) with 4.317° < 2θ < 39.08°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.857. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P -1, with Z = 2 for the formula unit, $C_{84}H_{50}B_2Cl_2F_{33}N_5OPd$. The final anisotropic full-matrix least-squares refinement on F^2 with 1161 variables converged at R1 = 9.74%, for the observed data and wR2 = 30.99% for all data. The goodness-of-fit was 0.994. The largest peak in the final difference electron density synthesis was 3.515 $e^-/Å^3$ and the largest hole was -1.430 $e^-/Å^3$ with an RMS deviation of 0.147 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.577 g/cm^3 and F(000), 1968 e^-. PLATON SQUEEZE was used to account for disordered solvent present in the

crystal that could not be modelled.

Table 1. Sample and crystal data for 5359.

Identification code	5359	
Chemical formula	$C_{84}H_{50}B_2Cl_2F_{33}N_5OPd$	
Formula weight	1971.21 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 14.1686(15) Å	α = 114.321(4)°
	b = 18.684(2) Å	β = 98.469(4)°
	c = 19.045(2) Å	γ = 107.830(4)°
Volume	4150.7(8) $Å^3$	
Z	2	
Density (calculated)	1.577 g/cm^3	
Absorption coefficient	0.412 mm^{-1}	
F(000)	1968	

Table 2. Data collection and structure refinement for 5359.

Theta range for data collection	1.31 to 28.33°	
Index ranges	-18<=h<=18, -24<=k<=24, -25<=l<=25	
Reflections collected	110269	
Independent reflections	20355 [R(int) = 0.2813]	
Coverage of independent reflections	98.3%	
Absorption correction	Multi-Scan	
Structure solution technique	direct methods	
Structure solution program	XT, VERSION 2014/5	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	20355 / 0 / 1161	
Goodness-of-fit on F^2	0.994	
Final R indices	7934 data; I>2σ(I)	R1 = 0.0974, wR2 = 0.2360
	all data	R1 = 0.2546, wR2 = 0.3099
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.1488P)^2]$ where $P=(F_o^2+2F_c^2)/3$	

Largest diff. peak and hole	3.515 and -1.430 eÅ^{-3}
R.M.S. deviation from mean	0.147 eÅ^{-3}

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 5359.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij}tensor.

	x/a	y/b	z/c	U(eq)
Pd1	0.80192(6)	0.13691(4)	0.45962(4)	0.0274(2)
Cl1	0.0593(2)	0.14658(18)	0.28783(17)	0.0546(7)
Cl2	0.9877(3)	0.9956(2)	0.12899(19)	0.0708(9)
F9	0.0201(4)	0.1866(3)	0.1186(3)	0.0307(12)
F19	0.4664(4)	0.2483(3)	0.0251(3)	0.0309(12)
F24	0.4070(4)	0.0808(3)	0.0187(3)	0.0268(11)
F15	0.2652(4)	0.5142(3)	0.1852(3)	0.0314(12)
F25	0.3884(4)	0.9220(3)	0.9826(3)	0.0309(12)
F4	0.2214(4)	0.3034(3)	0.2552(3)	0.0300(11)
F14	0.2332(4)	0.2665(3)	0.9527(3)	0.0318(12)
F8	0.0554(4)	0.4178(3)	0.1203(3)	0.0337(12)
F13	0.0576(4)	0.2949(3)	0.9338(3)	0.0352(13)
F33	0.6493(4)	0.4103(3)	0.3015(3)	0.0370(13)
F27	0.5403(4)	0.0184(3)	0.2596(3)	0.0350(12)
F28	0.5401(4)	0.1697(3)	0.2986(3)	0.0342(12)
F26	0.4623(4)	0.8903(3)	0.1027(3)	0.0343(12)
F23	0.6897(4)	0.2660(3)	0.2483(3)	0.0380(13)
F16	0.3746(4)	0.6120(3)	0.1337(3)	0.0374(13)
F7	0.9815(4)	0.4784(3)	0.2422(3)	0.0425(14)
F29	0.3406(4)	0.1897(3)	0.2666(3)	0.0368(13)
F5	0.1569(4)	0.3726(3)	0.3801(3)	0.0396(13)
F18	0.3455(5)	0.3678(3)	0.9031(3)	0.0440(14)
F10	0.8304(4)	0.0717(3)	0.0200(3)	0.0389(13)
F11	0.7541(4)	0.0636(4)	0.8754(3)	0.0491(15)
F17	0.4183(5)	0.5415(3)	0.9918(3)	0.0449(15)
F20	0.6282(5)	0.2879(3)	0.9720(3)	0.0464(15)
F6	0.0344(4)	0.4603(3)	0.3757(3)	0.0457(14)
F32	0.6637(5)	0.5001(4)	0.4548(3)	0.0545(16)
F31	0.5170(6)	0.4401(4)	0.5177(3)	0.0604(19)
F30	0.3529(5)	0.2837(4)	0.4198(3)	0.0581(18)
F22	0.8471(4)	0.2959(4)	0.1886(4)	0.0582(17)

	x/a	y/b	z/c	U(eq)
F12	0.8703(4)	0.1788(4)	0.8372(3)	0.0521(16)
F21	0.8201(5)	0.3087(4)	0.0510(4)	0.0603(18)
F1	0.6419(5)	0.6899(3)	0.3862(4)	0.0624(19)
N5	0.2404(5)	0.2623(4)	0.1025(4)	0.0223(15)
N4	0.3693(5)	0.2264(4)	0.1357(4)	0.0206(15)
N1	0.7821(5)	0.0993(4)	0.3385(4)	0.0272(16)
F3	0.6981(5)	0.6737(4)	0.2873(4)	0.076(2)
O1	0.7401(6)	0.9815(4)	0.4648(4)	0.051(2)
N2	0.8810(6)	0.2742(4)	0.6138(4)	0.0300(17)
N3	0.8446(6)	0.1772(5)	0.6474(4)	0.0306(17)
F2	0.5578(6)	0.6938(4)	0.2878(5)	0.098(3)
C28	0.7518(7)	0.0132(5)	0.4229(6)	0.029(2)
C56	0.3230(7)	0.4031(5)	0.9727(5)	0.030(2)
C53	0.9879(7)	0.1878(5)	0.0487(5)	0.027(2)
C83	0.4344(6)	0.0667(5)	0.0811(5)	0.0254(19)
C48	0.0546(7)	0.2453(5)	0.0313(5)	0.0252(19)
C60	0.1465(6)	0.3615(5)	0.1820(5)	0.0225(18)
C46	0.4218(6)	0.4385(5)	0.2650(5)	0.0227(18)
C39	0.2004(7)	0.1739(5)	0.0704(5)	0.0249(19)
C38	0.3426(7)	0.2920(5)	0.1412(5)	0.0243(19)
C54	0.2384(6)	0.3833(5)	0.0699(5)	0.0220(18)
C79	0.5017(6)	0.1124(5)	0.2192(5)	0.0234(19)
C55	0.2652(7)	0.3516(5)	0.9991(5)	0.027(2)
C72	0.5714(7)	0.2613(5)	0.1433(5)	0.0262(19)
C80	0.5025(7)	0.0334(6)	0.2001(5)	0.029(2)
C73	0.5614(7)	0.2650(5)	0.0720(5)	0.027(2)
C34	0.7469(7)	0.0121(5)	0.2913(5)	0.028(2)
C40	0.2785(6)	0.1528(5)	0.0913(5)	0.0229(18)
C57	0.3613(7)	0.4906(6)	0.0176(6)	0.033(2)
C78	0.4675(6)	0.1338(5)	0.1611(5)	0.0234(19)
C82	0.4296(7)	0.9852(5)	0.0616(5)	0.0260(19)
C67	0.4224(7)	0.2668(6)	0.3104(5)	0.028(2)
C45	0.4880(7)	0.5253(5)	0.3042(5)	0.029(2)
C81	0.4646(7)	0.9690(5)	0.1210(5)	0.027(2)
C64	0.1315(7)	0.3839(5)	0.3153(5)	0.031(2)
C42	0.4790(7)	0.4201(5)	0.1481(5)	0.028(2)
C66	0.4959(7)	0.2929(5)	0.2760(5)	0.0256(19)

	x/a	y/b	z/c	U(eq)
C59	0.2792(7)	0.4731(5)	0.1137(5)	0.0261(19)
C1	0.8388(7)	0.1894(5)	0.5823(6)	0.030(2)
C71	0.5758(7)	0.3744(6)	0.3277(5)	0.032(2)
C65	0.1674(7)	0.3515(5)	0.2506(5)	0.028(2)
C70	0.5837(8)	0.4234(6)	0.4081(6)	0.034(2)
C5	0.7850(7)	0.3154(5)	0.5292(5)	0.031(2)
C58	0.3378(7)	0.5261(5)	0.0886(5)	0.031(2)
C43	0.5452(7)	0.5065(5)	0.1880(5)	0.032(2)
C61	0.0838(7)	0.4061(5)	0.1839(5)	0.0260(19)
C77	0.6717(7)	0.2720(5)	0.1794(6)	0.029(2)
C44	0.5483(7)	0.5587(5)	0.2657(6)	0.032(2)
C63	0.0710(7)	0.4277(5)	0.3132(6)	0.033(2)
C41	0.4164(6)	0.3844(5)	0.1863(5)	0.0240(19)
C62	0.0462(7)	0.4385(5)	0.2468(6)	0.032(2)
C29	0.7275(7)	0.9639(5)	0.3329(5)	0.031(2)
C49	0.0077(7)	0.2401(6)	0.9586(5)	0.027(2)
C37	0.8007(7)	0.1473(6)	0.3016(6)	0.035(2)
C4	0.8794(7)	0.3109(5)	0.5590(5)	0.026(2)
C8	0.9626(7)	0.3677(5)	0.4825(5)	0.032(2)
C33	0.7295(7)	0.9725(6)	0.2085(6)	0.036(2)
C10	0.6924(7)	0.2929(6)	0.5575(5)	0.035(2)
C69	0.5092(10)	0.3928(7)	0.4383(6)	0.044(3)
C74	0.6419(8)	0.2822(5)	0.0402(6)	0.033(2)
C36	0.7847(8)	0.1121(6)	0.2180(6)	0.042(2)
C14	0.0669(7)	0.3275(6)	0.5687(5)	0.034(2)
C7	0.8707(8)	0.3738(6)	0.4525(6)	0.039(2)
C6	0.7832(9)	0.3466(6)	0.4743(6)	0.040(2)
C52	0.8882(7)	0.1279(6)	0.9992(6)	0.034(2)
C76	0.7524(7)	0.2875(6)	0.1498(6)	0.036(2)
C25	0.6403(8)	0.1381(6)	0.6664(6)	0.041(2)
C2	0.9162(8)	0.3170(6)	0.6983(5)	0.038(2)
C50	0.9087(7)	0.1806(6)	0.9078(5)	0.034(2)
C16	0.7937(8)	0.0975(6)	0.6474(6)	0.036(2)
C47	0.6113(8)	0.6540(6)	0.3072(6)	0.039(2)
C75	0.7390(8)	0.2938(6)	0.0800(7)	0.040(3)
C68	0.4266(9)	0.3154(7)	0.3903(6)	0.041(3)
C9	0.9684(7)	0.3355(6)	0.5357(6)	0.035(2)

	x/a	y/b	z/c	U(eq)
C51	0.8487(7)	0.1227(6)	0.9259(6)	0.037(2)
C20	0.7887(9)	0.9638(7)	0.6371(6)	0.049(3)
C32	0.6911(8)	0.8818(7)	0.1654(6)	0.050(3)
C27	0.6288(9)	0.1743(7)	0.7512(6)	0.049(3)
B2	0.4775(8)	0.2313(6)	0.1803(6)	0.027(2)
C31	0.6702(9)	0.8351(6)	0.2045(7)	0.052(3)
C30	0.6879(8)	0.8765(6)	0.2892(7)	0.047(3)
C21	0.8443(9)	0.0414(7)	0.6385(6)	0.045(3)
C3	0.8928(8)	0.2544(7)	0.7181(6)	0.045(3)
C15	0.1578(8)	0.4198(7)	0.6193(7)	0.064(4)
C17	0.6931(8)	0.0780(6)	0.6545(6)	0.038(2)
C35	0.7514(7)	0.0262(6)	0.1720(6)	0.041(2)
B1	0.1726(8)	0.3150(6)	0.0965(6)	0.022(2)
C84	0.0968(8)	0.0872(7)	0.2067(6)	0.049(3)
C12	0.6834(9)	0.3728(7)	0.6156(7)	0.054(3)
C22	0.9540(9)	0.0645(8)	0.6312(7)	0.053(3)
C19	0.6923(9)	0.9453(6)	0.6459(6)	0.049(3)
C13	0.0993(9)	0.2714(7)	0.5019(6)	0.051(3)
C18	0.6449(8)	0.0000(6)	0.6535(6)	0.046(3)
C11	0.5910(8)	0.2311(7)	0.4883(6)	0.048(3)
C24	0.9760(11)	0.9863(9)	0.5839(8)	0.072(4)
C26	0.5343(9)	0.0965(9)	0.6008(7)	0.068(4)
C23	0.0348(11)	0.1235(10)	0.7142(9)	0.086(4)

Table 4. Bond lengths (Å) for 5359.

Pd1-C28	1.962(8)	Pd1-C1	2.033(9)
Pd1-N1	2.060(7)	Cl1-C84	1.757(11)
Cl2-C84	1.768(11)	F9-C53	1.353(9)
F19-C73	1.366(10)	F24-C83	1.347(9)
F15-C59	1.340(9)	F25-C82	1.362(9)
F4-C65	1.367(10)	F14-C55	1.341(9)
F8-C61	1.343(9)	F13-C49	1.351(9)
F33-C71	1.335(10)	F27-C80	1.350(9)
F28-C79	1.339(9)	F26-C81	1.353(9)
F23-C77	1.358(10)	F16-C58	1.344(9)
F7-C62	1.361(10)	F29-C67	1.348(10)

F5-C64	1.352(10)	F18-C56	1.351(9)
F10-C52	1.356(10)	F11-C51	1.334(10)
F17-C57	1.351(9)	F20-C74	1.338(10)
F6-C63	1.355(10)	F32-C70	1.337(10)
F31-C69	1.367(10)	F30-C68	1.352(11)
F22-C76	1.361(10)	F12-C50	1.357(9)
F21-C75	1.350(10)	F1-C47	1.305(11)
N5-C38	1.343(10)	N5-C39	1.384(9)
N5-B1	1.595(11)	N4-C38	1.359(10)
N4-C40	1.378(10)	N4-B2	1.596(12)
N1-C37	1.340(11)	N1-C34	1.370(10)
F3-C47	1.330(11)	O1-C28	1.176(10)
N2-C1	1.327(10)	N2-C2	1.393(11)
N2-C4	1.466(10)	N3-C1	1.346(11)
N3-C3	1.374(12)	N3-C16	1.443(11)
F2-C47	1.323(12)	C28-C29	1.495(12)
C56-C57	1.366(12)	C56-C55	1.373(11)
C53-C52	1.381(12)	C53-C48	1.385(12)
C83-C82	1.388(12)	C83-C78	1.404(11)
C48-C49	1.396(11)	C48-B1	1.660(13)
C60-C61	1.388(11)	C60-C65	1.396(11)
C60-B1	1.658(12)	C46-C45	1.390(11)
C46-C41	1.395(11)	C46-H46	0.95
C39-C40	1.344(11)	C39-H39	0.95
C38-C41	1.491(11)	C54-C55	1.394(11)
C54-C59	1.398(11)	C54-B1	1.643(12)
C79-C80	1.370(12)	C79-C78	1.396(11)
C72-C73	1.377(12)	C72-C77	1.399(12)
C72-B2	1.651(13)	C80-C81	1.371(12)
C73-C74	1.381(12)	C34-C33	1.382(12)
C34-C29	1.418(12)	C40-H40	0.95
C57-C58	1.382(12)	C78-B2	1.657(12)
C82-C81	1.350(12)	C67-C66	1.380(12)
C67-C68	1.394(12)	C45-C44	1.376(12)
C45-H45	0.95	C64-C63	1.359(13)
C64-C65	1.379(12)	C42-C43	1.383(11)
C42-C41	1.411(11)	C42-H42	0.95
C66-C71	1.396(12)	C66-B2	1.633(13)

C59-C58	1.378(12)	C71-C70	1.389(13)
C70-C69	1.360(14)	C5-C6	1.393(12)
C5-C4	1.415(12)	C5-C10	1.498(13)
C43-C44	1.382(12)	C43-H43	0.95
C61-C62	1.370(12)	C77-C76	1.354(12)
C44-C47	1.501(12)	C63-C62	1.374(13)
C29-C30	1.363(12)	C49-C50	1.378(12)
C37-C36	1.401(13)	C37-H37	0.95
C4-C9	1.405(12)	C8-C9	1.379(12)
C8-C7	1.401(13)	C8-H8	0.95
C33-C32	1.415(13)	C33-C35	1.426(14)
C10-C12	1.506(14)	C10-C11	1.518(13)
C10-H10	1.0	C69-C68	1.363(15)
C74-C75	1.374(14)	C36-C35	1.350(13)
C36-H36	0.95	C14-C13	1.516(13)
C14-C9	1.521(13)	C14-C15	1.570(13)
C14-H14	1.0	C7-C6	1.381(14)
C7-H7	0.95	C6-H6	0.95
C52-C51	1.379(13)	C76-C75	1.374(14)
C25-C17	1.492(14)	C25-C27	1.529(14)
C25-C26	1.535(14)	C25-H25	1.0
C2-C3	1.334(13)	C2-H2	0.95
C50-C51	1.356(12)	C16-C17	1.400(14)
C16-C21	1.411(13)	C20-C19	1.356(15)
C20-C21	1.409(14)	C20-H20	0.95
C32-C31	1.357(15)	C32-H32	0.95
C27-H27A	0.98	C27-H27B	0.98
C27-H27C	0.98	C31-C30	1.414(15)
C31-H31	0.95	C30-H30	0.95
C21-C22	1.524(15)	C3-H3	0.95
C15-H15A	0.98	C15-H15B	0.98
C15-H15C	0.98	C17-C18	1.398(13)
C35-H35	0.95	C84-H84A	0.99
C84-H84B	0.99	C12-H12A	0.98
C12-H12B	0.98	C12-H12C	0.98
C22-C23	1.511(17)	C22-C24	1.523(17)
C22-H22	1.0	C19-C18	1.357(14)
C19-H19	0.95	C13-H13A	0.98

C13-H13B	0.98	C13-H13C	0.98
C18-H18	0.95	C11-H11A	0.98
C11-H11B	0.98	C11-H11C	0.98
C24-H24A	0.98	C24-H24B	0.98
C24-H24C	0.98	C26-H26A	0.98
C26-H26B	0.98	C26-H26C	0.98
C23-H23A	0.98	C23-H23B	0.98
C23-H23C	0.98		

Table 5. Bond angles (°) for 5359.

C28-Pd1-C1	102.8(3)	C28-Pd1-N1	84.1(3)
C1-Pd1-N1	171.8(3)	C38-N5-C39	106.4(7)
C38-N5-B1	129.0(7)	C39-N5-B1	124.6(7)
C38-N4-C40	105.6(7)	C38-N4-B2	128.6(7)
C40-N4-B2	125.3(6)	C37-N1-C34	117.5(7)
C37-N1-Pd1	129.6(6)	C34-N1-Pd1	112.9(6)
C1-N2-C2	112.5(7)	C1-N2-C4	118.8(7)
C2-N2-C4	128.5(7)	C1-N3-C3	110.9(7)
C1-N3-C16	126.6(7)	C3-N3-C16	121.8(8)
O1-C28-C29	124.3(8)	O1-C28-Pd1	125.4(7)
C29-C28-Pd1	110.3(6)	F18-C56-C57	119.1(8)
F18-C56-C55	120.3(7)	C57-C56-C55	120.6(8)
F9-C53-C52	114.7(7)	F9-C53-C48	119.8(7)
C52-C53-C48	125.5(8)	F24-C83-C82	117.0(7)
F24-C83-C78	119.6(7)	C82-C83-C78	123.5(8)
C53-C48-C49	112.3(8)	C53-C48-B1	120.8(7)
C49-C48-B1	126.8(7)	C61-C60-C65	113.5(8)
C61-C60-B1	118.1(7)	C65-C60-B1	127.7(7)
C45-C46-C41	120.2(8)	C45-C46-H46	119.9
C41-C46-H46	119.9	C40-C39-N5	108.1(7)
C40-C39-H39	125.9	N5-C39-H39	125.9
N5-C38-N4	110.8(7)	N5-C38-C41	124.9(7)
N4-C38-C41	124.3(7)	C55-C54-C59	113.8(7)
C55-C54-B1	118.7(7)	C59-C54-B1	127.3(7)
F28-C79-C80	115.1(7)	F28-C79-C78	121.5(7)
C80-C79-C78	123.4(8)	F14-C55-C56	116.8(7)
F14-C55-C54	119.6(7)	C56-C55-C54	123.5(7)

C73-C72-C77	112.9(8)	C73-C72-B2	127.7(8)
C77-C72-B2	118.6(8)	F27-C80-C79	119.9(8)
F27-C80-C81	119.5(7)	C79-C80-C81	120.6(8)
F19-C73-C72	120.7(7)	F19-C73-C74	114.5(8)
C72-C73-C74	124.8(9)	N1-C34-C33	122.9(8)
N1-C34-C29	115.5(7)	C33-C34-C29	121.5(8)
C39-C40-N4	109.1(7)	C39-C40-H40	125.5
N4-C40-H40	125.5	F17-C57-C56	120.8(8)
F17-C57-C58	120.5(8)	C56-C57-C58	118.6(8)
C79-C78-C83	113.3(7)	C79-C78-B2	125.1(7)
C83-C78-B2	121.1(7)	C81-C82-F25	120.8(7)
C81-C82-C83	119.9(8)	F25-C82-C83	119.3(7)
F29-C67-C66	120.2(8)	F29-C67-C68	115.7(8)
C66-C67-C68	124.1(9)	C44-C45-C46	120.4(8)
C44-C45-H45	119.8	C46-C45-H45	119.8
C82-C81-F26	120.4(7)	C82-C81-C80	119.2(8)
F26-C81-C80	120.4(8)	F5-C64-C63	120.7(8)
F5-C64-C65	120.1(8)	C63-C64-C65	119.2(8)
C43-C42-C41	120.8(8)	C43-C42-H42	119.6
C41-C42-H42	119.6	C67-C66-C71	114.4(8)
C67-C66-B2	118.6(8)	C71-C66-B2	126.9(8)
F15-C59-C58	114.8(7)	F15-C59-C54	121.5(7)
C58-C59-C54	123.7(8)	N2-C1-N3	104.1(8)
N2-C1-Pd1	107.6(6)	N3-C1-Pd1	148.1(6)
F33-C71-C70	115.9(8)	F33-C71-C66	121.2(8)
C70-C71-C66	122.9(9)	F4-C65-C64	115.3(8)
F4-C65-C60	120.6(7)	C64-C65-C60	124.0(8)
F32-C70-C69	120.7(9)	F32-C70-C71	119.9(9)
C69-C70-C71	119.4(9)	C6-C5-C4	116.5(9)
C6-C5-C10	120.3(9)	C4-C5-C10	123.1(8)
F16-C58-C59	120.6(7)	F16-C58-C57	119.7(8)
C59-C58-C57	119.7(8)	C44-C43-C42	119.5(8)
C44-C43-H43	120.3	C42-C43-H43	120.3
F8-C61-C62	116.6(8)	F8-C61-C60	119.4(7)
C62-C61-C60	124.0(8)	C76-C77-F23	117.4(8)
C76-C77-C72	124.3(9)	F23-C77-C72	118.3(8)
C45-C44-C43	120.7(8)	C45-C44-C47	118.7(8)
C43-C44-C47	120.5(8)	F6-C63-C64	120.7(8)

F6-C63-C62	119.6(8)	C64-C63-C62	119.7(8)
C46-C41-C42	118.4(7)	C46-C41-C38	121.5(7)
C42-C41-C38	120.1(7)	F7-C62-C61	120.1(8)
F7-C62-C63	120.2(8)	C61-C62-C63	119.6(8)
C30-C29-C34	118.7(9)	C30-C29-C28	124.0(9)
C34-C29-C28	117.2(7)	F13-C49-C50	115.4(7)
F13-C49-C48	121.2(7)	C50-C49-C48	123.4(8)
N1-C37-C36	123.1(9)	N1-C37-H37	118.5
C36-C37-H37	118.5	C9-C4-C5	123.6(8)
C9-C4-N2	119.1(8)	C5-C4-N2	117.2(7)
C9-C8-C7	120.6(9)	C9-C8-H8	119.7
C7-C8-H8	119.7	C34-C33-C32	118.2(9)
C34-C33-C35	117.5(8)	C32-C33-C35	124.3(9)
C5-C10-C12	110.9(8)	C5-C10-C11	113.3(8)
C12-C10-C11	111.6(9)	C5-C10-H10	106.9
C12-C10-H10	106.9	C11-C10-H10	106.9
C70-C69-C68	120.8(9)	C70-C69-F31	119.8(10)
C68-C69-F31	119.4(10)	F20-C74-C75	119.0(8)
F20-C74-C73	122.0(9)	C75-C74-C73	119.0(9)
C35-C36-C37	119.1(9)	C35-C36-H36	120.4
C37-C36-H36	120.4	C13-C14-C9	112.5(8)
C13-C14-C15	109.1(8)	C9-C14-C15	108.6(8)
C13-C14-H14	108.9	C9-C14-H14	108.9
C15-C14-H14	108.9	C6-C7-C8	121.0(8)
C6-C7-H7	119.5	C8-C7-H7	119.5
C7-C6-C5	121.0(10)	C7-C6-H6	119.5
C5-C6-H6	119.5	F10-C52-C51	119.5(8)
F10-C52-C53	121.2(8)	C51-C52-C53	119.3(8)
C77-C76-F22	120.1(9)	C77-C76-C75	120.2(9)
F22-C76-C75	119.7(9)	C17-C25-C27	111.5(8)
C17-C25-C26	112.3(9)	C27-C25-C26	110.8(9)
C17-C25-H25	107.3	C27-C25-H25	107.3
C26-C25-H25	107.3	C3-C2-N2	104.6(8)
C3-C2-H2	127.7	N2-C2-H2	127.7
C51-C50-F12	118.8(8)	C51-C50-C49	121.8(8)
F12-C50-C49	119.4(8)	C17-C16-C21	122.4(9)
C17-C16-N3	117.6(8)	C21-C16-N3	120.0(9)
F1-C47-F2	106.7(9)	F1-C47-F3	105.5(8)

F2-C47-F3	107.2(9)	F1-C47-C44	113.5(8)
F2-C47-C44	111.6(8)	F3-C47-C44	112.0(8)
F21-C75-C76	119.5(9)	F21-C75-C74	121.7(9)
C76-C75-C74	118.8(8)	F30-C68-C69	121.4(9)
F30-C68-C67	120.2(9)	C69-C68-C67	118.4(9)
C8-C9-C4	117.3(9)	C8-C9-C14	121.7(8)
C4-C9-C14	121.1(8)	F11-C51-C50	121.6(8)
F11-C51-C52	120.8(8)	C50-C51-C52	117.6(9)
C19-C20-C21	121.3(10)	C19-C20-H20	119.4
C21-C20-H20	119.4	C31-C32-C33	120.7(10)
C31-C32-H32	119.7	C33-C32-H32	119.7
C25-C27-H27A	109.5	C25-C27-H27B	109.5
H27A-C27-H27B	109.5	C25-C27-H27C	109.5
H27A-C27-H27C	109.5	H27B-C27-H27C	109.5
N4-B2-C66	103.1(7)	N4-B2-C72	112.6(7)
C66-B2-C72	117.0(7)	N4-B2-C78	110.2(7)
C66-B2-C78	112.0(7)	C72-B2-C78	102.1(7)
C32-C31-C30	120.4(9)	C32-C31-H31	119.8
C30-C31-H31	119.8	C29-C30-C31	120.4(10)
C29-C30-H30	119.8	C31-C30-H30	119.8
C20-C21-C16	116.8(9)	C20-C21-C22	122.2(10)
C16-C21-C22	121.1(9)	C2-C3-N3	107.8(8)
C2-C3-H3	126.1	N3-C3-H3	126.1
C14-C15-H15A	109.5	C14-C15-H15B	109.5
H15A-C15-H15B	109.5	C14-C15-H15C	109.5
H15A-C15-H15C	109.5	H15B-C15-H15C	109.5
C18-C17-C16	116.6(9)	C18-C17-C25	120.6(9)
C16-C17-C25	122.8(8)	C36-C35-C33	119.8(9)
C36-C35-H35	120.1	C33-C35-H35	120.1
N5-B1-C54	106.0(7)	N5-B1-C60	112.1(6)
C54-B1-C60	113.6(7)	N5-B1-C48	108.1(6)
C54-B1-C48	114.7(7)	C60-B1-C48	102.3(7)
Cl1-C84-Cl2	111.1(6)	Cl1-C84-H84A	109.4
Cl2-C84-H84A	109.4	Cl1-C84-H84B	109.4
Cl2-C84-H84B	109.4	H84A-C84-H84B	108.0
C10-C12-H12A	109.5	C10-C12-H12B	109.5
H12A-C12-H12B	109.5	C10-C12-H12C	109.5
H12A-C12-H12C	109.5	H12B-C12-H12C	109.5

C23-C22-C24	111.1(10)	C23-C22-C21	110.4(10)
C24-C22-C21	113.3(10)	C23-C22-H22	107.2
C24-C22-H22	107.2	C21-C22-H22	107.2
C20-C19-C18	120.7(9)	C20-C19-H19	119.6
C18-C19-H19	119.6	C14-C13-H13A	109.5
C14-C13-H13B	109.5	H13A-C13-H13B	109.5
C14-C13-H13C	109.5	H13A-C13-H13C	109.5
H13B-C13-H13C	109.5	C19-C18-C17	122.3(10)
C19-C18-H18	118.9	C17-C18-H18	118.9
C10-C11-H11A	109.5	C10-C11-H11B	109.5
H11A-C11-H11B	109.5	C10-C11-H11C	109.5
H11A-C11-H11C	109.5	H11B-C11-H11C	109.5
C22-C24-H24A	109.5	C22-C24-H24B	109.5
H24A-C24-H24B	109.5	C22-C24-H24C	109.5
H24A-C24-H24C	109.5	H24B-C24-H24C	109.5
C25-C26-H26A	109.5	C25-C26-H26B	109.5
H26A-C26-H26B	109.5	C25-C26-H26C	109.5
H26A-C26-H26C	109.5	H26B-C26-H26C	109.5
C22-C23-H23A	109.5	C22-C23-H23B	109.5
H23A-C23-H23B	109.5	C22-C23-H23C	109.5
H23A-C23-H23C	109.5	H23B-C23-H23C	109.5

Table 6. Anisotropic atomic displacement parameters (Å^2) for 5359.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pd1	0.0291(4)	0.0267(4)	0.0247(4)	0.0133(3)	0.0068(3)	0.0091(3)
Cl1	0.072(2)	0.0522(16)	0.0470(16)	0.0245(14)	0.0226(15)	0.0315(15)
Cl2	0.069(2)	0.0560(18)	0.059(2)	0.0049(16)	0.0068(17)	0.0293(17)
F9	0.034(3)	0.032(3)	0.031(3)	0.021(2)	0.009(2)	0.011(2)
F19	0.040(3)	0.029(3)	0.024(3)	0.012(2)	0.012(2)	0.013(2)
F24	0.034(3)	0.025(2)	0.021(3)	0.011(2)	0.009(2)	0.012(2)
F15	0.039(3)	0.022(2)	0.030(3)	0.012(2)	0.015(2)	0.007(2)
F25	0.033(3)	0.024(2)	0.027(3)	0.007(2)	0.008(2)	0.010(2)
F4	0.037(3)	0.034(3)	0.030(3)	0.022(2)	0.014(2)	0.018(2)
F14	0.043(3)	0.023(2)	0.034(3)	0.016(2)	0.018(2)	0.013(2)
F8	0.038(3)	0.040(3)	0.037(3)	0.024(3)	0.017(3)	0.024(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F13	0.035(3)	0.039(3)	0.030(3)	0.024(2)	0.005(2)	0.006(2)
F33	0.033(3)	0.026(3)	0.037(3)	0.006(2)	0.004(3)	0.009(2)
F27	0.042(3)	0.040(3)	0.040(3)	0.028(3)	0.015(3)	0.024(3)
F28	0.051(3)	0.033(3)	0.022(3)	0.013(2)	0.010(2)	0.024(3)
F26	0.045(3)	0.025(3)	0.042(3)	0.019(2)	0.015(3)	0.019(2)
F23	0.032(3)	0.034(3)	0.039(3)	0.014(3)	0.001(2)	0.013(2)
F16	0.052(3)	0.022(3)	0.041(3)	0.018(2)	0.020(3)	0.011(2)
F7	0.048(3)	0.030(3)	0.055(4)	0.017(3)	0.028(3)	0.022(3)
F29	0.044(3)	0.040(3)	0.038(3)	0.026(3)	0.022(3)	0.019(3)
F5	0.050(3)	0.042(3)	0.030(3)	0.021(3)	0.018(3)	0.016(3)
F18	0.068(4)	0.035(3)	0.040(3)	0.021(3)	0.035(3)	0.021(3)
F10	0.030(3)	0.043(3)	0.041(3)	0.027(3)	0.009(3)	0.004(2)
F11	0.025(3)	0.062(4)	0.045(3)	0.028(3)	0.000(3)	0.002(3)
F17	0.066(4)	0.035(3)	0.049(3)	0.029(3)	0.036(3)	0.020(3)
F20	0.064(4)	0.041(3)	0.050(4)	0.028(3)	0.038(3)	0.022(3)
F6	0.059(4)	0.041(3)	0.041(3)	0.018(3)	0.032(3)	0.021(3)
F32	0.068(4)	0.046(4)	0.025(3)	0.001(3)	-0.006(3)	0.025(3)
F31	0.118(6)	0.063(4)	0.025(3)	0.021(3)	0.028(3)	0.065(4)
F30	0.104(5)	0.068(4)	0.052(4)	0.044(3)	0.057(4)	0.060(4)
F22	0.025(3)	0.047(3)	0.101(5)	0.037(4)	0.017(3)	0.013(3)
F12	0.044(4)	0.069(4)	0.042(3)	0.036(3)	0.007(3)	0.013(3)
F21	0.050(4)	0.055(4)	0.106(5)	0.049(4)	0.056(4)	0.029(3)
F1	0.079(5)	0.029(3)	0.039(4)	0.005(3)	0.006(3)	-0.005(3)
N5	0.028(4)	0.016(3)	0.023(4)	0.011(3)	0.011(3)	0.006(3)
N4	0.023(4)	0.022(3)	0.022(4)	0.014(3)	0.007(3)	0.009(3)
N1	0.026(4)	0.029(4)	0.024(4)	0.009(3)	0.008(3)	0.011(3)
F3	0.063(5)	0.044(4)	0.075(5)	0.013(4)	0.029(4)	-0.015(3)
O1	0.067(5)	0.037(4)	0.054(5)	0.033(4)	0.018(4)	0.012(4)
N2	0.032(4)	0.029(4)	0.025(4)	0.015(3)	0.007(3)	0.006(3)
N3	0.032(4)	0.035(4)	0.031(4)	0.022(4)	0.012(4)	0.013(4)
F2	0.081(5)	0.033(4)	0.140(7)	0.043(4)	-0.029(5)	0.003(4)
C28	0.021(5)	0.023(4)	0.043(6)	0.020(4)	0.007(4)	0.005(4)
C56	0.044(6)	0.032(5)	0.023(5)	0.017(4)	0.018(4)	0.019(4)
C53	0.027(5)	0.027(5)	0.030(5)	0.014(4)	0.008(4)	0.015(4)
C83	0.018(4)	0.030(5)	0.030(5)	0.016(4)	0.008(4)	0.010(4)
C48	0.028(5)	0.024(4)	0.029(5)	0.013(4)	0.012(4)	0.016(4)
C60	0.021(4)	0.016(4)	0.025(5)	0.008(4)	0.007(4)	0.004(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C46	0.026(5)	0.022(4)	0.021(4)	0.013(4)	0.008(4)	0.008(4)
C39	0.030(5)	0.017(4)	0.025(5)	0.010(4)	0.009(4)	0.008(4)
C38	0.025(5)	0.030(5)	0.023(5)	0.019(4)	0.008(4)	0.008(4)
C54	0.026(5)	0.022(4)	0.021(4)	0.013(4)	0.007(4)	0.010(4)
C79	0.020(5)	0.025(4)	0.023(5)	0.012(4)	0.006(4)	0.006(4)
C55	0.039(5)	0.012(4)	0.025(5)	0.005(4)	0.012(4)	0.009(4)
C72	0.025(5)	0.023(4)	0.026(5)	0.006(4)	0.008(4)	0.013(4)
C80	0.032(5)	0.040(5)	0.030(5)	0.026(5)	0.015(4)	0.020(4)
C73	0.031(5)	0.023(4)	0.027(5)	0.013(4)	0.011(4)	0.009(4)
C34	0.021(5)	0.026(5)	0.018(4)	-0.001(4)	-0.010(4)	0.012(4)
C40	0.024(5)	0.017(4)	0.027(5)	0.009(4)	0.008(4)	0.009(4)
C57	0.040(6)	0.028(5)	0.041(6)	0.024(5)	0.018(5)	0.014(4)
C78	0.014(4)	0.017(4)	0.031(5)	0.009(4)	0.005(4)	0.001(3)
C82	0.024(5)	0.022(4)	0.026(5)	0.007(4)	0.008(4)	0.008(4)
C67	0.039(6)	0.032(5)	0.031(5)	0.025(4)	0.017(4)	0.019(4)
C45	0.033(5)	0.027(5)	0.027(5)	0.013(4)	0.005(4)	0.014(4)
C81	0.028(5)	0.022(4)	0.031(5)	0.012(4)	0.014(4)	0.011(4)
C64	0.040(6)	0.022(4)	0.026(5)	0.010(4)	0.013(4)	0.006(4)
C42	0.028(5)	0.033(5)	0.023(5)	0.016(4)	0.012(4)	0.009(4)
C66	0.026(5)	0.031(5)	0.021(4)	0.012(4)	0.003(4)	0.017(4)
C59	0.034(5)	0.029(5)	0.022(5)	0.014(4)	0.015(4)	0.017(4)
C1	0.022(5)	0.018(4)	0.042(6)	0.016(4)	0.004(4)	0.001(4)
C71	0.033(5)	0.030(5)	0.031(5)	0.011(4)	0.011(4)	0.015(4)
C65	0.031(5)	0.028(5)	0.027(5)	0.013(4)	0.013(4)	0.013(4)
C70	0.039(6)	0.027(5)	0.027(5)	0.005(4)	-0.003(5)	0.017(5)
C5	0.040(6)	0.022(4)	0.031(5)	0.014(4)	0.012(4)	0.009(4)
C58	0.044(6)	0.022(4)	0.023(5)	0.007(4)	0.010(4)	0.015(4)
C43	0.035(5)	0.024(4)	0.035(5)	0.018(4)	0.011(4)	0.005(4)
C61	0.031(5)	0.026(4)	0.024(5)	0.014(4)	0.011(4)	0.012(4)
C77	0.032(5)	0.020(4)	0.042(6)	0.018(4)	0.017(5)	0.012(4)
C44	0.031(5)	0.027(5)	0.035(5)	0.018(4)	0.006(4)	0.006(4)
C63	0.037(6)	0.024(5)	0.033(5)	0.008(4)	0.016(5)	0.010(4)
C41	0.025(5)	0.023(4)	0.026(5)	0.014(4)	0.007(4)	0.011(4)
C62	0.020(5)	0.026(5)	0.050(6)	0.016(4)	0.013(4)	0.011(4)
C29	0.031(5)	0.024(4)	0.029(5)	0.004(4)	0.004(4)	0.015(4)
C49	0.024(5)	0.042(5)	0.023(5)	0.022(4)	0.005(4)	0.014(4)
C37	0.046(6)	0.028(5)	0.034(5)	0.019(4)	0.010(5)	0.015(5)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C4	0.024(5)	0.022(4)	0.029(5)	0.013(4)	0.004(4)	0.005(4)
C8	0.041(6)	0.027(5)	0.032(5)	0.022(4)	0.013(4)	0.009(4)
C33	0.029(5)	0.036(5)	0.031(5)	0.005(4)	-0.001(4)	0.018(4)
C10	0.035(6)	0.046(6)	0.028(5)	0.020(5)	0.009(4)	0.018(5)
C69	0.082(8)	0.046(6)	0.021(5)	0.017(5)	0.021(6)	0.047(6)
C74	0.040(6)	0.023(4)	0.032(5)	0.012(4)	0.019(5)	0.004(4)
C36	0.049(7)	0.047(6)	0.031(6)	0.018(5)	0.015(5)	0.021(5)
C14	0.022(5)	0.045(6)	0.033(5)	0.023(5)	0.013(4)	0.003(4)
C7	0.065(7)	0.031(5)	0.028(5)	0.020(4)	0.015(5)	0.021(5)
C6	0.058(7)	0.034(5)	0.030(5)	0.016(5)	0.012(5)	0.021(5)
C52	0.036(6)	0.041(5)	0.034(5)	0.022(5)	0.019(5)	0.020(5)
C76	0.020(5)	0.025(5)	0.058(7)	0.016(5)	0.007(5)	0.010(4)
C25	0.043(6)	0.041(6)	0.052(6)	0.033(5)	0.024(5)	0.016(5)
C2	0.042(6)	0.034(5)	0.025(5)	0.017(4)	0.000(4)	0.003(5)
C50	0.038(6)	0.045(6)	0.026(5)	0.023(5)	0.006(4)	0.022(5)
C16	0.047(6)	0.034(5)	0.037(6)	0.024(5)	0.016(5)	0.018(5)
C47	0.038(6)	0.026(5)	0.042(6)	0.017(5)	0.005(5)	0.002(5)
C75	0.036(6)	0.027(5)	0.073(8)	0.030(5)	0.035(6)	0.016(4)
C68	0.064(7)	0.052(6)	0.032(6)	0.031(5)	0.026(5)	0.036(6)
C9	0.037(6)	0.029(5)	0.034(5)	0.016(4)	0.012(5)	0.007(4)
C51	0.030(6)	0.040(5)	0.035(6)	0.017(5)	0.010(5)	0.007(5)
C20	0.073(8)	0.055(7)	0.059(7)	0.047(6)	0.033(6)	0.043(6)
C32	0.050(7)	0.042(6)	0.035(6)	0.000(5)	-0.004(5)	0.025(5)
C27	0.060(7)	0.049(6)	0.056(7)	0.032(6)	0.030(6)	0.028(6)
B2	0.031(6)	0.022(5)	0.028(6)	0.013(4)	0.011(5)	0.009(4)
C31	0.067(8)	0.018(5)	0.052(7)	0.003(5)	0.006(6)	0.018(5)
C30	0.038(6)	0.031(5)	0.064(8)	0.023(6)	0.004(6)	0.011(5)
C21	0.055(7)	0.061(7)	0.046(6)	0.036(6)	0.028(6)	0.035(6)
C3	0.042(6)	0.052(6)	0.025(5)	0.015(5)	0.002(5)	0.010(5)
C15	0.040(7)	0.053(7)	0.067(8)	0.005(6)	0.007(6)	0.017(6)
C17	0.047(6)	0.040(5)	0.033(5)	0.024(5)	0.015(5)	0.016(5)
C35	0.032(6)	0.046(6)	0.025(5)	0.005(5)	-0.001(4)	0.013(5)
B1	0.031(6)	0.026(5)	0.023(5)	0.018(4)	0.011(4)	0.018(4)
C84	0.050(7)	0.063(7)	0.038(6)	0.024(6)	0.015(5)	0.027(6)
C12	0.052(7)	0.061(7)	0.056(7)	0.027(6)	0.025(6)	0.030(6)
C22	0.050(7)	0.077(8)	0.060(8)	0.050(7)	0.020(6)	0.035(7)
C19	0.070(8)	0.036(6)	0.053(7)	0.032(5)	0.028(6)	0.019(6)

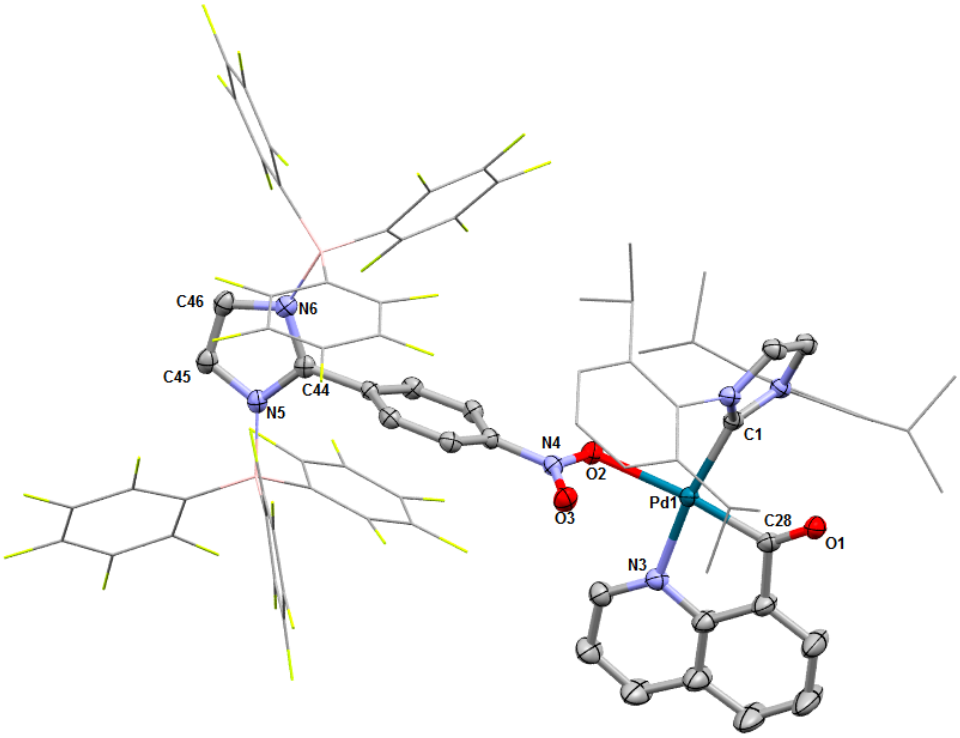
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C13	0.052(7)	0.044(6)	0.041(6)	0.010(5)	0.010(5)	0.017(5)
C18	0.041(6)	0.042(6)	0.050(7)	0.023(5)	0.013(5)	0.010(5)
C11	0.047(7)	0.053(7)	0.042(6)	0.022(5)	0.017(5)	0.019(6)
C24	0.081(10)	0.091(10)	0.087(10)	0.070(9)	0.046(8)	0.045(8)
C26	0.043(7)	0.093(10)	0.055(8)	0.024(7)	0.009(6)	0.035(7)
C23	0.064(9)	0.114(12)	0.101(12)	0.061(10)	0.039(9)	0.044(9)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 5359.

	x/a	y/b	z/c	U(eq)
H46	0.3802	0.4159	0.2919	0.027
H39	0.1301	0.1350	0.0391	0.03
H40	0.2721	0.0962	0.0778	0.027
H45	0.4916	0.5617	0.3580	0.035
H42	0.4757	0.3844	0.0942	0.033
H43	0.5882	0.5297	0.1622	0.038
H37	0.8259	0.2079	0.3337	0.042
H8	1.0216	0.3859	0.4661	0.038
H10	0.7054	0.2630	0.5885	0.042
H36	0.7971	0.1483	0.1939	0.05
H14	1.0543	0.3022	0.6053	0.041
H7	0.8685	0.3970	0.4166	0.047
H6	0.7209	0.3492	0.4515	0.048
H25	0.6861	0.1876	0.6619	0.049
H2	0.9494	0.3773	0.7340	0.045
H20	0.8193	-0.0764	0.6298	0.058
H32	0.6799	-0.1468	0.1086	0.06
H27A	0.5849	0.1272	0.7580	0.074
H27B	0.5962	0.2150	0.7579	0.074
H27C	0.6978	0.2040	0.7922	0.074
H31	0.6436	-0.2259	0.1747	0.063
H30	0.6720	-0.1568	0.3158	0.056
H3	0.9070	0.2620	0.7716	0.054
H15A	1.1639	0.4485	0.5861	0.096
H15B	1.2236	0.4151	0.6356	0.096
H15C	1.1425	0.4535	0.6679	0.096

	x/a	y/b	z/c	U(eq)
H35	0.7425	0.0016	0.1155	0.049
H84A	0.1485	0.0689	0.2267	0.059
H84B	0.1303	0.1241	0.1845	0.059
H12A	0.7464	0.4075	0.6631	0.081
H12B	0.6221	0.3566	0.6330	0.081
H12C	0.6757	0.4063	0.5886	0.081
H22	0.9601	0.0974	0.6007	0.064
H19	0.6575	-0.1064	0.6468	0.058
H13A	1.0398	0.2162	0.4657	0.076
H13B	1.1567	0.2613	0.5260	0.076
H13C	1.1225	0.3002	0.4708	0.076
H18	0.5767	-0.0152	0.6582	0.056
H11A	0.5755	0.2579	0.4560	0.072
H11B	0.5340	0.2171	0.5105	0.072
H11C	0.5980	0.1783	0.4538	0.072
H24A	0.9789	-0.0438	0.6153	0.107
H24B	1.0430	0.0050	0.5742	0.107
H24C	0.9202	-0.0525	0.5318	0.107
H26A	0.4853	0.0509	0.6068	0.101
H26B	0.5430	0.0718	0.5470	0.101
H26C	0.5068	0.1401	0.6067	0.101
H23A	1.0250	0.1770	0.7401	0.128
H23B	1.1048	0.1365	0.7087	0.128
H23C	1.0269	0.0952	0.7476	0.128

Crystal Structure Report for 1[IMP-NO_2]



Thermal ellipsoid plot of 5886. Ellipsoids shown at 50% probability, $B(C_6F_5)_3$ and diisopropylphenyl substituents shown in wireframe, toluene solvates and hydrogen atoms hidden for clarity.

A specimen of $C_{117}H_{88}B_2F_{30}N_6O_3Pd$ was used for the X-ray crystallographic analysis. The X-ray intensity data were measured(λ = 0.71073 Å). The integration of the data using a monoclinic unit cell yielded a total of 92615 reflections to a maximum θ angle of 27.93° (0.76Å resolution), of which 25071 were independent (average redundancy 3.694, completeness = 97.9%, R_{int} = 1.95%, R_{sig} =2.15%) and 20712 (82.61%) were greater than $2\sigma(F^2)$. The final cell constants of a = 18.6043(18) Å, b = 26.890(3) Å, c =21.779(2) Å, β = 101.862(2)°, volume = 10662.7(18) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The final anisotropic full-matrix least-squares refinement on F^2 with 1445 variables converged at R1 = 5.96%, for the observed data and wR2 = 19.78% for all data. The goodness-of-fit was 1.069. The largest peak in the final difference electron density synthesis was 3.911 $e^-/Å^3$ and the largest hole was -1.234 $e^-/Å^3$ with an RMS deviation of 0.128 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.448 g/cm^3 and F(000), 4728 e^-. While several disordered molecules of toluene were able to be modelled and refined, disordered pentane was not and was accounted for using PLATON SQUEEZE.

Table 1. Sample and crystal data for 5886.

Identification code	5886	
Chemical formula	$C_{117}H_{88}B_2F_{30}N_6O_3Pd$	
Formula weight	2323.95 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 18.6043(18) Å	α = 90°
	b = 26.890(3) Å	β = 101.862(2)°
	c = 21.779(2) Å	γ = 90°
Volume	10662.7(18) $Å^3$	
Z	4	
Density (calculated)	1.448 g/cm^3	
Absorption coefficient	0.283 mm^{-1}	
F(000)	4728	

Table 2. Data collection and structure refinement for 5886.

Theta range for data collection	1.35 to 27.93°	
Index ranges	-23<=h<=24, -32<=k<=35, -28<=l<=15	
Reflections collected	92615	
Independent reflections	25071 [R(int) = 0.0195]	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	25071 / 168 / 1445	
Goodness-of-fit on F^2	1.069	
Δ/σ_{max}	0.001	
Final R indices	20712 data; I>2σ(I)	R1 = 0.0596, wR2 = 0.1799
	all data	R1 = 0.0737, wR2 = 0.1978
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.1133P)^2+21.6492P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	3.911 and -1.234 $eÅ^{-3}$	
R.M.S. deviation from mean	0.128 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for 5886.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij}tensor.

	x/a	y/b	z/c	U(eq)
Pd1	0.23197(2)	0.45155(2)	0.17967(2)	0.01838(8)
F16	0.63321(10)	0.57344(7)	0.39993(8)	0.0245(4)
F11	0.63025(11)	0.29442(7)	0.41480(8)	0.0270(4)
F5	0.53592(10)	0.36315(7)	0.35275(8)	0.0251(4)
F1	0.67677(10)	0.44633(7)	0.52936(8)	0.0262(4)
F15	0.75966(10)	0.40089(7)	0.30204(9)	0.0260(4)
F17	0.51728(11)	0.63201(8)	0.38810(9)	0.0303(4)
F10	0.84764(10)	0.37178(8)	0.41993(9)	0.0290(4)
F6	0.67040(11)	0.34418(7)	0.54547(8)	0.0292(4)
F30	0.61147(11)	0.53448(8)	0.18058(9)	0.0305(4)
F3	0.42056(11)	0.44061(9)	0.49782(10)	0.0359(5)
F2	0.55332(12)	0.46833(8)	0.56787(9)	0.0324(4)
F4	0.41533(10)	0.38720(8)	0.39047(9)	0.0325(4)
F18	0.47283(12)	0.68805(8)	0.28335(10)	0.0376(5)
F13	0.67515(13)	0.24643(8)	0.21917(9)	0.0391(5)
F20	0.66755(12)	0.62498(8)	0.19991(9)	0.0344(5)
F9	0.94817(11)	0.32733(9)	0.50787(10)	0.0401(5)
F12	0.62041(12)	0.22652(7)	0.32450(9)	0.0347(4)
F19	0.54969(14)	0.68370(8)	0.18914(10)	0.0414(5)
F14	0.74397(12)	0.33514(8)	0.21088(9)	0.0356(5)
F26	0.85654(12)	0.50552(9)	0.28992(10)	0.0390(5)
F21	0.76502(11)	0.61467(8)	0.41954(10)	0.0354(5)
F7	0.77194(13)	0.30209(8)	0.63118(9)	0.0394(5)
F29	0.63124(14)	0.47053(9)	0.09345(10)	0.0440(5)
O2	0.34785(11)	0.46795(8)	0.23393(10)	0.0237(4)
F25	0.82797(14)	0.59860(9)	0.22002(11)	0.0453(6)
F8	0.91295(13)	0.29462(10)	0.61629(10)	0.0470(6)
O1	0.09747(13)	0.44625(9)	0.08818(11)	0.0291(5)
F27	0.87325(15)	0.43974(10)	0.20260(12)	0.0488(6)
F28	0.76079(17)	0.42061(9)	0.10392(10)	0.0514(6)
F22	0.85789(14)	0.69037(10)	0.44552(13)	0.0551(7)
O3	0.38843(13)	0.41364(9)	0.17539(11)	0.0290(5)
N2	0.25267(14)	0.51887(9)	0.07182(11)	0.0203(5)
N4	0.39870(14)	0.44408(9)	0.21775(12)	0.0213(5)
N1	0.17311(14)	0.54903(9)	0.12041(12)	0.0208(5)
N3	0.22486(15)	0.39040(10)	0.23710(12)	0.0239(5)

	x/a	y/b	z/c	U(eq)
F23	0.93210(17)	0.72397(13)	0.35883(19)	0.0793(11)
N6	0.73372(13)	0.51639(9)	0.35656(11)	0.0207(5)
N5	0.72161(14)	0.44531(9)	0.40554(11)	0.0202(5)
F24	0.91445(18)	0.67599(13)	0.24532(17)	0.0756(10)
C1	0.22141(16)	0.51110(11)	0.12206(13)	0.0194(5)
C41	0.61468(16)	0.46891(11)	0.31971(13)	0.0189(5)
C38	0.47375(16)	0.45349(11)	0.25254(13)	0.0197(5)
C64	0.54487(17)	0.38773(11)	0.40788(13)	0.0215(6)
C53	0.69085(16)	0.35276(11)	0.36213(13)	0.0208(5)
C39	0.48298(16)	0.48018(11)	0.30804(13)	0.0206(5)
C42	0.60276(16)	0.44283(11)	0.26292(13)	0.0204(5)
C59	0.61418(16)	0.40130(11)	0.44065(13)	0.0203(5)
C43	0.53179(16)	0.43482(11)	0.22880(13)	0.0205(5)
C17	0.38523(18)	0.51948(12)	0.08228(14)	0.0256(6)
C16	0.31872(17)	0.49443(12)	0.06177(13)	0.0229(6)
C54	0.65897(17)	0.30612(12)	0.36441(13)	0.0228(6)
C65	0.65263(17)	0.59220(11)	0.29752(14)	0.0226(6)
C58	0.72195(17)	0.35917(11)	0.30993(14)	0.0227(6)
C44	0.69006(15)	0.47657(11)	0.35893(13)	0.0191(5)
C28	0.13294(17)	0.43117(11)	0.13689(14)	0.0234(6)
C4	0.13113(18)	0.55878(12)	0.16833(15)	0.0245(6)
C2	0.17368(17)	0.57981(12)	0.06937(14)	0.0241(6)
C60	0.61291(17)	0.42980(11)	0.49409(13)	0.0224(6)
C40	0.55427(16)	0.48706(11)	0.34189(13)	0.0207(5)
C66	0.61357(17)	0.59825(11)	0.34506(14)	0.0221(6)
C3	0.22301(18)	0.56111(12)	0.03891(14)	0.0244(6)
C63	0.48033(17)	0.39996(12)	0.42623(14)	0.0250(6)
C25	0.39015(18)	0.57141(12)	0.11140(15)	0.0280(6)
C67	0.55413(17)	0.62975(11)	0.34112(14)	0.0236(6)
C71	0.79289(18)	0.60015(13)	0.31989(16)	0.0282(6)
C20	0.37999(19)	0.42584(13)	0.02539(16)	0.0304(7)
C48	0.73860(18)	0.34359(12)	0.53350(14)	0.0251(6)
C21	0.31419(18)	0.44786(12)	0.03249(14)	0.0240(6)
C47	0.75391(17)	0.36441(11)	0.47913(13)	0.0223(6)
C62	0.48265(18)	0.42733(13)	0.48039(15)	0.0269(6)
C18	0.44944(19)	0.49572(14)	0.07426(15)	0.0305(7)
C55	0.65291(18)	0.27008(12)	0.31813(15)	0.0259(6)

	x/a	y/b	z/c	U(eq)
C26	0.4309(2)	0.57166(14)	0.17995(16)	0.0328(7)
C22	0.24177(18)	0.42141(12)	0.00768(14)	0.0255(6)
C29	0.10585(19)	0.38925(14)	0.17194(16)	0.0328(7)
C5	0.17029(19)	0.57286(12)	0.22828(14)	0.0268(6)
C46	0.79452(17)	0.51033(12)	0.40423(15)	0.0263(6)
C51	0.87977(18)	0.33310(14)	0.51705(16)	0.0312(7)
C68	0.53173(18)	0.65857(12)	0.28847(16)	0.0275(6)
C81	0.67903(19)	0.51385(12)	0.18824(15)	0.0272(6)
C24	0.2304(2)	0.41384(14)	0.93653(15)	0.0317(7)
C70	0.62973(18)	0.62399(12)	0.24678(14)	0.0259(6)
C80	0.6874(2)	0.47978(14)	0.14198(15)	0.0330(7)
C57	0.71563(18)	0.32476(13)	0.26171(14)	0.0273(6)
C77	0.7988(2)	0.49828(14)	0.24194(16)	0.0314(7)
C61	0.55003(19)	0.44187(12)	0.51474(14)	0.0257(6)
C52	0.82616(17)	0.35634(12)	0.47246(14)	0.0254(6)
C56	0.6811(2)	0.27983(13)	0.26564(14)	0.0292(7)
C19	0.44689(19)	0.44934(13)	0.04612(16)	0.0313(7)
C45	0.78690(17)	0.46748(12)	0.43442(14)	0.0248(6)
C37	0.2727(2)	0.37259(13)	0.28526(15)	0.0309(7)
C69	0.5707(2)	0.65581(12)	0.24090(15)	0.0285(7)
C82	0.73337(18)	0.52420(12)	0.24032(14)	0.0263(6)
C13	0.25225(19)	0.58304(12)	0.24161(15)	0.0282(7)
C49	0.7909(2)	0.32048(13)	0.57965(15)	0.0303(7)
C34	0.15589(19)	0.36936(13)	0.22344(15)	0.0308(7)
C9	0.05423(19)	0.55621(13)	0.15228(17)	0.0297(7)
C94	0.8239(2)	0.18910(16)	0.56331(19)	0.0434(9)
C8	0.0161(2)	0.56632(15)	0.20031(19)	0.0385(8)
C6	0.1285(2)	0.58186(15)	0.27382(17)	0.0370(8)
C72	0.80356(18)	0.62682(13)	0.37566(18)	0.0322(7)
C76	0.8331(2)	0.61873(15)	0.27732(19)	0.0379(8)
C79	0.7530(2)	0.45446(14)	0.14716(16)	0.0364(8)
C50	0.8617(2)	0.31560(14)	0.57170(16)	0.0337(8)
C23	0.2380(2)	0.37159(13)	0.04121(16)	0.0317(7)
C119	0.0255(2)	0.70764(17)	0.17162(19)	0.0413(9)
C83	0.4112(2)	0.25585(15)	0.45399(17)	0.0356(8)
C78	0.8095(2)	0.46389(15)	0.19714(17)	0.0354(8)
C10	0.0115(2)	0.54624(13)	0.08623(18)	0.0337(7)

	x/a	y/b	z/c	U(eq)
C88	0.3950(3)	0.29597(15)	0.48863(18)	0.0420(9)
C73	0.8506(2)	0.66697(16)	0.3899(2)	0.0429(9)
C7	0.0528(2)	0.57818(17)	0.25986(19)	0.0447(10)
B2	0.69397(18)	0.39091(12)	0.42135(14)	0.0194(6)
C114	0.0813(2)	0.71309(16)	0.22318(18)	0.0397(8)
B1	0.7267(2)	0.55793(14)	0.30274(16)	0.0239(7)
C14	0.2913(3)	0.57261(18)	0.30917(18)	0.0469(10)
C36	0.2554(2)	0.33363(16)	0.32326(17)	0.0409(9)
C27	0.4256(3)	0.60797(15)	0.0730(2)	0.0463(10)
C84	0.3546(2)	0.22367(14)	0.42820(18)	0.0368(8)
C74	0.8886(2)	0.68377(18)	0.3463(3)	0.0537(12)
C85	0.2844(2)	0.23132(18)	0.4374(2)	0.0465(10)
C30	0.0360(2)	0.37049(19)	0.1564(2)	0.0523(12)
C33	0.1344(2)	0.33056(16)	0.25912(19)	0.0437(10)
C15	0.2656(2)	0.63670(14)	0.2238(2)	0.0409(9)
C95	0.7540(3)	0.19677(15)	0.52760(19)	0.0429(9)
C87	0.3242(3)	0.3036(2)	0.4973(2)	0.0583(13)
C93	0.8860(3)	0.19453(17)	0.5376(2)	0.0536(11)
C75	0.8794(2)	0.65978(18)	0.2900(2)	0.0515(11)
C90	0.7481(3)	0.20911(15)	0.4645(2)	0.0543(13)
C118	0.0066(2)	0.7465(2)	0.1289(2)	0.0486(10)
C115	0.1201(2)	0.75708(17)	0.2344(2)	0.0418(9)
C35	0.1875(3)	0.31286(17)	0.31060(19)	0.0481(11)
C12	0.9801(2)	0.59555(15)	0.05646(18)	0.0383(8)
C92	0.8773(4)	0.20761(16)	0.4749(3)	0.0609(14)
C117	0.0469(2)	0.7905(2)	0.1401(2)	0.0567(13)
C11	0.9492(2)	0.50851(16)	0.0838(3)	0.0496(11)
C86	0.2691(3)	0.2710(2)	0.4719(2)	0.0596(14)
C116	0.1028(2)	0.79590(18)	0.1924(2)	0.0497(11)
C96	0.6870(3)	0.1934(2)	0.5562(2)	0.0591(13)
C91	0.8088(4)	0.21490(16)	0.4388(2)	0.0618(15)
C32	0.0617(3)	0.3127(2)	0.2422(2)	0.0636(15)
C89	0.4871(3)	0.2482(3)	0.4439(3)	0.0664(16)
C31	0.0138(3)	0.3321(2)	0.1923(3)	0.0708(18)
C112	0.6135(5)	0.7786(3)	0.3737(4)	0.103(2)
C100	0.8617(5)	0.5452(2)	0.6581(3)	0.092(2)
C120	0.9439(3)	0.7416(3)	0.0733(2)	0.0718(17)

	x/a	y/b	z/c	U(eq)
C111	0.5497(6)	0.7958(3)	0.3379(3)	0.109(2)
C113	0.4838(5)	0.8094(3)	0.3689(4)	0.111(2)
C106	0.7561(4)	0.5568(3)	0.5833(5)	0.127(4)
C103	0.9371(7)	0.6007(4)	0.5931(4)	0.142(4)
C110	0.5451(6)	0.7984(3)	0.2761(4)	0.127(3)
C105	0.8305(5)	0.5656(3)	0.6051(3)	0.0857(18)
C104	0.8631(6)	0.5964(3)	0.5678(4)	0.108(3)
C109	0.6099(7)	0.7831(4)	0.2469(4)	0.139(4)
C101	0.9469(5)	0.5534(3)	0.6890(5)	0.100(2)
C107	0.6817(6)	0.7634(3)	0.3464(4)	0.134(3)
C108	0.6695(6)	0.7684(3)	0.2919(4)	0.142(3)
C102	0.9804(7)	0.5801(4)	0.6459(5)	0.133(3)

Table 4. Bond lengths (Å) for 5886.

Pd1-C28	1.964(3)	Pd1-C1	2.019(3)
Pd1-N3	2.087(3)	Pd1-O2	2.278(2)
F16-C66	1.352(3)	F11-C54	1.353(3)
F5-C64	1.351(3)	F1-C60	1.351(4)
F15-C58	1.353(4)	F17-C67	1.345(3)
F10-C52	1.353(4)	F6-C48	1.347(4)
F30-C81	1.353(4)	F3-C62	1.336(4)
F2-C61	1.349(3)	F4-C63	1.341(4)
F18-C68	1.339(4)	F13-C56	1.340(4)
F20-C70	1.354(4)	F9-C51	1.337(4)
F12-C55	1.338(4)	F19-C69	1.343(4)
F14-C57	1.350(4)	F26-C77	1.350(4)
F21-C72	1.347(4)	F7-C49	1.338(4)
F29-C80	1.348(4)	O2-N4	1.252(3)
F25-C76	1.346(5)	F8-C50	1.337(4)
O1-C28	1.199(4)	F27-C78	1.337(4)
F28-C79	1.339(4)	F22-C73	1.348(5)
O3-N4	1.219(3)	N2-C1	1.357(4)
N2-C3	1.395(4)	N2-C16	1.449(4)
N4-C38	1.467(4)	N1-C1	1.355(4)
N1-C2	1.388(4)	N1-C4	1.450(4)
N3-C37	1.318(4)	N3-C34	1.378(4)

F23-C74	1.345(5)	N6-C44	1.351(4)
N6-C46	1.379(4)	N6-B1	1.605(4)
N5-C44	1.355(4)	N5-C45	1.383(4)
N5-B2	1.611(4)	F24-C75	1.350(5)
C41-C40	1.399(4)	C41-C42	1.399(4)
C41-C44	1.499(4)	C38-C43	1.384(4)
C38-C39	1.386(4)	C64-C63	1.381(4)
C64-C59	1.388(4)	C53-C58	1.388(4)
C53-C54	1.393(4)	C53-B2	1.640(4)
C39-C40	1.391(4)	C39-H39	0.95
C42-C43	1.392(4)	C42-H42	0.95
C59-C60	1.398(4)	C59-B2	1.648(4)
C43-H43	0.95	C17-C18	1.397(5)
C17-C16	1.399(4)	C17-C25	1.529(5)
C16-C21	1.400(4)	C54-C55	1.386(4)
C65-C66	1.391(4)	C65-C70	1.393(4)
C65-B1	1.643(5)	C58-C57	1.386(4)
C28-C29	1.505(4)	C4-C9	1.403(5)
C4-C5	1.410(4)	C2-C3	1.336(5)
C2-H2	0.95	C60-C61	1.376(4)
C40-H40	0.95	C66-C67	1.382(4)
C3-H3	0.95	C63-C62	1.383(5)
C25-C27	1.525(5)	C25-C26	1.529(5)
C25-H25	1.0	C67-C68	1.376(5)
C71-C72	1.389(5)	C71-C76	1.398(5)
C71-B1	1.660(5)	C20-C19	1.386(5)
C20-C21	1.397(5)	C20-H20	0.95
C48-C47	1.391(4)	C48-C49	1.393(4)
C21-C22	1.521(4)	C47-C52	1.398(4)
C47-B2	1.661(4)	C62-C61	1.378(5)
C18-C19	1.386(5)	C18-H18	0.95
C55-C56	1.377(5)	C26-H26A	0.98
C26-H26B	0.98	C26-H26C	0.98
C22-C24	1.534(4)	C22-C23	1.534(5)
C22-H22	1.0	C29-C30	1.370(5)
C29-C34	1.408(5)	C5-C6	1.401(5)
C5-C13	1.517(5)	C46-C45	1.349(5)
C46-H46	0.95	C51-C50	1.384(5)

C51-C52	1.389(4)	C68-C69	1.383(5)
C81-C82	1.384(5)	C81-C80	1.394(5)
C24-H24A	0.98	C24-H24B	0.98
C24-H24C	0.98	C70-C69	1.378(5)
C80-C79	1.381(6)	C57-C56	1.379(5)
C77-C78	1.388(5)	C77-C82	1.397(5)
C19-H19	0.95	C45-H45	0.95
C37-C36	1.413(5)	C37-H37	0.95
C82-B1	1.660(5)	C13-C14	1.527(5)
C13-C15	1.527(5)	C13-H13	1.0
C49-C50	1.371(5)	C34-C33	1.407(5)
C9-C8	1.405(5)	C9-C10	1.518(5)
C94-C95	1.386(6)	C94-C93	1.391(7)
C94-H94	0.95	C8-C7	1.373(6)
C8-H8	0.95	C6-C7	1.381(6)
C6-H6	0.95	C72-C73	1.384(5)
C76-C75	1.392(6)	C79-C78	1.372(6)
C23-H23A	0.98	C23-H23B	0.98
C23-H23C	0.98	C119-C114	1.371(6)
C119-C118	1.395(6)	C119-H119	0.95
C83-C88	1.385(5)	C83-C84	1.390(5)
C83-C89	1.488(6)	C10-C11	1.532(5)
C10-C12	1.537(5)	C10-H10	1.0
C88-C87	1.383(7)	C88-H88	0.95
C73-C74	1.371(6)	C7-H7	0.95
C114-C115	1.381(6)	C114-H114	0.95
C14-H14A	0.98	C14-H14B	0.98
C14-H14C	0.98	C36-C35	1.357(6)
C36-H36	0.95	C27-H27A	0.98
C27-H27B	0.98	C27-H27C	0.98
C84-C85	1.375(6)	C84-H84	0.95
C74-C75	1.365(7)	C85-C86	1.370(8)
C85-H85	0.95	C30-C31	1.406(6)
C30-H30	0.95	C33-C32	1.410(6)
C33-C35	1.416(5)	C15-H15A	0.98
C15-H15B	0.98	C15-H15C	0.98
C95-C90	1.396(6)	C95-C96	1.507(7)
C87-C86	1.374(8)	C87-H87	0.95

C93-C92	1.387(7)	C93-H93	0.95
C90-C91	1.369(8)	C90-H90	0.95
C118-C117	1.394(7)	C118-C120	1.505(6)
C115-C116	1.381(6)	C115-H115	0.95
C35-H35	0.95	C12-H12A	0.98
C12-H12B	0.98	C12-H12C	0.98
C92-C91	1.367(8)	C92-H92	0.95
C117-C116	1.382(7)	C117-H117	0.95
C11-H11A	0.98	C11-H11B	0.98
C11-H11C	0.98	C86-H86	0.95
C116-H116	0.95	C96-H96A	0.98
C96-H96B	0.98	C96-H96C	0.98
C91-H91	0.95	C32-C31	1.361(7)
C32-H32	0.95	C89-H89A	0.98
C89-H89B	0.98	C89-H89C	0.98
C31-H31	0.95	C112-C111	1.361(12)
C112-C107	1.563(12)	C112-H112	0.95
C100-C105	1.304(9)	C100-C101	1.604(13)
C100-H100	0.95	C120-H12D	0.98
C120-H12E	0.98	C120-H12F	0.98
C111-C110	1.332(9)	C111-C113	1.560(13)
C113-H11D	0.98	C113-H11E	0.98
C113-H11F	0.98	C106-C105	1.387(10)
C106-H10A	0.98	C106-H10B	0.98
C106-H10C	0.98	C103-C102	1.377(13)
C103-C104	1.380(14)	C103-H103	0.95
C110-C109	1.532(15)	C110-H110	0.95
C105-C104	1.383(10)	C104-H104	0.95
C109-C108	1.379(12)	C109-H109	0.95
C101-C102	1.425(13)	C101-H101	0.95
C107-C108	1.170(11)	C107-H107	0.95
C108-H108	0.95	C102-H102	0.95

Table 5. Bond angles (°) for 5886.

C28-Pd1-C1	87.97(12)	C28-Pd1-N3	84.01(12)
C1-Pd1-N3	170.95(11)	C28-Pd1-O2	174.51(11)
C1-Pd1-O2	97.45(10)	N3-Pd1-O2	90.66(9)

N4-O2-Pd1	116.35(18)	C1-N2-C3	110.5(3)
C1-N2-C16	124.7(2)	C3-N2-C16	123.4(2)
O3-N4-O2	123.2(3)	O3-N4-C38	119.4(2)
O2-N4-C38	117.4(2)	C1-N1-C2	110.9(3)
C1-N1-C4	124.7(2)	C2-N1-C4	124.2(3)
C37-N3-C34	118.0(3)	C37-N3-Pd1	130.4(2)
C34-N3-Pd1	111.4(2)	C44-N6-C46	106.5(3)
C44-N6-B1	128.3(2)	C46-N6-B1	124.2(3)
C44-N5-C45	106.1(3)	C44-N5-B2	128.0(2)
C45-N5-B2	125.7(2)	N1-C1-N2	104.7(2)
N1-C1-Pd1	126.4(2)	N2-C1-Pd1	128.3(2)
C40-C41-C42	119.2(3)	C40-C41-C44	118.6(2)
C42-C41-C44	122.2(3)	C43-C38-C39	123.2(3)
C43-C38-N4	118.5(3)	C39-C38-N4	118.3(3)
F5-C64-C63	114.7(3)	F5-C64-C59	121.2(3)
C63-C64-C59	124.0(3)	C58-C53-C54	113.2(3)
C58-C53-B2	127.8(3)	C54-C53-B2	118.8(3)
C38-C39-C40	117.7(3)	C38-C39-H39	121.1
C40-C39-H39	121.1	C43-C42-C41	120.6(3)
C43-C42-H42	119.7	C41-C42-H42	119.7
C64-C59-C60	113.5(3)	C64-C59-B2	127.9(2)
C60-C59-B2	118.4(3)	C38-C43-C42	118.2(3)
C38-C43-H43	120.9	C42-C43-H43	120.9
C18-C17-C16	117.6(3)	C18-C17-C25	119.3(3)
C16-C17-C25	123.1(3)	C17-C16-C21	122.9(3)
C17-C16-N2	117.1(3)	C21-C16-N2	120.1(3)
F11-C54-C55	116.1(3)	F11-C54-C53	118.7(3)
C55-C54-C53	125.1(3)	C66-C65-C70	113.4(3)
C66-C65-B1	125.0(3)	C70-C65-B1	121.0(3)
F15-C58-C57	115.0(3)	F15-C58-C53	121.4(3)
C57-C58-C53	123.5(3)	N6-C44-N5	110.4(2)
N6-C44-C41	125.9(3)	N5-C44-C41	123.5(3)
O1-C28-C29	121.4(3)	O1-C28-Pd1	128.1(2)
C29-C28-Pd1	110.3(2)	C9-C4-C5	123.4(3)
C9-C4-N1	119.0(3)	C5-C4-N1	117.6(3)
C3-C2-N1	107.0(3)	C3-C2-H2	126.5
N1-C2-H2	126.5	F1-C60-C61	116.4(3)
F1-C60-C59	119.4(3)	C61-C60-C59	124.2(3)

C39-C40-C41	121.1(3)	C39-C40-H40	119.4
C41-C40-H40	119.4	F16-C66-C67	115.1(3)
F16-C66-C65	120.8(3)	C67-C66-C65	124.0(3)
C2-C3-N2	106.9(3)	C2-C3-H3	126.5
N2-C3-H3	126.5	F4-C63-C64	120.3(3)
F4-C63-C62	119.8(3)	C64-C63-C62	119.8(3)
C27-C25-C17	110.9(3)	C27-C25-C26	110.4(3)
C17-C25-C26	112.6(3)	C27-C25-H25	107.6
C17-C25-H25	107.6	C26-C25-H25	107.6
F17-C67-C68	119.6(3)	F17-C67-C66	120.5(3)
C68-C67-C66	119.9(3)	C72-C71-C76	113.3(3)
C72-C71-B1	121.1(3)	C76-C71-B1	124.6(3)
C19-C20-C21	121.3(3)	C19-C20-H20	119.4
C21-C20-H20	119.4	F6-C48-C47	121.7(3)
F6-C48-C49	114.3(3)	C47-C48-C49	124.0(3)
C20-C21-C16	117.2(3)	C20-C21-C22	119.7(3)
C16-C21-C22	123.1(3)	C48-C47-C52	113.3(3)
C48-C47-B2	126.5(3)	C52-C47-B2	119.9(3)
F3-C62-C61	120.9(3)	F3-C62-C63	120.5(3)
C61-C62-C63	118.6(3)	C19-C18-C17	121.0(3)
C19-C18-H18	119.5	C17-C18-H18	119.5
F12-C55-C56	120.6(3)	F12-C55-C54	120.5(3)
C56-C55-C54	118.8(3)	C25-C26-H26A	109.5
C25-C26-H26B	109.5	H26A-C26-H26B	109.5
C25-C26-H26C	109.5	H26A-C26-H26C	109.5
H26B-C26-H26C	109.5	C21-C22-C24	110.4(3)
C21-C22-C23	111.3(3)	C24-C22-C23	110.8(3)
C21-C22-H22	108.1	C24-C22-H22	108.1
C23-C22-H22	108.1	C30-C29-C34	119.7(3)
C30-C29-C28	123.4(3)	C34-C29-C28	116.9(3)
C6-C5-C4	116.5(3)	C6-C5-C13	121.0(3)
C4-C5-C13	122.2(3)	C45-C46-N6	108.4(3)
C45-C46-H46	125.8	N6-C46-H46	125.8
F9-C51-C50	119.7(3)	F9-C51-C52	121.1(3)
C50-C51-C52	119.2(3)	F18-C68-C67	120.4(3)
F18-C68-C69	121.0(3)	C67-C68-C69	118.6(3)
F30-C81-C82	121.5(3)	F30-C81-C80	114.8(3)
C82-C81-C80	123.6(3)	C22-C24-H24A	109.5

C22-C24-H24B	109.5	H24A-C24-H24B	109.5
C22-C24-H24C	109.5	H24A-C24-H24C	109.5
H24B-C24-H24C	109.5	F20-C70-C69	116.5(3)
F20-C70-C65	119.3(3)	C69-C70-C65	124.2(3)
F29-C80-C79	120.2(3)	F29-C80-C81	120.2(3)
C79-C80-C81	119.5(3)	F14-C57-C56	119.8(3)
F14-C57-C58	119.8(3)	C56-C57-C58	120.4(3)
F26-C77-C78	115.8(3)	F26-C77-C82	119.9(3)
C78-C77-C82	124.3(3)	F2-C61-C60	120.9(3)
F2-C61-C62	119.4(3)	C60-C61-C62	119.7(3)
F10-C52-C51	115.8(3)	F10-C52-C47	119.9(3)
C51-C52-C47	124.4(3)	F13-C56-C55	120.8(3)
F13-C56-C57	120.5(3)	C55-C56-C57	118.7(3)
C18-C19-C20	120.1(3)	C18-C19-H19	120.0
C20-C19-H19	120.0	C46-C45-N5	108.5(3)
C46-C45-H45	125.8	N5-C45-H45	125.8
N3-C37-C36	122.6(3)	N3-C37-H37	118.7
C36-C37-H37	118.7	F19-C69-C70	120.9(3)
F19-C69-C68	119.5(3)	C70-C69-C68	119.6(3)
C81-C82-C77	114.0(3)	C81-C82-B1	128.1(3)
C77-C82-B1	117.6(3)	C5-C13-C14	114.3(3)
C5-C13-C15	109.4(3)	C14-C13-C15	110.4(3)
C5-C13-H13	107.5	C14-C13-H13	107.5
C15-C13-H13	107.5	F7-C49-C50	119.7(3)
F7-C49-C48	120.4(3)	C50-C49-C48	119.9(3)
N3-C34-C33	122.9(3)	N3-C34-C29	116.7(3)
C33-C34-C29	120.3(3)	C4-C9-C8	116.7(3)
C4-C9-C10	123.6(3)	C8-C9-C10	119.5(3)
C95-C94-C93	121.3(4)	C95-C94-H94	119.3
C93-C94-H94	119.3	C7-C8-C9	121.3(4)
C7-C8-H8	119.4	C9-C8-H8	119.4
C7-C6-C5	121.4(4)	C7-C6-H6	119.3
C5-C6-H6	119.3	F21-C72-C73	115.8(3)
F21-C72-C71	119.6(3)	C73-C72-C71	124.6(3)
F25-C76-C75	115.2(3)	F25-C76-C71	121.7(3)
C75-C76-C71	123.1(4)	F28-C79-C78	120.5(4)
F28-C79-C80	119.9(4)	C78-C79-C80	119.5(3)
F8-C50-C49	120.6(3)	F8-C50-C51	120.3(3)

C49-C50-C51	119.1(3)	C22-C23-H23A	109.5
C22-C23-H23B	109.5	H23A-C23-H23B	109.5
C22-C23-H23C	109.5	H23A-C23-H23C	109.5
H23B-C23-H23C	109.5	C114-C119-C118	120.7(4)
C114-C119-H119	119.7	C118-C119-H119	119.7
C88-C83-C84	118.2(4)	C88-C83-C89	120.5(4)
C84-C83-C89	121.2(4)	F27-C78-C79	120.1(3)
F27-C78-C77	120.9(4)	C79-C78-C77	119.0(3)
C9-C10-C11	113.3(3)	C9-C10-C12	109.1(3)
C11-C10-C12	109.8(3)	C9-C10-H10	108.2
C11-C10-H10	108.2	C12-C10-H10	108.2
C87-C88-C83	120.6(4)	C87-C88-H88	119.7
C83-C88-H88	119.7	F22-C73-C74	119.9(4)
F22-C73-C72	120.5(4)	C74-C73-C72	119.6(4)
C8-C7-C6	120.7(4)	C8-C7-H7	119.6
C6-C7-H7	119.6	N5-B2-C53	111.2(2)
N5-B2-C59	104.1(2)	C53-B2-C59	114.8(2)
N5-B2-C47	110.9(2)	C53-B2-C47	103.7(2)
C59-B2-C47	112.3(2)	C119-C114-C115	121.1(4)
C119-C114-H114	119.5	C115-C114-H114	119.5
N6-B1-C65	112.4(2)	N6-B1-C71	111.5(3)
C65-B1-C71	101.8(3)	N6-B1-C82	102.1(2)
C65-B1-C82	116.9(3)	C71-B1-C82	112.4(3)
C13-C14-H14A	109.5	C13-C14-H14B	109.5
H14A-C14-H14B	109.5	C13-C14-H14C	109.5
H14A-C14-H14C	109.5	H14B-C14-H14C	109.5
C35-C36-C37	120.1(3)	C35-C36-H36	120.0
C37-C36-H36	120.0	C25-C27-H27A	109.5
C25-C27-H27B	109.5	H27A-C27-H27B	109.5
C25-C27-H27C	109.5	H27A-C27-H27C	109.5
H27B-C27-H27C	109.5	C85-C84-C83	120.8(4)
C85-C84-H84	119.6	C83-C84-H84	119.6
F23-C74-C75	121.4(4)	F23-C74-C73	119.9(4)
C75-C74-C73	118.6(4)	C86-C85-C84	120.5(4)
C86-C85-H85	119.8	C84-C85-H85	119.8
C29-C30-C31	120.4(4)	C29-C30-H30	119.8
C31-C30-H30	119.8	C34-C33-C32	118.4(4)
C34-C33-C35	117.1(4)	C32-C33-C35	124.6(4)

C13-C15-H15A	109.5	C13-C15-H15B	109.5
H15A-C15-H15B	109.5	C13-C15-H15C	109.5
H15A-C15-H15C	109.5	H15B-C15-H15C	109.5
C94-C95-C90	117.6(5)	C94-C95-C96	121.3(4)
C90-C95-C96	121.1(4)	C86-C87-C88	120.2(4)
C86-C87-H87	119.9	C88-C87-H87	119.9
C92-C93-C94	119.0(5)	C92-C93-H93	120.5
C94-C93-H93	120.5	F24-C75-C74	120.3(4)
F24-C75-C76	118.9(4)	C74-C75-C76	120.7(4)
C91-C90-C95	121.6(5)	C91-C90-H90	119.2
C95-C90-H90	119.2	C117-C118-C119	117.8(4)
C117-C118-C120	121.0(5)	C119-C118-C120	121.2(5)
C116-C115-C114	119.2(4)	C116-C115-H115	120.4
C114-C115-H115	120.4	C36-C35-C33	119.5(4)
C36-C35-H35	120.3	C33-C35-H35	120.3
C10-C12-H12A	109.5	C10-C12-H12B	109.5
H12A-C12-H12B	109.5	C10-C12-H12C	109.5
H12A-C12-H12C	109.5	H12B-C12-H12C	109.5
C91-C92-C93	120.6(5)	C91-C92-H92	119.7
C93-C92-H92	119.7	C116-C117-C118	121.3(4)
C116-C117-H117	119.3	C118-C117-H117	119.3
C10-C11-H11A	109.5	C10-C11-H11B	109.5
H11A-C11-H11B	109.5	C10-C11-H11C	109.5
H11A-C11-H11C	109.5	H11B-C11-H11C	109.5
C85-C86-C87	119.6(4)	C85-C86-H86	120.2
C87-C86-H86	120.2	C115-C116-C117	119.9(4)
C115-C116-H116	120.0	C117-C116-H116	120.0
C95-C96-H96A	109.5	C95-C96-H96B	109.5
H96A-C96-H96B	109.5	C95-C96-H96C	109.5
H96A-C96-H96C	109.5	H96B-C96-H96C	109.5
C92-C91-C90	119.9(4)	C92-C91-H91	120.0
C90-C91-H91	120.0	C31-C32-C33	120.9(4)
C31-C32-H32	119.6	C33-C32-H32	119.6
C83-C89-H89A	109.5	C83-C89-H89B	109.5
H89A-C89-H89B	109.5	C83-C89-H89C	109.5
H89A-C89-H89C	109.5	H89B-C89-H89C	109.5
C32-C31-C30	120.4(4)	C32-C31-H31	119.8
C30-C31-H31	119.8	C111-C112-C107	123.5(8)

C111-C112-H112	118.3	C107-C112-H112	118.3
C105-C100-C101	122.4(8)	C105-C100-H100	118.8
C101-C100-H100	118.8	C118-C120-H12D	109.5
C118-C120-H12E	109.5	H12D-C120-H12E	109.5
C118-C120-H12F	109.5	H12D-C120-H12F	109.5
H12E-C120-H12F	109.5	C110-C111-C112	117.7(11)
C110-C111-C113	122.1(10)	C112-C111-C113	120.1(7)
C111-C113-H11D	109.5	C111-C113-H11E	109.5
H11D-C113-H11E	109.5	C111-C113-H11F	109.5
H11D-C113-H11F	109.5	H11E-C113-H11F	109.5
C105-C106-H10A	109.5	C105-C106-H10B	109.5
H10A-C106-H10B	109.5	C105-C106-H10C	109.5
H10A-C106-H10C	109.5	H10B-C106-H10C	109.5
C102-C103-C104	131.6(11)	C102-C103-H103	114.2
C104-C103-H103	114.2	C111-C110-C109	120.9(10)
C111-C110-H110	119.6	C109-C110-H110	119.6
C100-C105-C104	127.1(9)	C100-C105-C106	117.5(9)
C104-C105-C106	115.4(9)	C103-C104-C105	109.8(9)
C103-C104-H104	125.1	C105-C104-H104	125.1
C108-C109-C110	111.6(9)	C108-C109-H109	124.2
C110-C109-H109	124.2	C102-C101-C100	108.8(8)
C102-C101-H101	125.6	C100-C101-H101	125.6
C108-C107-C112	110.7(11)	C108-C107-H107	124.6
C112-C107-H107	124.6	C107-C108-C109	135.6(13)
C107-C108-H108	112.2	C109-C108-H108	112.2
C103-C102-C101	119.5(12)	C103-C102-H102	120.2
C101-C102-H102	120.2		

Table 6. Anisotropic atomic displacement parameters (Å^2) for 5886.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pd1	0.02078(12)	0.01816(12)	0.01562(11)	-0.00011(7)	0.00240(8)	-0.00124(8)
F16	0.0300(9)	0.0268(9)	0.0178(8)	0.0019(7)	0.0074(7)	0.0018(7)
F11	0.0353(10)	0.0249(9)	0.0221(8)	-0.0014(7)	0.0092(7)	-0.0008(8)
F5	0.0254(9)	0.0318(9)	0.0169(8)	-0.0038(7)	0.0017(7)	-0.0004(7)
F1	0.0287(9)	0.0291(9)	0.0196(8)	-0.0065(7)	0.0021(7)	0.0026(7)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F15	0.0287(9)	0.0271(9)	0.0247(9)	-0.0011(7)	0.0115(7)	0.0023(7)
F17	0.0295(9)	0.0353(10)	0.0285(9)	-0.0025(8)	0.0110(8)	0.0041(8)
F10	0.0262(9)	0.0375(10)	0.0243(9)	-0.0012(8)	0.0076(7)	0.0075(8)
F6	0.0328(10)	0.0336(10)	0.0219(9)	0.0053(7)	0.0073(7)	0.0079(8)
F30	0.0336(10)	0.0339(10)	0.0244(9)	-0.0011(8)	0.0066(8)	-0.0027(8)
F3	0.0303(10)	0.0499(13)	0.0327(10)	0.0069(9)	0.0187(8)	0.0117(9)
F2	0.0429(11)	0.0350(10)	0.0217(9)	-0.0047(8)	0.0125(8)	0.0115(9)
F4	0.0209(9)	0.0472(12)	0.0285(9)	0.0050(9)	0.0028(7)	-0.0011(8)
F18	0.0355(11)	0.0327(11)	0.0411(11)	-0.0009(9)	0.0000(9)	0.0111(9)
F13	0.0602(14)	0.0336(11)	0.0219(9)	-0.0123(8)	0.0043(9)	0.0057(10)
F20	0.0492(12)	0.0323(10)	0.0264(9)	0.0058(8)	0.0186(9)	-0.0033(9)
F9	0.0267(10)	0.0542(14)	0.0376(11)	-0.0032(10)	0.0025(8)	0.0159(9)
F12	0.0468(12)	0.0242(9)	0.0307(10)	-0.0069(8)	0.0022(9)	-0.0050(9)
F19	0.0623(15)	0.0313(11)	0.0286(10)	0.0099(9)	0.0048(10)	0.0070(10)
F14	0.0506(12)	0.0393(11)	0.0204(9)	-0.0016(8)	0.0156(8)	0.0096(10)
F26	0.0336(11)	0.0471(13)	0.0383(11)	-0.0056(10)	0.0118(9)	0.0075(9)
F21	0.0360(11)	0.0386(11)	0.0342(10)	-0.0134(9)	0.0135(9)	-0.0092(9)
F7	0.0550(13)	0.0417(12)	0.0213(9)	0.0097(8)	0.0075(9)	0.0165(10)
F29	0.0609(15)	0.0473(13)	0.0232(10)	-0.0072(9)	0.0075(10)	-0.0057(11)
O2	0.0201(10)	0.0264(11)	0.0241(10)	-0.0021(9)	0.0034(8)	-0.0004(8)
F25	0.0518(14)	0.0479(13)	0.0457(13)	-0.0044(10)	0.0321(11)	-0.0129(11)
F8	0.0464(13)	0.0575(15)	0.0308(11)	0.0055(10)	-0.0065(9)	0.0266(11)
O1	0.0297(12)	0.0266(11)	0.0268(11)	0.0039(9)	-0.0043(9)	-0.0049(9)
F27	0.0572(15)	0.0523(14)	0.0437(13)	-0.0016(11)	0.0267(11)	0.0211(12)
F28	0.0883(19)	0.0436(13)	0.0295(11)	-0.0073(10)	0.0292(12)	0.0102(13)
F22	0.0457(14)	0.0551(15)	0.0647(17)	-0.0305(13)	0.0121(12)	-0.0201(12)
O3	0.0303(12)	0.0292(12)	0.0251(11)	-0.0065(9)	0.0002(9)	-0.0007(9)
N2	0.0254(12)	0.0186(11)	0.0167(11)	-0.0006(9)	0.0034(9)	-0.0015(9)
N4	0.0221(12)	0.0214(12)	0.0197(11)	0.0019(9)	0.0029(9)	-0.0009(9)
N1	0.0237(12)	0.0195(12)	0.0183(11)	-0.0020(9)	0.0026(9)	-0.0001(9)
N3	0.0292(13)	0.0237(12)	0.0181(11)	0.0020(10)	0.0033(10)	-0.0030(10)
F23	0.0561(17)	0.070(2)	0.120(3)	-0.0330(19)	0.0378(18)	-0.0448(16)
N6	0.0207(11)	0.0226(12)	0.0199(11)	-0.0034(9)	0.0067(9)	-0.0013(9)
N5	0.0198(11)	0.0237(12)	0.0164(11)	-0.0034(9)	0.0021(9)	0.0025(9)
F24	0.073(2)	0.074(2)	0.099(2)	-0.0123(18)	0.0612(19)	-0.0391(16)
C1	0.0224(13)	0.0184(13)	0.0164(12)	-0.0017(10)	0.0013(10)	-0.0029(10)
C41	0.0211(13)	0.0187(13)	0.0170(12)	0.0025(10)	0.0042(10)	0.0007(10)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C38	0.0204(13)	0.0205(13)	0.0174(13)	0.0014(10)	0.0021(10)	0.0003(10)
C64	0.0256(14)	0.0227(14)	0.0163(12)	0.0010(11)	0.0047(11)	0.0026(11)
C53	0.0231(13)	0.0232(14)	0.0152(12)	-0.0004(10)	0.0022(10)	0.0051(11)
C39	0.0213(13)	0.0222(14)	0.0188(13)	0.0007(11)	0.0055(10)	0.0031(11)
C42	0.0236(14)	0.0215(13)	0.0180(13)	0.0017(11)	0.0085(11)	0.0033(11)
C59	0.0256(14)	0.0194(13)	0.0163(12)	0.0000(10)	0.0052(10)	0.0038(11)
C43	0.0258(14)	0.0211(13)	0.0150(12)	0.0010(10)	0.0049(10)	-0.0008(11)
C17	0.0296(15)	0.0272(15)	0.0204(13)	-0.0001(12)	0.0062(12)	-0.0048(12)
C16	0.0273(14)	0.0242(14)	0.0179(13)	0.0000(11)	0.0062(11)	0.0004(12)
C54	0.0256(14)	0.0256(14)	0.0166(12)	-0.0011(11)	0.0030(11)	0.0042(12)
C65	0.0244(14)	0.0221(14)	0.0211(13)	-0.0005(11)	0.0042(11)	-0.0032(11)
C58	0.0249(14)	0.0229(14)	0.0201(13)	0.0010(11)	0.0043(11)	0.0056(11)
C44	0.0197(13)	0.0232(14)	0.0149(12)	-0.0035(10)	0.0047(10)	0.0022(11)
C28	0.0255(14)	0.0213(14)	0.0232(14)	-0.0028(11)	0.0044(11)	-0.0033(11)
C4	0.0277(15)	0.0230(14)	0.0238(14)	0.0027(11)	0.0075(12)	0.0036(12)
C2	0.0287(15)	0.0211(14)	0.0206(13)	0.0019(11)	0.0009(11)	-0.0003(12)
C60	0.0268(14)	0.0230(14)	0.0169(12)	0.0011(11)	0.0033(11)	0.0036(11)
C40	0.0232(13)	0.0221(13)	0.0173(12)	-0.0024(10)	0.0050(10)	0.0010(11)
C66	0.0252(14)	0.0217(14)	0.0191(13)	0.0004(11)	0.0034(11)	-0.0020(11)
C3	0.0331(16)	0.0220(14)	0.0172(13)	0.0016(11)	0.0026(11)	-0.0007(12)
C63	0.0246(14)	0.0282(15)	0.0228(14)	0.0073(12)	0.0063(11)	0.0003(12)
C25	0.0292(15)	0.0258(15)	0.0284(15)	-0.0022(12)	0.0043(12)	-0.0050(13)
C67	0.0241(14)	0.0234(14)	0.0239(14)	-0.0051(11)	0.0063(11)	-0.0038(11)
C71	0.0230(14)	0.0280(16)	0.0356(17)	-0.0022(13)	0.0103(13)	-0.0028(12)
C20	0.0342(17)	0.0297(16)	0.0278(15)	-0.0069(13)	0.0075(13)	0.0019(14)
C48	0.0297(15)	0.0241(14)	0.0201(13)	-0.0023(11)	0.0023(11)	0.0059(12)
C21	0.0275(15)	0.0249(15)	0.0196(13)	-0.0013(11)	0.0045(11)	-0.0017(12)
C47	0.0252(14)	0.0222(14)	0.0182(13)	-0.0028(11)	0.0012(11)	0.0047(11)
C62	0.0275(15)	0.0312(16)	0.0248(14)	0.0078(12)	0.0120(12)	0.0075(13)
C18	0.0288(16)	0.0363(18)	0.0271(15)	-0.0031(14)	0.0077(13)	-0.0051(14)
C55	0.0309(15)	0.0220(14)	0.0225(14)	-0.0036(12)	0.0000(12)	0.0025(12)
C26	0.0345(17)	0.0319(17)	0.0309(17)	-0.0026(14)	0.0037(14)	-0.0040(14)
C22	0.0307(15)	0.0222(14)	0.0238(14)	-0.0037(12)	0.0059(12)	-0.0039(12)
C29	0.0315(17)	0.0355(18)	0.0288(16)	0.0069(14)	-0.0001(13)	-0.0120(14)
C5	0.0372(17)	0.0217(14)	0.0213(14)	0.0024(11)	0.0057(12)	0.0071(13)
C46	0.0225(14)	0.0297(16)	0.0258(14)	-0.0065(12)	0.0029(12)	-0.0018(12)
C51	0.0263(15)	0.0358(17)	0.0288(16)	-0.0056(14)	-0.0006(12)	0.0109(13)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C68	0.0283(15)	0.0224(14)	0.0295(15)	-0.0025(12)	0.0005(12)	0.0023(12)
C81	0.0346(16)	0.0282(15)	0.0214(14)	0.0014(12)	0.0121(12)	-0.0013(13)
C24	0.0357(17)	0.0360(18)	0.0221(15)	-0.0029(13)	0.0028(13)	-0.0041(14)
C70	0.0345(16)	0.0224(14)	0.0226(14)	0.0000(11)	0.0099(12)	-0.0035(12)
C80	0.048(2)	0.0344(18)	0.0191(14)	-0.0008(13)	0.0133(14)	-0.0074(15)
C57	0.0328(16)	0.0326(16)	0.0165(13)	-0.0014(12)	0.0053(12)	0.0092(13)
C77	0.0357(17)	0.0343(17)	0.0278(16)	0.0004(14)	0.0149(14)	-0.0001(14)
C61	0.0350(16)	0.0265(15)	0.0172(13)	0.0001(11)	0.0092(12)	0.0086(13)
C52	0.0276(15)	0.0286(15)	0.0193(13)	-0.0044(12)	0.0033(11)	0.0047(12)
C56	0.0389(18)	0.0277(16)	0.0185(14)	-0.0069(12)	0.0001(12)	0.0096(14)
C19	0.0284(16)	0.0372(18)	0.0296(16)	-0.0031(14)	0.0089(13)	0.0036(14)
C45	0.0241(14)	0.0278(15)	0.0212(14)	-0.0048(12)	0.0016(11)	0.0013(12)
C37	0.0348(17)	0.0322(17)	0.0238(15)	0.0052(13)	0.0013(13)	-0.0041(14)
C69	0.0393(18)	0.0215(14)	0.0220(14)	0.0022(12)	0.0003(13)	-0.0009(13)
C82	0.0335(16)	0.0267(15)	0.0223(14)	0.0007(12)	0.0138(12)	-0.0029(13)
C13	0.0340(17)	0.0280(16)	0.0198(14)	-0.0045(12)	-0.0010(12)	0.0063(13)
C49	0.0430(19)	0.0278(16)	0.0180(14)	0.0008(12)	0.0014(13)	0.0088(14)
C34	0.0330(17)	0.0333(17)	0.0248(15)	0.0058(13)	0.0031(13)	-0.0097(14)
C9	0.0280(16)	0.0266(15)	0.0358(17)	0.0043(13)	0.0094(13)	0.0039(13)
C94	0.052(2)	0.042(2)	0.0320(18)	0.0082(16)	-0.0021(16)	0.0098(18)
C8	0.0334(18)	0.041(2)	0.044(2)	0.0074(17)	0.0169(16)	0.0088(16)
C6	0.050(2)	0.0387(19)	0.0242(16)	0.0046(14)	0.0119(15)	0.0146(17)
C72	0.0260(15)	0.0317(17)	0.0407(18)	-0.0059(14)	0.0115(14)	-0.0039(13)
C76	0.0323(17)	0.039(2)	0.048(2)	-0.0058(17)	0.0213(16)	-0.0093(15)
C79	0.060(2)	0.0323(18)	0.0229(16)	-0.0011(13)	0.0237(16)	0.0010(16)
C50	0.0377(18)	0.0364(18)	0.0220(15)	-0.0004(13)	-0.0052(13)	0.0145(15)
C23	0.0418(19)	0.0247(15)	0.0291(16)	-0.0019(13)	0.0089(14)	-0.0024(14)
C119	0.044(2)	0.048(2)	0.0366(19)	-0.0055(17)	0.0178(16)	-0.0028(18)
C83	0.0387(19)	0.0380(19)	0.0327(17)	-0.0016(15)	0.0136(15)	-0.0042(15)
C78	0.045(2)	0.0365(18)	0.0312(17)	0.0038(14)	0.0225(16)	0.0071(16)
C10	0.0277(16)	0.0310(17)	0.0404(19)	-0.0051(14)	0.0027(14)	-0.0010(13)
C88	0.062(3)	0.0340(19)	0.0288(17)	-0.0022(15)	0.0076(17)	-0.0058(18)
C73	0.0281(17)	0.043(2)	0.058(2)	-0.0192(19)	0.0111(17)	-0.0107(16)
C7	0.053(2)	0.049(2)	0.038(2)	0.0115(17)	0.0237(18)	0.0209(19)
B2	0.0210(14)	0.0217(15)	0.0154(13)	-0.0021(11)	0.0033(11)	0.0027(12)
C114	0.045(2)	0.041(2)	0.0364(19)	0.0077(16)	0.0162(16)	0.0040(17)
B1	0.0254(16)	0.0255(16)	0.0223(15)	-0.0012(13)	0.0084(13)	-0.0024(13)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C14	0.052(2)	0.056(3)	0.0254(17)	0.0002(17)	-0.0085(16)	0.006(2)
C36	0.047(2)	0.042(2)	0.0276(17)	0.0161(15)	-0.0051(15)	-0.0064(17)
C27	0.069(3)	0.0327(19)	0.040(2)	0.0009(16)	0.019(2)	-0.0129(19)
C84	0.043(2)	0.0273(17)	0.0389(19)	0.0014(14)	0.0053(16)	-0.0021(15)
C74	0.033(2)	0.050(2)	0.083(3)	-0.020(2)	0.025(2)	-0.0225(18)
C85	0.036(2)	0.058(3)	0.043(2)	0.023(2)	0.0034(16)	-0.0049(18)
C30	0.040(2)	0.063(3)	0.046(2)	0.022(2)	-0.0110(18)	-0.025(2)
C33	0.043(2)	0.047(2)	0.0362(19)	0.0159(17)	-0.0024(16)	-0.0167(18)
C15	0.042(2)	0.0309(18)	0.047(2)	0.0000(16)	0.0024(17)	-0.0012(16)
C95	0.057(2)	0.0327(18)	0.0335(19)	-0.0011(15)	-0.0031(17)	0.0135(18)
C87	0.084(4)	0.057(3)	0.038(2)	0.004(2)	0.021(2)	0.033(3)
C93	0.062(3)	0.037(2)	0.060(3)	0.008(2)	0.009(2)	0.013(2)
C75	0.041(2)	0.049(2)	0.074(3)	-0.007(2)	0.036(2)	-0.0167(19)
C90	0.092(4)	0.0314(19)	0.0310(19)	0.0000(16)	-0.008(2)	0.018(2)
C118	0.035(2)	0.076(3)	0.037(2)	0.009(2)	0.0119(16)	0.004(2)
C115	0.0343(19)	0.050(2)	0.042(2)	0.0112(18)	0.0099(16)	0.0005(17)
C35	0.055(2)	0.051(2)	0.0346(19)	0.0203(18)	-0.0009(18)	-0.017(2)
C12	0.0323(18)	0.040(2)	0.0370(19)	-0.0035(16)	-0.0053(15)	0.0010(15)
C92	0.102(4)	0.029(2)	0.063(3)	-0.002(2)	0.043(3)	0.008(2)
C117	0.042(2)	0.074(3)	0.056(3)	0.037(2)	0.015(2)	0.004(2)
C11	0.0311(19)	0.037(2)	0.080(3)	-0.007(2)	0.009(2)	-0.0049(16)
C86	0.045(2)	0.097(4)	0.041(2)	0.024(3)	0.0170(19)	0.023(3)
C116	0.035(2)	0.052(3)	0.062(3)	0.021(2)	0.0115(19)	-0.0057(18)
C96	0.049(3)	0.068(3)	0.053(3)	-0.015(2)	-0.006(2)	0.006(2)
C91	0.122(5)	0.030(2)	0.033(2)	-0.0008(17)	0.016(3)	0.009(3)
C32	0.053(3)	0.073(3)	0.057(3)	0.034(3)	-0.007(2)	-0.034(2)
C89	0.040(2)	0.105(5)	0.058(3)	-0.027(3)	0.019(2)	-0.012(3)
C31	0.047(3)	0.084(4)	0.069(3)	0.041(3)	-0.018(2)	-0.040(3)
C112	0.155(6)	0.061(4)	0.087(5)	0.030(3)	0.014(4)	-0.032(4)
C100	0.163(5)	0.074(4)	0.041(3)	0.007(2)	0.025(3)	0.073(4)
C120	0.044(3)	0.121(5)	0.046(3)	0.010(3)	0.001(2)	0.001(3)
C111	0.197(7)	0.068(4)	0.061(3)	-0.003(3)	0.023(4)	-0.087(4)
C113	0.131(6)	0.067(4)	0.115(6)	0.009(4)	-0.018(4)	-0.026(4)
C106	0.067(4)	0.136(7)	0.175(8)	-0.124(7)	0.017(4)	-0.008(4)
C103	0.199(8)	0.100(6)	0.093(5)	0.010(5)	-0.047(6)	-0.055(7)
C110	0.192(8)	0.093(5)	0.072(4)	0.027(4)	-0.026(4)	-0.072(5)
C105	0.105(5)	0.072(4)	0.076(4)	-0.007(3)	0.012(3)	-0.001(4)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C104	0.164(6)	0.077(4)	0.085(5)	0.000(4)	0.031(4)	-0.059(5)
C109	0.216(10)	0.125(7)	0.071(5)	0.004(4)	0.015(4)	-0.087(7)
C101	0.117(5)	0.061(4)	0.133(6)	0.021(4)	0.049(4)	0.026(4)
C107	0.184(7)	0.132(7)	0.080(5)	0.020(5)	0.009(5)	-0.091(6)
C108	0.207(8)	0.115(7)	0.090(5)	0.019(5)	-0.004(5)	-0.084(6)
C102	0.160(8)	0.118(7)	0.110(7)	0.002(5)	0.006(5)	-0.017(6)

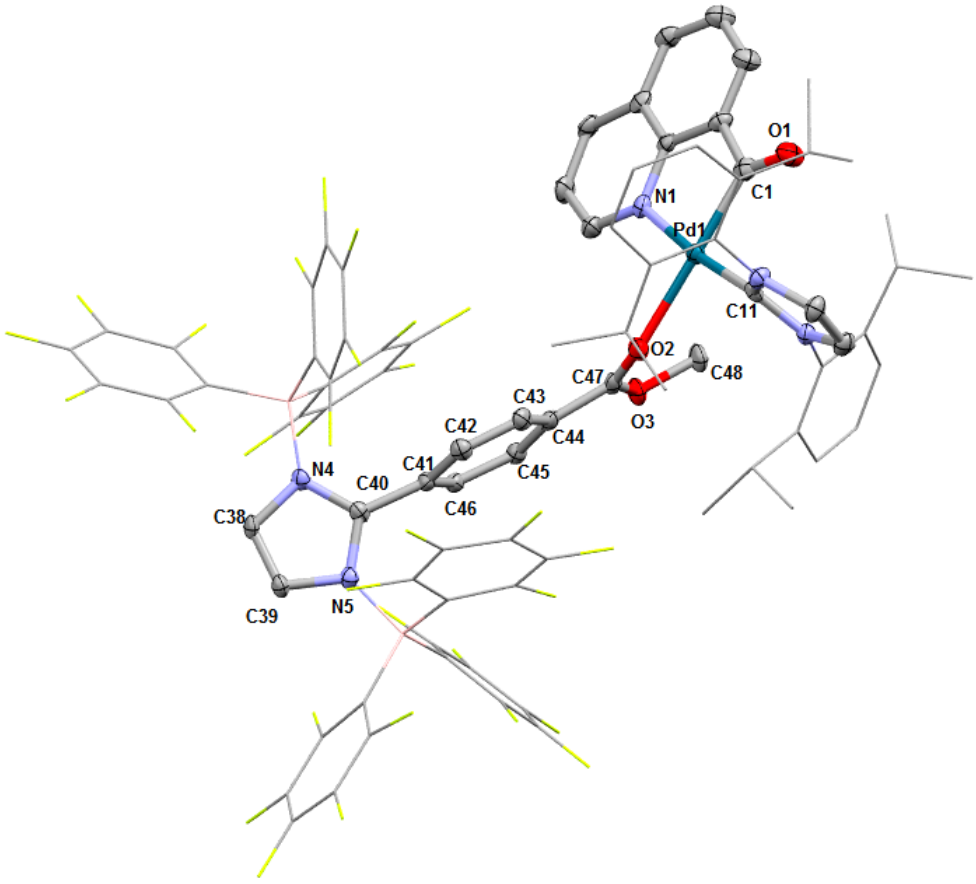
Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 5886.

	x/a	y/b	z/c	U(eq)
H39	0.4420	0.4933	0.3225	0.025
H42	0.6435	0.4305	0.2475	0.025
H43	0.5235	0.4170	0.1903	0.025
H2	0.1445	0.6087	0.0582	0.029
H40	0.5621	0.5044	0.3807	0.025
H3	0.2355	0.5741	0.0019	0.029
H25	0.3389	0.5831	0.1103	0.034
H20	0.3789	0.3941	0.0060	0.036
H18	0.4955	0.5116	0.0883	0.037
H26A	0.4039	0.5513	0.2050	0.049
H26B	0.4345	0.6059	0.1958	0.049
H26C	0.4803	0.5580	0.1830	0.049
H22	0.2012	0.4430	0.0161	0.031
H46	0.8349	0.5326	0.4141	0.032
H24A	0.2275	0.4463	-0.0843	0.048
H24B	0.1847	0.3955	-0.0785	0.048
H24C	0.2718	0.3949	-0.0731	0.048
H19	0.4910	0.4336	0.0410	0.038
H45	0.8207	0.4547	0.4696	0.03
H37	0.3206	0.3865	0.2948	0.037
H13	0.2745	0.5608	0.2137	0.034
H94	0.8295	0.1799	0.6062	0.052
H8	-0.0360	0.5649	0.1914	0.046
H6	0.1527	0.5907	0.3151	0.044
H23A	0.2750	0.3489	0.0310	0.047
H23B	0.1890	0.3570	0.0274	0.047

	x/a	y/b	z/c	U(eq)
H23C	0.2474	0.3771	0.0867	0.047
H119	0.9995	0.6771	0.1649	0.05
H10	0.0463	0.5328	0.0610	0.04
H88	0.4328	0.3185	0.5066	0.05
H7	0.0259	0.5839	0.2918	0.054
H114	1.0934	0.6862	0.2517	0.048
H14A	0.2735	0.5958	0.3374	0.07
H14B	0.3443	0.5769	0.3131	0.07
H14C	0.2810	0.5384	0.3203	0.07
H36	0.2913	0.3220	0.3577	0.049
H27A	0.4776	0.5995	0.0769	0.07
H27B	0.4215	0.6418	0.0887	0.07
H27C	0.4006	0.6061	0.0289	0.07
H84	0.3644	0.1961	0.4040	0.044
H85	0.2464	0.2089	0.4196	0.056
H30	0.0024	0.3835	0.1213	0.063
H15A	0.2409	0.6427	0.1802	0.061
H15B	0.3185	0.6423	0.2283	0.061
H15C	0.2461	0.6594	0.2516	0.061
H87	0.3137	0.3313	0.5209	0.07
H93	0.9336	0.1894	0.5627	0.064
H90	0.7007	0.2136	0.4387	0.065
H115	1.1583	0.7606	0.2705	0.05
H35	0.1757	0.2867	0.3361	0.058
H12A	-0.0543	0.6093	0.0805	0.057
H12B	-0.0456	0.5896	0.0131	0.057
H12C	0.0203	0.6192	0.0568	0.057
H92	0.9194	0.2115	0.4569	0.073
H117	1.0358	0.8172	0.1112	0.068
H11A	-0.0310	0.4779	0.1054	0.074
H11B	-0.0728	0.5009	0.0399	0.074
H11C	-0.0882	0.5225	0.1045	0.074
H86	0.2206	0.2761	0.4783	0.072
H116	1.1291	0.8263	0.1995	0.06
H96A	0.6830	0.1596	0.5722	0.089
H96B	0.6431	0.2010	0.5243	0.089
H96C	0.6913	0.2172	0.5908	0.089

	x/a	y/b	z/c	U(eq)
H91	0.8034	0.2240	0.3959	0.074
H32	0.0461	0.2867	0.2660	0.076
H89A	0.4882	0.2542	0.3997	0.1
H89B	0.5026	0.2140	0.4550	0.1
H89C	0.5206	0.2714	0.4703	0.1
H31	-0.0350	0.3197	0.1816	0.085
H112	0.6167	0.7756	0.4177	0.123
H100	0.8330	0.5246	0.6793	0.11
H12D	0.9299	0.7066	0.0672	0.108
H12E	0.9591	0.7542	0.0357	0.108
H12F	0.9019	0.7609	0.0808	0.108
H11D	0.4685	0.7799	0.3894	0.166
H11E	0.4426	0.8213	0.3366	0.166
H11F	0.4988	0.8356	0.4002	0.166
H10A	0.7490	0.5224	0.5684	0.191
H10B	0.7371	0.5796	0.5487	0.191
H10C	0.7299	0.5621	0.6174	0.191
H103	0.9630	0.6215	0.5698	0.171
H110	0.5010	0.8100	0.2499	0.152
H104	0.8382	0.6122	0.5305	0.129
H109	0.6092	0.7838	0.2031	0.167
H101	0.9710	0.5422	0.7294	0.121
H107	0.7269	0.7518	0.3708	0.161
H108	0.7108	0.7602	0.2744	0.171
H102	1.0323	0.5837	0.6535	0.159

Crystal Structure Report for 1[IMP-CO_2Me]



Thermal ellipsoid plot of 5839. Ellipsoids shown at 50% probability, $B(C_6F_5)_3$ and diisopropylphenyl substituents shown in wireframe, hydrogen atoms hidden for clarity.

A specimen of $C_{84}H_{51}B_2F_{30}N_5O_3Pd$ was used for the X-ray crystallographic analysis. The X-ray intensity data were measured(λ = 0.71073 Å). The integration of the data using a monoclinic unit cell yielded a total of 89474 reflections to a maximum θ angle of 27.91° (0.76Å resolution), of which 22568 were independent (average redundancy 3.965, completeness = 99.8%, R_{int} = 11.40%, R_{sig} =12.99%) and 12565 (55.68%) were greater than $2\sigma(F^2)$. The final cell constants of a = 22.722(2) Å, b = 18.9379(19) Å, c =22.844(2) Å, β = 105.759(2)°, volume = 9460.5(17) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The final anisotropic full-matrix least-squares refinement on F^2 with 1135 variables converged at R1 = 10.44%, for the observed data and wR2 = 35.45% for all data. The goodness-of-fit was 1.049. The largest peak in the final difference electron density synthesis was 4.392 $e^-/Å^3$ and the largest hole was -0.733 $e^-/Å^3$ with an RMS deviation of 0.239 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.317 g/cm^3 and F(000), 3760 e^-.

Table 1. Sample and crystal data for 5839.

Identification code	5839	
Chemical formula	$C_{84}H_{51}B_2F_{30}N_5O_3Pd$	
Formula weight	1876.32 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 22.722(2) Å	α = 90°
	b = 18.9379(19) Å	β = 105.759(2)°
	c = 22.844(2) Å	γ = 90°
Volume	9460.5(17) $Å^3$	
Z	4	
Density (calculated)	1.317 g/cm^3	
Absorption coefficient	0.301 mm^{-1}	
F(000)	3760	

Table 2. Data collection and structure refinement for 5839.

Theta range for data collection	1.12 to 27.91°	
Index ranges	-29<=h<=29, -24<=k<=13, -30<=l<=29	
Reflections collected	89474	
Independent reflections	22568 [R(int) = 0.1140]	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	22568 / 0 / 1135	
Goodness-of-fit on F^2	1.049	
Δ/σ_{max}	0.001	
Final R indices	12565 data; I>2σ(I)	R1 = 0.1044, wR2 = 0.3002
	all data	R1 = 0.1784, wR2 = 0.3545
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.1986P)^2+45.9409P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	4.392 and -0.733 $eÅ^{-3}$	
R.M.S. deviation from mean	0.239 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for 5839.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij}tensor.

	x/a	y/b	z/c	U(eq)
Pd1	0.54970(2)	0.46479(3)	0.37394(2)	0.01558(16)
F26	0.6056(2)	0.2385(2)	0.55849(19)	0.0224(9)
F16	0.81943(19)	0.1125(2)	0.70887(19)	0.0237(10)
F11	0.8764(2)	0.0991(2)	0.53102(19)	0.0245(10)
F10	0.65590(19)	0.9648(2)	0.45921(19)	0.0213(9)
F1	0.9045(2)	0.0423(2)	0.4287(2)	0.0289(10)
F25	0.80934(19)	0.1864(2)	0.5999(2)	0.0239(10)
F5	0.7620(2)	0.8822(2)	0.4751(2)	0.0257(10)
F30	0.6255(2)	0.0009(2)	0.6245(2)	0.0229(9)
F20	0.6119(2)	0.0927(3)	0.7130(2)	0.0283(10)
F15	0.7247(2)	0.1417(3)	0.3466(2)	0.0307(11)
F6	0.7729(2)	0.0229(3)	0.3238(2)	0.0310(11)
F21	0.6467(2)	0.2431(3)	0.6844(2)	0.0290(11)
F9	0.5670(2)	0.9183(2)	0.3659(2)	0.0304(11)
F12	0.9223(2)	0.2278(3)	0.5240(2)	0.0338(12)
F17	0.8544(2)	0.0756(3)	0.8242(2)	0.0332(12)
F27	0.4898(2)	0.2163(3)	0.5036(2)	0.0313(11)
F28	0.4375(2)	0.0884(3)	0.5081(2)	0.0352(12)
F19	0.6494(2)	0.0554(3)	0.8277(2)	0.0390(13)
F29	0.5063(2)	0.9816(3)	0.5731(2)	0.0331(11)
F2	0.9847(2)	0.9400(3)	0.4449(3)	0.0404(13)
O2	0.5838(2)	0.3531(3)	0.3768(2)	0.0217(11)
F18	0.7701(3)	0.0452(3)	0.8858(2)	0.0415(14)
F13	0.8748(2)	0.3104(3)	0.4251(3)	0.0421(14)
F4	0.8433(3)	0.7803(3)	0.4869(3)	0.0440(14)
F3	0.9570(3)	0.8070(3)	0.4736(3)	0.0519(16)
F14	0.7779(2)	0.2634(3)	0.3362(3)	0.0431(14)
F24	0.8540(3)	0.3142(3)	0.6257(3)	0.0510(16)
O3	0.5141(2)	0.2657(3)	0.3449(2)	0.0231(12)
O1	0.5219(3)	0.6105(3)	0.3473(3)	0.0291(13)
F8	0.5805(3)	0.9191(4)	0.2516(2)	0.0502(16)
F22	0.6938(3)	0.3718(3)	0.7117(3)	0.0522(16)
F7	0.6846(3)	0.9728(4)	0.2320(2)	0.0539(17)
N4	0.7256(3)	0.0793(3)	0.5896(3)	0.0160(12)
N1	0.4889(3)	0.4361(3)	0.4254(3)	0.0180(12)
N5	0.7592(3)	0.0375(3)	0.5133(3)	0.0169(12)

	x/a	y/b	z/c	U(eq)
N2	0.5905(3)	0.4896(3)	0.2613(3)	0.0183(12)
N3	0.6489(3)	0.5491(3)	0.3337(3)	0.0195(13)
F23	0.7973(3)	0.4103(3)	0.6814(4)	0.072(2)
C11	0.6020(3)	0.5017(4)	0.3220(3)	0.0153(14)
C39	0.7833(3)	0.9971(4)	0.5643(3)	0.0177(14)
C42	0.7051(3)	0.2078(4)	0.4826(3)	0.0188(15)
C45	0.5879(3)	0.1677(4)	0.4178(3)	0.0188(15)
C26	0.5457(3)	0.4405(4)	0.2263(3)	0.0206(15)
C38	0.7627(3)	0.0221(4)	0.6104(3)	0.0185(15)
C61	0.7993(3)	0.1102(4)	0.4376(3)	0.0193(15)
C40	0.7240(3)	0.0873(3)	0.5304(3)	0.0135(13)
C10	0.4808(4)	0.3752(4)	0.4507(3)	0.0227(16)
C7	0.4518(3)	0.4913(4)	0.4300(3)	0.0173(14)
C5	0.3704(3)	0.5446(4)	0.4643(3)	0.0218(16)
C55	0.8290(3)	0.9707(4)	0.4558(3)	0.0200(15)
C9	0.4351(4)	0.3646(4)	0.4795(4)	0.0283(18)
C60	0.8875(4)	0.9798(4)	0.4468(3)	0.0242(17)
C46	0.6252(3)	0.1206(4)	0.4562(3)	0.0163(14)
C84	0.7767(4)	0.2307(4)	0.6263(4)	0.0248(17)
C24	0.6283(3)	0.5291(4)	0.2356(3)	0.0205(15)
C25	0.6650(4)	0.5671(4)	0.2816(3)	0.0234(16)
C35	0.6284(4)	0.3452(4)	0.2448(4)	0.0260(17)
C8	0.3978(4)	0.4186(4)	0.4856(3)	0.0223(16)
C62	0.8498(3)	0.1386(4)	0.4824(3)	0.0221(16)
C66	0.7759(3)	0.1564(4)	0.3900(4)	0.0228(16)
C79	0.7230(3)	0.2092(4)	0.6378(3)	0.0196(15)
C12	0.6833(3)	0.5774(4)	0.3918(3)	0.0202(15)
C43	0.6666(4)	0.2558(4)	0.4445(3)	0.0216(16)
C31	0.4864(3)	0.4657(4)	0.2002(3)	0.0207(15)
C32	0.4684(4)	0.5419(4)	0.2043(4)	0.0245(16)
C67	0.7135(4)	0.0996(4)	0.7018(3)	0.0198(15)
C1	0.5105(4)	0.5588(4)	0.3705(4)	0.0235(16)
C41	0.6848(3)	0.1396(4)	0.4888(3)	0.0174(14)
C78	0.5839(3)	0.1738(4)	0.5658(3)	0.0197(15)
C6	0.4061(3)	0.4854(4)	0.4604(3)	0.0202(15)
C2	0.4604(3)	0.5554(4)	0.4020(3)	0.0191(15)
C71	0.6916(4)	0.0691(5)	0.7973(4)	0.0271(18)

	x/a	y/b	z/c	U(eq)
C47	0.5674(3)	0.2914(4)	0.3758(3)	0.0185(15)
C72	0.6733(3)	0.0873(4)	0.7365(4)	0.0223(16)
C13	0.6793(4)	0.6509(4)	0.4019(4)	0.0246(17)
C27	0.5645(3)	0.3719(4)	0.2170(3)	0.0208(15)
C44	0.6072(3)	0.2367(4)	0.4129(3)	0.0205(15)
C28	0.5209(4)	0.3274(4)	0.1803(4)	0.0264(17)
C56	0.8176(3)	0.9003(4)	0.4675(4)	0.0224(16)
C83	0.8018(4)	0.2979(5)	0.6387(5)	0.036(2)
C74	0.5927(3)	0.0560(4)	0.5965(3)	0.0198(15)
C77	0.5223(3)	0.1629(4)	0.5360(3)	0.0207(15)
C50	0.6648(3)	0.9719(4)	0.4032(3)	0.0193(15)
C30	0.4444(4)	0.4193(4)	0.1660(4)	0.0247(17)
C49	0.7168(3)	0.0016(4)	0.3957(3)	0.0181(15)
C68	0.7746(3)	0.0957(4)	0.7349(3)	0.0196(15)
C63	0.8742(4)	0.2037(5)	0.4789(4)	0.0273(18)
C18	0.7306(4)	0.4545(4)	0.4218(3)	0.0262(17)
C73	0.6219(3)	0.1212(4)	0.5978(3)	0.0169(14)
C59	0.9300(4)	0.9262(5)	0.4533(4)	0.0312(19)
C57	0.8595(4)	0.8457(4)	0.4737(4)	0.0290(18)
C48	0.4689(4)	0.3137(4)	0.3070(4)	0.0248(17)
C80	0.6982(4)	0.2590(4)	0.6680(4)	0.0247(17)
C70	0.7531(4)	0.0624(5)	0.8272(3)	0.0280(18)
C15	0.7550(4)	0.6351(5)	0.4982(4)	0.0286(18)
C54	0.7219(4)	0.9987(4)	0.3366(4)	0.0260(17)
C17	0.7228(4)	0.5329(4)	0.4341(3)	0.0215(15)
C19	0.7626(4)	0.4450(5)	0.3708(4)	0.0325(19)
C16	0.7580(4)	0.5641(5)	0.4876(4)	0.0279(18)
C64	0.8503(4)	0.2468(4)	0.4296(4)	0.0290(18)
C33	0.4105(4)	0.5489(5)	0.2262(4)	0.0310(19)
C14	0.7163(4)	0.6782(5)	0.4558(4)	0.0319(19)
C36	0.6710(4)	0.3597(5)	0.2035(4)	0.035(2)
C34	0.4587(5)	0.5775(5)	0.1418(4)	0.038(2)
C76	0.4960(3)	0.0987(5)	0.5379(4)	0.0247(17)
C37	0.6307(4)	0.2669(5)	0.2594(4)	0.0317(19)
C58	0.9164(4)	0.8591(5)	0.4675(4)	0.033(2)
C29	0.4617(4)	0.3504(4)	0.1560(4)	0.0264(17)
C51	0.6180(3)	0.9446(4)	0.3556(4)	0.0226(16)

	x/a	y/b	z/c	U(eq)
C20	0.7685(4)	0.4140(5)	0.4767(4)	0.0287(18)
C3	0.4255(4)	0.6128(4)	0.4060(4)	0.0280(18)
C65	0.8015(4)	0.2228(5)	0.3846(4)	0.0309(19)
C4	0.3801(4)	0.6080(4)	0.4378(4)	0.0289(18)
C21	0.6407(4)	0.7011(4)	0.3558(4)	0.0284(18)
C69	0.7952(4)	0.0781(5)	0.7962(4)	0.0277(18)
C75	0.5317(4)	0.0445(4)	0.5697(4)	0.0248(17)
C81	0.7214(4)	0.3256(4)	0.6828(4)	0.034(2)
C22	0.6014(5)	0.7475(5)	0.3848(5)	0.042(2)
C52	0.6244(4)	0.9462(5)	0.2981(4)	0.034(2)
B1	0.7755(4)	0.0312(4)	0.4496(4)	0.0182(16)
C53	0.6773(4)	0.9726(5)	0.2885(4)	0.036(2)
C23	0.6816(5)	0.7492(5)	0.3287(5)	0.046(3)
B2	0.6950(4)	0.1281(4)	0.6305(4)	0.0183(16)
C82	0.7735(5)	0.3449(5)	0.6683(5)	0.044(3)

Table 4. Bond lengths (Å) for 5839.

Pd1-C1	1.984(8)	Pd1-C11	2.019(7)
Pd1-N1	2.113(6)	Pd1-O2	2.247(5)
F26-C78	1.348(8)	F16-C68	1.350(9)
F11-C62	1.340(8)	F10-C50	1.356(8)
F1-C60	1.343(9)	F25-C84	1.364(9)
F5-C56	1.365(9)	F30-C74	1.339(8)
F20-C72	1.357(9)	F15-C66	1.337(9)
F6-C54	1.348(9)	F21-C80	1.355(9)
F9-C51	1.340(9)	F12-C63	1.360(9)
F17-C69	1.326(9)	F27-C77	1.350(8)
F28-C76	1.333(8)	F19-C71	1.353(9)
F29-C75	1.336(9)	F2-C59	1.335(10)
O2-C47	1.224(9)	F18-C70	1.329(9)
F13-C64	1.341(9)	F4-C57	1.349(10)
F3-C58	1.332(9)	F14-C65	1.334(9)
F24-C83	1.336(11)	O3-C47	1.319(9)
O3-C48	1.464(8)	O1-C1	1.174(10)
F8-C52	1.347(9)	F22-C81	1.350(10)
F7-C53	1.345(10)	N4-C40	1.351(9)

N4-C38	1.375(9)	N4-B2	1.600(10)
N1-C10	1.326(10)	N1-C7	1.366(9)
N5-C40	1.360(9)	N5-C39	1.376(9)
N5-B1	1.602(10)	N2-C11	1.358(9)
N2-C24	1.384(9)	N2-C26	1.448(10)
N3-C11	1.363(9)	N3-C25	1.379(10)
N3-C12	1.448(9)	F23-C82	1.351(10)
C39-C38	1.350(10)	C39-H39	0.95
C42-C41	1.392(10)	C42-C43	1.392(10)
C42-H42	0.95	C45-C46	1.370(10)
C45-C44	1.392(10)	C45-H45	0.95
C26-C31	1.400(10)	C26-C27	1.402(11)
C38-H38	0.95	C61-C66	1.384(10)
C61-C62	1.420(11)	C61-B1	1.639(11)
C40-C41	1.489(9)	C10-C9	1.385(11)
C10-H10	0.95	C7-C6	1.403(10)
C7-C2	1.409(10)	C5-C4	1.388(12)
C5-C6	1.401(10)	C5-H5	0.95
C55-C56	1.397(11)	C55-C60	1.408(11)
C55-B1	1.649(11)	C9-C8	1.360(11)
C9-H9	0.95	C60-C59	1.381(11)
C46-C41	1.403(10)	C46-H46	0.95
C84-C79	1.378(11)	C84-C83	1.391(11)
C24-C25	1.357(11)	C24-H24	0.95
C25-H25	0.95	C35-C27	1.507(11)
C35-C37	1.517(11)	C35-C36	1.547(12)
C35-H35	1.0	C8-C6	1.423(11)
C8-H8	0.95	C62-C63	1.363(12)
C66-C65	1.404(11)	C79-C80	1.375(11)
C79-B2	1.653(11)	C12-C17	1.406(11)
C12-C13	1.419(11)	C43-C44	1.394(11)
C43-H43	0.95	C31-C30	1.375(11)
C31-C32	1.511(11)	C32-C33	1.533(11)
C32-C34	1.540(12)	C32-H32	1.0
C67-C72	1.381(11)	C67-C68	1.392(10)
C67-B2	1.658(11)	C1-C2	1.505(11)
C78-C73	1.389(10)	C78-C77	1.395(11)
C2-C3	1.363(11)	C71-C72	1.381(11)

C71-C70	1.385(12)	C47-C44	1.482(10)
C13-C14	1.389(11)	C13-C21	1.510(12)
C27-C28	1.393(11)	C28-C29	1.379(12)
C28-H28	0.95	C56-C57	1.387(11)
C83-C82	1.378(14)	C74-C75	1.371(11)
C74-C73	1.398(10)	C77-C76	1.360(11)
C50-C49	1.361(11)	C50-C51	1.397(10)
C30-C29	1.401(11)	C30-H30	0.95
C49-C54	1.387(11)	C49-B1	1.648(11)
C68-C69	1.390(10)	C63-C64	1.377(12)
C18-C20	1.521(11)	C18-C17	1.530(11)
C18-C19	1.542(12)	C18-H18	1.0
C73-B2	1.632(11)	C59-C58	1.368(13)
C57-C58	1.361(12)	C48-H48A	0.98
C48-H48B	0.98	C48-H48C	0.98
C80-C81	1.373(11)	C70-C69	1.369(12)
C15-C16	1.371(12)	C15-C14	1.383(12)
C15-H15	0.95	C54-C53	1.369(12)
C17-C16	1.397(11)	C19-H19A	0.98
C19-H19B	0.98	C19-H19C	0.98
C16-H16	0.95	C64-C65	1.369(12)
C33-H33A	0.98	C33-H33B	0.98
C33-H33C	0.98	C14-H14	0.95
C36-H36A	0.98	C36-H36B	0.98
C36-H36C	0.98	C34-H34A	0.98
C34-H34B	0.98	C34-H34C	0.98
C76-C75	1.386(11)	C37-H37A	0.98
C37-H37B	0.98	C37-H37C	0.98
C29-H29	0.95	C51-C52	1.361(12)
C20-H20A	0.98	C20-H20B	0.98
C20-H20C	0.98	C3-C4	1.416(12)
C3-H3	0.95	C4-H4	0.95
C21-C22	1.527(13)	C21-C23	1.544(13)
C21-H21	1.0	C81-C82	1.364(14)
C22-H22A	0.98	C22-H22B	0.98
C22-H22C	0.98	C52-C53	1.374(13)
C23-H23A	0.98	C23-H23B	0.98
C23-H23C	0.98		

Table 5. Bond angles (°) for 5839.

C1-Pd1-C11	89.8(3)	C1-Pd1-N1	84.2(3)
C11-Pd1-N1	173.7(3)	C1-Pd1-O2	173.6(3)
C11-Pd1-O2	95.2(2)	N1-Pd1-O2	90.8(2)
C47-O2-Pd1	142.9(5)	C47-O3-C48	118.7(6)
C40-N4-C38	106.4(6)	C40-N4-B2	128.4(6)
C38-N4-B2	125.2(6)	C10-N1-C7	118.1(6)
C10-N1-Pd1	131.0(5)	C7-N1-Pd1	110.9(5)
C40-N5-C39	105.9(6)	C40-N5-B1	127.7(6)
C39-N5-B1	126.1(6)	C11-N2-C24	111.9(6)
C11-N2-C26	125.6(6)	C24-N2-C26	122.5(6)
C11-N3-C25	111.7(6)	C11-N3-C12	128.5(6)
C25-N3-C12	119.7(6)	N2-C11-N3	103.6(6)
N2-C11-Pd1	124.1(5)	N3-C11-Pd1	131.7(5)
C38-C39-N5	108.8(6)	C38-C39-H39	125.6
N5-C39-H39	125.6	C41-C42-C43	120.0(7)
C41-C42-H42	120.0	C43-C42-H42	120.0
C46-C45-C44	120.6(7)	C46-C45-H45	119.7
C44-C45-H45	119.7	C31-C26-C27	123.2(7)
C31-C26-N2	117.9(7)	C27-C26-N2	118.8(7)
C39-C38-N4	108.4(6)	C39-C38-H38	125.8
N4-C38-H38	125.8	C66-C61-C62	112.9(7)
C66-C61-B1	129.4(7)	C62-C61-B1	117.7(6)
N4-C40-N5	110.5(6)	N4-C40-C41	124.2(6)
N5-C40-C41	125.0(6)	N1-C10-C9	123.0(7)
N1-C10-H10	118.5	C9-C10-H10	118.5
N1-C7-C6	122.2(7)	N1-C7-C2	117.4(7)
C6-C7-C2	120.4(7)	C4-C5-C6	120.1(7)
C4-C5-H5	120.0	C6-C5-H5	120.0
C56-C55-C60	112.1(7)	C56-C55-B1	120.5(7)
C60-C55-B1	127.2(7)	C8-C9-C10	120.5(7)
C8-C9-H9	119.7	C10-C9-H9	119.7
F1-C60-C59	115.4(7)	F1-C60-C55	120.9(7)
C59-C60-C55	123.6(8)	C45-C46-C41	120.9(7)
C45-C46-H46	119.6	C41-C46-H46	119.6
F25-C84-C79	121.3(7)	F25-C84-C83	114.2(7)

C79-C84-C83	124.5(8)	C25-C24-N2	106.2(7)
C25-C24-H24	126.9	N2-C24-H24	126.9
C24-C25-N3	106.6(7)	C24-C25-H25	126.7
N3-C25-H25	126.7	C27-C35-C37	113.1(7)
C27-C35-C36	111.9(7)	C37-C35-C36	108.6(7)
C27-C35-H35	107.7	C37-C35-H35	107.7
C36-C35-H35	107.7	C9-C8-C6	118.2(7)
C9-C8-H8	120.9	C6-C8-H8	120.9
F11-C62-C63	117.1(7)	F11-C62-C61	118.6(7)
C63-C62-C61	124.2(7)	F15-C66-C61	121.5(7)
F15-C66-C65	114.7(7)	C61-C66-C65	123.7(7)
C80-C79-C84	113.4(7)	C80-C79-B2	119.3(7)
C84-C79-B2	126.2(7)	C17-C12-C13	122.3(7)
C17-C12-N3	119.5(7)	C13-C12-N3	118.0(7)
C42-C43-C44	120.7(7)	C42-C43-H43	119.7
C44-C43-H43	119.7	C30-C31-C26	117.7(7)
C30-C31-C32	119.1(7)	C26-C31-C32	123.0(7)
C31-C32-C33	112.0(7)	C31-C32-C34	109.5(7)
C33-C32-C34	110.2(7)	C31-C32-H32	108.4
C33-C32-H32	108.4	C34-C32-H32	108.4
C72-C67-C68	113.3(7)	C72-C67-B2	126.1(7)
C68-C67-B2	120.0(7)	O1-C1-C2	122.7(7)
O1-C1-Pd1	127.9(6)	C2-C1-Pd1	109.4(5)
C42-C41-C46	118.8(6)	C42-C41-C40	121.7(6)
C46-C41-C40	119.5(6)	F26-C78-C73	121.4(6)
F26-C78-C77	115.3(6)	C73-C78-C77	123.2(7)
C5-C6-C7	119.1(7)	C5-C6-C8	122.9(7)
C7-C6-C8	117.9(7)	C3-C2-C7	120.0(7)
C3-C2-C1	121.8(7)	C7-C2-C1	118.1(7)
F19-C71-C72	120.2(7)	F19-C71-C70	119.3(7)
C72-C71-C70	120.4(7)	O2-C47-O3	126.4(7)
O2-C47-C44	121.4(7)	O3-C47-C44	112.1(6)
F20-C72-C71	114.4(7)	F20-C72-C67	121.9(7)
C71-C72-C67	123.7(7)	C14-C13-C12	117.3(8)
C14-C13-C21	118.8(7)	C12-C13-C21	123.8(7)
C28-C27-C26	117.2(7)	C28-C27-C35	119.8(7)
C26-C27-C35	123.0(7)	C45-C44-C43	118.9(7)
C45-C44-C47	123.1(7)	C43-C44-C47	118.0(7)

C29-C28-C27	120.4(8)	C29-C28-H28	119.8
C27-C28-H28	119.8	F5-C56-C57	115.6(7)
F5-C56-C55	119.4(6)	C57-C56-C55	124.9(8)
F24-C83-C82	121.3(8)	F24-C83-C84	120.4(8)
C82-C83-C84	118.1(9)	F30-C74-C75	117.0(7)
F30-C74-C73	118.6(6)	C75-C74-C73	124.4(7)
F27-C77-C76	120.4(7)	F27-C77-C78	119.0(7)
C76-C77-C78	120.6(7)	F10-C50-C49	121.1(6)
F10-C50-C51	114.8(7)	C49-C50-C51	124.0(7)
C31-C30-C29	120.3(7)	C31-C30-H30	119.8
C29-C30-H30	119.8	C50-C49-C54	114.2(7)
C50-C49-B1	126.9(6)	C54-C49-B1	118.5(7)
F16-C68-C69	114.3(7)	F16-C68-C67	120.6(6)
C69-C68-C67	125.0(7)	F12-C63-C62	121.0(7)
F12-C63-C64	118.5(7)	C62-C63-C64	120.5(7)
C20-C18-C17	114.0(7)	C20-C18-C19	106.7(7)
C17-C18-C19	110.8(7)	C20-C18-H18	108.4
C17-C18-H18	108.4	C19-C18-H18	108.4
C78-C73-C74	113.5(6)	C78-C73-B2	126.4(6)
C74-C73-B2	119.9(6)	F2-C59-C58	119.7(8)
F2-C59-C60	119.5(8)	C58-C59-C60	120.8(8)
F4-C57-C58	121.3(8)	F4-C57-C56	119.1(8)
C58-C57-C56	119.7(8)	O3-C48-H48A	109.5
O3-C48-H48B	109.5	H48A-C48-H48B	109.5
O3-C48-H48C	109.5	H48A-C48-H48C	109.5
H48B-C48-H48C	109.5	F21-C80-C81	116.0(7)
F21-C80-C79	119.2(7)	C81-C80-C79	124.8(8)
F18-C70-C69	121.5(8)	F18-C70-C71	119.9(8)
C69-C70-C71	118.5(7)	C16-C15-C14	120.5(8)
C16-C15-H15	119.7	C14-C15-H15	119.7
F6-C54-C53	116.2(7)	F6-C54-C49	120.0(7)
C53-C54-C49	123.8(8)	C16-C17-C12	117.1(7)
C16-C17-C18	120.2(7)	C12-C17-C18	122.7(7)
C18-C19-H19A	109.5	C18-C19-H19B	109.5
H19A-C19-H19B	109.5	C18-C19-H19C	109.5
H19A-C19-H19C	109.5	H19B-C19-H19C	109.5
C15-C16-C17	121.6(8)	C15-C16-H16	119.2
C17-C16-H16	119.2	F13-C64-C65	120.6(8)

F13-C64-C63	120.9(8)	C65-C64-C63	118.4(8)
C32-C33-H33A	109.5	C32-C33-H33B	109.5
H33A-C33-H33B	109.5	C32-C33-H33C	109.5
H33A-C33-H33C	109.5	H33B-C33-H33C	109.5
C15-C14-C13	121.2(8)	C15-C14-H14	119.4
C13-C14-H14	119.4	C35-C36-H36A	109.5
C35-C36-H36B	109.5	H36A-C36-H36B	109.5
C35-C36-H36C	109.5	H36A-C36-H36C	109.5
H36B-C36-H36C	109.5	C32-C34-H34A	109.5
C32-C34-H34B	109.5	H34A-C34-H34B	109.5
C32-C34-H34C	109.5	H34A-C34-H34C	109.5
H34B-C34-H34C	109.5	F28-C76-C77	120.1(7)
F28-C76-C75	121.3(7)	C77-C76-C75	118.6(7)
C35-C37-H37A	109.5	C35-C37-H37B	109.5
H37A-C37-H37B	109.5	C35-C37-H37C	109.5
H37A-C37-H37C	109.5	H37B-C37-H37C	109.5
F3-C58-C57	120.0(8)	F3-C58-C59	121.2(8)
C57-C58-C59	118.7(8)	C28-C29-C30	121.1(8)
C28-C29-H29	119.5	C30-C29-H29	119.5
F9-C51-C52	120.1(7)	F9-C51-C50	121.0(7)
C52-C51-C50	118.9(8)	C18-C20-H20A	109.5
C18-C20-H20B	109.5	H20A-C20-H20B	109.5
C18-C20-H20C	109.5	H20A-C20-H20C	109.5
H20B-C20-H20C	109.5	C2-C3-C4	120.1(8)
C2-C3-H3	119.9	C4-C3-H3	119.9
F14-C65-C64	119.5(7)	F14-C65-C66	120.4(8)
C64-C65-C66	120.1(7)	C5-C4-C3	120.2(8)
C5-C4-H4	119.9	C3-C4-H4	119.9
C13-C21-C22	110.9(7)	C13-C21-C23	110.6(7)
C22-C21-C23	108.8(7)	C13-C21-H21	108.8
C22-C21-H21	108.8	C23-C21-H21	108.8
F17-C69-C70	120.2(7)	F17-C69-C68	121.0(7)
C70-C69-C68	118.8(7)	F29-C75-C74	121.0(7)
F29-C75-C76	119.4(7)	C74-C75-C76	119.6(7)
F22-C81-C82	119.6(8)	F22-C81-C80	121.2(8)
C82-C81-C80	119.2(8)	C21-C22-H22A	109.5
C21-C22-H22B	109.5	H22A-C22-H22B	109.5
C21-C22-H22C	109.5	H22A-C22-H22C	109.5

H22B-C22-H22C	109.5	F8-C52-C51	120.2(8)
F8-C52-C53	120.4(8)	C51-C52-C53	119.4(8)
N5-B1-C61	104.6(6)	N5-B1-C49	111.4(6)
C61-B1-C49	115.0(6)	N5-B1-C55	108.7(6)
C61-B1-C55	112.4(6)	C49-B1-C55	104.8(6)
F7-C53-C54	120.7(8)	F7-C53-C52	119.7(8)
C54-C53-C52	119.5(8)	C21-C23-H23A	109.5
C21-C23-H23B	109.5	H23A-C23-H23B	109.5
C21-C23-H23C	109.5	H23A-C23-H23C	109.5
H23B-C23-H23C	109.5	N4-B2-C73	103.7(6)
N4-B2-C79	112.4(6)	C73-B2-C79	115.9(6)
N4-B2-C67	110.6(6)	C73-B2-C67	112.2(6)
C79-B2-C67	102.4(6)	F23-C82-C81	120.9(9)
F23-C82-C83	119.3(9)	C81-C82-C83	119.7(8)

Table 6. Anisotropic atomic displacement parameters (Å^2) for 5839.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pd1	0.0148(3)	0.0187(3)	0.0139(3)	0.0016(2)	0.00512(19)	0.0005(2)
F26	0.021(2)	0.023(2)	0.022(2)	0.0050(17)	0.0029(18)	0.0026(17)
F16	0.018(2)	0.034(2)	0.019(2)	-0.0023(18)	0.0044(18)	0.0002(18)
F11	0.019(2)	0.034(2)	0.019(2)	0.0071(18)	0.0018(18)	-0.0003(18)
F10	0.019(2)	0.026(2)	0.019(2)	0.0014(17)	0.0052(17)	-0.0012(18)
F1	0.022(2)	0.040(3)	0.029(2)	0.003(2)	0.015(2)	0.000(2)
F25	0.016(2)	0.030(2)	0.026(2)	0.0002(18)	0.0067(19)	0.0008(18)
F5	0.023(2)	0.023(2)	0.032(3)	0.0021(19)	0.009(2)	0.0007(18)
F30	0.022(2)	0.021(2)	0.024(2)	0.0036(17)	0.0041(19)	0.0021(18)
F20	0.018(2)	0.045(3)	0.022(2)	0.001(2)	0.0062(19)	0.002(2)
F15	0.023(3)	0.036(3)	0.030(3)	0.012(2)	0.001(2)	0.002(2)
F6	0.021(2)	0.054(3)	0.022(2)	0.004(2)	0.0123(19)	0.004(2)
F21	0.026(3)	0.036(3)	0.027(2)	-0.005(2)	0.010(2)	0.009(2)
F9	0.024(3)	0.032(3)	0.033(3)	-0.012(2)	0.005(2)	-0.007(2)
F12	0.025(3)	0.032(3)	0.041(3)	0.004(2)	0.004(2)	-0.007(2)
F17	0.022(3)	0.054(3)	0.017(2)	0.000(2)	-0.0061(19)	0.002(2)
F27	0.018(2)	0.041(3)	0.032(3)	0.009(2)	0.002(2)	0.013(2)
F28	0.013(2)	0.053(3)	0.035(3)	0.001(2)	-0.002(2)	-0.003(2)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F19	0.036(3)	0.063(4)	0.023(3)	0.013(2)	0.018(2)	0.009(3)
F29	0.022(2)	0.038(3)	0.040(3)	-0.005(2)	0.010(2)	-0.013(2)
F2	0.018(3)	0.063(4)	0.044(3)	-0.004(3)	0.015(2)	0.011(2)
O2	0.019(3)	0.024(3)	0.023(3)	0.008(2)	0.006(2)	0.005(2)
F18	0.039(3)	0.070(4)	0.013(2)	0.012(2)	0.003(2)	0.012(3)
F13	0.030(3)	0.033(3)	0.062(4)	0.016(3)	0.010(3)	-0.006(2)
F4	0.041(3)	0.026(3)	0.068(4)	0.004(3)	0.019(3)	0.012(2)
F3	0.039(3)	0.045(3)	0.077(4)	0.003(3)	0.024(3)	0.024(3)
F14	0.032(3)	0.045(3)	0.048(3)	0.030(3)	0.004(3)	0.001(2)
F24	0.033(3)	0.037(3)	0.087(5)	-0.007(3)	0.023(3)	-0.015(2)
O3	0.016(3)	0.027(3)	0.024(3)	0.005(2)	0.001(2)	0.005(2)
O1	0.033(3)	0.021(3)	0.042(4)	0.005(2)	0.024(3)	0.000(2)
F8	0.033(3)	0.084(4)	0.027(3)	-0.025(3)	-0.002(2)	-0.009(3)
F22	0.040(3)	0.040(3)	0.069(4)	-0.026(3)	0.002(3)	0.009(3)
F7	0.040(3)	0.105(5)	0.018(3)	-0.012(3)	0.010(2)	0.001(3)
N4	0.014(3)	0.018(3)	0.016(3)	0.001(2)	0.003(2)	0.000(2)
N1	0.018(3)	0.022(3)	0.013(3)	0.004(2)	0.002(2)	-0.001(2)
N5	0.015(3)	0.020(3)	0.016(3)	0.001(2)	0.004(2)	-0.002(2)
N2	0.016(3)	0.024(3)	0.014(3)	0.005(2)	0.003(2)	0.001(2)
N3	0.020(3)	0.021(3)	0.020(3)	-0.001(2)	0.010(3)	-0.005(2)
F23	0.047(4)	0.027(3)	0.136(7)	-0.027(4)	0.015(4)	-0.015(3)
C11	0.008(3)	0.020(4)	0.016(3)	-0.001(3)	0.001(3)	0.002(3)
C39	0.017(4)	0.017(3)	0.019(4)	0.005(3)	0.007(3)	0.002(3)
C42	0.012(3)	0.024(4)	0.022(4)	0.003(3)	0.007(3)	-0.002(3)
C45	0.013(3)	0.026(4)	0.018(4)	0.001(3)	0.004(3)	0.000(3)
C26	0.015(4)	0.033(4)	0.017(4)	-0.001(3)	0.009(3)	-0.004(3)
C38	0.017(4)	0.025(4)	0.012(3)	0.005(3)	0.000(3)	0.001(3)
C61	0.016(4)	0.024(4)	0.021(4)	0.006(3)	0.009(3)	0.005(3)
C40	0.010(3)	0.014(3)	0.019(3)	0.003(3)	0.008(3)	0.001(2)
C10	0.026(4)	0.025(4)	0.022(4)	0.005(3)	0.015(3)	0.006(3)
C7	0.017(4)	0.022(3)	0.013(3)	-0.002(3)	0.003(3)	0.003(3)
C5	0.015(4)	0.027(4)	0.024(4)	-0.004(3)	0.006(3)	-0.002(3)
C55	0.017(4)	0.031(4)	0.011(3)	0.001(3)	0.003(3)	0.004(3)
C9	0.036(5)	0.027(4)	0.028(4)	0.010(3)	0.019(4)	0.005(3)
C60	0.028(4)	0.029(4)	0.017(4)	0.002(3)	0.009(3)	0.006(3)
C46	0.018(4)	0.018(3)	0.013(3)	0.001(3)	0.005(3)	0.000(3)
C84	0.023(4)	0.025(4)	0.027(4)	-0.001(3)	0.007(3)	-0.002(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C24	0.016(4)	0.027(4)	0.021(4)	0.003(3)	0.009(3)	-0.001(3)
C25	0.022(4)	0.030(4)	0.020(4)	0.003(3)	0.008(3)	-0.006(3)
C35	0.022(4)	0.029(4)	0.024(4)	0.004(3)	0.000(3)	0.005(3)
C8	0.019(4)	0.032(4)	0.019(4)	0.004(3)	0.011(3)	0.003(3)
C62	0.016(4)	0.034(4)	0.016(4)	0.008(3)	0.003(3)	0.009(3)
C66	0.012(4)	0.036(4)	0.021(4)	0.007(3)	0.005(3)	0.000(3)
C79	0.017(4)	0.020(3)	0.021(4)	0.003(3)	0.004(3)	0.002(3)
C12	0.021(4)	0.025(4)	0.017(4)	-0.002(3)	0.010(3)	-0.007(3)
C43	0.025(4)	0.020(4)	0.022(4)	0.007(3)	0.009(3)	0.001(3)
C31	0.014(3)	0.033(4)	0.016(3)	0.004(3)	0.005(3)	0.004(3)
C32	0.020(4)	0.024(4)	0.029(4)	0.000(3)	0.004(3)	0.002(3)
C67	0.021(4)	0.023(4)	0.015(3)	-0.001(3)	0.004(3)	0.005(3)
C1	0.020(4)	0.028(4)	0.021(4)	-0.002(3)	0.004(3)	-0.002(3)
C41	0.016(4)	0.022(4)	0.014(3)	0.002(3)	0.004(3)	0.004(3)
C78	0.016(4)	0.025(4)	0.021(4)	0.000(3)	0.008(3)	0.002(3)
C6	0.019(4)	0.027(4)	0.015(3)	-0.003(3)	0.006(3)	0.000(3)
C2	0.016(4)	0.024(4)	0.019(4)	-0.006(3)	0.008(3)	-0.006(3)
C71	0.023(4)	0.041(5)	0.019(4)	0.005(3)	0.009(3)	0.004(3)
C47	0.014(4)	0.027(4)	0.015(3)	0.006(3)	0.006(3)	0.005(3)
C72	0.016(4)	0.029(4)	0.022(4)	0.002(3)	0.006(3)	0.004(3)
C13	0.028(4)	0.023(4)	0.025(4)	-0.001(3)	0.010(3)	-0.007(3)
C27	0.019(4)	0.024(4)	0.020(4)	0.004(3)	0.007(3)	0.001(3)
C44	0.019(4)	0.025(4)	0.018(4)	0.001(3)	0.004(3)	0.004(3)
C28	0.028(4)	0.029(4)	0.020(4)	-0.004(3)	0.004(3)	0.002(3)
C56	0.016(4)	0.028(4)	0.022(4)	-0.001(3)	0.002(3)	0.004(3)
C83	0.027(5)	0.027(4)	0.050(6)	-0.006(4)	0.004(4)	-0.011(4)
C74	0.019(4)	0.024(4)	0.018(4)	-0.001(3)	0.007(3)	0.000(3)
C77	0.021(4)	0.028(4)	0.015(3)	0.003(3)	0.006(3)	0.008(3)
C50	0.019(4)	0.022(4)	0.015(3)	0.000(3)	0.003(3)	0.005(3)
C30	0.019(4)	0.033(4)	0.020(4)	0.000(3)	0.001(3)	0.001(3)
C49	0.016(4)	0.024(4)	0.013(3)	0.002(3)	0.003(3)	0.008(3)
C68	0.020(4)	0.021(4)	0.019(4)	0.001(3)	0.007(3)	0.000(3)
C63	0.012(4)	0.037(5)	0.030(4)	0.004(3)	0.002(3)	-0.002(3)
C18	0.022(4)	0.038(5)	0.018(4)	-0.004(3)	0.004(3)	-0.003(3)
C73	0.013(3)	0.020(3)	0.017(3)	0.000(3)	0.003(3)	0.001(3)
C59	0.014(4)	0.053(6)	0.025(4)	-0.002(4)	0.004(3)	0.007(4)
C57	0.030(5)	0.024(4)	0.035(5)	-0.005(3)	0.011(4)	0.004(3)

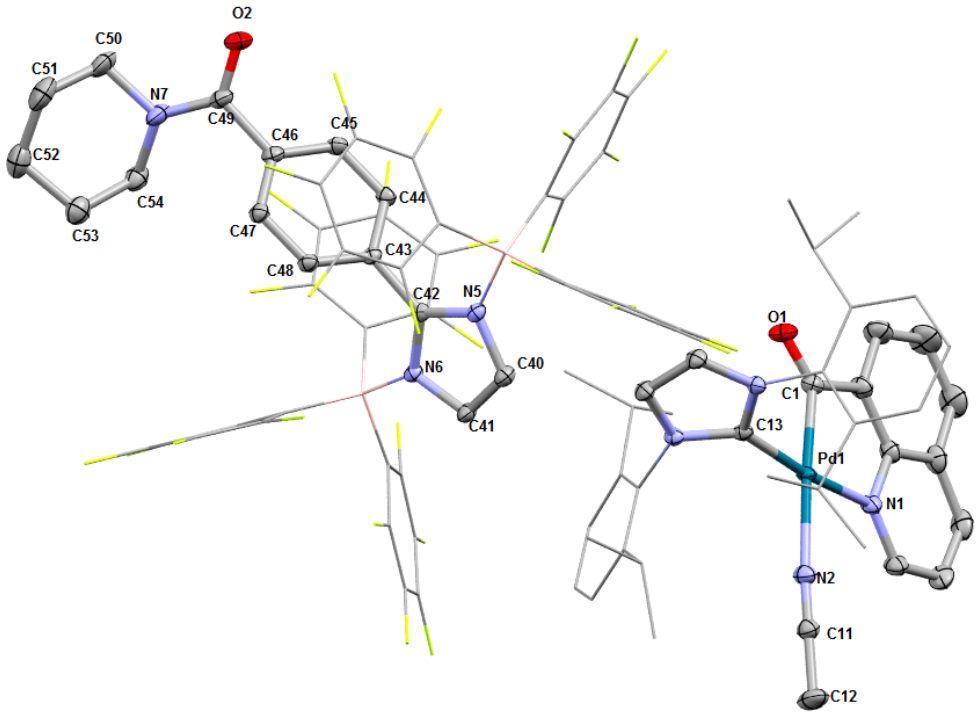
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C48	0.021(4)	0.031(4)	0.019(4)	0.011(3)	0.000(3)	0.010(3)
C80	0.019(4)	0.027(4)	0.026(4)	-0.003(3)	0.003(3)	0.003(3)
C70	0.030(5)	0.041(5)	0.012(3)	0.002(3)	0.003(3)	0.005(4)
C15	0.030(5)	0.037(5)	0.017(4)	-0.006(3)	0.004(3)	-0.012(4)
C54	0.022(4)	0.034(5)	0.024(4)	0.003(3)	0.009(3)	0.007(3)
C17	0.022(4)	0.030(4)	0.016(3)	0.001(3)	0.011(3)	-0.002(3)
C19	0.031(5)	0.036(5)	0.032(5)	-0.007(4)	0.012(4)	0.006(4)
C16	0.023(4)	0.041(5)	0.021(4)	0.001(3)	0.008(3)	-0.003(4)
C64	0.017(4)	0.025(4)	0.046(5)	0.008(4)	0.010(4)	-0.001(3)
C33	0.018(4)	0.034(5)	0.040(5)	-0.008(4)	0.008(4)	0.003(3)
C14	0.036(5)	0.032(4)	0.029(4)	-0.008(4)	0.011(4)	-0.007(4)
C36	0.029(5)	0.040(5)	0.041(5)	0.007(4)	0.019(4)	0.003(4)
C34	0.039(6)	0.042(5)	0.033(5)	0.012(4)	0.009(4)	0.015(4)
C76	0.007(3)	0.042(5)	0.023(4)	-0.002(3)	0.001(3)	-0.003(3)
C37	0.034(5)	0.036(5)	0.023(4)	0.001(3)	0.004(4)	0.010(4)
C58	0.022(4)	0.040(5)	0.037(5)	0.002(4)	0.008(4)	0.015(4)
C29	0.026(4)	0.032(4)	0.022(4)	-0.004(3)	0.008(3)	-0.004(3)
C51	0.015(4)	0.027(4)	0.023(4)	-0.009(3)	0.001(3)	0.004(3)
C20	0.024(4)	0.032(4)	0.029(4)	0.005(3)	0.007(4)	0.007(3)
C3	0.035(5)	0.019(4)	0.034(5)	0.003(3)	0.017(4)	0.003(3)
C65	0.024(4)	0.035(5)	0.036(5)	0.016(4)	0.010(4)	0.000(3)
C4	0.024(4)	0.030(4)	0.035(5)	-0.006(3)	0.013(4)	0.002(3)
C21	0.032(5)	0.021(4)	0.034(5)	0.001(3)	0.012(4)	-0.004(3)
C69	0.023(4)	0.040(5)	0.019(4)	0.006(3)	0.003(3)	0.008(3)
C75	0.020(4)	0.027(4)	0.028(4)	0.001(3)	0.007(3)	-0.006(3)
C81	0.026(5)	0.024(4)	0.047(5)	-0.017(4)	0.004(4)	0.005(3)
C22	0.052(6)	0.032(5)	0.039(5)	-0.005(4)	0.008(5)	0.002(4)
C52	0.016(4)	0.057(6)	0.025(4)	-0.015(4)	-0.003(3)	0.002(4)
B1	0.016(4)	0.020(4)	0.019(4)	0.004(3)	0.004(3)	0.006(3)
C53	0.032(5)	0.061(6)	0.018(4)	-0.008(4)	0.010(4)	0.005(4)
C23	0.059(7)	0.034(5)	0.049(6)	0.006(4)	0.023(5)	-0.006(5)
B2	0.014(4)	0.022(4)	0.019(4)	-0.001(3)	0.004(3)	0.001(3)
C82	0.037(6)	0.023(4)	0.069(7)	-0.012(4)	0.006(5)	-0.005(4)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 5839.

	x/a	y/b	z/c	U(eq)
H39	0.8100	-0.0420	0.5666	0.021
H42	0.7453	0.2215	0.5044	0.023
H45	0.5486	0.1532	0.3944	0.023
H38	0.7721	0.0033	0.6504	0.022
H10	0.5074	0.3371	0.4490	0.027
H5	0.3396	0.5414	0.4852	0.026
H9	0.4299	0.3192	0.4951	0.034
H46	0.6106	0.0745	0.4607	0.02
H24	0.6285	0.5295	0.1941	0.025
H25	0.6958	0.5996	0.2786	0.028
H35	0.6453	0.3712	0.2839	0.031
H8	0.3670	0.4119	0.5061	0.027
H43	0.6809	0.3021	0.4400	0.026
H32	0.5026	0.5666	0.2341	0.029
H28	0.5322	0.2809	0.1718	0.032
H30	0.4033	0.4341	0.1490	0.03
H18	0.6892	0.4324	0.4084	0.031
H48A	0.4465	0.2892	0.2699	0.037
H48B	0.4899	0.3549	0.2962	0.037
H48C	0.4403	0.3292	0.3297	0.037
H15	0.7796	0.6549	0.5349	0.034
H19A	0.7366	0.4643	0.3327	0.049
H19B	0.7696	0.3946	0.3655	0.049
H19C	0.8018	0.4699	0.3817	0.049
H16	0.7847	0.5354	0.5174	0.033
H33A	0.3757	0.5284	0.1958	0.047
H33B	0.4025	0.5990	0.2318	0.047
H33C	0.4164	0.5239	0.2649	0.047
H14	0.7150	0.7273	0.4638	0.038
H36A	0.6551	0.3354	0.1646	0.053
H36B	0.7122	0.3424	0.2234	0.053
H36C	0.6726	0.4107	0.1964	0.053
H34A	0.4972	0.5772	0.1303	0.057
H34B	0.4452	0.6264	0.1440	0.057
H34C	0.4274	0.5517	0.1113	0.057
H37A	0.6003	0.2560	0.2815	0.048
H37B	0.6716	0.2545	0.2848	0.048

	x/a	y/b	z/c	U(eq)
H37C	0.6216	0.2397	0.2216	0.048
H29	0.4322	0.3189	0.1322	0.032
H20A	0.8102	0.4329	0.4887	0.043
H20B	0.7697	0.3639	0.4661	0.043
H20C	0.7500	0.4190	0.5105	0.043
H3	0.4316	0.6560	0.3875	0.034
H4	0.3561	0.6482	0.4409	0.035
H21	0.6133	0.6731	0.3222	0.034
H22A	0.5778	0.7176	0.4051	0.063
H22B	0.5734	0.7757	0.3532	0.063
H22C	0.6278	0.7791	0.4147	0.063
H23A	0.7077	0.7781	0.3611	0.068
H23B	0.6558	0.7800	0.2977	0.068
H23C	0.7072	0.7199	0.3101	0.068

Crystal Structure Report for [1(MeCN)][IMP-pipA]



Thermal ellipsoid plot of 6038. Ellipsoids shown at 50% probability, $B(C_6F_5)_3$ and diisopropylphenyl substituents shown in wireframe. Hydrogen atoms and DCM solvate hidden for clarity.

A specimen of $C_{91}H_{63}B_2Cl_2F_{30}N_7O_2Pd$ was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å). The integration of the data using a triclinic unit cell yielded a total of 83372 reflections to a maximum θ angle of 27.92° (0.76 Å resolution), of which 22304 were independent (average redundancy 3.738, completeness = 99.0%, R_{int} = 1.72%, R_{sig} =1.55%) and 20376 (91.36%) were greater than $2\sigma(F^2)$. The final cell constants of a = 15.857(3) Å, b = 19.087(4) Å, c =19.142(4) Å, α = 115.371(3)°, β = 106.919(3)°, γ = 99.963(4)°, volume = 4701.8(16) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The final anisotropic full-matrix least-squares refinement on F^2 with 1225 variables converged at R1 = 6.98%, for the observed data and wR2 = 22.86% for all data. The goodness-of-fit was 1.069. The largest peak in the final difference electron density synthesis was 4.585 $e^-/Å^3$ and the largest hole was -2.494 $e^-/Å^3$ with an RMS deviation of 0.187 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.452 g/cm^3 and F(000), 2068 e^-. PLATON SQUEEZE was used to account for disordered solvent present in the crystal that could not be modelled.

Table 1. Sample and crystal data for 6038.

Identification code	6038	
Chemical formula	$C_{91}H_{63}B_2Cl_2F_{30}N_7O_2Pd$	
Formula weight	2055.40 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 15.857(3) Å	α = 115.371(3)°
	b = 19.087(4) Å	β = 106.919(3)°
	c = 19.142(4) Å	γ = 99.963(4)°
Volume	4701.8(16) $Å^3$	
Z	2	
Density (calculated)	1.452 g/cm^3	
Absorption coefficient	0.364 mm^{-1}	
F(000)	2068	

Table 2. Data collection and structure refinement for 6038.

Theta range for data collection	1.26 to 27.92°	
Index ranges	-20<=h<=20, -25<=k<=24, -25<=l<=25	
Reflections collected	83372	
Independent reflections	22304 [R(int) = 0.0172]	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	22304 / 0 / 1225	
Goodness-of-fit on F^2	1.069	
Δ/σ_{max}	0.001	
Final R indices	20376 data; I>2σ(I)	R1 = 0.0698, wR2 = 0.2234
	all data	R1 = 0.0741, wR2 = 0.2286
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.1393P)^2+18.3561P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	4.585 and -2.494 $eÅ^{-3}$	
R.M.S. deviation from mean	0.187 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for 6038.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij}tensor.

	x/a	y/b	z/c	U(eq)
Pd1	0.09993(2)	0.15823(2)	0.45396(2)	0.01364(9)
F15	0.12873(15)	0.33931(13)	0.20418(14)	0.0206(4)
F26	0.53731(15)	0.41775(14)	0.17793(13)	0.0217(4)
F10	0.43052(14)	0.57594(14)	0.24052(13)	0.0201(4)
F11	0.12449(16)	0.49569(14)	0.06665(13)	0.0211(4)
F5	0.39376(15)	0.59831(14)	0.38954(13)	0.0206(4)
F6	0.13216(15)	0.59699(14)	0.22368(15)	0.0219(4)
F1	0.06264(15)	0.46895(15)	0.26783(14)	0.0237(5)
F4	0.39189(17)	0.66582(15)	0.54291(14)	0.0275(5)
F30	0.30883(16)	0.19839(14)	0.90895(14)	0.0233(5)
F16	0.19514(16)	0.21600(15)	0.10891(16)	0.0254(5)
F28	0.52278(18)	0.41474(15)	0.92861(15)	0.0300(5)
F2	0.06281(18)	0.54203(17)	0.41855(17)	0.0320(6)
F21	0.36402(16)	0.19464(15)	0.20736(15)	0.0231(5)
F25	0.59282(17)	0.28350(18)	0.12009(18)	0.0319(6)
F22	0.48437(19)	0.15073(17)	0.29328(17)	0.0320(5)
F3	0.22675(19)	0.63953(15)	0.56063(15)	0.0303(5)
F14	0.96682(18)	0.22531(14)	0.07585(16)	0.0297(5)
F20	0.39324(18)	0.11787(15)	0.97558(17)	0.0305(5)
F27	0.60122(16)	0.48848(14)	0.10096(14)	0.0256(5)
F29	0.37762(18)	0.26782(15)	0.83562(14)	0.0307(5)
F12	0.96256(18)	0.38575(16)	0.94464(15)	0.0313(5)
F7	0.1825(2)	0.73908(15)	0.22616(17)	0.0316(5)
F9	0.47494(18)	0.71304(15)	0.23339(16)	0.0302(5)
F13	0.87888(17)	0.24954(15)	0.94621(16)	0.0317(5)
F8	0.3529(2)	0.79763(16)	0.2278(2)	0.0399(7)
F17	0.07035(18)	0.06568(19)	0.0187(2)	0.0419(7)
O1	0.98150(19)	0.05443(17)	0.27428(16)	0.0231(5)
F18	0.0998(2)	0.93787(18)	0.9029(2)	0.0528(9)
F23	0.6610(2)	0.1747(2)	0.2978(2)	0.0457(7)
O2	0.1465(2)	0.30576(19)	0.76224(18)	0.0325(7)
F24	0.7110(2)	0.2421(3)	0.2092(2)	0.0517(9)
N4	0.1607(2)	0.24788(17)	0.37043(18)	0.0142(5)
F19	0.2636(3)	0.96655(17)	0.8819(2)	0.0516(8)
N3	0.1980(2)	0.13821(17)	0.33411(18)	0.0140(5)
N1	0.0192(2)	0.11951(18)	0.50827(19)	0.0179(6)
N2	0.2083(2)	0.24992(19)	0.5773(2)	0.0201(6)

	x/a	y/b	z/c	U(eq)
N5	0.36127(19)	0.33609(18)	0.16575(18)	0.0136(5)
N6	0.30243(19)	0.43482(17)	0.21818(18)	0.0139(5)
N7	0.1396(2)	0.4347(2)	0.8264(2)	0.0245(7)
C43	0.2688(2)	0.3737(2)	0.0639(2)	0.0136(6)
C55	0.2297(2)	0.5246(2)	0.3189(2)	0.0143(6)
C74	0.4952(2)	0.3774(2)	0.0921(2)	0.0164(6)
C72	0.1339(2)	0.4255(2)	0.1449(2)	0.0148(6)
C7	0.9386(3)	0.0535(2)	0.4484(2)	0.0194(7)
C44	0.1912(2)	0.3067(2)	0.9948(2)	0.0158(6)
C60	0.3097(2)	0.5792(2)	0.3936(2)	0.0165(6)
C67	0.0894(2)	0.3531(2)	0.1405(2)	0.0174(6)
C59	0.3110(3)	0.6164(2)	0.4742(2)	0.0191(7)
C58	0.2269(3)	0.6030(2)	0.4831(2)	0.0217(7)
C73	0.4222(2)	0.3017(2)	0.0483(2)	0.0152(6)
C78	0.3837(2)	0.2687(2)	0.9610(2)	0.0173(6)
C13	0.1618(2)	0.1849(2)	0.3859(2)	0.0140(6)
C41	0.3534(2)	0.4250(2)	0.2831(2)	0.0168(6)
C2	0.9217(3)	0.0258(2)	0.3625(2)	0.0204(7)
C61	0.2757(2)	0.5753(2)	0.2255(2)	0.0157(6)
C40	0.3894(2)	0.3653(2)	0.2513(2)	0.0164(6)
C48	0.3100(2)	0.4379(2)	0.0541(2)	0.0154(6)
C57	0.1453(3)	0.5530(2)	0.4122(3)	0.0220(7)
C1	0.9939(2)	0.0717(2)	0.3455(2)	0.0170(6)
C16	0.2261(2)	0.0717(2)	0.3387(2)	0.0151(6)
C47	0.2729(2)	0.4370(2)	0.9781(2)	0.0169(6)
C46	0.1939(2)	0.3713(2)	0.9104(2)	0.0166(6)
C71	0.0877(2)	0.4322(2)	0.0755(2)	0.0176(6)
C75	0.5296(2)	0.4156(2)	0.0541(2)	0.0191(7)
C28	0.1393(2)	0.3187(2)	0.4204(2)	0.0164(6)
C21	0.3030(2)	0.0920(2)	0.4124(2)	0.0185(7)
C33	0.0459(3)	0.3150(2)	0.3966(2)	0.0197(7)
C81	0.5112(3)	0.1849(3)	0.2514(3)	0.0245(7)
C14	0.1919(3)	0.2392(2)	0.3072(2)	0.0181(6)
C37	0.9670(3)	0.2433(2)	0.3168(2)	0.0214(7)
C62	0.2182(3)	0.6232(2)	0.2256(2)	0.0194(7)
C68	0.0057(3)	0.2934(2)	0.0754(2)	0.0207(7)
C66	0.3636(2)	0.6110(2)	0.2319(2)	0.0174(6)

	x/a	y/b	z/c	U(eq)
C56	0.1476(2)	0.5145(2)	0.3327(2)	0.0176(6)
C42	0.3089(2)	0.3801(2)	0.1476(2)	0.0128(6)
C79	0.4706(2)	0.2449(2)	0.1602(2)	0.0174(6)
C29	0.2145(3)	0.3875(2)	0.4924(2)	0.0186(7)
C27	0.1459(3)	0.9558(2)	0.1194(2)	0.0248(8)
C17	0.1806(2)	0.9911(2)	0.2688(2)	0.0173(6)
C84	0.5613(3)	0.2535(3)	0.1632(3)	0.0232(7)
C15	0.2156(2)	0.1705(2)	0.2850(2)	0.0174(6)
C8	0.8961(3)	0.0473(3)	0.5581(3)	0.0284(8)
C30	0.1916(3)	0.4537(2)	0.5416(3)	0.0252(8)
C24	0.4177(3)	0.1934(3)	0.5672(3)	0.0293(8)
C45	0.1547(2)	0.3052(2)	0.9184(2)	0.0179(6)
C25	0.1049(3)	0.9706(2)	0.1858(2)	0.0190(7)
C11	0.2615(3)	0.2955(2)	0.6450(2)	0.0210(7)
C63	0.2421(3)	0.6967(2)	0.2263(2)	0.0236(7)
C85	0.3001(2)	0.1759(2)	0.0440(2)	0.0181(6)
C65	0.3897(3)	0.6839(2)	0.2310(2)	0.0228(7)
C69	0.9616(3)	0.3052(2)	0.0097(2)	0.0227(7)
C23	0.4260(3)	0.2209(3)	0.4526(3)	0.0276(8)
C70	0.0030(3)	0.3746(2)	0.0094(2)	0.0213(7)
C76	0.4904(3)	0.3788(2)	0.9670(2)	0.0212(7)
C80	0.4503(2)	0.2086(2)	0.2057(2)	0.0191(7)
C22	0.3598(3)	0.1815(2)	0.4812(2)	0.0206(7)
C90	0.2162(3)	0.1571(2)	0.0525(3)	0.0218(7)
C10	0.0362(3)	0.1486(2)	0.5893(2)	0.0233(7)
C38	0.8867(3)	0.2082(3)	0.3354(3)	0.0265(8)
C49	0.1563(3)	0.3677(2)	0.8266(2)	0.0204(7)
C9	0.9746(3)	0.1138(3)	0.6160(3)	0.0280(8)
C64	0.3286(3)	0.7270(2)	0.2280(3)	0.0270(8)
C54	0.1314(3)	0.5035(3)	0.8956(3)	0.0254(8)
C20	0.3296(3)	0.0275(2)	0.4165(3)	0.0247(8)
C6	0.8754(3)	0.0149(2)	0.4706(3)	0.0251(8)
C77	0.4167(3)	0.3045(2)	0.9204(2)	0.0209(7)
C26	0.0200(3)	0.8948(2)	0.1533(3)	0.0250(8)
C39	0.9305(3)	0.2703(3)	0.2522(3)	0.0306(9)
C18	0.2113(3)	0.9289(2)	0.2756(2)	0.0232(7)
C88	0.1639(3)	0.0141(3)	0.9475(3)	0.0364(10)

	x/a	y/b	z/c	U(eq)
C36	0.3611(3)	0.4216(3)	0.4695(3)	0.0332(9)
C53	0.1972(3)	0.5863(3)	0.9185(3)	0.0280(8)
C83	0.6249(3)	0.2308(3)	0.2090(3)	0.0324(9)
B2	0.3876(3)	0.2649(2)	0.1028(2)	0.0142(6)
C86	0.3123(3)	0.1078(2)	0.9861(3)	0.0248(8)
C12	0.3299(3)	0.3535(3)	0.7322(3)	0.0357(10)
C52	0.1765(3)	0.5954(3)	0.8399(3)	0.0333(9)
C32	0.0274(3)	0.3831(2)	0.4494(3)	0.0260(8)
C89	0.1492(3)	0.0782(3)	0.0058(3)	0.0289(9)
C34	0.3160(3)	0.3911(2)	0.5159(2)	0.0216(7)
C82	0.6006(3)	0.1967(3)	0.2536(3)	0.0305(9)
C87	0.2464(4)	0.0285(3)	0.9373(3)	0.0342(10)
C19	0.2835(3)	0.9465(2)	0.3488(3)	0.0277(8)
C3	0.8425(3)	0.9598(3)	0.2994(3)	0.0313(9)
C31	0.0989(3)	0.4508(3)	0.5206(3)	0.0296(9)
C50	0.1154(3)	0.4395(3)	0.7486(3)	0.0328(9)
C35	0.3761(3)	0.4462(3)	0.6115(3)	0.0385(11)
C4	0.7794(3)	0.9194(3)	0.3207(3)	0.0417(12)
C5	0.7952(3)	0.9461(3)	0.4036(3)	0.0366(10)
B1	0.2358(3)	0.4897(2)	0.2254(2)	0.0137(6)
C51	0.1789(4)	0.5211(3)	0.7670(3)	0.0378(10)
Cl1	0.3246(3)	0.7940(3)	0.4498(3)	0.1437(14)
C91	0.2307(17)	0.782(3)	0.434(2)	0.36(2)
Cl2	0.1501(6)	0.7648(5)	0.4662(5)	0.282(4)

Table 4. Bond lengths (Å) for 6038.

Pd1-C1	1.984(3)	Pd1-C13	2.015(3)
Pd1-N1	2.091(3)	Pd1-N2	2.155(3)
F15-C67	1.353(4)	F26-C74	1.355(4)
F10-C66	1.356(4)	F11-C71	1.351(4)
F5-C60	1.353(4)	F6-C62	1.354(4)
F1-C56	1.345(4)	F4-C59	1.342(4)
F30-C78	1.348(4)	F16-C90	1.357(5)
F28-C76	1.343(4)	F2-C57	1.338(4)
F21-C80	1.360(4)	F25-C84	1.344(4)
F22-C81	1.342(5)	F3-C58	1.343(4)

F14-C68	1.343(4)	F20-C86	1.350(5)
F27-C75	1.349(4)	F29-C77	1.341(4)
F12-C70	1.344(4)	F7-C63	1.346(5)
F9-C65	1.349(4)	F13-C69	1.345(4)
F8-C64	1.339(4)	F17-C89	1.344(5)
O1-C1	1.202(4)	F18-C88	1.341(5)
F23-C82	1.336(5)	O2-C49	1.232(5)
F24-C83	1.344(5)	N4-C13	1.356(4)
N4-C14	1.394(4)	N4-C28	1.447(4)
F19-C87	1.343(6)	N3-C13	1.363(4)
N3-C15	1.390(4)	N3-C16	1.444(4)
N1-C10	1.324(5)	N1-C7	1.374(5)
N2-C11	1.137(5)	N5-C42	1.356(4)
N5-C40	1.378(4)	N5-B2	1.598(5)
N6-C42	1.356(4)	N6-C41	1.378(4)
N6-B1	1.606(5)	N7-C49	1.351(5)
N7-C54	1.471(5)	N7-C50	1.473(5)
C43-C44	1.399(4)	C43-C48	1.399(5)
C43-C42	1.482(4)	C55-C60	1.397(5)
C55-C56	1.399(5)	C55-B1	1.662(5)
C74-C75	1.382(5)	C74-C73	1.396(5)
C72-C71	1.390(5)	C72-C67	1.394(5)
C72-B1	1.653(5)	C7-C6	1.409(5)
C7-C2	1.415(5)	C44-C45	1.393(5)
C60-C59	1.387(5)	C67-C68	1.383(5)
C59-C58	1.387(5)	C58-C57	1.367(6)
C73-C78	1.391(5)	C73-B2	1.646(5)
C78-C77	1.382(5)	C41-C40	1.352(5)
C2-C3	1.373(5)	C2-C1	1.516(5)
C61-C66	1.387(5)	C61-C62	1.397(5)
C61-B1	1.646(5)	C48-C47	1.394(5)
C57-C56	1.393(5)	C16-C17	1.404(5)
C16-C21	1.412(5)	C47-C46	1.392(5)
C46-C45	1.397(5)	C46-C49	1.507(5)
C71-C70	1.385(5)	C75-C76	1.379(5)
C28-C33	1.396(5)	C28-C29	1.414(5)
C21-C20	1.395(5)	C21-C22	1.520(5)
C33-C32	1.406(5)	C33-C37	1.509(5)

C81-C80	1.379(5)	C81-C82	1.381(6)
C14-C15	1.352(5)	C37-C39	1.536(6)
C37-C38	1.539(5)	C62-C63	1.382(5)
C68-C69	1.381(6)	C66-C65	1.391(5)
C79-C80	1.396(5)	C79-C84	1.401(5)
C79-B2	1.665(5)	C29-C30	1.397(5)
C29-C34	1.521(5)	C27-C25	1.535(5)
C17-C18	1.400(5)	C17-C25	1.520(5)
C84-C83	1.391(6)	C8-C9	1.355(6)
C8-C6	1.421(6)	C30-C31	1.390(6)
C24-C22	1.526(5)	C25-C26	1.535(5)
C11-C12	1.461(5)	C63-C64	1.379(6)
C85-C86	1.391(5)	C85-C90	1.391(5)
C85-B2	1.648(5)	C65-C64	1.378(6)
C69-C70	1.375(6)	C23-C22	1.544(5)
C76-C77	1.381(5)	C90-C89	1.391(5)
C10-C9	1.420(5)	C54-C53	1.532(6)
C20-C19	1.394(6)	C6-C5	1.421(6)
C18-C19	1.383(6)	C88-C89	1.369(7)
C88-C87	1.377(7)	C36-C34	1.519(6)
C53-C52	1.534(6)	C83-C82	1.371(6)
C86-C87	1.388(5)	C52-C51	1.521(7)
C32-C31	1.377(6)	C34-C35	1.534(6)
C3-C4	1.415(6)	C50-C51	1.530(7)
C4-C5	1.368(7)	Cl1-C91	1.385(18)
C91-Cl2	1.610(17)		

Table 5. Bond angles (°) for 6038.

C1-Pd1-C13	88.19(14)	C1-Pd1-N1	83.76(14)
C13-Pd1-N1	171.88(12)	C1-Pd1-N2	175.08(13)
C13-Pd1-N2	96.70(12)	N1-Pd1-N2	91.33(12)
C13-N4-C14	111.3(3)	C13-N4-C28	123.2(3)
C14-N4-C28	125.2(3)	C13-N3-C15	110.5(3)
C13-N3-C16	124.1(3)	C15-N3-C16	124.8(3)
C10-N1-C7	118.3(3)	C10-N1-Pd1	129.3(3)
C7-N1-Pd1	112.3(2)	C11-N2-Pd1	174.4(3)
C42-N5-C40	106.3(3)	C42-N5-B2	128.2(3)

C40-N5-B2	125.5(3)	C42-N6-C41	106.2(3)
C42-N6-B1	128.4(3)	C41-N6-B1	124.6(3)
C49-N7-C54	126.2(3)	C49-N7-C50	120.7(3)
C54-N7-C50	112.7(3)	C44-C43-C48	118.8(3)
C44-C43-C42	122.8(3)	C48-C43-C42	118.3(3)
C60-C55-C56	112.7(3)	C60-C55-B1	120.4(3)
C56-C55-B1	126.3(3)	F26-C74-C75	115.9(3)
F26-C74-C73	119.6(3)	C75-C74-C73	124.5(3)
C71-C72-C67	113.8(3)	C71-C72-B1	127.1(3)
C67-C72-B1	119.0(3)	N1-C7-C6	122.2(3)
N1-C7-C2	116.6(3)	C6-C7-C2	121.2(3)
C45-C44-C43	120.3(3)	F5-C60-C59	115.7(3)
F5-C60-C55	119.3(3)	C59-C60-C55	124.9(3)
F15-C67-C68	116.4(3)	F15-C67-C72	119.0(3)
C68-C67-C72	124.5(3)	F4-C59-C60	120.9(3)
F4-C59-C58	120.1(3)	C60-C59-C58	119.0(3)
F3-C58-C57	121.2(3)	F3-C58-C59	119.8(3)
C57-C58-C59	119.0(3)	C78-C73-C74	113.3(3)
C78-C73-B2	127.8(3)	C74-C73-B2	118.8(3)
F30-C78-C77	114.6(3)	F30-C78-C73	121.5(3)
C77-C78-C73	123.9(3)	N4-C13-N3	104.7(3)
N4-C13-Pd1	125.6(2)	N3-C13-Pd1	128.8(2)
C40-C41-N6	108.5(3)	C3-C2-C7	119.6(4)
C3-C2-C1	123.4(4)	C7-C2-C1	117.0(3)
C66-C61-C62	113.7(3)	C66-C61-B1	128.3(3)
C62-C61-B1	117.8(3)	C41-C40-N5	108.5(3)
C47-C48-C43	120.9(3)	F2-C57-C58	120.2(3)
F2-C57-C56	119.7(3)	C58-C57-C56	120.1(3)
O1-C1-C2	120.6(3)	O1-C1-Pd1	129.2(3)
C2-C1-Pd1	110.1(2)	C17-C16-C21	122.6(3)
C17-C16-N3	119.4(3)	C21-C16-N3	117.8(3)
C46-C47-C48	120.0(3)	C47-C46-C45	119.5(3)
C47-C46-C49	120.3(3)	C45-C46-C49	120.0(3)
F11-C71-C70	114.8(3)	F11-C71-C72	121.5(3)
C70-C71-C72	123.7(3)	F27-C75-C76	119.4(3)
F27-C75-C74	120.9(3)	C76-C75-C74	119.6(3)
C33-C28-C29	123.3(3)	C33-C28-N4	118.8(3)
C29-C28-N4	117.9(3)	C20-C21-C16	117.5(3)

C20-C21-C22	121.2(3)	C16-C21-C22	121.1(3)
C28-C33-C32	117.1(3)	C28-C33-C37	122.9(3)
C32-C33-C37	120.0(3)	F22-C81-C80	120.6(3)
F22-C81-C82	120.2(4)	C80-C81-C82	119.2(4)
C15-C14-N4	106.1(3)	C33-C37-C39	109.9(3)
C33-C37-C38	111.5(3)	C39-C37-C38	110.6(3)
F6-C62-C63	116.1(3)	F6-C62-C61	119.4(3)
C63-C62-C61	124.6(4)	F14-C68-C69	120.2(3)
F14-C68-C67	121.1(3)	C69-C68-C67	118.8(3)
F10-C66-C61	120.8(3)	F10-C66-C65	115.8(3)
C61-C66-C65	123.4(3)	F1-C56-C57	114.4(3)
F1-C56-C55	121.4(3)	C57-C56-C55	124.1(3)
N6-C42-N5	110.5(3)	N6-C42-C43	124.0(3)
N5-C42-C43	125.4(3)	C80-C79-C84	112.4(3)
C80-C79-B2	120.3(3)	C84-C79-B2	127.0(3)
C30-C29-C28	116.7(3)	C30-C29-C34	120.8(3)
C28-C29-C34	122.4(3)	C18-C17-C16	117.4(3)
C18-C17-C25	119.8(3)	C16-C17-C25	122.7(3)
F25-C84-C83	114.8(3)	F25-C84-C79	121.7(3)
C83-C84-C79	123.6(4)	C14-C15-N3	107.3(3)
C9-C8-C6	118.8(4)	C31-C30-C29	121.2(4)
C44-C45-C46	120.4(3)	C17-C25-C27	109.6(3)
C17-C25-C26	111.4(3)	C27-C25-C26	110.4(3)
N2-C11-C12	179.6(5)	F7-C63-C64	120.0(3)
F7-C63-C62	120.9(4)	C64-C63-C62	119.1(4)
C86-C85-C90	113.7(3)	C86-C85-B2	119.1(3)
C90-C85-B2	126.7(3)	F9-C65-C64	119.7(3)
F9-C65-C66	120.2(4)	C64-C65-C66	120.1(4)
F13-C69-C70	120.0(4)	F13-C69-C68	120.6(4)
C70-C69-C68	119.4(3)	F12-C70-C69	120.2(3)
F12-C70-C71	120.1(4)	C69-C70-C71	119.7(3)
F28-C76-C75	120.7(3)	F28-C76-C77	121.0(3)
C75-C76-C77	118.4(3)	F21-C80-C81	115.0(3)
F21-C80-C79	119.4(3)	C81-C80-C79	125.6(3)
C21-C22-C24	114.4(3)	C21-C22-C23	109.9(3)
C24-C22-C23	108.9(3)	F16-C90-C85	121.1(3)
F16-C90-C89	115.4(3)	C85-C90-C89	123.5(4)
N1-C10-C9	122.4(4)	O2-C49-N7	123.1(3)

O2-C49-C46	118.7(3)	N7-C49-C46	118.2(3)
C8-C9-C10	120.2(4)	F8-C64-C65	120.8(4)
F8-C64-C63	120.2(4)	C65-C64-C63	118.9(3)
N7-C54-C53	110.4(3)	C19-C20-C21	120.7(4)
C7-C6-C5	117.5(4)	C7-C6-C8	118.0(4)
C5-C6-C8	124.5(4)	F29-C77-C76	119.2(3)
F29-C77-C78	120.6(3)	C76-C77-C78	120.2(3)
C19-C18-C17	121.0(3)	F18-C88-C89	120.2(5)
F18-C88-C87	120.6(5)	C89-C88-C87	119.2(4)
C54-C53-C52	110.3(4)	F24-C83-C82	119.7(4)
F24-C83-C84	119.5(4)	C82-C83-C84	120.7(4)
N5-B2-C73	105.1(3)	N5-B2-C85	112.3(3)
C73-B2-C85	114.2(3)	N5-B2-C79	108.7(3)
C73-B2-C79	113.4(3)	C85-B2-C79	103.2(3)
F20-C86-C87	116.6(4)	F20-C86-C85	118.9(3)
C87-C86-C85	124.5(4)	C51-C52-C53	110.9(4)
C31-C32-C33	121.1(4)	F17-C89-C88	120.6(4)
F17-C89-C90	119.3(4)	C88-C89-C90	120.1(4)
C36-C34-C29	111.8(3)	C36-C34-C35	108.7(3)
C29-C34-C35	112.3(4)	F23-C82-C83	121.4(4)
F23-C82-C81	120.2(4)	C83-C82-C81	118.4(4)
F19-C87-C88	120.5(4)	F19-C87-C86	120.4(4)
C88-C87-C86	119.1(4)	C18-C19-C20	120.6(4)
C2-C3-C4	119.9(4)	C32-C31-C30	120.6(4)
N7-C50-C51	110.1(4)	C5-C4-C3	120.8(4)
C4-C5-C6	121.0(4)	N6-B1-C61	114.8(3)
N6-B1-C72	103.8(3)	C61-B1-C72	113.3(3)
N6-B1-C55	109.7(3)	C61-B1-C55	102.6(3)
C72-B1-C55	113.0(3)	C52-C51-C50	112.0(4)
Cl1-C91-Cl2	145.3(16)		

Table 6. Anisotropic atomic displacement parameters (Å^2) for 6038.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Pd1	0.01447(14)	0.01284(14)	0.01035(13)	0.00389(10)	0.00577(10)	0.00176(10)
F15	0.0227(10)	0.0206(10)	0.0210(10)	0.0131(9)	0.0092(8)	0.0060(8)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F26	0.0205(10)	0.0215(10)	0.0117(9)	0.0037(8)	0.0053(8)	-0.0029(8)
F10	0.0157(9)	0.0236(10)	0.0171(10)	0.0088(8)	0.0062(8)	0.0036(8)
F11	0.0254(11)	0.0217(10)	0.0174(10)	0.0120(9)	0.0072(8)	0.0084(9)
F5	0.0155(9)	0.0230(10)	0.0164(10)	0.0066(8)	0.0059(8)	0.0014(8)
F6	0.0215(10)	0.0207(10)	0.0258(11)	0.0115(9)	0.0110(9)	0.0107(8)
F1	0.0151(10)	0.0287(11)	0.0218(11)	0.0085(9)	0.0086(8)	0.0054(9)
F4	0.0284(12)	0.0257(11)	0.0136(10)	0.0036(9)	0.0048(9)	0.0005(9)
F30	0.0213(10)	0.0188(10)	0.0156(10)	0.0037(8)	0.0041(8)	-0.0049(8)
F16	0.0185(10)	0.0290(12)	0.0392(13)	0.0220(11)	0.0173(10)	0.0092(9)
F28	0.0361(13)	0.0278(12)	0.0212(11)	0.0124(10)	0.0138(10)	-0.0032(10)
F2	0.0279(12)	0.0384(14)	0.0325(13)	0.0133(11)	0.0238(11)	0.0105(11)
F21	0.0206(10)	0.0315(12)	0.0322(12)	0.0225(10)	0.0176(9)	0.0131(9)
F25	0.0205(11)	0.0496(15)	0.0448(15)	0.0330(13)	0.0214(11)	0.0160(11)
F22	0.0385(14)	0.0419(14)	0.0382(14)	0.0312(12)	0.0221(12)	0.0233(12)
F3	0.0433(14)	0.0269(12)	0.0186(11)	0.0061(9)	0.0203(10)	0.0094(11)
F14	0.0309(12)	0.0176(11)	0.0293(12)	0.0069(9)	0.0119(10)	-0.0024(9)
F20	0.0349(13)	0.0225(11)	0.0349(13)	0.0093(10)	0.0233(11)	0.0102(10)
F27	0.0248(11)	0.0187(10)	0.0188(10)	0.0036(9)	0.0086(9)	-0.0080(9)
F29	0.0359(13)	0.0293(12)	0.0116(10)	0.0062(9)	0.0060(9)	-0.0049(10)
F12	0.0313(13)	0.0316(13)	0.0190(11)	0.0100(10)	-0.0016(9)	0.0130(10)
F7	0.0426(14)	0.0213(11)	0.0343(13)	0.0158(10)	0.0135(11)	0.0177(11)
F9	0.0302(12)	0.0272(12)	0.0274(12)	0.0129(10)	0.0138(10)	-0.0040(10)
F13	0.0193(11)	0.0245(12)	0.0256(12)	0.0002(10)	-0.0004(9)	0.0012(9)
F8	0.0574(18)	0.0229(12)	0.0472(16)	0.0237(12)	0.0249(14)	0.0089(12)
F17	0.0174(11)	0.0445(16)	0.068(2)	0.0399(16)	0.0124(12)	-0.0009(11)
O1	0.0212(12)	0.0256(13)	0.0129(11)	0.0041(10)	0.0061(10)	0.0040(10)
F18	0.0464(17)	0.0239(14)	0.0535(19)	0.0146(13)	0.0014(15)	-0.0172(12)
F23	0.0320(14)	0.069(2)	0.0581(19)	0.0471(18)	0.0163(13)	0.0304(15)
O2	0.0475(18)	0.0261(15)	0.0131(12)	0.0051(11)	0.0090(12)	0.0082(13)
F24	0.0213(13)	0.091(3)	0.079(2)	0.062(2)	0.0280(15)	0.0322(15)
N4	0.0156(13)	0.0148(13)	0.0127(12)	0.0064(11)	0.0071(10)	0.0054(10)
F19	0.070(2)	0.0174(12)	0.0446(17)	0.0003(12)	0.0244(16)	0.0043(13)
N3	0.0149(12)	0.0124(12)	0.0133(12)	0.0051(10)	0.0069(10)	0.0036(10)
N1	0.0222(14)	0.0158(13)	0.0169(14)	0.0072(11)	0.0120(12)	0.0052(11)
N2	0.0220(15)	0.0179(14)	0.0155(14)	0.0059(12)	0.0078(12)	0.0030(12)
N5	0.0119(12)	0.0167(13)	0.0138(13)	0.0086(11)	0.0063(10)	0.0044(10)
N6	0.0135(12)	0.0155(13)	0.0134(12)	0.0076(11)	0.0065(10)	0.0040(10)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N7	0.0296(17)	0.0317(17)	0.0164(14)	0.0146(13)	0.0095(13)	0.0137(14)
C43	0.0129(14)	0.0160(14)	0.0120(14)	0.0064(12)	0.0065(12)	0.0049(12)
C55	0.0161(15)	0.0135(14)	0.0149(15)	0.0073(12)	0.0077(12)	0.0062(12)
C74	0.0162(15)	0.0171(15)	0.0122(14)	0.0048(12)	0.0069(12)	0.0029(12)
C72	0.0150(14)	0.0156(15)	0.0132(14)	0.0066(12)	0.0060(12)	0.0056(12)
C7	0.0181(16)	0.0175(16)	0.0225(17)	0.0098(14)	0.0098(14)	0.0048(13)
C44	0.0154(14)	0.0137(14)	0.0153(15)	0.0061(12)	0.0065(12)	0.0019(12)
C60	0.0184(15)	0.0162(15)	0.0161(15)	0.0080(13)	0.0088(13)	0.0060(12)
C67	0.0172(15)	0.0172(15)	0.0165(15)	0.0071(13)	0.0077(13)	0.0058(13)
C59	0.0247(17)	0.0152(15)	0.0142(15)	0.0058(13)	0.0078(13)	0.0045(13)
C58	0.033(2)	0.0184(16)	0.0176(16)	0.0080(14)	0.0169(15)	0.0102(14)
C73	0.0137(14)	0.0165(15)	0.0151(15)	0.0068(12)	0.0084(12)	0.0039(12)
C78	0.0155(15)	0.0148(15)	0.0154(15)	0.0044(13)	0.0061(12)	0.0010(12)
C13	0.0126(14)	0.0140(14)	0.0121(14)	0.0052(12)	0.0046(11)	0.0024(11)
C41	0.0196(15)	0.0204(16)	0.0132(14)	0.0096(13)	0.0077(12)	0.0084(13)
C2	0.0177(16)	0.0180(16)	0.0201(17)	0.0077(14)	0.0064(13)	0.0022(13)
C61	0.0189(15)	0.0145(14)	0.0118(14)	0.0064(12)	0.0055(12)	0.0036(12)
C40	0.0158(15)	0.0205(16)	0.0150(15)	0.0100(13)	0.0069(12)	0.0074(13)
C48	0.0142(14)	0.0165(15)	0.0127(14)	0.0066(12)	0.0050(12)	0.0021(12)
C57	0.0246(18)	0.0228(17)	0.0259(18)	0.0124(15)	0.0182(15)	0.0106(14)
C1	0.0158(15)	0.0162(15)	0.0157(15)	0.0060(13)	0.0060(12)	0.0049(12)
C16	0.0153(14)	0.0138(15)	0.0164(15)	0.0071(13)	0.0080(12)	0.0044(12)
C47	0.0181(15)	0.0172(15)	0.0141(15)	0.0082(13)	0.0069(13)	0.0022(12)
C46	0.0180(15)	0.0198(16)	0.0101(14)	0.0067(13)	0.0056(12)	0.0053(13)
C71	0.0186(15)	0.0165(15)	0.0165(15)	0.0073(13)	0.0066(13)	0.0076(13)
C75	0.0170(15)	0.0145(15)	0.0173(16)	0.0038(13)	0.0076(13)	-0.0028(12)
C28	0.0219(16)	0.0154(15)	0.0151(15)	0.0079(13)	0.0108(13)	0.0075(13)
C21	0.0170(15)	0.0178(16)	0.0169(16)	0.0067(13)	0.0063(13)	0.0044(13)
C33	0.0227(17)	0.0176(16)	0.0204(16)	0.0089(14)	0.0113(14)	0.0082(13)
C81	0.0275(19)	0.0293(19)	0.0254(18)	0.0174(16)	0.0138(15)	0.0141(16)
C14	0.0227(16)	0.0196(16)	0.0166(15)	0.0106(13)	0.0119(13)	0.0073(13)
C37	0.0177(16)	0.0234(17)	0.0225(17)	0.0096(15)	0.0093(14)	0.0097(14)
C62	0.0216(16)	0.0177(16)	0.0165(15)	0.0078(13)	0.0069(13)	0.0060(13)
C68	0.0196(16)	0.0158(16)	0.0215(17)	0.0053(14)	0.0101(14)	0.0029(13)
C66	0.0193(16)	0.0176(15)	0.0134(15)	0.0076(13)	0.0060(12)	0.0044(13)
C56	0.0187(16)	0.0174(15)	0.0176(16)	0.0082(13)	0.0091(13)	0.0070(13)
C42	0.0118(13)	0.0135(14)	0.0136(14)	0.0069(12)	0.0067(11)	0.0027(11)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C79	0.0147(15)	0.0175(15)	0.0200(16)	0.0086(13)	0.0085(13)	0.0059(12)
C29	0.0240(17)	0.0159(15)	0.0165(15)	0.0085(13)	0.0100(13)	0.0044(13)
C27	0.0302(19)	0.0209(17)	0.0190(17)	0.0073(14)	0.0108(15)	0.0056(15)
C17	0.0185(15)	0.0147(15)	0.0157(15)	0.0057(13)	0.0072(13)	0.0045(12)
C84	0.0183(16)	0.0293(19)	0.0289(19)	0.0169(16)	0.0138(15)	0.0104(14)
C15	0.0198(16)	0.0176(15)	0.0159(15)	0.0078(13)	0.0107(13)	0.0048(13)
C8	0.035(2)	0.030(2)	0.039(2)	0.0241(19)	0.0270(19)	0.0144(17)
C30	0.033(2)	0.0184(17)	0.0203(17)	0.0062(14)	0.0135(15)	0.0055(15)
C24	0.0244(19)	0.032(2)	0.0188(18)	0.0087(16)	0.0026(15)	0.0034(16)
C45	0.0165(15)	0.0157(15)	0.0140(15)	0.0044(12)	0.0038(12)	0.0014(12)
C25	0.0206(16)	0.0142(15)	0.0149(15)	0.0038(13)	0.0055(13)	0.0025(13)
C11	0.0234(17)	0.0207(17)	0.0165(17)	0.0087(14)	0.0077(14)	0.0052(14)
C63	0.033(2)	0.0166(16)	0.0191(17)	0.0081(14)	0.0083(15)	0.0099(15)
C85	0.0162(15)	0.0163(15)	0.0200(16)	0.0096(13)	0.0065(13)	0.0024(12)
C65	0.0262(18)	0.0200(17)	0.0154(16)	0.0072(14)	0.0084(14)	-0.0018(14)
C69	0.0156(16)	0.0200(17)	0.0178(16)	0.0004(14)	0.0034(13)	0.0043(13)
C23	0.0211(17)	0.0267(19)	0.0249(19)	0.0097(16)	0.0072(15)	-0.0010(15)
C70	0.0190(16)	0.0243(17)	0.0148(15)	0.0063(14)	0.0035(13)	0.0104(14)
C76	0.0239(17)	0.0206(17)	0.0185(17)	0.0095(14)	0.0121(14)	0.0018(14)
C80	0.0169(15)	0.0211(16)	0.0222(17)	0.0105(14)	0.0109(13)	0.0091(13)
C22	0.0165(15)	0.0191(16)	0.0173(16)	0.0050(13)	0.0047(13)	0.0021(13)
C90	0.0163(16)	0.0230(17)	0.0294(19)	0.0178(16)	0.0076(14)	0.0048(14)
C10	0.0307(19)	0.0199(17)	0.0188(17)	0.0077(14)	0.0138(15)	0.0068(15)
C38	0.0228(18)	0.0260(19)	0.030(2)	0.0124(16)	0.0125(16)	0.0087(15)
C49	0.0203(16)	0.0249(17)	0.0116(15)	0.0082(14)	0.0047(13)	0.0042(14)
C9	0.041(2)	0.030(2)	0.0251(19)	0.0158(17)	0.0240(18)	0.0141(18)
C64	0.040(2)	0.0165(17)	0.0230(18)	0.0117(15)	0.0111(16)	0.0046(15)
C54	0.0275(19)	0.033(2)	0.0253(19)	0.0183(17)	0.0146(16)	0.0160(16)
C20	0.0221(17)	0.0252(19)	0.0232(18)	0.0116(16)	0.0052(14)	0.0093(15)
C6	0.0234(18)	0.0245(18)	0.031(2)	0.0167(17)	0.0143(16)	0.0056(15)
C77	0.0223(17)	0.0203(16)	0.0121(15)	0.0049(13)	0.0063(13)	0.0007(14)
C26	0.0226(17)	0.0179(17)	0.0240(18)	0.0065(14)	0.0062(15)	0.0011(14)
C39	0.0254(19)	0.043(2)	0.030(2)	0.0223(19)	0.0123(16)	0.0152(18)
C18	0.0269(18)	0.0155(16)	0.0225(18)	0.0067(14)	0.0090(15)	0.0072(14)
C88	0.032(2)	0.0198(19)	0.037(2)	0.0143(18)	-0.0007(18)	-0.0082(17)
C36	0.030(2)	0.040(2)	0.033(2)	0.021(2)	0.0169(18)	0.0071(18)
C53	0.0273(19)	0.031(2)	0.029(2)	0.0177(17)	0.0111(16)	0.0127(16)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C83	0.0183(18)	0.049(3)	0.041(2)	0.027(2)	0.0161(17)	0.0170(18)
B2	0.0123(15)	0.0152(16)	0.0157(16)	0.0077(14)	0.0076(13)	0.0032(13)
C86	0.0273(19)	0.0174(17)	0.0255(19)	0.0089(15)	0.0115(15)	0.0030(14)
C12	0.037(2)	0.035(2)	0.0154(18)	0.0079(17)	0.0029(17)	-0.0053(18)
C52	0.028(2)	0.041(2)	0.043(2)	0.031(2)	0.0130(18)	0.0124(18)
C32	0.0279(19)	0.0241(18)	0.033(2)	0.0129(16)	0.0198(17)	0.0144(16)
C89	0.0175(17)	0.028(2)	0.041(2)	0.0245(19)	0.0049(16)	-0.0005(15)
C34	0.0215(17)	0.0175(16)	0.0216(17)	0.0105(14)	0.0051(14)	0.0032(13)
C82	0.0242(19)	0.040(2)	0.035(2)	0.0229(19)	0.0108(17)	0.0184(17)
C87	0.045(3)	0.0159(18)	0.028(2)	0.0056(16)	0.0114(19)	0.0015(17)
C19	0.033(2)	0.0211(18)	0.029(2)	0.0129(16)	0.0096(17)	0.0135(16)
C3	0.0239(19)	0.030(2)	0.0249(19)	0.0108(17)	0.0026(16)	-0.0034(16)
C31	0.038(2)	0.0197(18)	0.031(2)	0.0067(16)	0.0216(18)	0.0119(16)
C50	0.040(2)	0.044(2)	0.0191(18)	0.0205(18)	0.0080(17)	0.018(2)
C35	0.031(2)	0.042(3)	0.028(2)	0.018(2)	0.0022(18)	-0.0039(19)
C4	0.028(2)	0.035(2)	0.040(3)	0.014(2)	0.0045(19)	-0.0113(18)
C5	0.028(2)	0.034(2)	0.043(3)	0.021(2)	0.0146(19)	-0.0025(18)
B1	0.0144(15)	0.0140(16)	0.0137(16)	0.0078(13)	0.0058(13)	0.0048(13)
C51	0.043(3)	0.055(3)	0.035(2)	0.035(2)	0.020(2)	0.021(2)
Cl1	0.142(3)	0.162(4)	0.167(4)	0.112(3)	0.059(3)	0.072(3)
C91	0.26(2)	0.81(7)	0.61(5)	0.66(6)	0.34(3)	0.40(4)
Cl2	0.482(10)	0.360(8)	0.483(11)	0.378(9)	0.419(10)	0.378(8)

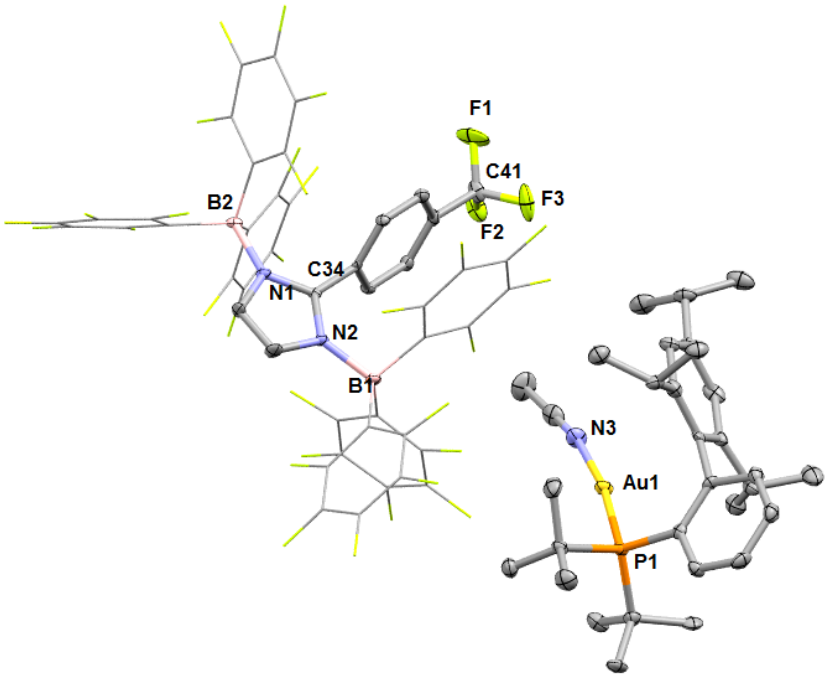
Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 6038.

	x/a	y/b	z/c	U(eq)
H44	0.1633	0.2619	0.0000	0.019
H41	0.3618	0.4551	0.3405	0.02
H40	0.4276	0.3466	0.2827	0.02
H48	0.3641	0.4828	0.1000	0.018
H47	0.3015	0.4811	-0.0276	0.02
H14	0.1957	0.2744	0.2843	0.022
H37	-0.0077	0.1987	0.2916	0.026
H27A	0.1971	0.0060	0.1393	0.037
H27B	0.0967	-0.0583	0.0657	0.037
H27C	0.1701	-0.0897	0.1108	0.037

	x/a	y/b	z/c	U(eq)
H15	0.2399	0.1484	0.2436	0.021
H8	-0.1445	0.0227	0.5756	0.034
H30	0.2401	0.5014	0.5901	0.03
H24A	0.3772	0.1644	0.5836	0.044
H24B	0.4446	0.2524	0.6098	0.044
H24C	0.4683	0.1710	0.5633	0.044
H45	0.1027	0.2590	-0.1285	0.021
H25	0.0833	0.0189	0.1959	0.023
H23A	0.4711	0.1922	0.4449	0.041
H23B	0.4598	0.2793	0.4958	0.041
H23C	0.3890	0.2161	0.3988	0.041
H22	0.3149	0.2120	0.4889	0.025
H10	0.0916	0.1944	0.6310	0.028
H38A	-0.0883	0.1931	0.3780	0.04
H38B	-0.1609	0.1592	0.2831	0.04
H38C	-0.1417	0.2500	0.3568	0.04
H9	-0.0115	0.1372	0.6747	0.034
H54A	0.1476	0.4970	-0.0540	0.03
H54B	0.0658	0.5025	-0.1220	0.03
H20	0.3796	0.0388	0.4660	0.03
H26A	-0.0303	-0.1131	0.1035	0.037
H26B	-0.0025	-0.0965	0.1979	0.037
H26C	0.0385	-0.1543	0.1377	0.037
H39A	-0.0967	0.3129	0.2749	0.046
H39B	-0.1177	0.2226	0.1991	0.046
H39C	-0.0175	0.2928	0.2414	0.046
H18	0.1822	-0.1263	0.2293	0.028
H36A	0.3238	0.3864	0.4082	0.05
H36B	0.4249	0.4195	0.4831	0.05
H36C	0.3639	0.4786	0.4872	0.05
H53A	0.2632	0.5894	-0.0588	0.034
H53B	0.1885	0.6321	-0.0370	0.034
H12A	0.3930	0.3537	0.7363	0.054
H12B	0.3151	0.3366	0.7702	0.054
H12C	0.3275	0.4090	0.7486	0.054
H52A	0.1138	0.6007	-0.1775	0.04
H52B	0.2236	0.6462	-0.1459	0.04

	x/a	y/b	z/c	U(eq)
H32	-0.0354	0.3824	0.4358	0.031
H34	0.3166	0.3338	0.4987	0.026
H19	0.3017	-0.0969	0.3529	0.033
H3	-0.1698	-0.0586	0.2416	0.038
H31	0.0848	0.4960	0.5556	0.036
H50A	0.0490	0.4357	-0.2730	0.039
H50B	0.1232	0.3927	-0.2956	0.039
H35A	0.3879	0.5043	0.6277	0.058
H35B	0.4360	0.4367	0.6254	0.058
H35C	0.3428	0.4329	0.6424	0.058
H4	-0.2747	-0.1269	0.2768	0.05
H5	-0.2481	-0.0819	0.4165	0.044
H51A	0.2442	0.5213	-0.2189	0.045
H51B	0.1585	0.5256	-0.2845	0.045
H91A	0.2005	0.7357	0.3746	0.436
H91B	0.2248	0.8308	0.4303	0.436

Crystal Structure Report for 2[IMP-CF_3]



Thermal ellipsoid plot of 5778. Ellipsoids shown at 50% probability, C_6F_5 rings shown in wireframe, DCM solvent and hydrogen atoms hidden for clarity.

A specimen of $C_{79}H_{58}AuB_2Cl_4F_{33}N_3P$, approximate dimensions 0.032 mm x 0.098 mm x 0.112 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The total exposure time was 10.06 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 37557 reflections to a maximum θ angle of 27.97° (0.76 Å resolution), of which 18286 were independent (average redundancy 2.054, completeness = 99.7%, R_{int} = 4.11%, R_{sig} = 10.70%) and 14639 (80.06%) were greater than $2\sigma(F^2)$. The final cell constants of a = 11.2277(11) Å, b = 21.034(2) Å, c = 17.1640(18) Å, β = 98.416(2)°, volume = 4009.9(7) $Å^3$, are based upon the refinement of the XYZ-centroids of 9181 reflections above 20 σ(I) with 4.555° < 2θ < 49.51°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.836. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.7980 and 0.9350. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21 1, with Z = 2 for the formula unit, $C_{79}H_{58}AuB_2Cl_4F_{33}N_3P$. The final anisotropic full-matrix least-squares refinement on F^2 with 1122 variables converged at R1 = 3.61%, for the observed data and wR2 = 7.59% for all data. The goodness-of-fit was 0.790. The largest peak in the final difference electron density synthesis was 1.011 $e^-/Å^3$ and the largest hole was -1.516 $e^-/Å^3$ with an RMS deviation of 0.098 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.713 g/cm^3 and F(000), 2044 e^-.

Table 1. Sample and crystal data for 5778.

Identification code	5778	
Chemical formula	$C_{79}H_{58}AuB_2Cl_4F_{33}N_3P$	
Formula weight	2067.64 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.032 x 0.098 x 0.112 mm	
Crystal system	monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 11.2277(11) Å	α = 90°
	b = 21.034(2) Å	β = 98.416(2)°
	c = 17.1640(18) Å	γ = 90°
Volume	4009.9(7) $Å^3$	
Z	2	
Density (calculated)	1.713 g/cm^3	
Absorption coefficient	2.112 mm^{-1}	
F(000)	2044	

Table 2. Data collection and structure refinement for 5778.

Theta range for data collection	1.54 to 27.97°	
Index ranges	-14<=h<=14, -27<=k<=27, -22<=l<=22	
Reflections collected	37557	
Independent reflections	18286 [R(int) = 0.0411]	
Coverage of independent reflections	99.7%	
Absorption correction	Multi-Scan	
Max. and min. transmission	0.9350 and 0.7980	
Structure solution technique	direct methods	
Structure solution program	XT, VERSION 2014/5	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	18286 / 1 / 1122	
Goodness-of-fit on F^2	0.790	
Final R indices	14639 data; I>2σ(I)	R1 = 0.0361, wR2 = 0.0692
	all data	R1 = 0.0561, wR2 = 0.0759
Weighting scheme	$w=1/[\sigma^2(F_o^2)]$ where $P=(F_o^2+2F_c^2)/3$	
Absolute structure parameter	0.003(4)	
Largest diff. peak and hole	1.011 and -1.516 $eÅ^{-3}$	
R.M.S. deviation from mean	0.098 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 5778.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Au1	0.72308(2)	0.61228(2)	0.14826(2)	0.01762(6)
P1	0.66174(15)	0.69651(7)	0.07307(10)	0.0128(3)
Cl3	0.1098(2)	0.28036(10)	0.20316(14)	0.0484(6)
Cl4	0.1516(2)	0.17002(12)	0.30281(14)	0.0553(7)
Cl2	0.1369(2)	0.57932(11)	0.74423(14)	0.0501(6)
F29	0.0254(3)	0.37851(16)	0.3886(2)	0.0181(8)
F23	0.1957(3)	0.39928(17)	0.7428(2)	0.0162(8)
F18	0.4117(3)	0.55602(16)	0.5418(2)	0.0174(8)
F10	0.1475(3)	0.70743(17)	0.1457(2)	0.0219(9)
F9	0.2307(3)	0.59498(14)	0.1915(2)	0.0174(8)
F28	0.3114(3)	0.27482(15)	0.5518(2)	0.0156(8)
F13	0.2838(3)	0.66747(16)	0.4569(2)	0.0177(8)
Cl1	0.2648(3)	0.67326(14)	0.84874(19)	0.0764(9)
F24	0.3041(3)	0.48420(15)	0.6542(2)	0.0176(8)
F12	0.2033(3)	0.78033(16)	0.4066(2)	0.0209(8)
F14	0.5057(3)	0.6080(2)	0.28888(17)	0.0177(7)
F2	0.6992(4)	0.2787(2)	0.4298(2)	0.0294(10)
F19	0.9005(3)	0.42669(17)	0.5167(2)	0.0175(8)
F17	0.6240(3)	0.59983(19)	0.60579(19)	0.0256(10)
F11	0.1285(3)	0.80166(16)	0.2508(2)	0.0213(9)
F32	0.0170(3)	0.17254(16)	0.5772(2)	0.0196(8)
F26	0.6489(3)	0.35735(18)	0.7082(2)	0.0252(9)
F27	0.5325(3)	0.26108(16)	0.6227(2)	0.0213(9)
F21	0.8049(3)	0.46023(19)	0.7692(2)	0.0245(9)
F33	0.1237(3)	0.27787(16)	0.6367(2)	0.0146(8)
F7	0.5331(3)	0.48057(17)	0.3115(2)	0.0196(8)
F8	0.5132(3)	0.39413(18)	0.1982(2)	0.0254(9)
F15	0.7187(3)	0.65329(18)	0.3558(2)	0.0244(9)
F20	0.7417(3)	0.45742(18)	0.6091(2)	0.0210(9)
F31	0.9087(4)	0.16828(18)	0.4244(2)	0.0265(9)
F30	0.9128(3)	0.2733(2)	0.3326(2)	0.0246(9)
F5	0.0937(4)	0.42163(18)	0.1525(2)	0.0277(9)
F25	0.5331(3)	0.47068(17)	0.7192(2)	0.0226(9)
F6	0.1091(3)	0.50649(17)	0.2685(2)	0.0184(8)
F22	0.0350(3)	0.42746(18)	0.8320(2)	0.0226(9)
F4	0.2953(4)	0.36427(18)	0.1159(2)	0.0298(10)
F16	0.7818(4)	0.64830(19)	0.5156(2)	0.0290(10)
F3	0.6174(4)	0.2835(2)	0.3101(3)	0.0431(13)

	x/a	y/b	z/c	U(eq)
F1	0.5548(4)	0.21589(19)	0.3875(3)	0.0492(14)
C17	0.6729(7)	0.5548(3)	0.9838(4)	0.0150(16)
C43	0.2133(6)	0.4803(3)	0.2528(4)	0.0149(14)
N3	0.7714(6)	0.5440(3)	0.2316(3)	0.0238(14)
C3	0.7774(6)	0.7612(3)	0.0889(4)	0.0180(15)
C34	0.2483(5)	0.4625(3)	0.4539(3)	0.0092(12)
N2	0.2387(5)	0.5214(2)	0.4230(3)	0.0108(10)
C55	0.2475(6)	0.6742(3)	0.3789(4)	0.0137(13)
N1	0.1674(4)	0.4541(2)	0.5035(3)	0.0115(10)
C16	0.6450(5)	0.6156(4)	0.9375(3)	0.0136(11)
C37	0.5426(6)	0.3741(3)	0.4525(4)	0.0137(13)
C56	0.2061(6)	0.7336(3)	0.3548(4)	0.0162(14)
C75	0.9642(6)	0.2211(3)	0.4532(4)	0.0176(14)
C65	0.3593(6)	0.3247(3)	0.5962(4)	0.0115(13)
C54	0.2572(5)	0.6223(3)	0.3286(3)	0.0117(14)
C36	0.4596(6)	0.4195(3)	0.4688(4)	0.0125(13)
C40	0.3023(6)	0.3621(3)	0.3886(3)	0.0116(12)
C47	0.4204(6)	0.4689(3)	0.2735(4)	0.0143(13)
C32	0.1460(6)	0.5509(3)	0.4538(4)	0.0173(14)
C69	0.8881(6)	0.4451(3)	0.7226(4)	0.0153(13)
C52	0.6418(6)	0.6279(2)	0.4010(3)	0.0146(14)
C42	0.3223(6)	0.5002(3)	0.2948(4)	0.0131(13)
C63	0.5342(5)	0.3651(3)	0.6740(4)	0.0151(13)
C70	0.0017(6)	0.4299(3)	0.7535(4)	0.0149(13)
C35	0.3390(6)	0.4137(3)	0.4368(3)	0.0116(13)
C62	0.4752(6)	0.4222(3)	0.6801(4)	0.0145(13)
C22	0.5791(6)	0.5128(3)	0.9938(4)	0.0180(14)
C19	0.8176(7)	0.4770(3)	0.0414(4)	0.0221(17)
C46	0.4137(6)	0.4232(3)	0.2154(4)	0.0177(14)
C58	0.1788(6)	0.6962(3)	0.2233(4)	0.0149(13)
C68	0.8551(6)	0.4446(3)	0.6417(4)	0.0148(13)
C6	0.8411(6)	0.7571(3)	0.1748(4)	0.0227(15)
C57	0.1702(6)	0.7441(3)	0.2753(4)	0.0142(14)
C26	0.7547(7)	0.3694(3)	0.0885(4)	0.0229(16)
C5	0.7280(7)	0.8288(3)	0.0756(4)	0.0206(16)
C33	0.1040(6)	0.5098(3)	0.5027(4)	0.0163(14)
C50	0.5942(5)	0.6011(3)	0.5268(3)	0.0169(15)
C71	0.0868(5)	0.4152(3)	0.7043(4)	0.0112(12)
C39	0.3852(6)	0.3172(3)	0.3727(4)	0.0163(14)
C30	0.9485(7)	0.5528(4)	0.9188(5)	0.0333(19)
C66	0.0606(6)	0.4151(3)	0.6230(4)	0.0117(13)

	x/a	y/b	z/c	U(eq)
C76	0.0194(6)	0.2238(3)	0.5308(4)	0.0148(13)
C14	0.5972(6)	0.6581(3)	0.8057(4)	0.0213(15)
C15	0.6265(5)	0.6081(5)	0.8557(3)	0.0187(12)
C41	0.5933(6)	0.2755(3)	0.3838(4)	0.0205(15)
C59	0.2216(6)	0.6370(3)	0.2492(4)	0.0145(13)
C53	0.5336(5)	0.6034(3)	0.3681(3)	0.0147(14)
C77	0.0753(5)	0.2784(3)	0.5590(4)	0.0128(13)
C51	0.6740(6)	0.6261(3)	0.4813(4)	0.0185(16)
C64	0.4746(6)	0.3168(3)	0.6309(4)	0.0144(13)
C29	0.8984(6)	0.5774(3)	0.9909(4)	0.0184(14)
C23	0.4482(6)	0.5270(3)	0.9635(4)	0.0177(14)
C11	0.6353(6)	0.6770(3)	0.9690(4)	0.0137(15)
C45	0.3032(7)	0.4071(3)	0.1744(4)	0.0217(15)
C73	0.0282(6)	0.3277(3)	0.4383(4)	0.0147(13)
C72	0.0869(6)	0.3328(3)	0.5147(4)	0.0130(13)
C9	0.5326(6)	0.7446(3)	0.1869(4)	0.0233(16)
C49	0.4859(6)	0.5778(3)	0.4910(4)	0.0142(13)
B2	0.1539(6)	0.3948(3)	0.5606(4)	0.0104(13)
C74	0.9695(6)	0.2746(3)	0.4074(4)	0.0179(14)
C61	0.3581(6)	0.4278(3)	0.6450(4)	0.0147(14)
C48	0.4496(6)	0.5766(3)	0.4107(4)	0.0130(13)
C31	0.9991(7)	0.5825(3)	0.0597(4)	0.0278(16)
C18	0.7938(6)	0.5363(3)	0.0071(4)	0.0166(14)
C13	0.5862(6)	0.7188(3)	0.8352(4)	0.0230(15)
C21	0.6097(6)	0.4536(3)	0.0293(4)	0.0186(14)
C12	0.6053(6)	0.7276(3)	0.9157(4)	0.0165(14)
C60	0.2916(5)	0.3801(3)	0.6024(3)	0.0116(13)
C27	0.8014(7)	0.3732(3)	0.1771(4)	0.0315(18)
C20	0.7261(6)	0.4345(3)	0.0542(4)	0.0189(14)
C25	0.3629(7)	0.5095(3)	0.0227(4)	0.0270(17)
C7	0.5130(6)	0.7216(3)	0.1015(4)	0.0165(14)
C4	0.8731(6)	0.7499(3)	0.0353(4)	0.0224(16)
C8	0.4444(7)	0.7721(3)	0.0485(4)	0.0281(17)
C10	0.4366(6)	0.6612(3)	0.0944(4)	0.0265(16)
C2	0.8192(8)	0.4749(4)	0.3567(4)	0.037(2)
C67	0.9403(6)	0.4284(3)	0.5951(4)	0.0123(13)
C44	0.2013(6)	0.4363(3)	0.1934(4)	0.0177(14)
C28	0.8461(7)	0.3332(3)	0.0457(5)	0.0324(19)
C78	0.0927(8)	0.1981(4)	0.2089(5)	0.040(2)
C24	0.4087(7)	0.4920(3)	0.8862(4)	0.0259(16)
B1	0.3174(7)	0.5544(3)	0.3640(4)	0.0124(14)

	x/a	y/b	z/c	U(eq)
C38	0.5044(6)	0.3237(3)	0.4042(4)	0.0154(14)
C1	0.7913(6)	0.5138(3)	0.2859(5)	0.0263(16)
C79	0.2598(8)	0.6313(4)	0.7589(6)	0.052(3)

Table 4. Bond lengths (Å) for 5778.

Au1-N3	2.044(6)	Au1-P1	2.2402(16)
P1-C11	1.814(7)	P1-C3	1.873(7)
P1-C7	1.882(7)	Cl3-C78	1.745(8)
Cl4-C78	1.753(8)	Cl2-C79	1.749(8)
F29-C73	1.365(7)	F23-C71	1.344(7)
F18-C49	1.370(6)	F10-C58	1.348(7)
F9-C59	1.343(7)	F28-C65	1.360(6)
F13-C55	1.350(7)	Cl1-C79	1.771(10)
F24-C61	1.352(7)	F12-C56	1.328(7)
F14-C53	1.353(6)	F2-C41	1.329(7)
F19-C67	1.355(7)	F17-C50	1.348(7)
F11-C57	1.344(7)	F32-C76	1.344(7)
F26-C63	1.345(7)	F27-C64	1.358(7)
F21-C69	1.353(7)	F33-C77	1.364(7)
F7-C47	1.357(7)	F8-C46	1.343(7)
F15-C52	1.352(6)	F20-C68	1.340(7)
F31-C75	1.332(7)	F30-C74	1.346(7)
F5-C44	1.342(7)	F25-C62	1.336(7)
F6-C43	1.356(7)	F22-C70	1.345(7)
F4-C45	1.341(7)	F16-C51	1.350(7)
F3-C41	1.341(8)	F1-C41	1.330(8)
C17-C22	1.405(9)	C17-C18	1.413(9)
C17-C16	1.513(10)	C43-C44	1.368(9)
C43-C42	1.390(9)	N3-C1	1.123(9)
C3-C4	1.532(9)	C3-C5	1.532(9)
C3-C6	1.544(9)	C34-N1	1.345(7)
C34-N2	1.346(7)	C34-C35	1.505(8)
N2-C32	1.381(8)	N2-B1	1.597(8)
C55-C56	1.376(8)	C55-C54	1.405(9)
N1-C33	1.370(7)	N1-B2	1.606(8)
C16-C15	1.398(7)	C16-C11	1.412(11)
C37-C38	1.375(9)	C37-C36	1.391(8)
C37-H37	0.95	C56-C57	1.382(9)
C75-C74	1.380(9)	C75-C76	1.385(9)
C65-C64	1.353(9)	C65-C60	1.404(8)

C54-C59	1.396(8)	C54-B1	1.658(9)
C36-C35	1.390(9)	C36-H36	0.95
C40-C39	1.381(8)	C40-C35	1.390(8)
C40-H40	0.95	C47-C42	1.378(8)
C47-C46	1.380(9)	C32-C33	1.338(8)
C32-H32	0.95	C69-C70	1.347(9)
C69-C68	1.384(9)	C52-C53	1.363(8)
C52-C51	1.373(8)	C42-B1	1.653(9)
C63-C64	1.372(9)	C63-C62	1.382(9)
C70-C71	1.399(8)	C62-C61	1.369(9)
C22-C21	1.406(9)	C22-C23	1.515(9)
C19-C18	1.389(9)	C19-C20	1.403(10)
C19-H19	0.95	C46-C45	1.377(10)
C58-C57	1.359(9)	C58-C59	1.383(8)
C68-C67	1.376(8)	C6-H6A	0.98
C6-H6B	0.98	C6-H6C	0.98
C26-C20	1.506(9)	C26-C27	1.535(11)
C26-C28	1.548(10)	C26-H26	1.0
C5-H5A	0.98	C5-H5B	0.98
C5-H5C	0.98	C33-H33	0.95
C50-C49	1.371(8)	C50-C51	1.376(8)
C71-C66	1.383(8)	C39-C38	1.376(9)
C39-H39	0.95	C30-C29	1.523(9)
C30-H30A	0.98	C30-H30B	0.98
C30-H30C	0.98	C66-C67	1.394(9)
C66-B2	1.659(9)	C76-C77	1.363(8)
C14-C15	1.366(10)	C14-C13	1.387(10)
C14-H14	0.95	C15-H15	0.95
C41-C38	1.500(8)	C53-C48	1.395(8)
C77-C72	1.390(8)	C29-C31	1.514(9)
C29-C18	1.515(9)	C29-H29	1.0
C23-C24	1.525(9)	C23-C25	1.539(9)
C23-H23	1.0	C11-C12	1.411(9)
C45-C44	1.380(9)	C73-C74	1.365(9)
C73-C72	1.383(9)	C72-B2	1.648(9)
C9-C7	1.529(9)	C9-H9A	0.98
C9-H9B	0.98	C9-H9C	0.98
C49-C48	1.379(9)	B2-C60	1.636(9)
C61-C60	1.392(9)	C48-B1	1.648(10)
C31-H31A	0.98	C31-H31B	0.98
C31-H31C	0.98	C13-C12	1.380(9)
C13-H13	0.95	C21-C20	1.374(9)

C21-H21	0.95	C12-H12	0.95
C27-H27A	0.98	C27-H27B	0.98
C27-H27C	0.98	C25-H25A	0.98
C25-H25B	0.98	C25-H25C	0.98
C7-C10	1.528(9)	C7-C8	1.529(9)
C4-H4A	0.98	C4-H4B	0.98
C4-H4C	0.98	C8-H8A	0.98
C8-H8B	0.98	C8-H8C	0.98
C10-H10A	0.98	C10-H10B	0.98
C10-H10C	0.98	C2-C1	1.460(10)
C2-H2A	0.98	C2-H2B	0.98
C2-H2C	0.98	C28-H28A	0.98
C28-H28B	0.98	C28-H28C	0.98
C78-H78A	0.99	C78-H78B	0.99
C24-H24A	0.98	C24-H24B	0.98
C24-H24C	0.98	C79-H79A	0.99
C79-H79B	0.99		

Table 5. Bond angles (°) for 5778.

N3-Au1-P1	170.66(16)	C11-P1-C3	108.5(3)
C11-P1-C7	107.2(3)	C3-P1-C7	112.4(3)
C11-P1-Au1	112.4(2)	C3-P1-Au1	110.0(2)
C7-P1-Au1	106.4(2)	C22-C17-C18	119.9(6)
C22-C17-C16	119.7(6)	C18-C17-C16	119.8(6)
F6-C43-C44	115.4(6)	F6-C43-C42	119.6(5)
C44-C43-C42	125.0(6)	C1-N3-Au1	168.2(6)
C4-C3-C5	109.0(5)	C4-C3-C6	107.3(6)
C5-C3-C6	107.5(5)	C4-C3-P1	109.5(5)
C5-C3-P1	115.1(5)	C6-C3-P1	108.2(4)
N1-C34-N2	110.5(5)	N1-C34-C35	124.9(5)
N2-C34-C35	124.6(5)	C34-N2-C32	106.4(5)
C34-N2-B1	129.1(5)	C32-N2-B1	124.5(5)
F13-C55-C56	115.6(6)	F13-C55-C54	119.3(5)
C56-C55-C54	125.1(6)	C34-N1-C33	106.1(5)
C34-N1-B2	128.5(5)	C33-N1-B2	125.1(5)
C15-C16-C11	118.6(7)	C15-C16-C17	115.0(8)
C11-C16-C17	126.4(5)	C38-C37-C36	119.4(6)
C38-C37-H37	120.3	C36-C37-H37	120.3
F12-C56-C55	120.8(6)	F12-C56-C57	120.7(5)
C55-C56-C57	118.5(6)	F31-C75-C74	121.7(6)
F31-C75-C76	120.7(6)	C74-C75-C76	117.6(6)

C64-C65-F28	115.2(5)	C64-C65-C60	124.2(6)
F28-C65-C60	120.6(5)	C59-C54-C55	113.0(5)
C59-C54-B1	126.2(5)	C55-C54-B1	120.5(5)
C35-C36-C37	120.2(6)	C35-C36-H36	119.9
C37-C36-H36	119.9	C39-C40-C35	120.2(6)
C39-C40-H40	119.9	C35-C40-H40	119.9
F7-C47-C42	120.8(6)	F7-C47-C46	114.9(5)
C42-C47-C46	124.2(6)	C33-C32-N2	107.7(5)
C33-C32-H32	126.1	N2-C32-H32	126.1
C70-C69-F21	121.2(6)	C70-C69-C68	119.5(5)
F21-C69-C68	119.2(6)	F15-C52-C53	121.1(5)
F15-C52-C51	119.3(6)	C53-C52-C51	119.6(5)
C47-C42-C43	113.4(6)	C47-C42-B1	129.1(6)
C43-C42-B1	117.5(5)	F26-C63-C64	120.4(5)
F26-C63-C62	120.7(6)	C64-C63-C62	118.9(6)
F22-C70-C69	120.8(5)	F22-C70-C71	118.8(6)
C69-C70-C71	120.4(6)	C36-C35-C40	119.3(5)
C36-C35-C34	120.7(5)	C40-C35-C34	120.0(6)
F25-C62-C61	121.4(6)	F25-C62-C63	119.9(6)
C61-C62-C63	118.8(6)	C17-C22-C21	118.0(6)
C17-C22-C23	122.7(6)	C21-C22-C23	119.1(6)
C18-C19-C20	122.6(7)	C18-C19-H19	118.7
C20-C19-H19	118.7	F8-C46-C45	119.4(6)
F8-C46-C47	121.1(6)	C45-C46-C47	119.4(6)
F10-C58-C57	119.1(6)	F10-C58-C59	120.3(6)
C57-C58-C59	120.6(6)	F20-C68-C67	120.4(6)
F20-C68-C69	121.0(5)	C67-C68-C69	118.5(6)
C3-C6-H6A	109.5	C3-C6-H6B	109.5
H6A-C6-H6B	109.5	C3-C6-H6C	109.5
H6A-C6-H6C	109.5	H6B-C6-H6C	109.5
F11-C57-C58	121.1(6)	F11-C57-C56	119.4(6)
C58-C57-C56	119.5(6)	C20-C26-C27	111.2(6)
C20-C26-C28	112.4(6)	C27-C26-C28	109.9(6)
C20-C26-H26	107.7	C27-C26-H26	107.7
C28-C26-H26	107.7	C3-C5-H5A	109.5
C3-C5-H5B	109.5	H5A-C5-H5B	109.5
C3-C5-H5C	109.5	H5A-C5-H5C	109.5
H5B-C5-H5C	109.5	C32-C33-N1	109.2(5)
C32-C33-H33	125.4	N1-C33-H33	125.4
F17-C50-C49	121.1(5)	F17-C50-C51	119.5(6)
C49-C50-C51	119.3(6)	F23-C71-C66	122.6(5)
F23-C71-C70	114.3(5)	C66-C71-C70	123.1(6)

C38-C39-C40	119.9(6)	C38-C39-H39	120.0
C40-C39-H39	120.0	C29-C30-H30A	109.5
C29-C30-H30B	109.5	H30A-C30-H30B	109.5
C29-C30-H30C	109.5	H30A-C30-H30C	109.5
H30B-C30-H30C	109.5	C71-C66-C67	113.5(5)
C71-C66-B2	126.2(6)	C67-C66-B2	120.1(5)
F32-C76-C77	120.8(6)	F32-C76-C75	119.4(5)
C77-C76-C75	119.7(6)	C15-C14-C13	120.4(6)
C15-C14-H14	119.8	C13-C14-H14	119.8
C14-C15-C16	122.1(8)	C14-C15-H15	118.9
C16-C15-H15	118.9	F2-C41-F1	106.8(6)
F2-C41-F3	105.5(5)	F1-C41-F3	106.0(6)
F2-C41-C38	113.2(6)	F1-C41-C38	113.2(6)
F3-C41-C38	111.6(6)	F9-C59-C58	114.5(5)
F9-C59-C54	122.1(5)	C58-C59-C54	123.3(6)
F14-C53-C52	116.8(5)	F14-C53-C48	118.7(5)
C52-C53-C48	124.4(6)	C76-C77-F33	116.0(5)
C76-C77-C72	125.0(6)	F33-C77-C72	119.0(6)
F16-C51-C52	121.1(5)	F16-C51-C50	120.0(6)
C52-C51-C50	118.9(6)	C65-C64-F27	120.1(6)
C65-C64-C63	120.4(5)	F27-C64-C63	119.4(6)
C31-C29-C18	114.0(6)	C31-C29-C30	109.6(6)
C18-C29-C30	110.1(5)	C31-C29-H29	107.6
C18-C29-H29	107.6	C30-C29-H29	107.6
C22-C23-C24	110.3(5)	C22-C23-C25	113.1(5)
C24-C23-C25	109.2(6)	C22-C23-H23	108.0
C24-C23-H23	108.0	C25-C23-H23	108.0
C12-C11-C16	117.8(6)	C12-C11-P1	117.2(5)
C16-C11-P1	125.0(5)	F4-C45-C46	120.2(6)
F4-C45-C44	120.7(6)	C46-C45-C44	119.1(6)
F29-C73-C74	115.6(6)	F29-C73-C72	119.8(5)
C74-C73-C72	124.6(6)	C73-C72-C77	112.7(6)
C73-C72-B2	129.4(5)	C77-C72-B2	117.6(6)
C7-C9-H9A	109.5	C7-C9-H9B	109.5
H9A-C9-H9B	109.5	C7-C9-H9C	109.5
H9A-C9-H9C	109.5	H9B-C9-H9C	109.5
F18-C49-C50	114.6(5)	F18-C49-C48	120.7(6)
C50-C49-C48	124.7(6)	N1-B2-C60	104.3(4)
N1-B2-C72	113.6(5)	C60-B2-C72	113.3(5)
N1-B2-C66	108.6(5)	C60-B2-C66	114.3(5)
C72-B2-C66	103.0(5)	F30-C74-C73	121.4(6)
F30-C74-C75	118.3(6)	C73-C74-C75	120.3(6)

F24-C61-C62	116.2(6)	F24-C61-C60	118.6(6)
C62-C61-C60	125.2(6)	C49-C48-C53	113.1(6)
C49-C48-B1	127.3(5)	C53-C48-B1	119.3(5)
C29-C31-H31A	109.5	C29-C31-H31B	109.5
H31A-C31-H31B	109.5	C29-C31-H31C	109.5
H31A-C31-H31C	109.5	H31B-C31-H31C	109.5
C19-C18-C17	119.0(6)	C19-C18-C29	119.0(6)
C17-C18-C29	121.9(6)	C12-C13-C14	118.7(6)
C12-C13-H13	120.7	C14-C13-H13	120.7
C20-C21-C22	123.7(6)	C20-C21-H21	118.2
C22-C21-H21	118.2	C13-C12-C11	122.4(6)
C13-C12-H12	118.8	C11-C12-H12	118.8
C61-C60-C65	112.5(6)	C61-C60-B2	119.6(5)
C65-C60-B2	127.7(5)	C26-C27-H27A	109.5
C26-C27-H27B	109.5	H27A-C27-H27B	109.5
C26-C27-H27C	109.5	H27A-C27-H27C	109.5
H27B-C27-H27C	109.5	C21-C20-C19	116.7(6)
C21-C20-C26	121.7(6)	C19-C20-C26	121.4(6)
C23-C25-H25A	109.5	C23-C25-H25B	109.5
H25A-C25-H25B	109.5	C23-C25-H25C	109.5
H25A-C25-H25C	109.5	H25B-C25-H25C	109.5
C10-C7-C8	107.6(6)	C10-C7-C9	109.8(5)
C8-C7-C9	109.9(5)	C10-C7-P1	104.8(4)
C8-C7-P1	115.4(5)	C9-C7-P1	109.2(5)
C3-C4-H4A	109.5	C3-C4-H4B	109.5
H4A-C4-H4B	109.5	C3-C4-H4C	109.5
H4A-C4-H4C	109.5	H4B-C4-H4C	109.5
C7-C8-H8A	109.5	C7-C8-H8B	109.5
H8A-C8-H8B	109.5	C7-C8-H8C	109.5
H8A-C8-H8C	109.5	H8B-C8-H8C	109.5
C7-C10-H10A	109.5	C7-C10-H10B	109.5
H10A-C10-H10B	109.5	C7-C10-H10C	109.5
H10A-C10-H10C	109.5	H10B-C10-H10C	109.5
C1-C2-H2A	109.5	C1-C2-H2B	109.5
H2A-C2-H2B	109.5	C1-C2-H2C	109.5
H2A-C2-H2C	109.5	H2B-C2-H2C	109.5
F19-C67-C68	115.3(6)	F19-C67-C66	119.9(5)
C68-C67-C66	124.9(6)	F5-C44-C43	122.0(6)
F5-C44-C45	119.2(6)	C43-C44-C45	118.9(6)
C26-C28-H28A	109.5	C26-C28-H28B	109.5
H28A-C28-H28B	109.5	C26-C28-H28C	109.5
H28A-C28-H28C	109.5	H28B-C28-H28C	109.5

Cl3-C78-Cl4	110.9(5)	Cl3-C78-H78A	109.5
Cl4-C78-H78A	109.5	Cl3-C78-H78B	109.5
Cl4-C78-H78B	109.5	H78A-C78-H78B	108.1
C23-C24-H24A	109.5	C23-C24-H24B	109.5
H24A-C24-H24B	109.5	C23-C24-H24C	109.5
H24A-C24-H24C	109.5	H24B-C24-H24C	109.5
N2-B1-C48	110.9(5)	N2-B1-C42	103.6(5)
C48-B1-C42	115.0(5)	N2-B1-C54	111.9(5)
C48-B1-C54	103.0(5)	C42-B1-C54	112.7(5)
C37-C38-C39	120.9(6)	C37-C38-C41	120.2(6)
C39-C38-C41	118.9(6)	N3-C1-C2	179.0(9)
Cl2-C79-Cl1	111.2(5)	Cl2-C79-H79A	109.4
Cl1-C79-H79A	109.4	Cl2-C79-H79B	109.4
Cl1-C79-H79B	109.4	H79A-C79-H79B	108.0

Table 6. Anisotropic atomic displacement parameters (Å^2) for 5778.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au1	0.02463(12)	0.01209(9)	0.01520(10)	0.00221(16)	-0.00026(8)	0.00359(16)
P1	0.0155(9)	0.0101(7)	0.0121(8)	0.0002(6)	-0.0001(6)	0.0011(7)
Cl3	0.0481(15)	0.0339(11)	0.0670(16)	0.0059(11)	0.0209(12)	0.0017(10)
Cl4	0.0472(15)	0.0698(16)	0.0495(14)	0.0247(13)	0.0086(11)	0.0156(13)
Cl2	0.0506(15)	0.0395(12)	0.0624(15)	-0.0043(11)	0.0158(12)	0.0010(11)
F29	0.016(2)	0.0194(19)	0.018(2)	0.0050(16)	0.0007(15)	0.0042(16)
F23	0.0105(19)	0.0204(18)	0.0174(19)	0.0003(16)	0.0018(14)	0.0048(16)
F18	0.021(2)	0.0173(18)	0.0152(19)	0.0012(15)	0.0058(16)	-0.0050(16)
F10	0.026(2)	0.0179(19)	0.019(2)	0.0042(16)	-0.0058(16)	0.0024(17)
F9	0.025(2)	0.012(2)	0.0147(18)	-0.0004(13)	0.0008(15)	0.0008(14)
F28	0.0137(19)	0.0092(16)	0.024(2)	-0.0029(15)	0.0015(15)	0.0027(14)
F13	0.027(2)	0.0136(18)	0.0134(19)	-0.0017(15)	0.0058(16)	0.0009(16)
Cl1	0.0539(19)	0.0660(17)	0.102(2)	-0.0195(17)	-0.0114(16)	-0.0019(15)
F24	0.020(2)	0.0087(16)	0.024(2)	-0.0015(15)	0.0056(16)	0.0006(15)
F12	0.028(2)	0.0083(17)	0.028(2)	-0.0028(16)	0.0085(18)	0.0016(16)
F14	0.0177(17)	0.0215(18)	0.0138(15)	0.004(2)	0.0022(12)	-0.001(2)
F2	0.018(2)	0.038(2)	0.030(2)	-0.006(2)	-0.0025(17)	0.0142(19)
F19	0.0118(19)	0.0237(19)	0.0166(19)	0.0046(16)	0.0012(15)	0.0041(16)
F17	0.028(2)	0.034(3)	0.0140(17)	-0.0033(17)	0.0002(14)	-0.0101(19)
F11	0.019(2)	0.0076(17)	0.035(2)	0.0020(16)	-0.0052(17)	0.0015(15)
F32	0.020(2)	0.0093(17)	0.030(2)	0.0015(16)	0.0058(17)	-0.0062(15)
F26	0.012(2)	0.027(2)	0.034(2)	0.0030(18)	-0.0053(17)	0.0020(17)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F27	0.012(2)	0.0161(18)	0.035(2)	0.0023(17)	0.0022(17)	0.0083(15)
F21	0.015(2)	0.033(2)	0.027(2)	-0.0080(18)	0.0078(17)	0.0037(18)
F33	0.016(2)	0.0121(17)	0.0151(19)	0.0032(15)	0.0006(15)	-0.0015(15)
F7	0.015(2)	0.0195(19)	0.025(2)	0.0001(16)	0.0048(16)	0.0028(16)
F8	0.026(2)	0.022(2)	0.031(2)	-0.0008(18)	0.0130(18)	0.0073(18)
F15	0.021(2)	0.028(2)	0.025(2)	0.0030(17)	0.0063(17)	-0.0120(18)
F20	0.009(2)	0.027(2)	0.027(2)	-0.0022(18)	0.0028(16)	0.0021(17)
F31	0.029(2)	0.022(2)	0.029(2)	-0.0102(18)	0.0045(18)	-0.0137(18)
F30	0.018(2)	0.037(2)	0.016(2)	-0.0025(19)	-0.0052(16)	-0.0021(19)
F5	0.025(2)	0.023(2)	0.032(2)	-0.0065(18)	-0.0082(18)	-0.0021(18)
F25	0.014(2)	0.023(2)	0.031(2)	-0.0078(17)	0.0017(17)	-0.0057(17)
F6	0.013(2)	0.0145(18)	0.027(2)	-0.0046(16)	0.0006(16)	0.0014(16)
F22	0.023(2)	0.030(2)	0.016(2)	-0.0022(17)	0.0052(17)	0.0041(17)
F4	0.046(3)	0.021(2)	0.024(2)	-0.0104(18)	0.009(2)	-0.0005(19)
F16	0.023(2)	0.035(2)	0.027(2)	-0.0003(19)	-0.0031(18)	-0.0109(19)
F3	0.038(3)	0.072(3)	0.021(2)	-0.002(2)	0.008(2)	0.034(3)
F1	0.033(3)	0.014(2)	0.102(4)	-0.010(2)	0.015(3)	0.009(2)
C17	0.024(4)	0.008(3)	0.013(4)	-0.004(3)	0.004(3)	-0.001(3)
C43	0.014(4)	0.008(3)	0.023(4)	0.001(3)	0.005(3)	0.003(3)
N3	0.031(4)	0.021(3)	0.018(3)	0.005(3)	-0.001(3)	0.008(3)
C3	0.021(4)	0.015(3)	0.018(4)	0.002(3)	0.003(3)	0.002(3)
C34	0.006(3)	0.008(3)	0.013(3)	-0.002(2)	-0.001(2)	0.000(2)
N2	0.012(3)	0.008(2)	0.013(3)	0.002(2)	0.002(2)	0.001(2)
C55	0.009(3)	0.013(3)	0.019(4)	0.003(3)	0.005(3)	0.000(3)
N1	0.010(3)	0.008(2)	0.016(3)	0.002(2)	0.002(2)	0.001(2)
C16	0.014(3)	0.014(3)	0.012(2)	0.006(4)	0.000(2)	0.000(4)
C37	0.012(3)	0.014(3)	0.015(3)	0.004(3)	0.004(3)	0.004(3)
C56	0.015(3)	0.009(3)	0.026(4)	-0.001(3)	0.007(3)	-0.001(3)
C75	0.015(3)	0.016(3)	0.023(4)	-0.009(3)	0.004(3)	-0.006(3)
C65	0.012(3)	0.008(3)	0.015(3)	-0.001(2)	0.004(3)	-0.005(2)
C54	0.009(3)	0.010(4)	0.016(3)	0.002(2)	0.003(2)	-0.001(2)
C36	0.015(3)	0.008(3)	0.015(3)	0.000(2)	0.003(3)	0.000(2)
C40	0.010(3)	0.011(3)	0.013(3)	0.000(2)	0.001(2)	-0.001(2)
C47	0.015(3)	0.013(3)	0.014(3)	0.003(3)	0.001(3)	0.000(3)
C32	0.019(4)	0.010(3)	0.024(4)	0.007(3)	0.007(3)	0.005(3)
C69	0.016(3)	0.015(3)	0.016(3)	-0.003(3)	0.009(3)	-0.003(3)
C52	0.020(3)	0.010(3)	0.016(3)	0.002(2)	0.009(3)	-0.004(2)
C42	0.014(3)	0.009(3)	0.017(3)	0.003(2)	0.004(3)	0.001(2)
C63	0.006(3)	0.023(3)	0.016(3)	0.004(3)	0.001(2)	0.000(3)
C70	0.024(4)	0.013(3)	0.009(3)	-0.002(2)	0.007(3)	0.002(3)
C35	0.017(3)	0.008(3)	0.011(3)	0.005(2)	0.006(3)	0.001(2)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C62	0.011(3)	0.016(3)	0.016(3)	-0.001(3)	0.002(3)	-0.004(3)
C22	0.021(4)	0.017(3)	0.016(3)	-0.002(3)	0.001(3)	0.004(3)
C19	0.016(4)	0.022(4)	0.025(4)	-0.007(3)	-0.009(3)	0.005(3)
C46	0.022(4)	0.016(3)	0.017(3)	0.001(3)	0.008(3)	0.008(3)
C58	0.011(3)	0.015(3)	0.017(3)	0.006(3)	-0.004(3)	-0.002(3)
C68	0.006(3)	0.018(3)	0.019(3)	0.001(3)	0.001(3)	0.000(3)
C6	0.022(4)	0.020(3)	0.024(4)	-0.005(3)	-0.005(3)	0.005(3)
C57	0.003(3)	0.007(3)	0.031(4)	0.006(3)	-0.001(3)	0.002(3)
C26	0.022(4)	0.013(3)	0.032(4)	0.004(3)	0.000(3)	0.002(3)
C5	0.029(4)	0.009(3)	0.022(4)	0.002(3)	-0.001(3)	0.000(3)
C33	0.018(4)	0.010(3)	0.022(4)	0.003(3)	0.010(3)	0.007(3)
C50	0.016(3)	0.019(4)	0.014(3)	-0.001(3)	-0.003(2)	-0.001(3)
C71	0.006(3)	0.006(3)	0.019(3)	0.002(2)	-0.006(2)	0.001(2)
C39	0.021(4)	0.012(3)	0.016(3)	0.001(3)	0.005(3)	0.000(3)
C30	0.025(4)	0.033(4)	0.042(5)	-0.014(4)	0.008(4)	-0.009(4)
C66	0.015(3)	0.003(3)	0.018(3)	0.000(2)	0.005(3)	-0.001(2)
C76	0.012(3)	0.012(3)	0.021(3)	0.001(3)	0.005(3)	-0.001(3)
C14	0.023(4)	0.027(4)	0.014(3)	-0.001(3)	0.003(3)	-0.003(3)
C15	0.020(3)	0.021(3)	0.015(3)	-0.004(4)	0.003(2)	-0.001(4)
C41	0.013(4)	0.026(4)	0.021(4)	-0.004(3)	-0.001(3)	0.009(3)
C59	0.011(3)	0.010(3)	0.023(4)	-0.001(3)	0.005(3)	-0.002(2)
C53	0.016(3)	0.014(4)	0.014(3)	0.000(3)	0.002(2)	0.001(3)
C77	0.009(3)	0.014(3)	0.016(3)	-0.001(3)	0.003(2)	0.004(2)
C51	0.014(3)	0.017(4)	0.023(3)	-0.004(3)	-0.002(2)	-0.011(2)
C64	0.010(3)	0.011(3)	0.023(4)	0.002(3)	0.006(3)	0.006(3)
C29	0.014(4)	0.016(3)	0.025(4)	-0.006(3)	0.002(3)	0.000(3)
C23	0.020(4)	0.015(3)	0.018(3)	0.003(3)	0.000(3)	-0.004(3)
C11	0.009(3)	0.017(3)	0.015(4)	0.001(3)	0.002(3)	0.000(3)
C45	0.034(4)	0.015(3)	0.017(4)	-0.004(3)	0.007(3)	-0.002(3)
C73	0.014(3)	0.014(3)	0.018(3)	0.004(3)	0.007(3)	0.004(3)
C72	0.011(3)	0.009(3)	0.019(3)	0.003(3)	0.003(3)	0.004(2)
C9	0.027(4)	0.024(4)	0.020(4)	-0.001(3)	0.007(3)	0.003(3)
C49	0.015(3)	0.009(3)	0.020(3)	0.002(3)	0.006(3)	-0.002(2)
B2	0.009(3)	0.007(3)	0.014(4)	0.001(3)	-0.002(3)	-0.001(3)
C74	0.013(4)	0.025(4)	0.016(3)	-0.006(3)	0.001(3)	0.001(3)
C61	0.020(4)	0.010(3)	0.015(3)	0.001(3)	0.005(3)	0.001(3)
C48	0.015(3)	0.009(3)	0.016(3)	0.001(2)	0.004(3)	-0.001(2)
C31	0.024(4)	0.027(4)	0.032(4)	-0.003(3)	0.003(3)	0.001(3)
C18	0.014(3)	0.014(3)	0.021(4)	-0.005(3)	0.002(3)	-0.001(3)
C13	0.027(4)	0.024(4)	0.017(4)	0.008(3)	0.001(3)	-0.006(3)
C21	0.021(4)	0.013(3)	0.021(4)	0.000(3)	-0.001(3)	0.000(3)

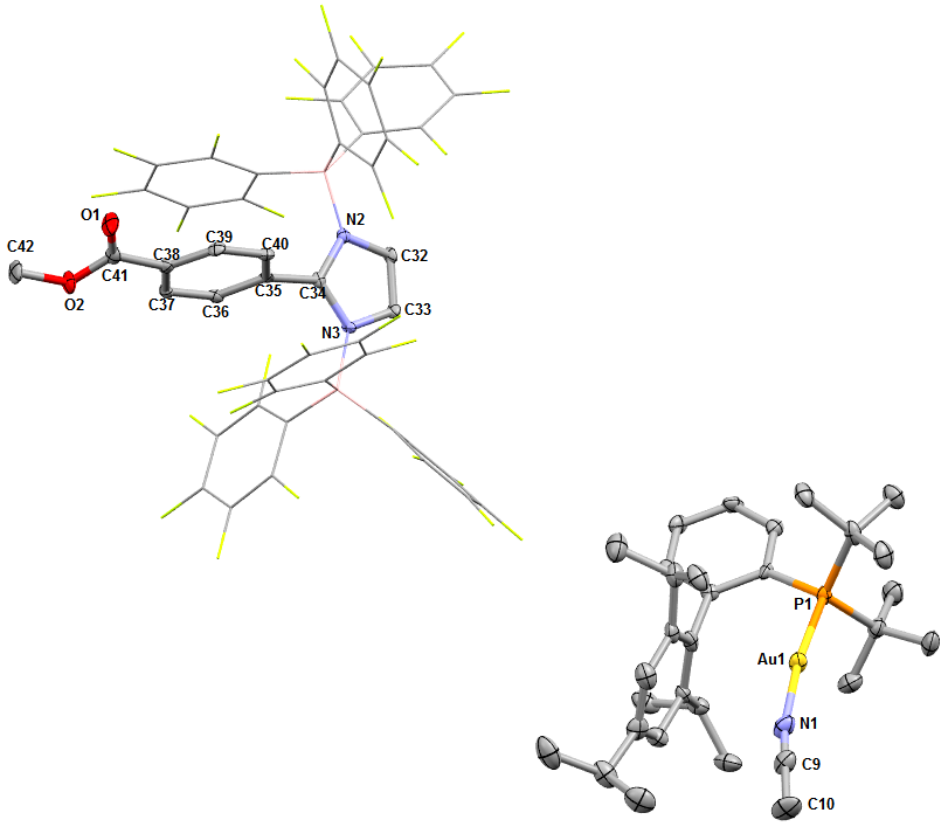
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C12	0.018(4)	0.015(3)	0.016(3)	-0.001(3)	0.000(3)	0.003(3)
C60	0.013(3)	0.009(3)	0.014(3)	0.004(2)	0.007(2)	-0.002(2)
C27	0.028(4)	0.025(4)	0.040(5)	0.011(3)	0.000(3)	0.005(3)
C20	0.020(4)	0.012(3)	0.024(4)	0.001(3)	0.002(3)	0.002(3)
C25	0.026(4)	0.027(4)	0.028(4)	0.005(3)	0.002(3)	0.000(3)
C7	0.019(4)	0.013(3)	0.017(3)	0.000(3)	0.002(3)	0.003(3)
C4	0.022(4)	0.017(3)	0.027(4)	-0.004(3)	0.000(3)	-0.009(3)
C8	0.025(4)	0.024(4)	0.035(4)	0.003(3)	0.003(3)	0.008(3)
C10	0.020(4)	0.032(4)	0.029(4)	-0.002(3)	0.008(3)	-0.004(3)
C2	0.039(5)	0.047(5)	0.024(4)	0.017(4)	-0.003(4)	0.011(4)
C67	0.013(3)	0.010(3)	0.014(3)	0.004(2)	0.001(3)	0.001(3)
C44	0.019(4)	0.011(3)	0.022(4)	0.002(3)	-0.003(3)	-0.002(3)
C28	0.028(5)	0.021(4)	0.045(5)	-0.003(3)	-0.006(4)	0.006(3)
C78	0.037(5)	0.034(4)	0.048(6)	0.008(4)	0.004(4)	0.002(4)
C24	0.025(4)	0.024(4)	0.028(4)	0.001(3)	-0.002(3)	-0.004(3)
B1	0.015(4)	0.007(3)	0.015(4)	0.002(3)	0.002(3)	0.001(3)
C38	0.015(3)	0.015(3)	0.018(3)	0.002(3)	0.008(3)	0.005(3)
C1	0.018(4)	0.025(4)	0.036(5)	-0.001(3)	0.001(3)	0.008(3)
C79	0.035(5)	0.041(6)	0.075(7)	0.024(5)	-0.001(5)	-0.006(4)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 5778.

	x/a	y/b	z/c	U(eq)
H37	0.6250	0.3780	0.4744	0.016
H36	0.4853	0.4545	0.5020	0.015
H40	0.2200	0.3576	0.3667	0.014
H32	0.1172	0.5928	0.4423	0.021
H19	0.8991	0.4647	0.0568	0.027
H6A	0.7815	0.7616	0.2108	0.034
H6B	0.9008	0.7912	0.1846	0.034
H6C	0.8815	0.7158	0.1835	0.034
H26	0.6782	0.3444	0.0819	0.027
H5A	0.6843	0.8325	0.0221	0.031
H5B	0.7948	0.8592	0.0827	0.031
H5C	0.6731	0.8380	0.1137	0.031
H33	0.0404	0.5180	0.5322	0.02
H39	0.3599	0.2818	0.3399	0.02
H30A	1.0154	0.5800	-0.0915	0.05
H30B	0.8850	0.5536	-0.1269	0.05
H30C	0.9773	0.5092	-0.0716	0.05

	x/a	y/b	z/c	U(eq)
H14	0.5844	0.6512	-0.2496	0.026
H15	0.6345	0.5670	-0.1658	0.022
H29	0.8666	0.6212	-0.0215	0.022
H23	0.4405	0.5736	-0.0471	0.021
H9A	0.5820	0.7137	0.2199	0.035
H9B	0.4546	0.7491	0.2055	0.035
H9C	0.5738	0.7858	0.1901	0.035
H31A	1.0387	0.5411	0.0690	0.042
H31B	0.9658	0.5955	0.1069	0.042
H31C	1.0579	0.6141	0.0477	0.042
H13	0.5658	0.7537	-0.1994	0.028
H21	0.5464	0.4253	0.0366	0.022
H12	0.5981	0.7692	-0.0640	0.02
H27A	0.8725	0.4008	0.1857	0.047
H27B	0.8231	0.3306	0.1973	0.047
H27C	0.7384	0.3908	0.2047	0.047
H25A	0.3564	0.4631	0.0258	0.04
H25B	0.2831	0.5277	0.0051	0.04
H25C	0.3948	0.5265	0.0747	0.04
H4A	0.9062	0.7070	0.0440	0.034
H4B	0.9379	0.7812	0.0473	0.034
H4C	0.8365	0.7544	-0.0199	0.034
H8A	0.4935	0.8107	0.0493	0.042
H8B	0.3687	0.7820	0.0679	0.042
H8C	0.4272	0.7559	-0.0055	0.042
H10A	0.4269	0.6459	0.0399	0.04
H10B	0.3574	0.6706	0.1091	0.04
H10C	0.4767	0.6285	0.1296	0.04
H2A	0.8164	0.4298	0.3421	0.056
H2B	0.7600	0.4833	0.3921	0.056
H2C	0.8999	0.4855	0.3834	0.056
H28A	0.9235	0.3556	0.0536	0.049
H28B	0.8157	0.3309	-0.0107	0.049
H28C	0.8570	0.2900	0.0672	0.049
H78A	0.1347	0.1772	0.1689	0.048
H78B	0.0062	0.1871	0.1973	0.048
H24A	0.4575	0.5063	-0.1534	0.039
H24B	0.3236	0.5011	-0.1324	0.039
H24C	0.4194	0.4461	-0.1055	0.039
H79A	0.2537	0.6619	-0.2853	0.062
H79B	0.3352	0.6068	-0.2405	0.062

Crystal Structure Report for 2[IMP-CO_2Me]



Thermal ellipsoid plot for 5864. Ellipsoids shown at 50% probability, $B(C_6F_5)_3$ substituents shown in wireframe, hydrogen atoms hidden for clarity.

A specimen of $C_{78}H_{57}AuB_2F_{30}N_3O_2P$ was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å). The integration of the data using a monoclinic unit cell yielded a total of 37159 reflections to a maximum θ angle of 27.96° (0.76Å resolution), of which 16341 were independent (average redundancy 2.274, completeness = 99.2%, R_{int} = 2.76%, R_{sig} =7.54%) and 14278 (87.38%) were greater than $2\sigma(F^2)$. The final cell constants of a = 11.4352(19) Å, b = 20.494(3) Å, c =17.462(3) Å, β = 98.794(4)°, volume = 4044.2(12) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The final anisotropic full-matrix least-squares refinement on F^2 with 1068 variables converged at R1 = 6.54%, for the observed data and wR2 = 18.89% for all data. The goodness-of-fit was 1.051. The largest peak in the final difference electron density synthesis was 9.775 $e^-/Å^3$ and the largest hole was -1.038 $e^-/Å^3$ with an RMS deviation of 0.220 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.550 g/cm^3 and F(000), 1872 e^-. PLATON SQUEEZE was used to model disordered solvent present in the crystal.

Table 1. Sample and crystal data for 5864.

Identification code	5864	
Chemical formula	$C_{78}H_{57}AuB_2F_{30}N_3O_2P$	
Formula weight	1887.82 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 11.4352(19) Å	α = 90°
	b = 20.494(3) Å	β = 98.794(4)°
	c = 17.462(3) Å	γ = 90°
Volume	4044.2(12) $Å^3$	
Z	2	
Density (calculated)	1.550 g/cm^3	
Absorption coefficient	1.955 mm^{-1}	
F(000)	1872	

Table 2. Data collection and structure refinement for 5864.

Theta range for data collection	1.18 to 27.96°	
Index ranges	-15<=h<=15, -27<=k<=22, -22<=l<=22	
Reflections collected	37159	
Independent reflections	16341 [R(int) = 0.0276]	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	16341 / 16 / 1068	
Goodness-of-fit on F^2	1.051	
Final R indices	14278 data; I>2σ(I)	R1 = 0.0654, wR2 = 0.1831
	all data	R1 = 0.0732, wR2 = 0.1889
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.1366P)^2]$ where $P=(F_o^2+2F_c^2)/3$	
Absolute structure parameter	0.014(3)	
Largest diff. peak and hole	9.775 and -1.038 $eÅ^{-3}$	
R.M.S. deviation from mean	0.220 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for 5864.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij}tensor.

	x/a	y/b	z/c	U(eq)
Au1	0.78001(3)	0.35628(3)	0.34133(2)	0.02101(13)
P1	0.8344(2)	0.27429(14)	0.42393(15)	0.0159(5)
F5	0.3702(5)	0.6778(3)	0.8495(3)	0.0156(12)
F1	0.4570(5)	0.5758(3)	0.0957(3)	0.0166(12)
F4	0.4766(5)	0.7866(3)	0.9081(4)	0.0190(13)
F20	0.9926(4)	0.3551(4)	0.2058(3)	0.0198(11)
F15	0.1884(5)	0.4661(3)	0.8343(4)	0.0179(13)
F30	0.3841(5)	0.4582(3)	0.2153(4)	0.0215(14)
F25	0.2611(6)	0.3699(3)	0.2996(3)	0.0213(15)
F16	0.0809(5)	0.3950(3)	0.9531(3)	0.0175(12)
F21	0.2097(6)	0.2855(3)	0.0418(4)	0.0201(14)
F6	0.5847(5)	0.5247(3)	0.9711(4)	0.0190(13)
F2	0.5623(6)	0.6849(4)	0.1537(4)	0.0234(16)
F10	0.2961(5)	0.5543(3)	0.7464(3)	0.0164(12)
F11	0.1819(5)	0.6824(3)	0.9298(4)	0.0149(12)
F19	0.7816(6)	0.3063(3)	0.1424(4)	0.0228(14)
F3	0.5714(6)	0.7924(3)	0.0617(4)	0.0244(15)
F22	0.2961(6)	0.1726(3)	0.0975(4)	0.0263(15)
F26	0.9670(5)	0.4829(3)	0.1774(4)	0.0209(13)
F13	0.8488(6)	0.5952(4)	0.7781(4)	0.0282(16)
F12	0.9645(5)	0.6956(3)	0.8609(4)	0.0205(13)
F24	0.3479(6)	0.2566(3)	0.3512(4)	0.0250(14)
F8	0.6809(6)	0.4963(4)	0.7225(4)	0.0290(16)
F9	0.4550(6)	0.5291(4)	0.6601(4)	0.0252(15)
F17	0.8724(5)	0.3481(4)	0.8935(4)	0.0281(16)
F14	0.9631(6)	0.4795(3)	0.7694(4)	0.0243(14)
F23	0.3731(6)	0.1564(3)	0.2524(5)	0.0274(16)
O1	0.7839(7)	0.6647(4)	0.0870(5)	0.0248(18)
F7	0.7425(5)	0.4961(4)	0.8811(4)	0.0236(15)
F27	0.9906(7)	0.5807(4)	0.2781(4)	0.0339(18)
F18	0.7182(6)	0.3045(4)	0.9852(4)	0.0288(16)
F29	0.4061(7)	0.5578(4)	0.3161(5)	0.0330(17)
F28	0.2084(8)	0.6193(4)	0.3495(5)	0.0385(19)
N3	0.3219(7)	0.4994(4)	0.9837(5)	0.0092(15)
O2	0.9334(7)	0.7331(4)	0.1310(5)	0.0213(17)
N2	0.2512(7)	0.4349(4)	0.0673(5)	0.0125(17)

	x/a	y/b	z/c	U(eq)
C78	0.2845(10)	0.4878(6)	0.2304(7)	0.019(2)
C1	0.7158(12)	0.2099(6)	0.4149(7)	0.024(3)
C34	0.2396(8)	0.4939(5)	0.0319(6)	0.0115(18)
C46	0.9598(9)	0.5876(6)	0.8128(6)	0.018(2)
C39	0.9482(8)	0.5812(5)	0.0310(6)	0.014(2)
C71	0.2922(9)	0.2219(5)	0.1472(7)	0.019(2)
C63	0.9010(8)	0.3503(7)	0.9710(6)	0.0173(19)
C36	0.1867(9)	0.5988(5)	0.0900(6)	0.0143(19)
N1	0.7373(10)	0.4246(5)	0.2560(6)	0.027(2)
C61	0.0459(8)	0.3811(5)	0.0841(5)	0.0123(18)
C49	0.4025(8)	0.6230(5)	0.9699(6)	0.0116(19)
C62	0.0099(9)	0.3756(5)	0.0033(6)	0.016(2)
C65	0.8564(9)	0.3289(6)	0.0969(6)	0.018(2)
C72	0.2465(9)	0.2818(5)	0.1203(6)	0.0138(19)
C50	0.4155(9)	0.6786(5)	0.9256(6)	0.014(2)
C41	0.8887(9)	0.6782(5)	0.0976(6)	0.016(2)
C47	0.0190(9)	0.6385(5)	0.8533(6)	0.0134(19)
C29	0.0413(10)	0.4530(6)	0.5162(7)	0.024(2)
C16	0.8431(8)	0.3669(5)	0.5473(5)	0.014(2)
C73	0.1746(9)	0.4633(5)	0.1920(6)	0.0131(19)
C66	0.9638(8)	0.3563(7)	0.1268(5)	0.0154(16)
C48	0.1360(9)	0.6295(5)	0.8884(6)	0.015(2)
C38	0.9858(10)	0.6339(5)	0.0779(6)	0.016(2)
C15	0.8577(10)	0.3815(6)	0.6273(6)	0.021(2)
C58	0.6010(9)	0.5087(6)	0.7690(6)	0.018(2)
C59	0.6310(9)	0.5097(5)	0.8475(7)	0.018(2)
C68	0.2715(9)	0.3248(5)	0.2449(7)	0.019(2)
C14	0.8847(11)	0.3359(5)	0.6832(7)	0.022(2)
C53	0.5146(9)	0.6834(5)	0.0780(7)	0.017(2)
C67	0.2386(8)	0.3366(5)	0.1658(6)	0.013(2)
C32	0.3459(9)	0.4034(5)	0.0416(6)	0.016(2)
C22	0.7018(10)	0.4446(6)	0.4678(6)	0.020(2)
C52	0.5207(10)	0.7369(5)	0.0317(7)	0.020(2)
C43	0.2013(9)	0.5742(5)	0.8830(6)	0.0127(19)
C33	0.3840(9)	0.4430(5)	0.9887(6)	0.0131(19)
C18	0.9142(10)	0.4673(5)	0.4832(6)	0.018(2)
C12	0.8886(10)	0.2551(6)	0.5835(6)	0.020(2)

	x/a	y/b	z/c	U(eq)
C37	0.1008(10)	0.6437(5)	0.1048(6)	0.017(2)
C74	0.0776(9)	0.4977(5)	0.2121(6)	0.017(2)
C11	0.8597(10)	0.3009(6)	0.5234(6)	0.019(2)
C57	0.4848(9)	0.5246(6)	0.7360(6)	0.018(2)
C17	0.8169(11)	0.4259(6)	0.4943(7)	0.021(2)
C54	0.4568(9)	0.6275(5)	0.0460(6)	0.0128(19)
C2	0.7611(13)	0.1408(7)	0.4375(10)	0.034(3)
C75	0.0874(11)	0.5490(6)	0.2628(7)	0.022(2)
C44	0.1356(9)	0.5243(5)	0.8414(6)	0.015(2)
C69	0.3181(9)	0.2658(6)	0.2746(7)	0.020(2)
C40	0.0318(9)	0.5358(5)	0.0143(6)	0.0143(19)
C45	0.0195(10)	0.5300(6)	0.8082(6)	0.019(2)
C76	0.1981(12)	0.5695(6)	0.2994(7)	0.025(2)
C20	0.7737(12)	0.5460(7)	0.4186(7)	0.027(3)
C56	0.4026(8)	0.5378(5)	0.7843(6)	0.0116(18)
C64	0.8257(9)	0.3269(6)	0.0176(7)	0.022(2)
C13	0.9033(11)	0.2682(6)	0.6598(7)	0.024(2)
C19	0.8891(11)	0.5270(6)	0.4455(7)	0.026(2)
C23	0.5953(11)	0.4041(6)	0.4831(8)	0.027(3)
C42	0.8474(11)	0.7778(6)	0.1564(8)	0.027(3)
C30	0.0756(13)	0.4915(7)	0.5934(8)	0.036(3)
C3	0.6616(13)	0.2061(7)	0.3270(8)	0.034(3)
C60	0.5462(9)	0.5238(5)	0.8932(6)	0.0121(19)
C55	0.4271(9)	0.5367(5)	0.8644(6)	0.010(2)
C70	0.3293(9)	0.2142(5)	0.2247(7)	0.018(2)
C24	0.5046(11)	0.3955(7)	0.4109(8)	0.030(3)
B2	0.3356(10)	0.5591(5)	0.9265(6)	0.010(2)
C51	0.4699(9)	0.7340(5)	0.9540(6)	0.015(2)
C6	0.0459(13)	0.1957(7)	0.4600(8)	0.032(3)
B1	0.1753(10)	0.4056(6)	0.1272(6)	0.012(2)
C7	0.0600(11)	0.3036(7)	0.4004(8)	0.032(3)
C8	0.9618(13)	0.2127(7)	0.3210(7)	0.031(3)
C4	0.6225(13)	0.2278(7)	0.4618(9)	0.035(3)
C5	0.9802(10)	0.2436(6)	0.4014(7)	0.024(2)
C31	0.1277(12)	0.4659(7)	0.4602(8)	0.032(3)
C35	0.1510(9)	0.5439(5)	0.0447(6)	0.0120(18)
C77	0.2974(11)	0.5377(6)	0.2815(7)	0.024(2)

	x/a	y/b	z/c	U(eq)
C26	0.7467(11)	0.6126(7)	0.3836(8)	0.030(3)
C27	0.7064(13)	0.6082(7)	0.2971(9)	0.039(3)
C10	0.6895(14)	0.4925(9)	0.1295(8)	0.042(4)
C21	0.6809(13)	0.5041(7)	0.4310(9)	0.030(3)
C28	0.6598(15)	0.6525(8)	0.4240(10)	0.044(4)
C9	0.7178(11)	0.4557(7)	0.2015(8)	0.030(3)
C25	0.5378(13)	0.4369(8)	0.5465(9)	0.041(3)

Table 4. Bond lengths (Å) for 5864.

Au1-N1	2.050(11)	Au1-P1	2.240(3)
P1-C11	1.802(11)	P1-C5	1.879(11)
P1-C1	1.882(14)	F5-C50	1.351(12)
F1-C54	1.369(12)	F4-C51	1.352(11)
F20-C66	1.368(10)	F15-C44	1.350(12)
F30-C78	1.352(12)	F25-C68	1.346(12)
F16-C62	1.344(11)	F21-C72	1.374(12)
F6-C60	1.365(12)	F2-C53	1.350(13)
F10-C56	1.338(11)	F11-C48	1.365(12)
F19-C65	1.336(11)	F3-C52	1.346(12)
F22-C71	1.338(13)	F26-C74	1.352(13)
F13-C46	1.329(12)	F12-C47	1.343(12)
F24-C69	1.342(13)	F8-C58	1.336(11)
F9-C57	1.321(13)	F17-C63	1.343(11)
F14-C45	1.345(13)	F23-C70	1.347(13)
O1-C41	1.216(13)	F7-C59	1.349(12)
F27-C75	1.345(13)	F18-C64	1.353(12)
F29-C77	1.360(14)	F28-C76	1.337(14)
N3-C33	1.353(12)	N3-C34	1.361(12)
N3-B2	1.600(12)	O2-C41	1.333(14)
O2-C42	1.463(13)	N2-C34	1.356(14)
N2-C32	1.392(12)	N2-B1	1.575(13)
C78-C77	1.351(17)	C78-C73	1.422(16)
C1-C4	1.487(19)	C1-C2	1.539(18)
C1-C3	1.566(18)	C34-C35	1.482(13)
C46-C45	1.373(17)	C46-C47	1.377(15)
C39-C38	1.384(16)	C39-C40	1.397(14)

C39-H39	0.95	C71-C70	1.365(17)
C71-C72	1.387(15)	C63-C64	1.359(15)
C63-C62	1.387(15)	C36-C37	1.399(14)
C36-C35	1.400(15)	C36-H36	0.95
N1-C9	1.137(17)	C61-C66	1.383(13)
C61-C62	1.412(14)	C61-B1	1.633(15)
C49-C54	1.382(14)	C49-C50	1.398(14)
C49-B2	1.642(15)	C65-C64	1.376(15)
C65-C66	1.379(15)	C72-C67	1.387(14)
C50-C51	1.352(15)	C41-C38	1.514(14)
C47-C48	1.396(14)	C29-C18	1.509(16)
C29-C31	1.516(16)	C29-C30	1.559(18)
C29-H29	1.0	C16-C15	1.414(13)
C16-C11	1.435(15)	C16-C17	1.525(15)
C73-C74	1.404(14)	C73-B1	1.637(15)
C48-C43	1.368(14)	C38-C37	1.342(16)
C15-C14	1.354(17)	C15-H15	0.95
C58-C59	1.361(16)	C58-C57	1.403(15)
C59-C60	1.377(14)	C68-C69	1.389(15)
C68-C67	1.396(15)	C14-C13	1.471(15)
C14-H14	0.95	C53-C52	1.371(16)
C53-C54	1.397(14)	C67-B1	1.681(15)
C32-C33	1.351(14)	C32-H32	0.95
C22-C17	1.381(17)	C22-C21	1.383(18)
C22-C23	1.531(17)	C52-C51	1.394(16)
C43-C44	1.405(15)	C43-B2	1.635(15)
C33-H33	0.95	C18-C19	1.397(17)
C18-C17	1.436(16)	C12-C13	1.344(15)
C12-C11	1.410(16)	C12-H12	0.95
C37-H37	0.95	C74-C75	1.366(16)
C57-C56	1.382(13)	C2-H2A	0.98
C2-H2B	0.98	C2-H2C	0.98
C75-C76	1.393(18)	C44-C45	1.370(15)
C69-C70	1.389(17)	C40-C35	1.395(14)
C40-H40	0.95	C76-C77	1.385(18)
C20-C19	1.387(18)	C20-C21	1.41(2)
C20-C26	1.508(19)	C56-C55	1.384(14)
C13-H13	0.95	C19-H19	0.95

C23-C24	1.516(17)	C23-C25	1.526(19)
C23-H23	1.0	C42-H42A	0.98
C42-H42B	0.98	C42-H42C	0.98
C30-H30A	0.98	C30-H30B	0.98
C30-H30C	0.98	C3-H3A	0.98
C3-H3B	0.98	C3-H3C	0.98
C60-C55	1.402(14)	C55-B2	1.683(14)
C24-H24A	0.98	C24-H24B	0.98
C24-H24C	0.98	C6-C5	1.530(18)
C6-H6A	0.98	C6-H6B	0.98
C6-H6C	0.98	C7-C5	1.533(19)
C7-H7A	0.98	C7-H7B	0.98
C7-H7C	0.98	C8-C5	1.525(17)
C8-H8A	0.98	C8-H8B	0.98
C8-H8C	0.98	C4-H4A	0.98
C4-H4B	0.98	C4-H4C	0.98
C31-H31A	0.98	C31-H31B	0.98
C31-H31C	0.98	C26-C27	1.51(2)
C26-C28	1.54(2)	C26-H26	1.0
C27-H27A	0.98	C27-H27B	0.98
C27-H27C	0.98	C10-C9	1.460(18)
C10-H10A	0.98	C10-H10B	0.98
C10-H10C	0.98	C21-H21	0.95
C28-H28A	0.98	C28-H28B	0.98
C28-H28C	0.98	C25-H25A	0.98
C25-H25B	0.98	C25-H25C	0.98

Table 5. Bond angles (°) for 5864.

N1-Au1-P1	173.2(3)	C11-P1-C5	106.7(5)
C11-P1-C1	107.5(5)	C5-P1-C1	113.5(6)
C11-P1-Au1	112.4(4)	C5-P1-Au1	106.5(4)
C1-P1-Au1	110.3(4)	C33-N3-C34	107.1(8)
C33-N3-B2	126.4(7)	C34-N3-B2	126.3(8)
C41-O2-C42	115.5(9)	C34-N2-C32	107.0(8)
C34-N2-B1	128.0(8)	C32-N2-B1	124.9(8)
C77-C78-F30	117.3(11)	C77-C78-C73	125.3(10)
F30-C78-C73	117.4(10)	C4-C1-C2	109.2(12)

C4-C1-C3	110.0(11)	C2-C1-C3	105.8(11)
C4-C1-P1	110.4(9)	C2-C1-P1	114.5(9)
C3-C1-P1	106.8(9)	N2-C34-N3	109.1(8)
N2-C34-C35	124.8(9)	N3-C34-C35	126.1(9)
F13-C46-C45	121.5(10)	F13-C46-C47	120.4(10)
C45-C46-C47	118.2(10)	C38-C39-C40	118.9(10)
C38-C39-H39	120.5	C40-C39-H39	120.5
F22-C71-C70	121.3(10)	F22-C71-C72	119.9(10)
C70-C71-C72	118.8(10)	F17-C63-C64	120.9(9)
F17-C63-C62	119.2(9)	C64-C63-C62	119.9(9)
C37-C36-C35	118.8(10)	C37-C36-H36	120.6
C35-C36-H36	120.6	C9-N1-Au1	170.0(11)
C66-C61-C62	113.0(9)	C66-C61-B1	120.4(8)
C62-C61-B1	126.2(8)	C54-C49-C50	114.0(9)
C54-C49-B2	127.3(9)	C50-C49-B2	118.5(9)
F16-C62-C63	116.1(9)	F16-C62-C61	121.0(9)
C63-C62-C61	123.0(9)	F19-C65-C64	120.0(9)
F19-C65-C66	122.0(9)	C64-C65-C66	118.0(9)
F21-C72-C67	119.4(9)	F21-C72-C71	115.3(9)
C67-C72-C71	125.3(9)	F5-C50-C51	117.1(9)
F5-C50-C49	118.5(9)	C51-C50-C49	124.4(9)
O1-C41-O2	124.2(9)	O1-C41-C38	124.7(10)
O2-C41-C38	111.0(9)	F12-C47-C46	120.8(9)
F12-C47-C48	120.0(9)	C46-C47-C48	119.2(9)
C18-C29-C31	113.9(10)	C18-C29-C30	109.4(10)
C31-C29-C30	111.6(11)	C18-C29-H29	107.2
C31-C29-H29	107.2	C30-C29-H29	107.2
C15-C16-C11	119.1(10)	C15-C16-C17	114.4(9)
C11-C16-C17	126.5(9)	C74-C73-C78	112.3(10)
C74-C73-B1	128.6(10)	C78-C73-B1	118.9(9)
F20-C66-C65	116.0(9)	F20-C66-C61	118.2(9)
C65-C66-C61	125.8(9)	F11-C48-C43	121.7(9)
F11-C48-C47	113.1(9)	C43-C48-C47	125.2(10)
C37-C38-C39	121.5(9)	C37-C38-C41	123.0(10)
C39-C38-C41	115.5(10)	C14-C15-C16	123.0(11)
C14-C15-H15	118.5	C16-C15-H15	118.5
F8-C58-C59	121.6(9)	F8-C58-C57	119.2(9)
C59-C58-C57	119.1(9)	F7-C59-C58	120.7(9)

F7-C59-C60	119.6(10)	C58-C59-C60	119.7(10)
F25-C68-C69	113.7(10)	F25-C68-C67	122.9(10)
C69-C68-C67	123.4(10)	C15-C14-C13	118.6(10)
C15-C14-H14	120.7	C13-C14-H14	120.7
F2-C53-C52	120.7(10)	F2-C53-C54	120.4(10)
C52-C53-C54	119.0(10)	C72-C67-C68	113.2(9)
C72-C67-B1	120.9(9)	C68-C67-B1	125.3(9)
C33-C32-N2	106.9(9)	C33-C32-H32	126.5
N2-C32-H32	126.5	C17-C22-C21	119.2(11)
C17-C22-C23	122.3(10)	C21-C22-C23	118.3(11)
F3-C52-C53	120.3(10)	F3-C52-C51	120.4(10)
C53-C52-C51	119.3(10)	C48-C43-C44	112.6(9)
C48-C43-B2	127.5(9)	C44-C43-B2	119.5(9)
C32-C33-N3	109.7(8)	C32-C33-H33	125.2
N3-C33-H33	125.2	C19-C18-C17	118.3(11)
C19-C18-C29	117.8(10)	C17-C18-C29	123.7(10)
C13-C12-C11	125.7(11)	C13-C12-H12	117.1
C11-C12-H12	117.1	C38-C37-C36	121.0(10)
C38-C37-H37	119.5	C36-C37-H37	119.5
F26-C74-C75	116.3(9)	F26-C74-C73	119.7(10)
C75-C74-C73	124.0(11)	C12-C11-C16	116.0(10)
C12-C11-P1	120.0(9)	C16-C11-P1	123.8(8)
F9-C57-C56	120.2(9)	F9-C57-C58	120.8(9)
C56-C57-C58	119.0(10)	C22-C17-C18	120.6(11)
C22-C17-C16	120.8(10)	C18-C17-C16	117.8(11)
F1-C54-C49	121.0(9)	F1-C54-C53	115.2(9)
C49-C54-C53	123.8(10)	C1-C2-H2A	109.5
C1-C2-H2B	109.5	H2A-C2-H2B	109.5
C1-C2-H2C	109.5	H2A-C2-H2C	109.5
H2B-C2-H2C	109.5	F27-C75-C74	120.7(11)
F27-C75-C76	118.8(11)	C74-C75-C76	120.5(10)
F15-C44-C45	117.0(10)	F15-C44-C43	118.6(9)
C45-C44-C43	124.3(10)	F24-C69-C68	121.3(10)
F24-C69-C70	118.9(10)	C68-C69-C70	119.7(10)
C35-C40-C39	120.0(10)	C35-C40-H40	120.0
C39-C40-H40	120.0	F14-C45-C44	120.4(10)
F14-C45-C46	119.2(10)	C44-C45-C46	120.4(10)
F28-C76-C77	120.9(12)	F28-C76-C75	120.9(11)

C77-C76-C75	118.2(11)	C19-C20-C21	118.5(12)
C19-C20-C26	121.1(12)	C21-C20-C26	120.1(12)
F10-C56-C57	113.6(9)	F10-C56-C55	122.2(8)
C57-C56-C55	124.1(9)	F18-C64-C63	119.1(10)
F18-C64-C65	120.5(10)	C63-C64-C65	120.3(10)
C12-C13-C14	117.5(11)	C12-C13-H13	121.2
C14-C13-H13	121.2	C20-C19-C18	121.4(12)
C20-C19-H19	119.3	C18-C19-H19	119.3
C24-C23-C25	109.8(11)	C24-C23-C22	112.3(11)
C25-C23-C22	109.3(11)	C24-C23-H23	108.4
C25-C23-H23	108.4	C22-C23-H23	108.4
O2-C42-H42A	109.5	O2-C42-H42B	109.5
H42A-C42-H42B	109.5	O2-C42-H42C	109.5
H42A-C42-H42C	109.5	H42B-C42-H42C	109.5
C29-C30-H30A	109.5	C29-C30-H30B	109.5
H30A-C30-H30B	109.5	C29-C30-H30C	109.5
H30A-C30-H30C	109.5	H30B-C30-H30C	109.5
C1-C3-H3A	109.5	C1-C3-H3B	109.5
H3A-C3-H3B	109.5	C1-C3-H3C	109.5
H3A-C3-H3C	109.5	H3B-C3-H3C	109.5
F6-C60-C59	115.6(9)	F6-C60-C55	120.2(9)
C59-C60-C55	124.2(10)	C56-C55-C60	113.7(9)
C56-C55-B2	126.7(9)	C60-C55-B2	119.0(9)
F23-C70-C71	120.0(11)	F23-C70-C69	120.7(10)
C71-C70-C69	119.3(10)	C23-C24-H24A	109.5
C23-C24-H24B	109.5	H24A-C24-H24B	109.5
C23-C24-H24C	109.5	H24A-C24-H24C	109.5
H24B-C24-H24C	109.5	N3-B2-C43	105.1(7)
N3-B2-C49	113.8(8)	C43-B2-C49	113.6(8)
N3-B2-C55	108.9(7)	C43-B2-C55	112.7(8)
C49-B2-C55	102.9(7)	F4-C51-C50	121.2(9)
F4-C51-C52	119.3(10)	C50-C51-C52	119.5(10)
C5-C6-H6A	109.5	C5-C6-H6B	109.5
H6A-C6-H6B	109.5	C5-C6-H6C	109.5
H6A-C6-H6C	109.5	H6B-C6-H6C	109.5
N2-B1-C61	111.3(8)	N2-B1-C73	104.2(8)
C61-B1-C73	116.1(8)	N2-B1-C67	109.8(7)
C61-B1-C67	103.3(8)	C73-B1-C67	112.1(8)

C5-C7-H7A	109.5	C5-C7-H7B	109.5
H7A-C7-H7B	109.5	C5-C7-H7C	109.5
H7A-C7-H7C	109.5	H7B-C7-H7C	109.5
C5-C8-H8A	109.5	C5-C8-H8B	109.5
H8A-C8-H8B	109.5	C5-C8-H8C	109.5
H8A-C8-H8C	109.5	H8B-C8-H8C	109.5
C1-C4-H4A	109.5	C1-C4-H4B	109.5
H4A-C4-H4B	109.5	C1-C4-H4C	109.5
H4A-C4-H4C	109.5	H4B-C4-H4C	109.5
C8-C5-C6	109.5(10)	C8-C5-C7	108.8(10)
C6-C5-C7	106.8(11)	C8-C5-P1	109.3(9)
C6-C5-P1	115.8(8)	C7-C5-P1	106.4(8)
C29-C31-H31A	109.5	C29-C31-H31B	109.5
H31A-C31-H31B	109.5	C29-C31-H31C	109.5
H31A-C31-H31C	109.5	H31B-C31-H31C	109.5
C40-C35-C36	119.6(9)	C40-C35-C34	120.7(9)
C36-C35-C34	119.6(9)	C78-C77-F29	121.5(11)
C78-C77-C76	119.7(11)	F29-C77-C76	118.8(11)
C20-C26-C27	111.2(12)	C20-C26-C28	113.7(12)
C27-C26-C28	111.7(12)	C20-C26-H26	106.6
C27-C26-H26	106.6	C28-C26-H26	106.6
C26-C27-H27A	109.5	C26-C27-H27B	109.5
H27A-C27-H27B	109.5	C26-C27-H27C	109.5
H27A-C27-H27C	109.5	H27B-C27-H27C	109.5
C9-C10-H10A	109.5	C9-C10-H10B	109.5
H10A-C10-H10B	109.5	C9-C10-H10C	109.5
H10A-C10-H10C	109.5	H10B-C10-H10C	109.5
C22-C21-C20	121.9(13)	C22-C21-H21	119.0
C20-C21-H21	119.0	C26-C28-H28A	109.5
C26-C28-H28B	109.5	H28A-C28-H28B	109.5
C26-C28-H28C	109.5	H28A-C28-H28C	109.5
H28B-C28-H28C	109.5	N1-C9-C10	176.9(17)
C23-C25-H25A	109.5	C23-C25-H25B	109.5
H25A-C25-H25B	109.5	C23-C25-H25C	109.5
H25A-C25-H25C	109.5	H25B-C25-H25C	109.5

Table 6. Anisotropic atomic displacement parameters ($Å^2$) for 5864.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au1	0.0292(2)	0.0197(2)	0.01313(18)	0.0009(2)	-0.00006(13)	0.0054(2)
P1	0.0199(13)	0.0160(13)	0.0111(12)	-0.0003(10)	0.0003(10)	0.0038(10)
F5	0.018(3)	0.012(3)	0.016(3)	0.003(2)	0.002(2)	0.000(2)
F1	0.014(3)	0.018(3)	0.018(3)	0.004(2)	0.002(2)	0.007(2)
F4	0.014(3)	0.013(3)	0.029(3)	0.005(3)	0.004(2)	-0.004(2)
F20	0.019(2)	0.024(3)	0.018(3)	0.008(4)	0.005(2)	-0.002(4)
F15	0.015(3)	0.011(3)	0.028(3)	-0.002(3)	0.004(2)	0.002(2)
F30	0.013(3)	0.014(3)	0.037(4)	0.000(3)	0.001(3)	0.001(2)
F25	0.031(3)	0.016(4)	0.014(3)	0.003(2)	-0.003(2)	0.000(2)
F16	0.021(3)	0.019(3)	0.014(3)	0.003(2)	0.006(2)	-0.001(2)
F21	0.028(4)	0.016(3)	0.018(3)	-0.001(3)	0.008(3)	-0.003(3)
F6	0.015(3)	0.025(4)	0.017(3)	0.002(3)	0.004(2)	0.001(3)
F2	0.019(3)	0.033(4)	0.018(4)	-0.007(3)	0.002(3)	-0.001(3)
F10	0.011(3)	0.021(3)	0.017(3)	0.002(2)	0.001(2)	0.002(2)
F11	0.014(3)	0.008(3)	0.022(3)	-0.003(2)	0.000(2)	0.001(2)
F19	0.021(3)	0.024(4)	0.026(3)	-0.002(3)	0.011(3)	-0.009(3)
F3	0.022(3)	0.020(4)	0.031(4)	-0.008(3)	0.003(3)	-0.013(3)
F22	0.026(4)	0.013(3)	0.042(4)	-0.003(3)	0.015(3)	0.004(3)
F26	0.016(3)	0.020(3)	0.028(4)	0.005(3)	0.006(3)	0.006(3)
F13	0.020(3)	0.033(4)	0.030(4)	0.001(3)	-0.003(3)	0.006(3)
F12	0.016(3)	0.018(3)	0.027(3)	0.004(3)	0.002(2)	0.010(3)
F24	0.026(4)	0.023(4)	0.022(3)	0.008(3)	-0.009(3)	0.002(3)
F8	0.015(3)	0.046(5)	0.029(4)	-0.012(3)	0.011(3)	0.000(3)
F9	0.020(3)	0.039(4)	0.018(3)	-0.003(3)	0.006(3)	0.003(3)
F17	0.026(3)	0.034(5)	0.022(3)	-0.005(3)	-0.003(2)	-0.010(3)
F14	0.022(3)	0.022(4)	0.027(4)	-0.008(3)	-0.003(3)	-0.009(3)
F23	0.023(4)	0.010(3)	0.046(4)	0.009(3)	-0.006(3)	0.002(3)
O1	0.016(4)	0.026(5)	0.034(5)	-0.007(4)	0.009(3)	0.005(3)
F7	0.009(3)	0.033(4)	0.029(4)	-0.001(3)	0.001(2)	0.005(3)
F27	0.037(4)	0.035(5)	0.032(4)	-0.003(3)	0.015(3)	0.019(3)
F18	0.014(3)	0.039(4)	0.032(4)	0.002(3)	-0.003(3)	-0.011(3)
F29	0.031(4)	0.027(4)	0.038(4)	-0.007(3)	-0.008(3)	0.000(3)
F28	0.052(5)	0.026(4)	0.035(4)	-0.013(3)	0.001(4)	0.004(4)
N3	0.009(4)	0.007(4)	0.013(4)	0.003(3)	0.007(3)	0.002(3)
O2	0.017(4)	0.018(4)	0.031(4)	-0.004(3)	0.010(3)	0.008(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N2	0.007(4)	0.011(4)	0.020(5)	0.005(3)	0.006(3)	0.003(3)
C78	0.019(6)	0.013(5)	0.025(6)	-0.002(4)	0.003(5)	0.004(4)
C1	0.031(7)	0.019(6)	0.019(6)	0.002(5)	-0.007(5)	0.004(5)
C34	0.006(4)	0.016(5)	0.011(4)	-0.001(4)	-0.003(3)	0.003(4)
C46	0.014(5)	0.027(6)	0.012(5)	-0.001(4)	-0.001(4)	-0.003(4)
C39	0.007(4)	0.014(5)	0.021(5)	0.001(4)	0.002(4)	0.003(4)
C71	0.014(5)	0.014(5)	0.030(6)	-0.004(4)	0.009(4)	-0.001(4)
C63	0.021(4)	0.011(5)	0.021(4)	-0.002(5)	0.004(3)	0.003(5)
C36	0.011(4)	0.013(5)	0.019(5)	0.003(4)	0.004(4)	-0.002(4)
N1	0.040(6)	0.029(6)	0.014(5)	0.001(4)	0.006(4)	0.008(5)
C61	0.011(4)	0.013(4)	0.011(4)	0.006(4)	-0.002(3)	0.003(4)
C49	0.008(4)	0.014(5)	0.013(5)	0.000(4)	0.002(3)	0.002(4)
C62	0.018(5)	0.016(5)	0.014(5)	-0.002(3)	0.004(4)	-0.004(4)
C65	0.020(5)	0.018(5)	0.019(5)	0.001(4)	0.007(4)	-0.005(4)
C72	0.016(5)	0.010(5)	0.016(5)	0.001(4)	0.003(4)	-0.002(4)
C50	0.011(5)	0.018(5)	0.015(5)	0.000(4)	0.005(4)	0.002(4)
C41	0.014(5)	0.021(5)	0.014(5)	0.003(4)	0.005(4)	0.002(4)
C47	0.015(5)	0.009(5)	0.016(5)	0.001(4)	0.002(4)	-0.001(4)
C29	0.024(6)	0.018(6)	0.029(6)	0.006(5)	0.000(5)	0.002(4)
C16	0.016(4)	0.017(6)	0.009(4)	-0.002(4)	-0.001(3)	-0.001(4)
C73	0.021(5)	0.009(5)	0.011(4)	0.002(4)	0.006(4)	0.000(4)
C66	0.015(4)	0.018(4)	0.013(4)	0.002(6)	0.003(3)	0.007(6)
C48	0.011(5)	0.017(5)	0.016(5)	0.002(4)	0.002(4)	0.002(4)
C38	0.019(5)	0.010(5)	0.021(5)	0.005(4)	0.008(4)	0.005(4)
C15	0.030(6)	0.024(6)	0.008(5)	-0.003(4)	0.002(4)	-0.013(5)
C58	0.011(5)	0.026(6)	0.018(5)	-0.010(4)	0.006(4)	0.002(4)
C59	0.011(5)	0.016(5)	0.028(6)	0.003(4)	0.004(4)	0.002(4)
C68	0.018(5)	0.013(5)	0.027(6)	-0.001(4)	0.003(4)	-0.001(4)
C14	0.033(6)	0.011(5)	0.019(6)	-0.008(4)	0.000(4)	-0.002(4)
C53	0.009(4)	0.015(5)	0.027(6)	-0.009(4)	0.001(4)	0.004(4)
C67	0.009(4)	0.012(5)	0.020(5)	0.003(3)	0.003(4)	0.000(3)
C32	0.010(4)	0.013(5)	0.027(6)	-0.003(4)	0.008(4)	0.003(4)
C22	0.029(6)	0.018(6)	0.010(5)	-0.001(4)	-0.002(4)	0.000(4)
C52	0.016(5)	0.015(5)	0.030(6)	-0.012(4)	0.005(4)	-0.010(4)
C43	0.013(5)	0.016(5)	0.011(5)	0.003(4)	0.007(4)	0.000(4)
C33	0.015(5)	0.009(5)	0.017(5)	0.002(4)	0.007(4)	0.001(4)
C18	0.019(5)	0.014(5)	0.020(5)	-0.004(4)	0.000(4)	0.000(4)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C12	0.023(5)	0.019(6)	0.018(5)	0.000(4)	0.004(4)	-0.005(4)
C37	0.024(5)	0.006(5)	0.023(5)	0.000(4)	0.005(4)	0.004(4)
C74	0.020(5)	0.013(5)	0.019(5)	0.006(4)	0.007(4)	0.004(4)
C11	0.026(6)	0.017(6)	0.013(5)	-0.007(4)	0.001(4)	-0.002(5)
C57	0.010(4)	0.020(5)	0.024(6)	-0.009(4)	0.002(4)	-0.008(4)
C17	0.036(7)	0.014(5)	0.013(5)	-0.003(4)	0.001(5)	-0.001(5)
C54	0.013(5)	0.013(5)	0.012(5)	0.001(4)	0.003(4)	0.000(4)
C2	0.029(7)	0.019(7)	0.054(9)	-0.003(6)	0.002(6)	0.012(5)
C75	0.030(6)	0.016(6)	0.021(6)	0.004(4)	0.010(5)	0.007(5)
C44	0.015(5)	0.014(5)	0.016(5)	0.001(4)	0.004(4)	0.006(4)
C69	0.014(5)	0.016(5)	0.029(6)	0.006(4)	0.001(4)	0.000(4)
C40	0.011(4)	0.013(5)	0.020(5)	0.004(4)	0.007(4)	0.000(4)
C45	0.021(5)	0.025(6)	0.011(5)	-0.005(4)	0.001(4)	-0.001(4)
C76	0.042(7)	0.011(5)	0.021(6)	0.000(4)	0.002(5)	0.003(5)
C20	0.031(7)	0.026(7)	0.021(6)	0.002(5)	-0.011(5)	-0.001(5)
C56	0.012(4)	0.010(5)	0.012(5)	-0.002(4)	-0.002(4)	0.006(4)
C64	0.013(5)	0.026(6)	0.025(6)	-0.001(5)	-0.005(4)	-0.008(4)
C13	0.038(7)	0.015(6)	0.018(5)	-0.004(4)	0.006(5)	-0.002(5)
C19	0.028(6)	0.027(6)	0.021(6)	0.001(5)	0.001(5)	0.004(5)
C23	0.027(6)	0.020(6)	0.031(7)	-0.007(5)	-0.006(5)	-0.001(5)
C42	0.020(6)	0.022(6)	0.040(7)	-0.002(5)	0.007(5)	0.012(5)
C30	0.034(7)	0.032(7)	0.037(8)	0.004(6)	-0.008(6)	-0.007(6)
C3	0.036(7)	0.026(7)	0.034(7)	-0.010(5)	-0.014(6)	0.000(6)
C60	0.013(5)	0.007(4)	0.016(5)	0.002(4)	0.000(4)	0.003(4)
C55	0.011(5)	0.012(5)	0.008(5)	0.003(4)	0.001(4)	0.003(4)
C70	0.010(5)	0.010(5)	0.034(6)	0.009(4)	0.001(4)	-0.001(4)
C24	0.026(6)	0.026(7)	0.035(7)	-0.005(5)	-0.008(5)	-0.003(5)
B2	0.012(5)	0.003(5)	0.015(5)	0.003(4)	0.003(4)	-0.002(4)
C51	0.015(5)	0.012(5)	0.020(5)	0.005(4)	0.014(4)	0.001(4)
C6	0.036(7)	0.028(7)	0.032(7)	0.004(5)	0.008(6)	0.013(6)
B1	0.011(5)	0.013(5)	0.014(5)	-0.002(4)	0.006(4)	0.002(4)
C7	0.026(6)	0.035(7)	0.037(7)	0.002(6)	0.017(5)	0.001(5)
C8	0.045(8)	0.030(7)	0.019(6)	0.002(5)	0.008(5)	0.016(6)
C4	0.033(7)	0.027(7)	0.045(8)	-0.009(6)	0.001(6)	0.000(6)
C5	0.025(6)	0.025(6)	0.024(6)	-0.001(5)	0.012(5)	0.006(5)
C31	0.027(6)	0.035(7)	0.034(7)	0.015(6)	0.007(5)	0.001(5)
C35	0.015(4)	0.013(5)	0.010(4)	0.009(3)	0.006(3)	0.003(4)

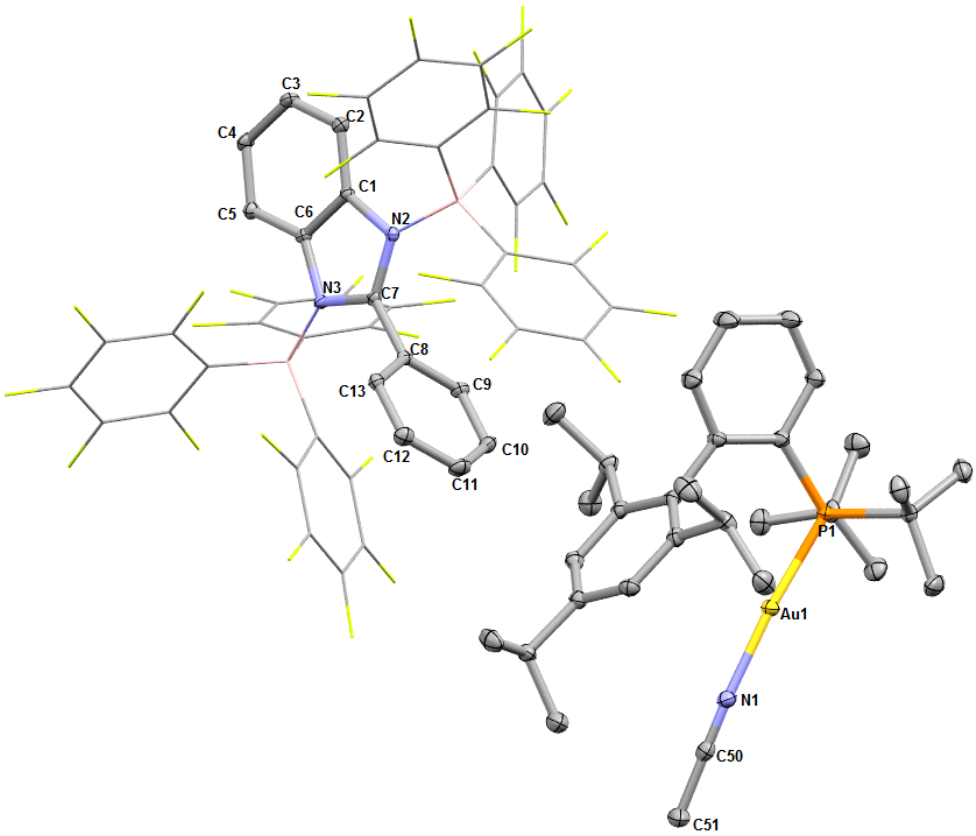
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C77	0.024(6)	0.020(6)	0.023(6)	0.001(5)	-0.008(4)	-0.006(5)
C26	0.024(6)	0.027(7)	0.036(7)	0.001(5)	-0.007(5)	0.003(5)
C27	0.038(8)	0.029(7)	0.044(8)	0.017(6)	-0.008(6)	0.001(6)
C10	0.044(8)	0.056(10)	0.025(7)	0.028(7)	-0.001(6)	0.016(7)
C21	0.029(7)	0.026(7)	0.033(8)	0.001(6)	-0.003(6)	0.006(6)
C28	0.046(9)	0.027(8)	0.058(10)	-0.001(7)	-0.002(7)	0.010(6)
C9	0.023(6)	0.036(7)	0.029(7)	0.005(6)	-0.005(5)	0.010(5)
C25	0.032(7)	0.050(10)	0.040(8)	-0.005(7)	0.007(6)	0.003(7)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 5864.

	x/a	y/b	z/c	U(eq)
H39	-0.1331	0.5760	1.0105	0.017
H36	0.2677	0.6055	1.1103	0.017
H29	1.0465	0.4055	0.5294	0.029
H15	0.8481	0.4255	0.6425	0.025
H14	0.8915	0.3473	0.7364	0.026
H32	0.3776	0.3620	1.0581	0.019
H33	0.4452	0.4328	0.9595	0.016
H12	0.8986	0.2110	0.5688	0.024
H37	0.1242	0.6817	1.1344	0.021
H2A	0.7992	0.1224	0.3957	0.052
H2B	0.6944	0.1130	0.4458	0.052
H2C	0.8184	0.1428	0.4852	0.052
H40	0.0074	0.4993	0.9822	0.017
H13	0.9249	0.2349	0.6972	0.028
H19	0.9525	0.5551	0.4380	0.031
H23	0.6240	0.3600	0.5019	0.033
H42A	-0.2031	0.7960	1.1111	0.04
H42B	-0.1108	0.8133	1.1868	0.04
H42C	-0.2016	0.7541	1.1886	0.04
H30A	1.0532	0.5375	0.5851	0.054
H30B	1.1611	0.4884	0.6102	0.054
H30C	1.0339	0.4730	0.6333	0.054
H3A	0.6122	0.2446	0.3129	0.051
H3B	0.6131	0.1666	0.3177	0.051

	x/a	y/b	z/c	U(eq)
H3C	0.7255	0.2046	0.2956	0.051
H24A	0.4836	0.4383	0.3877	0.046
H24B	0.4337	0.3745	0.4246	0.046
H24C	0.5380	0.3681	0.3736	0.046
H6A	1.0534	0.2145	0.5121	0.048
H6B	1.1249	0.1872	0.4469	0.048
H6C	1.0016	0.1546	0.4585	0.048
H7A	1.0326	0.3298	0.3542	0.047
H7B	1.1416	0.2894	0.3994	0.047
H7C	1.0568	0.3298	0.4470	0.047
H8A	0.9284	0.1688	0.3239	0.047
H8B	1.0379	0.2097	0.3019	0.047
H8C	0.9072	0.2396	0.2855	0.047
H4A	0.6570	0.2296	0.5167	0.053
H4B	0.5593	0.1951	0.4543	0.053
H4C	0.5898	0.2707	0.4453	0.053
H31A	1.0996	0.4445	0.4106	0.048
H31B	1.2057	0.4485	0.4817	0.048
H31C	1.1338	0.5130	0.4520	0.048
H26	0.8231	0.6373	0.3910	0.036
H27A	0.7717	0.5922	0.2718	0.058
H27B	0.6820	0.6515	0.2768	0.058
H27C	0.6394	0.5780	0.2867	0.058
H10A	0.7375	0.4763	0.0916	0.064
H10B	0.7066	0.5389	0.1397	0.064
H10C	0.6054	0.4871	0.1089	0.064
H21	0.6016	0.5172	0.4136	0.036
H28A	0.5795	0.6355	0.4089	0.067
H28B	0.6625	0.6983	0.4085	0.067
H28C	0.6822	0.6490	0.4803	0.067
H25A	0.5983	0.4459	0.5913	0.061
H25B	0.4775	0.4078	0.5620	0.061
H25C	0.5008	0.4779	0.5268	0.061

Crystal Structure Report for 2[BIMP]



Thermal ellipsoid plot of 5790. Ellipsoids shown at 50% probability, $B(C_6F_5)_3$ substituents shown in wireframe, hydrogen atoms and DCM solvates hidden for clarity.

A specimen of $C_{83}H_{63}AuB_2Cl_6F_{30}N_3P$, approximate dimensions 0.051 mm x 0.157 mm x 0.353 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å). The integration of the data using a triclinic unit cell yielded a total of 79278 reflections to a maximum θ angle of 28.01° (0.76 Å resolution), of which 20755 were independent (average redundancy 3.820, completeness = 98.7%, R_{int} = 3.05%, R_{sig} =3.09%) and 18789 (90.53%) were greater than $2\sigma(F^2)$. The final cell constants of a = 15.447(3) Å, b = 17.053(3) Å, c =18.040(3) Å, α = 67.410(3)°, β = 82.920(4)°, γ = 84.125(4)°, volume = 4346.2(13) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.5380 and 0.9050. The final anisotropic full-matrix least-squares refinement on F^2 with 1148 variables converged at R1 = 3.55%, for the observed data and wR2 = 9.52% for all data. The goodness-of-fit was 1.038. The largest peak in the final difference electron density synthesis was 2.345 $e^-/Å^3$ and the largest hole was -2.295 $e^-/Å^3$ with an RMS deviation of 0.107 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.631 g/cm^3 and F(000), 2116 e^-. PLATON SQUEEZE was used to account for disordered solvent within the crystal that could not be modelled.

Table 1. Sample and crystal data for 5790.

Identification code	5790	
Chemical formula	$C_{83}H_{63}AuB_2Cl_6F_{30}N_3P$	
Formula weight	2134.62 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.051 x 0.157 x 0.353 mm	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 15.447(3) Å	α = 67.410(3)°
	b = 17.053(3) Å	β = 82.920(4)°
	c = 18.040(3) Å	γ = 84.125(4)°
Volume	4346.2(13) $Å^3$	
Z	2	
Density (calculated)	1.631 g/cm^3	
Absorption coefficient	2.006 mm^{-1}	
F(000)	2116	

Table 2. Data collection and structure refinement for 5790.

Theta range for data collection	1.73 to 28.01°	
Index ranges	-20<=h<=20, -18<=k<=22, -23<=l<=23	
Reflections collected	79278	
Independent reflections	20755 [R(int) = 0.0305]	
Max. and min. transmission	0.9050 and 0.5380	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	20755 / 0 / 1148	
Goodness-of-fit on F^2	1.038	
Δ/σ_{max}	0.003	
Final R indices	18789 data; I>2σ(I)	R1 = 0.0355, wR2 = 0.0931
	all data	R1 = 0.0405, wR2 = 0.0952
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0540P)^2+7.5803P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	2.345 and -2.295 $eÅ^{-3}$	
R.M.S. deviation from mean	0.107 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for 5790.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij}tensor.

	x/a	y/b	z/c	U(eq)
Au1	0.24171(2)	0.19865(2)	0.79675(2)	0.01376(4)
P1	0.10950(5)	0.17996(5)	0.76786(4)	0.01216(14)
Cl4	0.35567(7)	0.62410(7)	0.41598(6)	0.0410(2)
Cl3	0.18461(9)	0.57674(11)	0.49829(9)	0.0661(4)
Cl1	0.22514(9)	0.92453(12)	0.24187(10)	0.0679(4)
Cl2	0.15248(11)	0.85947(13)	0.40838(10)	0.0844(6)
F6	0.71924(12)	0.71704(11)	0.57650(10)	0.0160(3)
F21	0.35161(11)	0.49726(10)	0.97406(10)	0.0143(3)
F15	0.39970(12)	0.76677(11)	0.63365(10)	0.0173(4)
F11	0.62824(12)	0.65391(11)	0.49576(10)	0.0162(3)
F5	0.64219(12)	0.61031(11)	0.81034(10)	0.0159(3)
F12	0.56000(13)	0.74136(12)	0.35986(10)	0.0216(4)
F30	0.24627(12)	0.72793(11)	0.73360(10)	0.0166(3)
F25	0.12066(11)	0.69338(11)	0.85540(10)	0.0165(3)
F26	0.11802(12)	0.47171(11)	0.77633(10)	0.0164(3)
F10	0.59130(12)	0.46667(11)	0.76036(10)	0.0178(4)
F24	0.11205(13)	0.75172(12)	0.97171(11)	0.0208(4)
F16	0.37473(12)	0.38769(11)	0.88710(10)	0.0170(4)
F22	0.34363(13)	0.56088(12)	0.08838(10)	0.0214(4)
F20	0.08627(12)	0.50035(12)	0.91918(11)	0.0191(4)
F23	0.22474(15)	0.68914(13)	0.08828(11)	0.0270(5)
F8	0.88174(13)	0.45598(13)	0.65685(12)	0.0258(4)
F7	0.86997(12)	0.62709(13)	0.57157(11)	0.0243(4)
F1	0.54315(13)	0.85719(11)	0.59713(10)	0.0193(4)
F9	0.73899(13)	0.37842(11)	0.74997(12)	0.0235(4)
F29	0.15452(15)	0.80820(12)	0.60820(12)	0.0282(5)
F27	0.03053(13)	0.55203(13)	0.65049(11)	0.0229(4)
F2	0.61702(15)	0.95126(12)	0.65299(12)	0.0270(4)
F17	0.32799(15)	0.23642(12)	0.98846(11)	0.0268(4)
F14	0.33124(13)	0.85215(13)	0.49525(12)	0.0270(4)
F4	0.71189(13)	0.70841(13)	0.86660(11)	0.0257(4)
F13	0.41052(14)	0.84156(13)	0.35549(11)	0.0274(4)

	x/a	y/b	z/c	U(eq)
F19	0.04066(14)	0.34672(14)	0.02103(12)	0.0285(5)
F28	0.04506(14)	0.72161(13)	0.56350(12)	0.0293(5)
F3	0.70604(15)	0.88074(14)	0.78607(14)	0.0319(5)
F18	0.16062(17)	0.21221(13)	0.05693(12)	0.0334(5)
Cl6	0.89955(15)	0.4867(2)	0.83086(13)	0.1237(9)
N2	0.34803(15)	0.55780(14)	0.78756(13)	0.0093(4)
N3	0.47478(16)	0.60373(14)	0.71478(13)	0.0096(4)
N1	0.35922(18)	0.23384(16)	0.81075(15)	0.0163(5)
Cl5	0.8882(2)	0.6698(3)	0.7583(3)	0.1896(18)
C7	0.41676(18)	0.60597(17)	0.77645(15)	0.0097(5)
C49	0.4428(2)	0.75857(18)	0.56709(16)	0.0134(5)
C14	0.23135(19)	0.45205(18)	0.89376(16)	0.0125(5)
C5	0.47656(19)	0.52209(18)	0.62229(16)	0.0128(5)
C25	0.19317(19)	0.68131(19)	0.71528(17)	0.0136(5)
C20	0.18748(19)	0.59579(18)	0.76353(16)	0.0120(5)
C1	0.36382(18)	0.52126(17)	0.72919(16)	0.0098(5)
C6	0.44178(18)	0.54971(17)	0.68423(16)	0.0104(5)
C38	0.58493(19)	0.72629(18)	0.70151(16)	0.0113(5)
C31	0.18058(19)	0.65928(18)	0.90917(17)	0.0137(5)
C52	0.0980(2)	0.07061(18)	0.77756(17)	0.0143(6)
C59	0.3233(2)	0.02297(18)	0.73815(17)	0.0140(5)
C27	0.29384(19)	0.56386(17)	0.96851(16)	0.0117(5)
C46	0.5208(2)	0.74827(19)	0.42817(17)	0.0154(6)
C37	0.72095(19)	0.63235(18)	0.61994(16)	0.0131(5)
C26	0.24283(18)	0.59659(18)	0.90327(16)	0.0110(5)
C2	0.31682(19)	0.46423(18)	0.71420(17)	0.0134(5)
C32	0.64478(19)	0.59646(18)	0.66436(16)	0.0118(5)
C12	0.4945(2)	0.64527(19)	0.94731(17)	0.0153(6)
C58	0.25950(19)	0.01577(17)	0.80316(17)	0.0131(5)
C70	0.2994(2)	0.02371(19)	0.65833(17)	0.0164(6)
C44	0.52041(19)	0.70846(17)	0.57382(16)	0.0108(5)
C30	0.1740(2)	0.69072(19)	0.96997(17)	0.0155(6)
C10	0.4129(2)	0.77181(19)	0.86915(18)	0.0167(6)
C9	0.39870(19)	0.73370(18)	0.81626(17)	0.0129(5)
C8	0.43153(18)	0.65048(17)	0.82990(16)	0.0105(5)
C67	0.5342(2)	0.01031(19)	0.83421(18)	0.0166(6)
C4	0.4291(2)	0.46704(19)	0.60666(17)	0.0141(6)

	x/a	y/b	z/c	U(eq)
C57	0.1660(2)	0.00563(18)	0.79602(17)	0.0139(5)
C11	0.4603(2)	0.7273(2)	0.93476(18)	0.0180(6)
C60	0.4111(2)	0.02232(18)	0.74963(17)	0.0153(6)
C53	0.0145(2)	0.0498(2)	0.7714(2)	0.0200(6)
C43	0.5824(2)	0.81438(19)	0.66530(17)	0.0143(6)
C45	0.55610(19)	0.70426(18)	0.50059(17)	0.0127(5)
C13	0.48069(19)	0.60704(18)	0.89491(16)	0.0122(5)
C61	0.4381(2)	0.01371(18)	0.82309(18)	0.0152(6)
C63	0.2863(2)	0.00538(18)	0.87915(17)	0.0151(6)
C15	0.2898(2)	0.38136(18)	0.91580(17)	0.0142(6)
C28	0.2901(2)	0.59387(19)	0.02936(16)	0.0151(6)
C64	0.2220(2)	0.9856(2)	0.95448(18)	0.0190(6)
C3	0.3501(2)	0.43841(19)	0.65192(17)	0.0143(6)
C19	0.1483(2)	0.43609(19)	0.93296(17)	0.0158(6)
C29	0.2298(2)	0.65924(19)	0.02933(17)	0.0179(6)
C47	0.4454(2)	0.7988(2)	0.42535(17)	0.0187(6)
C56	0.1450(2)	0.92316(19)	0.8090(2)	0.0209(6)
C33	0.6563(2)	0.50994(18)	0.70906(17)	0.0135(5)
C42	0.6212(2)	0.8669(2)	0.69295(19)	0.0187(6)
C39	0.63112(19)	0.69498(18)	0.76997(16)	0.0132(5)
C24	0.1466(2)	0.7246(2)	0.64956(18)	0.0184(6)
C41	0.6654(2)	0.8313(2)	0.7607(2)	0.0207(6)
C40	0.6692(2)	0.7443(2)	0.80012(18)	0.0188(6)
C34	0.7341(2)	0.46242(19)	0.70657(18)	0.0167(6)
C48	0.4053(2)	0.8037(2)	0.49620(18)	0.0173(6)
C73	0.0213(2)	0.2052(2)	0.83880(18)	0.0168(6)
C79	0.0993(2)	0.3449(2)	0.6506(2)	0.0232(7)
C36	0.7995(2)	0.5876(2)	0.61659(18)	0.0174(6)
C18	0.1231(2)	0.3572(2)	0.98675(18)	0.0199(6)
C62	0.3747(2)	0.00591(19)	0.88652(18)	0.0157(6)
C21	0.13011(19)	0.55584(19)	0.73795(17)	0.0145(6)
C77	0.1005(2)	0.25116(19)	0.65987(18)	0.0172(6)
C23	0.0910(2)	0.6814(2)	0.62753(18)	0.0202(6)
C78	0.1836(2)	0.2302(2)	0.61355(18)	0.0216(7)
C35	0.8061(2)	0.5010(2)	0.65996(18)	0.0173(6)
C22	0.0827(2)	0.5962(2)	0.67194(18)	0.0178(6)
C54	0.9958(2)	0.9674(2)	0.7847(2)	0.0267(7)

	x/a	y/b	z/c	U(eq)
C16	0.2674(2)	0.30129(19)	0.96953(18)	0.0195(6)
C74	0.0130(2)	0.1266(2)	0.91795(19)	0.0241(7)
C69	0.5619(2)	0.9274(2)	0.9014(2)	0.0243(7)
C50	0.4223(2)	0.26502(19)	0.80555(18)	0.0164(6)
C80	0.0221(2)	0.2378(2)	0.6232(2)	0.0253(7)
C65	0.2369(2)	0.8914(2)	0.0085(2)	0.0283(8)
C75	0.9315(2)	0.2336(2)	0.8058(2)	0.0231(7)
C17	0.1838(2)	0.2889(2)	0.00504(18)	0.0214(7)
C66	0.2299(2)	0.0423(2)	0.00095(19)	0.0245(7)
C51	0.5023(2)	0.3063(2)	0.7970(2)	0.0246(7)
C71	0.3169(3)	0.9349(2)	0.6552(2)	0.0255(7)
C72	0.3488(2)	0.0882(2)	0.58486(19)	0.0219(7)
C55	0.0620(2)	0.9036(2)	0.8042(2)	0.0268(7)
C76	0.0514(2)	0.2782(2)	0.8579(2)	0.0263(7)
C68	0.5565(2)	0.0867(2)	0.8505(2)	0.0255(7)
B1	0.2524(2)	0.55131(19)	0.83717(18)	0.0101(6)
B2	0.5562(2)	0.65879(19)	0.66475(17)	0.0094(5)
C82	0.2760(3)	0.6331(3)	0.4912(3)	0.0371(9)
C81	0.2115(3)	0.9383(3)	0.3325(3)	0.0453(11)
C83	0.8956(5)	0.5819(7)	0.8434(5)	0.120(4)

Table 4. Bond lengths (Å) for 5790.

Au1-N1	2.042(3)	Au1-P1	2.2509(8)
P1-C52	1.830(3)	P1-C77	1.872(3)
P1-C73	1.884(3)	Cl4-C82	1.757(4)
Cl3-C82	1.752(4)	Cl1-C81	1.725(5)
Cl2-C81	1.744(5)	F6-C37	1.352(3)
F21-C27	1.350(3)	F15-C49	1.348(3)
F11-C45	1.351(3)	F5-C39	1.348(3)
F12-C46	1.346(3)	F30-C25	1.348(3)
F25-C31	1.347(3)	F26-C21	1.354(3)
F10-C33	1.344(3)	F24-C30	1.346(3)
F16-C15	1.348(4)	F22-C28	1.340(3)
F20-C19	1.347(4)	F23-C29	1.336(3)
F8-C35	1.339(3)	F7-C36	1.345(4)
F1-C43	1.348(3)	F9-C34	1.342(3)

F29-C24	1.342(4)	F27-C22	1.339(4)
F2-C42	1.337(4)	F17-C16	1.340(4)
F14-C48	1.339(4)	F4-C40	1.341(4)
F13-C47	1.338(3)	F19-C18	1.343(4)
F28-C23	1.342(3)	F3-C41	1.338(4)
F18-C17	1.337(4)	Cl6-C83	1.718(10)
N2-C7	1.357(4)	N2-C1	1.402(3)
N2-B1	1.621(4)	N3-C7	1.350(3)
N3-C6	1.403(3)	N3-B2	1.609(4)
N1-C50	1.134(4)	Cl5-C83	1.690(10)
C7-C8	1.487(4)	C49-C48	1.378(4)
C49-C44	1.389(4)	C14-C19	1.386(4)
C14-C15	1.387(4)	C14-B1	1.648(4)
C5-C4	1.376(4)	C5-C6	1.401(4)
C5-H5	0.95	C25-C24	1.378(4)
C25-C20	1.387(4)	C20-C21	1.389(4)
C20-B1	1.657(4)	C1-C6	1.386(4)
C1-C2	1.393(4)	C38-C43	1.387(4)
C38-C39	1.397(4)	C38-B2	1.651(4)
C31-C30	1.383(4)	C31-C26	1.389(4)
C52-C53	1.400(4)	C52-C57	1.416(4)
C59-C60	1.395(4)	C59-C58	1.411(4)
C59-C70	1.525(4)	C27-C28	1.371(4)
C27-C26	1.397(4)	C46-C47	1.369(5)
C46-C45	1.381(4)	C37-C36	1.373(4)
C37-C32	1.393(4)	C26-B1	1.637(4)
C2-C3	1.383(4)	C2-H2	0.95
C32-C33	1.388(4)	C32-B2	1.646(4)
C12-C13	1.384(4)	C12-C11	1.386(4)
C12-H12	0.95	C58-C63	1.422(4)
C58-C57	1.499(4)	C70-C71	1.532(4)
C70-C72	1.534(4)	C70-H70	1.0
C44-C45	1.393(4)	C44-B2	1.666(4)
C30-C29	1.367(4)	C10-C11	1.387(4)
C10-C9	1.392(4)	C10-H10	0.95
C9-C8	1.395(4)	C9-H9	0.95
C8-C13	1.392(4)	C67-C61	1.514(4)
C67-C68	1.520(4)	C67-C69	1.529(4)

C67-H67	1.0	C4-C3	1.401(4)
C4-H4	0.95	C57-C56	1.399(4)
C11-H11	0.95	C60-C61	1.388(4)
C60-H60	0.95	C53-C54	1.386(4)
C53-H53	0.95	C43-C42	1.392(4)
C13-H13	0.95	C61-C62	1.385(4)
C63-C62	1.389(4)	C63-C64	1.527(4)
C15-C16	1.386(4)	C28-C29	1.378(4)
C64-C66	1.523(5)	C64-C65	1.536(5)
C64-H64	1.0	C3-H3	0.95
C19-C18	1.383(4)	C47-C48	1.379(4)
C56-C55	1.379(5)	C56-H56	0.95
C33-C34	1.385(4)	C42-C41	1.371(5)
C39-C40	1.371(4)	C24-C23	1.369(5)
C41-C40	1.375(5)	C34-C35	1.367(5)
C73-C75	1.536(4)	C73-C74	1.540(4)
C73-C76	1.540(4)	C79-C77	1.540(4)
C79-H79A	0.98	C79-H79B	0.98
C79-H79C	0.98	C36-C35	1.381(4)
C18-C17	1.379(5)	C62-H62	0.95
C21-C22	1.382(4)	C77-C80	1.526(5)
C77-C78	1.531(4)	C23-C22	1.374(5)
C78-H78A	0.98	C78-H78B	0.98
C78-H78C	0.98	C54-C55	1.386(5)
C54-H54	0.95	C16-C17	1.367(5)
C74-H74A	0.98	C74-H74B	0.98
C74-H74C	0.98	C69-H69A	0.98
C69-H69B	0.98	C69-H69C	0.98
C50-C51	1.447(5)	C80-H80A	0.98
C80-H80B	0.98	C80-H80C	0.98
C65-H65A	0.98	C65-H65B	0.98
C65-H65C	0.98	C75-H75A	0.98
C75-H75B	0.98	C75-H75C	0.98
C66-H66A	0.98	C66-H66B	0.98
C66-H66C	0.98	C51-H51A	0.98
C51-H51B	0.98	C51-H51C	0.98
C71-H71A	0.98	C71-H71B	0.98
C71-H71C	0.98	C72-H72A	0.98

C72-H72B	0.98	C72-H72C	0.98
C55-H55	0.95	C76-H76A	0.98
C76-H76B	0.98	C76-H76C	0.98
C68-H68A	0.98	C68-H68B	0.98
C68-H68C	0.98	C82-H82A	0.99
C82-H82B	0.99	C81-H81A	0.99
C81-H81B	0.99	C83-H83A	0.99
C83-H83B	0.99		

Table 5. Bond angles (°) for 5790.

N1-Au1-P1	171.41(7)	C52-P1-C77	108.00(14)
C52-P1-C73	107.34(14)	C77-P1-C73	112.98(14)
C52-P1-Au1	112.58(10)	C77-P1-Au1	105.95(11)
C73-P1-Au1	110.08(10)	C7-N2-C1	105.8(2)
C7-N2-B1	134.1(2)	C1-N2-B1	118.8(2)
C7-N3-C6	105.9(2)	C7-N3-B2	134.3(2)
C6-N3-B2	118.7(2)	C50-N1-Au1	167.6(3)
N3-C7-N2	112.4(2)	N3-C7-C8	123.0(2)
N2-C7-C8	124.4(2)	F15-C49-C48	115.5(3)
F15-C49-C44	119.3(2)	C48-C49-C44	125.2(3)
C19-C14-C15	113.6(3)	C19-C14-B1	118.1(3)
C15-C14-B1	127.8(3)	C4-C5-C6	117.3(3)
C4-C5-H5	121.4	C6-C5-H5	121.4
F30-C25-C24	115.9(3)	F30-C25-C20	119.1(2)
C24-C25-C20	125.0(3)	C25-C20-C21	112.9(3)
C25-C20-B1	119.4(2)	C21-C20-B1	127.5(3)
C6-C1-C2	121.1(3)	C6-C1-N2	107.9(2)
C2-C1-N2	130.9(3)	C1-C6-C5	121.4(3)
C1-C6-N3	108.0(2)	C5-C6-N3	130.6(3)
C43-C38-C39	112.5(3)	C43-C38-B2	127.6(2)
C39-C38-B2	119.0(2)	F25-C31-C30	114.8(3)
F25-C31-C26	121.5(3)	C30-C31-C26	123.7(3)
C53-C52-C57	118.8(3)	C53-C52-P1	116.8(2)
C57-C52-P1	124.3(2)	C60-C59-C58	118.9(3)
C60-C59-C70	119.2(3)	C58-C59-C70	121.6(3)
F21-C27-C28	115.9(2)	F21-C27-C26	119.1(2)
C28-C27-C26	125.1(3)	F12-C46-C47	119.5(3)

F12-C46-C45	120.1(3)	C47-C46-C45	120.3(3)
F6-C37-C36	116.4(3)	F6-C37-C32	119.0(3)
C36-C37-C32	124.6(3)	C31-C26-C27	112.9(2)
C31-C26-B1	127.4(2)	C27-C26-B1	119.2(2)
C3-C2-C1	117.5(3)	C3-C2-H2	121.3
C1-C2-H2	121.3	C33-C32-C37	113.3(3)
C33-C32-B2	127.5(3)	C37-C32-B2	119.0(2)
C13-C12-C11	120.1(3)	C13-C12-H12	119.9
C11-C12-H12	119.9	C59-C58-C63	119.3(3)
C59-C58-C57	120.2(3)	C63-C58-C57	119.8(3)
C59-C70-C71	110.3(2)	C59-C70-C72	112.9(3)
C71-C70-C72	109.3(3)	C59-C70-H70	108.1
C71-C70-H70	108.1	C72-C70-H70	108.1
C49-C44-C45	112.8(2)	C49-C44-B2	118.6(2)
C45-C44-B2	128.6(3)	F24-C30-C29	119.5(3)
F24-C30-C31	120.4(3)	C29-C30-C31	120.1(3)
C11-C10-C9	119.9(3)	C11-C10-H10	120.0
C9-C10-H10	120.0	C10-C9-C8	119.8(3)
C10-C9-H9	120.1	C8-C9-H9	120.1
C13-C8-C9	119.7(3)	C13-C8-C7	118.1(2)
C9-C8-C7	122.2(2)	C61-C67-C68	111.6(3)
C61-C67-C69	111.2(3)	C68-C67-C69	110.6(3)
C61-C67-H67	107.7	C68-C67-H67	107.7
C69-C67-H67	107.7	C5-C4-C3	121.4(3)
C5-C4-H4	119.3	C3-C4-H4	119.3
C56-C57-C52	117.7(3)	C56-C57-C58	115.7(3)
C52-C57-C58	126.6(3)	C12-C11-C10	120.2(3)
C12-C11-H11	119.9	C10-C11-H11	119.9
C61-C60-C59	122.3(3)	C61-C60-H60	118.8
C59-C60-H60	118.8	C54-C53-C52	122.1(3)
C54-C53-H53	118.9	C52-C53-H53	118.9
F1-C43-C38	121.9(3)	F1-C43-C42	113.4(3)
C38-C43-C42	124.6(3)	F11-C45-C46	114.5(2)
F11-C45-C44	121.6(2)	C46-C45-C44	123.9(3)
C12-C13-C8	120.1(3)	C12-C13-H13	119.9
C8-C13-H13	119.9	C62-C61-C60	118.0(3)
C62-C61-C67	121.0(3)	C60-C61-C67	120.9(3)
C62-C63-C58	118.9(3)	C62-C63-C64	119.0(3)

C58-C63-C64	121.9(3)	F16-C15-C16	115.4(3)
F16-C15-C14	120.9(3)	C16-C15-C14	123.7(3)
F22-C28-C27	121.4(3)	F22-C28-C29	119.8(3)
C27-C28-C29	118.9(3)	C66-C64-C63	112.9(3)
C66-C64-C65	110.5(3)	C63-C64-C65	108.6(3)
C66-C64-H64	108.3	C63-C64-H64	108.3
C65-C64-H64	108.3	C2-C3-C4	121.3(3)
C2-C3-H3	119.3	C4-C3-H3	119.3
F20-C19-C18	116.1(3)	F20-C19-C14	119.4(3)
C18-C19-C14	124.5(3)	F23-C29-C30	121.0(3)
F23-C29-C28	119.9(3)	C30-C29-C28	119.1(3)
F13-C47-C46	120.8(3)	F13-C47-C48	120.5(3)
C46-C47-C48	118.7(3)	C55-C56-C57	122.7(3)
C55-C56-H56	118.6	C57-C56-H56	118.6
F10-C33-C34	115.1(3)	F10-C33-C32	121.0(3)
C34-C33-C32	123.8(3)	F2-C42-C41	120.2(3)
F2-C42-C43	120.4(3)	C41-C42-C43	119.4(3)
F5-C39-C40	115.4(3)	F5-C39-C38	119.7(2)
C40-C39-C38	124.9(3)	F29-C24-C23	120.3(3)
F29-C24-C25	120.5(3)	C23-C24-C25	119.2(3)
F3-C41-C42	120.0(3)	F3-C41-C40	121.1(3)
C42-C41-C40	118.9(3)	F4-C40-C39	120.6(3)
F4-C40-C41	119.6(3)	C39-C40-C41	119.7(3)
F9-C34-C35	119.9(3)	F9-C34-C33	120.0(3)
C35-C34-C33	120.1(3)	F14-C48-C49	121.0(3)
F14-C48-C47	119.9(3)	C49-C48-C47	119.0(3)
C75-C73-C74	109.8(3)	C75-C73-C76	107.6(3)
C74-C73-C76	108.0(3)	C75-C73-P1	115.2(2)
C74-C73-P1	108.6(2)	C76-C73-P1	107.5(2)
C77-C79-H79A	109.5	C77-C79-H79B	109.5
H79A-C79-H79B	109.5	C77-C79-H79C	109.5
H79A-C79-H79C	109.5	H79B-C79-H79C	109.5
F7-C36-C37	120.9(3)	F7-C36-C35	119.7(3)
C37-C36-C35	119.4(3)	F19-C18-C17	120.0(3)
F19-C18-C19	120.8(3)	C17-C18-C19	119.2(3)
C61-C62-C63	122.4(3)	C61-C62-H62	118.8
C63-C62-H62	118.8	F26-C21-C22	114.5(3)
F26-C21-C20	121.2(3)	C22-C21-C20	124.2(3)

C80-C77-C78	108.0(3)	C80-C77-C79	109.7(3)
C78-C77-C79	108.7(3)	C80-C77-P1	114.8(2)
C78-C77-P1	105.5(2)	C79-C77-P1	109.8(2)
F28-C23-C24	120.6(3)	F28-C23-C22	120.3(3)
C24-C23-C22	119.1(3)	C77-C78-H78A	109.5
C77-C78-H78B	109.5	H78A-C78-H78B	109.5
C77-C78-H78C	109.5	H78A-C78-H78C	109.5
H78B-C78-H78C	109.5	F8-C35-C34	120.8(3)
F8-C35-C36	120.4(3)	C34-C35-C36	118.7(3)
F27-C22-C23	120.3(3)	F27-C22-C21	120.1(3)
C23-C22-C21	119.6(3)	C55-C54-C53	119.0(3)
C55-C54-H54	120.5	C53-C54-H54	120.5
F17-C16-C17	119.8(3)	F17-C16-C15	120.1(3)
C17-C16-C15	120.0(3)	C73-C74-H74A	109.5
C73-C74-H74B	109.5	H74A-C74-H74B	109.5
C73-C74-H74C	109.5	H74A-C74-H74C	109.5
H74B-C74-H74C	109.5	C67-C69-H69A	109.5
C67-C69-H69B	109.5	H69A-C69-H69B	109.5
C67-C69-H69C	109.5	H69A-C69-H69C	109.5
H69B-C69-H69C	109.5	N1-C50-C51	178.6(4)
C77-C80-H80A	109.5	C77-C80-H80B	109.5
H80A-C80-H80B	109.5	C77-C80-H80C	109.5
H80A-C80-H80C	109.5	H80B-C80-H80C	109.5
C64-C65-H65A	109.5	C64-C65-H65B	109.5
H65A-C65-H65B	109.5	C64-C65-H65C	109.5
H65A-C65-H65C	109.5	H65B-C65-H65C	109.5
C73-C75-H75A	109.5	C73-C75-H75B	109.5
H75A-C75-H75B	109.5	C73-C75-H75C	109.5
H75A-C75-H75C	109.5	H75B-C75-H75C	109.5
F18-C17-C16	121.0(3)	F18-C17-C18	120.0(3)
C16-C17-C18	118.9(3)	C64-C66-H66A	109.5
C64-C66-H66B	109.5	H66A-C66-H66B	109.5
C64-C66-H66C	109.5	H66A-C66-H66C	109.5
H66B-C66-H66C	109.5	C50-C51-H51A	109.5
C50-C51-H51B	109.5	H51A-C51-H51B	109.5
C50-C51-H51C	109.5	H51A-C51-H51C	109.5
H51B-C51-H51C	109.5	C70-C71-H71A	109.5
C70-C71-H71B	109.5	H71A-C71-H71B	109.5

C70-C71-H71C	109.5	H71A-C71-H71C	109.5
H71B-C71-H71C	109.5	C70-C72-H72A	109.5
C70-C72-H72B	109.5	H72A-C72-H72B	109.5
C70-C72-H72C	109.5	H72A-C72-H72C	109.5
H72B-C72-H72C	109.5	C56-C55-C54	119.6(3)
C56-C55-H55	120.2	C54-C55-H55	120.2
C73-C76-H76A	109.5	C73-C76-H76B	109.5
H76A-C76-H76B	109.5	C73-C76-H76C	109.5
H76A-C76-H76C	109.5	H76B-C76-H76C	109.5
C67-C68-H68A	109.5	C67-C68-H68B	109.5
H68A-C68-H68B	109.5	C67-C68-H68C	109.5
H68A-C68-H68C	109.5	H68B-C68-H68C	109.5
N2-B1-C26	113.7(2)	N2-B1-C14	111.8(2)
C26-B1-C14	102.4(2)	N2-B1-C20	101.9(2)
C26-B1-C20	114.2(2)	C14-B1-C20	113.2(2)
N3-B2-C32	110.7(2)	N3-B2-C38	115.1(2)
C32-B2-C38	104.3(2)	N3-B2-C44	102.0(2)
C32-B2-C44	113.1(2)	C38-B2-C44	112.0(2)
Cl3-C82-Cl4	111.2(2)	Cl3-C82-H82A	109.4
Cl4-C82-H82A	109.4	Cl3-C82-H82B	109.4
Cl4-C82-H82B	109.4	H82A-C82-H82B	108.0
Cl1-C81-Cl2	113.1(3)	Cl1-C81-H81A	109.0
Cl2-C81-H81A	109.0	Cl1-C81-H81B	109.0
Cl2-C81-H81B	109.0	H81A-C81-H81B	107.8
Cl5-C83-Cl6	115.4(4)	Cl5-C83-H83A	108.4
Cl6-C83-H83A	108.4	Cl5-C83-H83B	108.4
Cl6-C83-H83B	108.4	H83A-C83-H83B	107.5

Table 6. Anisotropic atomic displacement parameters (Å^2) for 5790.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au1	0.01304(6)	0.01393(6)	0.01537(6)	-0.00635(4)	-0.00072(4)	-0.00291(4)
P1	0.0108(3)	0.0118(3)	0.0148(3)	-0.0060(3)	-0.0005(3)	-0.0014(3)
Cl4	0.0367(6)	0.0517(6)	0.0423(5)	-0.0266(5)	0.0028(4)	-0.0095(5)
Cl3	0.0436(7)	0.1112(12)	0.0715(8)	-0.0660(9)	0.0194(6)	-0.0309(7)
Cl1	0.0335(6)	0.1122(12)	0.0816(10)	-0.0636(9)	0.0008(6)	-0.0071(7)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl2	0.0614(9)	0.1061(13)	0.0642(9)	0.0060(8)	-0.0224(7)	-0.0428(9)
F6	0.0149(9)	0.0138(8)	0.0162(8)	-0.0029(7)	0.0022(6)	-0.0031(7)
F21	0.0157(9)	0.0115(8)	0.0158(8)	-0.0057(6)	-0.0036(6)	0.0036(6)
F15	0.0175(9)	0.0206(9)	0.0125(8)	-0.0068(7)	0.0004(6)	0.0050(7)
F11	0.0165(9)	0.0201(9)	0.0134(8)	-0.0093(7)	0.0007(6)	0.0028(7)
F5	0.0196(9)	0.0158(8)	0.0126(8)	-0.0052(7)	-0.0045(7)	0.0007(7)
F12	0.0297(11)	0.0267(10)	0.0095(8)	-0.0091(7)	0.0003(7)	-0.0005(8)
F30	0.0177(9)	0.0134(8)	0.0186(8)	-0.0045(7)	-0.0034(7)	-0.0044(7)
F25	0.0135(9)	0.0188(9)	0.0185(8)	-0.0092(7)	-0.0040(7)	0.0049(7)
F26	0.0161(9)	0.0143(8)	0.0202(8)	-0.0073(7)	-0.0027(7)	-0.0031(7)
F10	0.0177(9)	0.0139(8)	0.0183(8)	-0.0007(7)	-0.0033(7)	-0.0046(7)
F24	0.0218(10)	0.0184(9)	0.0233(9)	-0.0123(8)	0.0016(7)	0.0074(7)
F16	0.0169(9)	0.0156(8)	0.0179(8)	-0.0068(7)	-0.0020(7)	0.0037(7)
F22	0.0330(11)	0.0202(9)	0.0126(8)	-0.0069(7)	-0.0105(7)	0.0042(8)
F20	0.0118(9)	0.0224(9)	0.0229(9)	-0.0097(8)	0.0029(7)	-0.0013(7)
F23	0.0447(13)	0.0258(10)	0.0159(9)	-0.0156(8)	-0.0044(8)	0.0076(9)
F8	0.0177(10)	0.0303(11)	0.0296(10)	-0.0138(9)	-0.0062(8)	0.0117(8)
F7	0.0108(9)	0.0338(11)	0.0216(9)	-0.0047(8)	0.0032(7)	0.0002(8)
F1	0.0277(10)	0.0118(8)	0.0176(8)	-0.0034(7)	-0.0061(7)	-0.0015(7)
F9	0.0300(11)	0.0127(8)	0.0267(10)	-0.0052(7)	-0.0117(8)	0.0054(8)
F29	0.0362(12)	0.0167(9)	0.0250(10)	0.0025(8)	-0.0121(9)	-0.0023(8)
F27	0.0189(10)	0.0319(11)	0.0228(9)	-0.0128(8)	-0.0076(7)	-0.0060(8)
F2	0.0371(12)	0.0134(9)	0.0326(11)	-0.0102(8)	0.0000(9)	-0.0087(8)
F17	0.0435(13)	0.0137(9)	0.0209(9)	-0.0041(7)	-0.0093(9)	0.0063(8)
F14	0.0208(10)	0.0344(11)	0.0222(9)	-0.0091(8)	-0.0079(8)	0.0149(9)
F4	0.0262(11)	0.0370(11)	0.0222(9)	-0.0182(9)	-0.0120(8)	0.0007(9)
F13	0.0319(12)	0.0339(11)	0.0129(8)	-0.0044(8)	-0.0097(8)	0.0060(9)
F19	0.0269(11)	0.0365(12)	0.0227(9)	-0.0111(9)	0.0099(8)	-0.0198(9)
F28	0.0315(12)	0.0314(11)	0.0219(9)	-0.0034(8)	-0.0166(8)	0.0016(9)
F3	0.0347(12)	0.0340(12)	0.0423(12)	-0.0280(10)	-0.0080(10)	-0.0093(10)
F18	0.0572(15)	0.0172(10)	0.0209(10)	0.0007(8)	0.0008(9)	-0.0180(10)
Cl6	0.0844(15)	0.204(3)	0.0747(12)	-0.0383(15)	0.0016(10)	-0.0424(16)
N2	0.0090(11)	0.0097(10)	0.0094(10)	-0.0039(8)	-0.0001(8)	-0.0008(8)
N3	0.0111(11)	0.0100(10)	0.0096(10)	-0.0056(9)	-0.0007(8)	-0.0013(9)
N1	0.0178(13)	0.0150(12)	0.0185(12)	-0.0087(10)	-0.0001(10)	-0.0033(10)
Cl5	0.090(2)	0.241(4)	0.280(5)	-0.171(4)	0.068(3)	-0.009(2)
C7	0.0109(13)	0.0097(12)	0.0092(11)	-0.0043(10)	-0.0019(10)	0.0009(10)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C49	0.0155(14)	0.0141(13)	0.0107(12)	-0.0052(10)	0.0011(10)	-0.0019(11)
C14	0.0144(14)	0.0135(13)	0.0106(12)	-0.0055(10)	-0.0001(10)	-0.0030(11)
C5	0.0134(14)	0.0138(13)	0.0121(12)	-0.0063(11)	0.0007(10)	-0.0010(11)
C25	0.0114(14)	0.0158(14)	0.0143(12)	-0.0059(11)	-0.0017(10)	-0.0021(11)
C20	0.0099(13)	0.0146(13)	0.0126(12)	-0.0068(11)	-0.0001(10)	-0.0004(10)
C1	0.0101(13)	0.0097(12)	0.0102(11)	-0.0044(10)	-0.0022(10)	0.0006(10)
C6	0.0116(13)	0.0094(12)	0.0109(12)	-0.0044(10)	-0.0015(10)	-0.0014(10)
C38	0.0115(13)	0.0133(13)	0.0108(12)	-0.0067(10)	0.0023(10)	-0.0037(10)
C31	0.0126(14)	0.0135(13)	0.0134(12)	-0.0033(11)	-0.0006(10)	-0.0012(11)
C52	0.0139(14)	0.0125(13)	0.0165(13)	-0.0050(11)	-0.0032(11)	-0.0005(11)
C59	0.0159(15)	0.0102(12)	0.0155(13)	-0.0041(11)	-0.0040(11)	0.0007(11)
C27	0.0115(13)	0.0106(12)	0.0123(12)	-0.0044(10)	0.0005(10)	0.0002(10)
C46	0.0217(16)	0.0162(14)	0.0103(12)	-0.0073(11)	-0.0002(11)	-0.0025(12)
C37	0.0143(14)	0.0141(13)	0.0106(12)	-0.0041(10)	-0.0012(10)	-0.0015(11)
C26	0.0098(13)	0.0123(13)	0.0104(11)	-0.0044(10)	0.0020(10)	-0.0023(10)
C2	0.0129(14)	0.0136(13)	0.0154(13)	-0.0075(11)	-0.0019(10)	-0.0002(11)
C32	0.0126(14)	0.0138(13)	0.0104(12)	-0.0059(10)	-0.0026(10)	0.0003(10)
C12	0.0169(15)	0.0177(14)	0.0118(12)	-0.0059(11)	-0.0021(10)	-0.0015(11)
C58	0.0134(14)	0.0093(12)	0.0162(13)	-0.0035(10)	-0.0046(11)	0.0000(10)
C70	0.0195(15)	0.0153(14)	0.0160(13)	-0.0071(11)	-0.0050(11)	0.0016(12)
C44	0.0120(13)	0.0101(12)	0.0106(12)	-0.0039(10)	-0.0006(10)	-0.0033(10)
C30	0.0167(15)	0.0136(13)	0.0155(13)	-0.0068(11)	0.0027(11)	0.0022(11)
C10	0.0203(16)	0.0133(13)	0.0197(14)	-0.0099(12)	-0.0004(12)	-0.0016(11)
C9	0.0145(14)	0.0128(13)	0.0129(12)	-0.0060(10)	-0.0018(10)	-0.0017(11)
C8	0.0105(13)	0.0119(12)	0.0099(11)	-0.0052(10)	0.0021(10)	-0.0035(10)
C67	0.0137(14)	0.0173(14)	0.0193(14)	-0.0064(12)	-0.0034(11)	-0.0020(11)
C4	0.0170(15)	0.0166(14)	0.0119(12)	-0.0094(11)	0.0006(10)	-0.0015(11)
C57	0.0133(14)	0.0138(13)	0.0147(13)	-0.0047(11)	-0.0038(10)	-0.0016(11)
C11	0.0218(16)	0.0206(15)	0.0164(13)	-0.0117(12)	-0.0008(11)	-0.0048(12)
C60	0.0146(14)	0.0143(13)	0.0159(13)	-0.0046(11)	-0.0002(11)	-0.0012(11)
C53	0.0156(15)	0.0136(14)	0.0305(16)	-0.0070(13)	-0.0071(12)	0.0008(12)
C43	0.0158(14)	0.0149(13)	0.0129(12)	-0.0063(11)	0.0014(10)	-0.0035(11)
C45	0.0127(14)	0.0124(13)	0.0141(12)	-0.0065(11)	0.0005(10)	-0.0017(10)
C13	0.0112(13)	0.0131(13)	0.0128(12)	-0.0055(10)	0.0001(10)	-0.0017(10)
C61	0.0133(14)	0.0123(13)	0.0194(14)	-0.0047(11)	-0.0039(11)	-0.0001(11)
C63	0.0163(15)	0.0123(13)	0.0148(13)	-0.0034(11)	-0.0011(11)	-0.0005(11)
C15	0.0186(15)	0.0141(13)	0.0114(12)	-0.0064(11)	-0.0015(10)	-0.0010(11)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C28	0.0185(15)	0.0157(14)	0.0092(12)	-0.0024(11)	-0.0025(10)	0.0007(11)
C64	0.0137(15)	0.0252(16)	0.0154(13)	-0.0043(12)	-0.0009(11)	-0.0030(12)
C3	0.0151(14)	0.0150(13)	0.0168(13)	-0.0097(11)	-0.0030(11)	-0.0020(11)
C19	0.0183(15)	0.0180(14)	0.0132(12)	-0.0077(11)	-0.0007(11)	-0.0044(12)
C29	0.0290(17)	0.0150(14)	0.0107(12)	-0.0075(11)	0.0011(11)	0.0009(12)
C47	0.0266(17)	0.0190(15)	0.0102(12)	-0.0032(11)	-0.0071(11)	-0.0025(13)
C56	0.0207(16)	0.0114(14)	0.0298(16)	-0.0056(12)	-0.0078(13)	0.0010(12)
C33	0.0142(14)	0.0146(13)	0.0132(12)	-0.0061(11)	-0.0025(10)	-0.0027(11)
C42	0.0223(16)	0.0148(14)	0.0226(15)	-0.0116(12)	0.0027(12)	-0.0043(12)
C39	0.0146(14)	0.0144(13)	0.0119(12)	-0.0068(11)	0.0012(10)	-0.0018(11)
C24	0.0200(16)	0.0163(14)	0.0147(13)	-0.0014(11)	-0.0015(11)	-0.0003(12)
C41	0.0215(17)	0.0233(16)	0.0263(16)	-0.0188(13)	0.0006(13)	-0.0070(13)
C40	0.0168(15)	0.0272(16)	0.0173(14)	-0.0136(13)	-0.0028(11)	-0.0004(12)
C34	0.0230(16)	0.0128(13)	0.0162(13)	-0.0071(11)	-0.0082(11)	0.0044(12)
C48	0.0153(15)	0.0179(14)	0.0175(14)	-0.0056(12)	-0.0033(11)	0.0020(12)
C73	0.0134(14)	0.0179(14)	0.0209(14)	-0.0104(12)	0.0025(11)	-0.0013(11)
C79	0.0260(18)	0.0140(14)	0.0253(16)	-0.0032(12)	-0.0007(13)	-0.0006(13)
C36	0.0120(14)	0.0249(16)	0.0150(13)	-0.0076(12)	-0.0006(11)	0.0003(12)
C18	0.0234(17)	0.0251(16)	0.0143(13)	-0.0098(12)	0.0047(12)	-0.0135(13)
C62	0.0156(15)	0.0171(14)	0.0153(13)	-0.0062(11)	-0.0041(11)	-0.0017(11)
C21	0.0123(14)	0.0152(14)	0.0160(13)	-0.0068(11)	0.0006(11)	-0.0006(11)
C77	0.0179(15)	0.0148(14)	0.0166(13)	-0.0039(11)	-0.0037(11)	0.0032(11)
C23	0.0188(16)	0.0278(17)	0.0123(13)	-0.0053(12)	-0.0066(11)	0.0030(13)
C78	0.0235(17)	0.0230(16)	0.0155(14)	-0.0056(12)	-0.0001(12)	0.0019(13)
C35	0.0150(15)	0.0214(15)	0.0182(13)	-0.0111(12)	-0.0067(11)	0.0077(12)
C22	0.0144(15)	0.0252(16)	0.0181(14)	-0.0123(12)	-0.0043(11)	-0.0005(12)
C54	0.0206(17)	0.0177(16)	0.043(2)	-0.0093(15)	-0.0127(15)	-0.0042(13)
C16	0.0324(19)	0.0143(14)	0.0141(13)	-0.0064(11)	-0.0069(12)	-0.0007(13)
C74	0.0203(17)	0.0296(18)	0.0186(15)	-0.0069(13)	0.0026(12)	0.0010(14)
C69	0.0177(16)	0.0216(16)	0.0292(17)	-0.0035(14)	-0.0080(13)	0.0004(13)
C50	0.0193(16)	0.0137(13)	0.0164(13)	-0.0063(11)	-0.0025(11)	0.0015(12)
C80	0.0253(18)	0.0262(17)	0.0227(15)	-0.0059(14)	-0.0103(13)	0.0019(14)
C65	0.0253(19)	0.0265(18)	0.0252(16)	-0.0005(14)	-0.0002(14)	-0.0059(14)
C75	0.0160(16)	0.0218(16)	0.0291(16)	-0.0084(13)	0.0020(13)	0.0004(13)
C17	0.039(2)	0.0138(14)	0.0114(13)	-0.0027(11)	-0.0013(12)	-0.0113(13)
C66	0.0210(17)	0.0377(19)	0.0182(14)	-0.0144(14)	0.0003(12)	-0.0034(14)
C51	0.0175(16)	0.0204(16)	0.0387(19)	-0.0143(15)	-0.0001(14)	-0.0038(13)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C71	0.033(2)	0.0195(16)	0.0295(17)	-0.0144(14)	-0.0103(14)	0.0050(14)
C72	0.0239(17)	0.0233(16)	0.0164(14)	-0.0056(12)	-0.0016(12)	0.0003(13)
C55	0.0247(18)	0.0135(15)	0.043(2)	-0.0077(14)	-0.0125(15)	-0.0037(13)
C76	0.0245(18)	0.0286(18)	0.0343(18)	-0.0231(15)	0.0072(14)	-0.0059(14)
C68	0.0182(17)	0.0232(17)	0.0382(19)	-0.0145(15)	-0.0043(14)	-0.0019(13)
B1	0.0084(14)	0.0099(13)	0.0115(13)	-0.0034(11)	-0.0002(11)	-0.0013(11)
B2	0.0109(14)	0.0091(13)	0.0083(12)	-0.0032(11)	-0.0010(10)	-0.0010(11)
C82	0.036(2)	0.042(2)	0.042(2)	-0.0266(19)	-0.0012(18)	-0.0009(18)
C81	0.040(3)	0.045(3)	0.045(2)	-0.006(2)	-0.015(2)	-0.005(2)
C83	0.088(5)	0.226(11)	0.098(5)	-0.125(7)	-0.067(5)	0.093(6)

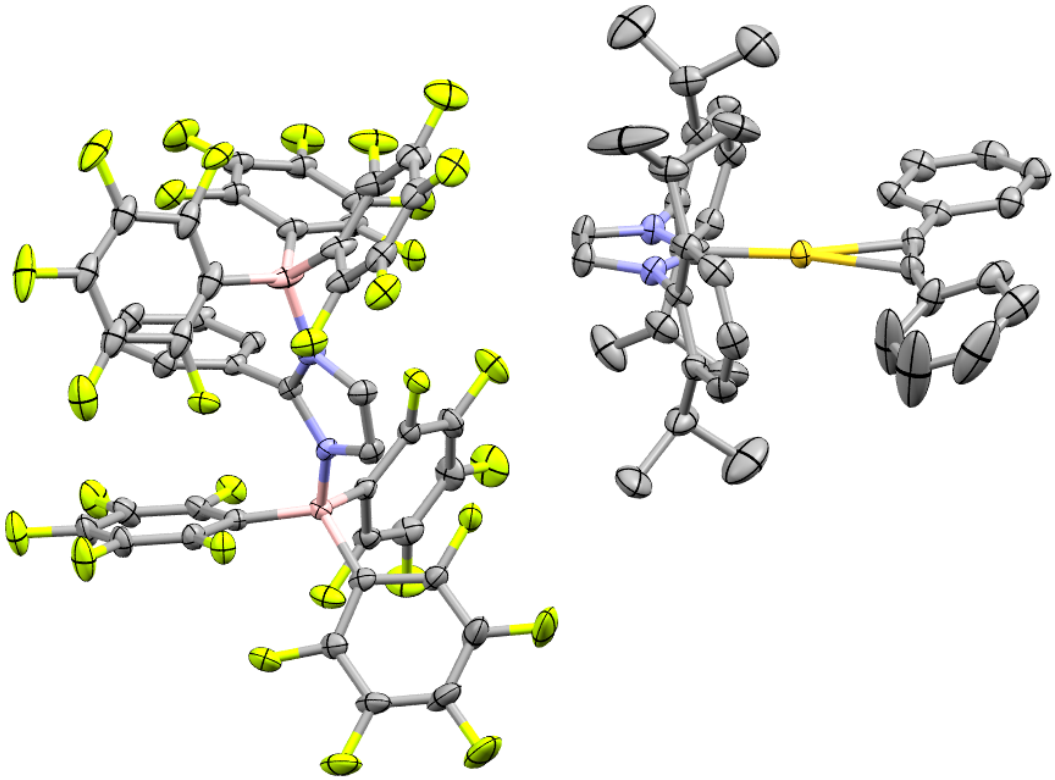
Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 5790.

	x/a	y/b	z/c	U(eq)
H5	0.5307	0.5406	0.5923	0.015
H2	0.2639	0.4438	0.7456	0.016
H12	0.5276	0.6152	0.9920	0.018
H70	0.2354	1.0394	0.6550	0.02
H10	0.3902	0.8283	0.8603	0.02
H9	0.3667	0.7643	0.7710	0.016
H67	0.5683	1.0120	0.7828	0.02
H4	0.4503	0.4481	0.5643	0.017
H11	0.4694	0.7531	0.9712	0.022
H60	0.4539	1.0280	0.7056	0.018
H53	-0.0308	1.0936	0.7576	0.024
H13	0.5048	0.5511	0.9033	0.015
H64	0.1614	0.9948	0.9374	0.023
H3	0.3189	0.4005	0.6396	0.017
H56	0.1899	0.8788	0.8217	0.025
H79A	0.0445	1.3601	0.6769	0.035
H79B	0.1039	1.3814	0.5932	0.035
H79C	0.1487	1.3528	0.6757	0.035
H62	0.3923	1.0007	0.9369	0.019
H78A	0.2348	1.2437	0.6326	0.032
H78B	0.1818	1.2641	0.5558	0.032
H78C	0.1874	1.1696	0.6226	0.032

	x/a	y/b	z/c	U(eq)
H54	-0.0615	0.9549	0.7806	0.032
H74A	-0.0107	1.0807	0.9081	0.036
H74B	-0.0262	1.1413	0.9582	0.036
H74C	0.0708	1.1077	0.9379	0.036
H69A	0.5293	0.9240	0.9526	0.036
H69B	0.6246	0.9260	0.9059	0.036
H69C	0.5495	0.8789	0.8886	0.036
H80A	0.0245	1.1788	0.6270	0.038
H80B	0.0233	1.2763	0.5664	0.038
H80C	-0.0320	1.2499	0.6526	0.038
H65A	0.2307	0.8559	0.9780	0.042
H65B	0.1936	0.8770	1.0555	0.042
H65C	0.2958	0.8813	1.0265	0.042
H75A	-0.0636	1.2856	0.7573	0.035
H75B	-0.1102	1.2447	0.8468	0.035
H75C	-0.0891	1.1886	0.7924	0.035
H66A	0.2860	1.0285	1.0246	0.037
H66B	0.1821	1.0326	1.0440	0.037
H66C	0.2267	1.1021	0.9642	0.037
H51A	0.5468	1.2875	0.7627	0.037
H51B	0.5230	1.2913	0.8502	0.037
H51C	0.4912	1.3682	0.7722	0.037
H71A	0.3795	0.9185	0.6577	0.038
H71B	0.2986	0.9357	0.6048	0.038
H71C	0.2838	0.8938	0.7011	0.038
H72A	0.3452	1.1432	0.5909	0.033
H72B	0.3225	1.0949	0.5359	0.033
H72C	0.4102	1.0678	0.5809	0.033
H55	0.0503	0.8466	0.8143	0.032
H76A	0.1078	1.2611	0.8809	0.039
H76B	0.0080	1.2911	0.8967	0.039
H76C	0.0576	1.3288	0.8082	0.039
H68A	0.5458	1.1388	0.8035	0.038
H68B	0.6181	1.0808	0.8606	0.038
H68C	0.5198	1.0897	0.8978	0.038
H82A	0.3014	0.6108	0.5437	0.044
H82B	0.2576	0.6939	0.4785	0.044

	x/a	y/b	z/c	U(eq)
H81A	0.1808	0.9944	0.3246	0.054
H81B	0.2697	0.9385	0.3501	0.054
H83A	0.8447	0.5839	0.8819	0.144
H83B	0.9488	0.5837	0.8681	0.144

Crystal Structure Report for 3[IMP-H]



Thermal ellipsoid plot of 5504. Ellipsoids are shown at 50% probability, hydrogens and solvent molecules omitted for clarity.

A specimen of $C_{88}H_{56.69}AuB_2Cl_4F_{30}N_4$, approximate dimensions 0.073 mm x 0.193 mm x 0.272 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The integration of the data using a triclinic unit cell yielded a total of 73125 reflections to a maximum θ angle of 28.05° (0.76 Å resolution), of which 19326 were independent (average redundancy 3.784, completeness = 98.5%, R_{int} = 4.32%, R_{sig} = 4.44%) and 16549 (85.63%) were greater than $2\sigma(F^2)$. The final cell constants of a = 13.708(2) Å, b = 18.136(3) Å, c = 18.494(3) Å, α = 113.739(3)°, β = 97.758(3)°, γ = 99.532(3)°, volume = 4045.8(10) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6405 and 0.7456. The final anisotropic full-matrix least-squares refinement on F^2 with 1401 variables converged at R1 = 4.42%, for the observed data and wR2 = 12.76% for all data. The goodness-of-fit was 1.042. The largest peak in the final difference electron density synthesis was 1.699 $e^-/Å^3$ and the largest hole was -2.366 $e^-/Å^3$ with an RMS deviation of 0.129 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.724 g/cm^3 and F(000), 2079 e^-.

Table 1. Sample and crystal data for 5504.

Identification code	5504
Chemical formula	$C_{88}H_{56.69}AuB_2Cl_4F_{30}N_4$
Formula weight	2100.44 g/mol
Wavelength	0.71073 Å

Crystal size	0.073 x 0.193 x 0.272 mm	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 13.708(2) Å	α = 113.739(3)°
	b = 18.136(3) Å	β = 97.758(3)°
	c = 18.494(3) Å	γ = 99.532(3)°
Volume	4045.8(10) $Å^3$	
Z	2	
Density (calculated)	1.724 g/cm^3	
Absorption coefficient	2.071 mm^{-1}	
F(000)	2079	

Table 2. Data collection and structure refinement for 5504.

Theta range for data collection	1.23 to 28.05°	
Index ranges	-18<=h<=18, -23<=k<=23, -24<=l<=24	
Reflections collected	73125	
Independent reflections	19326 [R(int) = 0.0432]	
Max. and min. transmission	0.7456 and 0.6405	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	XL (Sheldrick, 2008)	
Function minimized	$\Sigma\ w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	19326 / 96 / 1401	
Goodness-of-fit on F^2	1.042	
Δ/σ_{max}	0.005	
Final R indices	16549 data; I>2σ(I)	R1 = 0.0442, wR2 = 0.1206
	all data	R1 = 0.0557, wR2 = 0.1276
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0738P)^2+7.3333P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	1.699 and -2.366 $eÅ^{-3}$	
R.M.S. deviation from mean	0.129 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for 5504.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Au1	0.68210(2)	0.37783(2)	0.05308(2)	0.02301(6)
F15	0.3547(2)	0.97665(15)	0.36955(14)	0.0284(5)
F11	0.29762(19)	0.20977(14)	0.58165(15)	0.0271(5)
Cl2	0.1938(3)	0.2290(2)	0.9895(4)	0.0705(19)
Cl1	0.9805(8)	0.2400(5)	0.9583(5)	0.046(4)

	x/a	y/b	z/c	U(eq)
F10	0.39399(19)	0.18458(16)	0.29264(15)	0.0278(5)
F5	0.4786(2)	0.18027(19)	0.62538(16)	0.0380(6)
F6	0.5464(2)	0.07092(17)	0.45560(15)	0.0322(6)
F1	0.55186(19)	0.29645(17)	0.44508(15)	0.0335(6)
F25	0.2322(17)	0.2537(14)	0.2377(13)	0.027(3)
F12	0.1726(2)	0.10725(18)	0.61753(18)	0.0446(8)
F30	0.1131(2)	0.41018(16)	0.48845(16)	0.0343(6)
F16	0.104(2)	0.2607(19)	0.5094(16)	0.030(3)
F29	0.0937(2)	0.55461(15)	0.49402(18)	0.0376(6)
F26	0.0459(3)	0.29755(18)	0.20182(17)	0.0489(8)
F14	0.2296(3)	0.87867(16)	0.40553(18)	0.0420(7)
F28	0.0505(2)	0.57366(17)	0.3558(2)	0.0445(7)
F7	0.6596(2)	0.0133(2)	0.34898(18)	0.0465(8)
F9	0.5049(3)	0.1235(2)	0.18701(17)	0.0456(7)
F8	0.6404(3)	0.0387(2)	0.21341(19)	0.0527(9)
F4	0.6337(2)	0.2916(2)	0.73536(17)	0.0494(8)
F13	0.1346(3)	0.94102(18)	0.5296(2)	0.0489(8)
F21	0.927(2)	0.0897(18)	0.2440(14)	0.033(3)
N2	0.3292(2)	0.22031(19)	0.43561(19)	0.0180(6)
F27	0.0284(3)	0.4418(2)	0.2106(2)	0.0521(8)
F3	0.7558(2)	0.4037(3)	0.70331(19)	0.0650(11)
Cl3	0.4688(3)	0.4946(2)	0.4707(2)	0.1443(14)
N1	0.1959(2)	0.2565(2)	0.3908(2)	0.0207(7)
Cl4	0.3214(3)	0.4406(3)	0.3238(3)	0.1570(15)
F2	0.7124(3)	0.4011(3)	0.5552(2)	0.0741(13)
N4	0.5254(3)	0.3336(2)	0.1393(2)	0.0246(7)
F22	0.9335(18)	0.9725(16)	0.1081(15)	0.046(3)
F17	0.9492(13)	0.2424(8)	0.5765(9)	0.049(3)
F24	0.2413(11)	0.1283(12)	0.1048(12)	0.039(3)
F23	0.0913(15)	0.9839(14)	0.0352(13)	0.043(3)
N3	0.5300(3)	0.2273(2)	0.0335(2)	0.0242(7)
F20	0.8839(8)	0.2363(6)	0.2795(8)	0.036(2)
C28	0.3358(3)	0.0997(2)	0.4751(2)	0.0197(7)
C3	0.2329(3)	0.1921(2)	0.3911(2)	0.0184(7)
C40	0.5012(3)	0.2344(3)	0.5288(2)	0.0224(8)
C33	0.2849(3)	0.1275(2)	0.5372(2)	0.0224(8)
C64	0.6186(3)	0.0873(3)	0.8220(3)	0.0312(10)
C4	0.1761(3)	0.1037(2)	0.3499(2)	0.0194(7)
C34	0.4608(3)	0.1275(2)	0.3787(2)	0.0199(7)
C5	0.2019(3)	0.0482(2)	0.2816(2)	0.0219(8)
C45	0.5302(3)	0.2351(3)	0.6038(3)	0.0269(9)

	x/a	y/b	z/c	U(eq)
C6	0.1473(3)	0.9659(3)	0.2426(3)	0.0270(9)
C1	0.2712(3)	0.3268(2)	0.4366(3)	0.0257(8)
C74	0.7953(3)	0.4239(3)	0.9983(3)	0.0282(9)
C65	0.5459(4)	0.1309(3)	0.8187(3)	0.0337(10)
C10	0.9979(18)	0.2424(16)	0.3921(17)	0.0375(19)
C29	0.3142(3)	0.0140(3)	0.4330(2)	0.0232(8)
C2	0.3518(3)	0.3056(2)	0.4644(2)	0.0234(8)
C32	0.2189(4)	0.0760(3)	0.5562(3)	0.0293(9)
C63	0.6613(3)	0.0890(3)	0.8954(3)	0.0292(9)
C54	0.4850(3)	0.4678(3)	0.1868(3)	0.0283(9)
C62	0.6320(3)	0.1342(3)	0.9662(3)	0.0261(8)
C73	0.7954(4)	0.4821(3)	0.0600(3)	0.0311(10)
C46	0.5729(3)	0.3091(2)	0.0772(2)	0.0236(8)
C39	0.4561(3)	0.1396(3)	0.3097(2)	0.0231(8)
C49	0.5457(3)	0.4183(2)	0.1997(2)	0.0226(8)
C48	0.4561(3)	0.2010(3)	0.0670(3)	0.0312(10)
C61	0.5586(3)	0.1771(2)	0.9600(3)	0.0247(8)
C30	0.2479(4)	0.9609(3)	0.4503(3)	0.0303(9)
C17	0.0839(3)	0.4907(3)	0.4218(3)	0.0313(10)
C35	0.5324(3)	0.0843(3)	0.3890(2)	0.0253(8)
C81	0.8196(3)	0.3737(3)	0.9226(3)	0.0282(9)
C41	0.5679(3)	0.2932(3)	0.5167(3)	0.0277(9)
F19	0.7267(5)	0.2179(6)	0.3467(11)	0.055(3)
C21	0.0854(3)	0.3446(3)	0.3447(3)	0.0306(10)
C67	0.6818(4)	0.1367(3)	0.0462(3)	0.0363(11)
C47	0.4529(3)	0.2676(3)	0.1335(3)	0.0303(9)
C20	0.0624(4)	0.3589(3)	0.2770(3)	0.0356(11)
C9	0.0965(3)	0.0755(3)	0.3785(3)	0.0263(8)
C86	0.7804(4)	0.2888(3)	0.8809(3)	0.0301(9)
C66	0.5131(3)	0.1761(3)	0.8876(3)	0.0293(9)
C11	0.0126(17)	0.2497(14)	0.4654(15)	0.0374(19)
C50	0.6267(3)	0.4462(3)	0.2668(3)	0.0278(9)
C8	0.0428(3)	0.9927(3)	0.3398(3)	0.0331(10)
C7	0.0687(3)	0.9383(3)	0.2716(3)	0.0327(10)
C16	0.0939(3)	0.4144(3)	0.4172(3)	0.0297(9)
C51	0.6463(4)	0.5290(3)	0.3225(3)	0.0342(10)
C75	0.8114(4)	0.5636(3)	0.1258(3)	0.0385(11)
F18	0.7583(9)	0.2175(6)	0.4968(12)	0.062(4)
C31	0.2000(4)	0.9918(3)	0.5129(3)	0.0329(10)
C23	0.1536(15)	0.1819(12)	0.2061(13)	0.026(2)
C43	0.6748(3)	0.3487(4)	0.6472(3)	0.0422(13)

	x/a	y/b	z/c	U(eq)
C18	0.0620(3)	0.5004(3)	0.3527(3)	0.0333(10)
C42	0.6513(4)	0.3490(4)	0.5730(3)	0.0416(12)
C22	0.081(2)	0.1804(18)	0.2508(19)	0.026(2)
C38	0.5145(4)	0.1104(3)	0.2538(3)	0.0300(9)
C85	0.8059(4)	0.2445(3)	0.8084(3)	0.0365(11)
C37	0.5833(4)	0.0678(3)	0.2668(3)	0.0339(10)
C19	0.0514(4)	0.4344(3)	0.2795(3)	0.0358(10)
B1	0.0868(4)	0.2537(3)	0.3449(3)	0.0300(11)
C82	0.8859(4)	0.4146(3)	0.8916(3)	0.0333(10)
C52	0.5886(4)	0.5805(3)	0.3102(3)	0.0382(11)
C70	0.4295(4)	0.2208(3)	0.8816(3)	0.0358(10)
C58	0.3974(4)	0.4349(4)	0.1135(3)	0.0405(12)
C24	0.1633(14)	0.1226(13)	0.1428(14)	0.026(2)
B2	0.4048(3)	0.1683(3)	0.4538(3)	0.0178(8)
C80	0.8444(4)	0.6325(3)	0.1117(4)	0.0475(13)
C36	0.5919(3)	0.0543(3)	0.3351(3)	0.0313(10)
C44	0.6141(3)	0.2926(3)	0.6631(3)	0.0347(11)
C84	0.8712(4)	0.2850(3)	0.7777(3)	0.0381(11)
C25	0.0876(13)	0.0497(12)	0.1033(13)	0.026(2)
C55	0.6875(4)	0.3894(4)	0.2812(4)	0.0448(13)
C27	0.0030(17)	0.1034(12)	0.2085(12)	0.026(2)
C53	0.5093(4)	0.5505(3)	0.2439(3)	0.0370(11)
C83	0.9105(4)	0.3695(4)	0.8190(3)	0.0391(11)
C15	0.9081(13)	0.2376(9)	0.3536(12)	0.0375(19)
C68	0.7917(5)	0.1855(4)	0.0737(4)	0.0564(16)
C71	0.4579(6)	0.2820(4)	0.8459(4)	0.0615(17)
C26	0.0065(15)	0.0405(14)	0.1379(14)	0.026(2)
C69	0.6728(6)	0.0494(4)	0.0411(4)	0.0586(17)
C12	0.9300(12)	0.2410(9)	0.5043(11)	0.0375(19)
C59	0.4317(6)	0.4609(4)	0.0495(4)	0.0594(17)
C13	0.8342(11)	0.2268(9)	0.4602(13)	0.0375(19)
C72	0.3298(5)	0.1573(4)	0.8330(5)	0.072(2)
C14	0.8247(10)	0.2282(7)	0.3873(11)	0.0377(19)
C79	0.8659(5)	0.7102(4)	0.1730(5)	0.0621(19)
C56	0.7987(5)	0.4184(5)	0.2908(6)	0.078(2)
C78	0.8550(6)	0.7222(5)	0.2479(6)	0.091(3)
C88	0.0751(7)	0.2227(5)	0.0227(5)	0.076(2)
C76	0.7963(8)	0.5779(5)	0.2005(4)	0.102(4)
C77	0.8180(9)	0.6589(6)	0.2616(5)	0.127(5)
C60	0.3032(6)	0.4611(9)	0.1352(5)	0.132(5)
C87	0.4336(9)	0.4253(8)	0.3665(7)	0.120(4)

	x/a	y/b	z/c	U(eq)
C57	0.6831(8)	0.3985(7)	0.3718(6)	0.054(3)
Cl1A	0.1819(12)	0.270(3)	0.044(3)	0.221(17)
Cl2A	0.9946(11)	0.2635(17)	0.9807(16)	0.139(4)
F21A	0.911(2)	0.0905(19)	0.261(2)	0.055(6)
C27A	0.987(2)	0.1038(13)	0.2253(13)	0.040(6)
C26A	0.983(3)	0.0373(16)	0.1522(15)	0.053(7)
F22A	0.912(3)	0.9660(17)	0.119(2)	0.088(9)
F23A	0.065(3)	0.976(2)	0.0450(17)	0.094(9)
C25A	0.056(3)	0.0392(16)	0.1122(11)	0.053(7)
C24A	0.134(3)	0.109(2)	0.1370(15)	0.056(8)
F24A	0.211(3)	0.1172(19)	0.1039(15)	0.074(7)
C23A	0.138(2)	0.1812(16)	0.2166(11)	0.049(7)
F25A	0.212(2)	0.2459(18)	0.2441(16)	0.037(5)
C22A	0.0609(16)	0.1749(16)	0.2577(18)	0.032(5)
C57A	0.6386(15)	0.3320(15)	0.3065(19)	0.068(9)
F20A	0.8657(10)	0.2374(8)	0.3083(10)	0.039(3)
C15A	0.8950(11)	0.2373(8)	0.3773(11)	0.028(4)
C10A	0.0028(19)	0.2422(17)	0.3992(16)	0.035(4)
C11A	0.0215(16)	0.2455(12)	0.4805(10)	0.023(3)
F16A	0.119(3)	0.254(2)	0.5213(19)	0.025(4)
C12A	0.9560(12)	0.2451(9)	0.5274(13)	0.034(4)
F17A	0.9802(12)	0.2522(11)	0.6054(10)	0.041(3)
C13A	0.8551(11)	0.2425(9)	0.5004(15)	0.037(4)
F18A	0.7873(10)	0.2460(10)	0.5500(13)	0.057(4)
F19A	0.7304(7)	0.2368(8)	0.3987(14)	0.057(4)
C14A	0.8240(8)	0.2385(8)	0.4260(14)	0.031(4)

Table 4. Bond lengths (Å) for 5504.

Au1-C74	2.193(4)	Au1-C73	2.186(4)
Au1-C46	2.001(4)	F15-C29	1.343(4)
F11-C33	1.349(4)	Cl2-C88	1.816(10)
Cl1-C88	1.794(12)	F10-C39	1.363(5)
F5-C45	1.345(5)	F6-C35	1.343(5)
F1-C41	1.339(5)	F25-C23	1.40(2)
F12-C32	1.344(5)	F30-C16	1.343(5)
F16-C11	1.33(3)	F29-C17	1.341(5)
F26-C20	1.344(5)	F14-C30	1.341(5)
F28-C18	1.343(5)	F7-C36	1.340(5)
F9-C38	1.341(5)	F8-C37	1.340(5)
F4-C44	1.336(5)	F13-C31	1.333(5)

F21-C27	1.35(2)	N2-C3	1.352(5)
N2-C2	1.380(5)	N2-B2	1.601(5)
F27-C19	1.336(6)	F3-C43	1.339(5)
Cl3-Cl3	1.212(7)	Cl3-C87	1.768(12)
N1-C3	1.350(5)	N1-C1	1.366(5)
N1-B1	1.600(6)	Cl4-C87	1.747(12)
F2-C42	1.329(6)	N4-C46	1.351(5)
N4-C49	1.442(5)	N4-C47	1.381(6)
F22-C26	1.31(3)	F17-C12	1.316(18)
F24-C24	1.37(3)	F23-C25	1.36(3)
N3-C46	1.349(5)	N3-C48	1.372(5)
N3-C61	1.448(5)	F20-C15	1.35(2)
C28-C33	1.388(5)	C28-C29	1.387(5)
C28-B2	1.643(6)	C3-C4	1.482(5)
C40-C45	1.385(6)	C40-C41	1.396(6)
C40-B2	1.658(6)	C33-C32	1.373(6)
C64-H64	0.95	C64-C65	1.380(7)
C64-C63	1.391(7)	C4-C5	1.396(5)
C4-C9	1.386(6)	C34-C39	1.375(6)
C34-C35	1.391(6)	C34-B2	1.647(5)
C5-H5	0.95	C5-C6	1.387(6)
C45-C44	1.399(7)	C6-H6	0.95
C6-C7	1.376(6)	C1-H1	0.95
C1-C2	1.335(6)	C74-C73	1.202(6)
C74-C81	1.450(6)	C65-H65	0.95
C65-C66	1.390(6)	C10-C11	1.29(3)
C10-B1	1.62(2)	C10-C15	1.31(3)
C29-C30	1.375(6)	C2-H2	0.95
C32-C31	1.366(6)	C63-H63	0.95
C63-C62	1.391(6)	C54-C49	1.386(6)
C54-C58	1.518(7)	C54-C53	1.393(7)
C62-C61	1.390(6)	C62-C67	1.524(6)
C73-C75	1.444(6)	C39-C38	1.384(6)
C49-C50	1.402(6)	C48-H48	0.95
C48-C47	1.345(6)	C61-C66	1.390(6)
C30-C31	1.374(6)	C17-C16	1.382(6)
C17-C18	1.361(7)	C35-C36	1.373(6)
C81-C86	1.383(6)	C81-C82	1.401(6)
C41-C42	1.365(6)	F19-C14	1.392(16)
C21-C20	1.383(7)	C21-C16	1.399(6)
C21-B1	1.654(7)	C67-H67	1.0
C67-C68	1.517(8)	C67-C69	1.531(7)

C47-H47	0.95	C20-C19	1.386(7)
C9-H9	0.95	C9-C8	1.392(6)
C86-H86	0.95	C86-C85	1.385(6)
C66-C70	1.526(6)	C11-C12	1.44(3)
C50-C51	1.391(6)	C50-C55	1.506(7)
C8-H8	0.95	C8-C7	1.387(7)
C7-H7	0.95	C51-H51	0.95
C51-C52	1.385(7)	C75-C80	1.393(8)
C75-C76	1.352(8)	F18-C13	1.339(15)
C23-C22	1.38(2)	C23-C24	1.27(3)
C43-C42	1.369(7)	C43-C44	1.355(8)
C18-C19	1.367(7)	C22-B1	1.69(3)
C22-C27	1.45(3)	C38-C37	1.369(7)
C85-H85	0.95	C85-C84	1.385(7)
C37-C36	1.374(7)	B1-C22A	1.61(3)
B1-C10A	1.67(3)	C82-H82	0.95
C82-C83	1.384(7)	C52-H52	0.95
C52-C53	1.374(8)	C70-H70	1.0
C70-C71	1.528(8)	C70-C72	1.522(8)
C58-H58	1.0	C58-C59	1.538(8)
C58-C60	1.499(9)	C24-C25	1.39(2)
C80-H80	0.95	C80-C79	1.358(8)
C84-H84	0.95	C84-C83	1.377(8)
C25-C26	1.376(19)	C55-H55	1.0
C55-C56	1.490(8)	C55-C57	1.627(11)
C55-C57A	1.415(18)	C27-C26	1.36(3)
C53-H53	0.95	C83-H83	0.95
C15-C14	1.391(15)	C68-H68A	0.98
C68-H68B	0.98	C68-H68C	0.98
C71-H71A	0.98	C71-H71B	0.98
C71-H71C	0.98	C69-H69A	0.98
C69-H69B	0.98	C69-H69C	0.98
C12-C13	1.374(19)	C59-H59A	0.98
C59-H59B	0.98	C59-H59C	0.98
C13-C14	1.349(19)	C72-H72A	0.98
C72-H72B	0.98	C72-H72C	0.98
C79-H79	0.95	C79-C78	1.346(12)
C56-H56A	0.98	C56-H56B	0.98
C56-H56C	0.98	C78-H78	0.95
C78-C77	1.311(13)	C88-H88A	0.99
C88-H88B	0.99	C88-H88C	0.99
C88-H88D	0.99	C88-Cl1A	1.479(14)

C88-Cl2A	1.694(11)	C76-H76	0.95
C76-C77	1.396(10)	C77-H77	0.95
C60-H60A	0.98	C60-H60B	0.98
C60-H60C	0.98	C87-H87A	0.99
C87-H87B	0.99	C57-H57A	0.98
C57-H57B	0.98	C57-H57C	0.98
F21A-C27A	1.35(3)	C27A-C26A	1.389(18)
C27A-C22A	1.35(3)	C26A-F22A	1.33(3)
C26A-C25A	1.33(2)	F23A-C25A	1.35(3)
C25A-C24A	1.38(3)	C24A-F24A	1.31(3)
C24A-C23A	1.51(3)	C23A-F25A	1.29(3)
C23A-C22A	1.40(2)	C57A-H57D	0.98
C57A-H57E	0.98	C57A-H57F	0.98
F20A-C15A	1.28(2)	C15A-C10A	1.46(3)
C15A-C14A	1.410(17)	C10A-C11A	1.46(3)
C11A-F16A	1.40(3)	C11A-C12A	1.33(3)
C12A-F17A	1.38(2)	C12A-C13A	1.392(15)
C13A-F18A	1.383(17)	C13A-C14A	1.35(2)
F19A-C14A	1.304(15)		

Table 5. Bond angles (°) for 5504.

C73-Au1-C74	31.85(17)	C46-Au1-C74	165.39(16)
C46-Au1-C73	162.71(17)	C3-N2-C2	106.3(3)
C3-N2-B2	128.5(3)	C2-N2-B2	125.2(3)
Cl3-Cl3-C87	136.8(7)	C3-N1-C1	106.8(3)
C3-N1-B1	128.0(3)	C1-N1-B1	125.2(3)
C46-N4-C49	123.5(4)	C46-N4-C47	110.6(4)
C47-N4-C49	125.9(3)	C46-N3-C48	110.9(3)
C46-N3-C61	122.6(3)	C48-N3-C61	126.4(3)
C33-C28-B2	118.8(3)	C29-C28-C33	113.8(4)
C29-C28-B2	127.2(3)	N2-C3-C4	125.0(3)
N1-C3-N2	109.8(3)	N1-C3-C4	125.2(3)
C45-C40-C41	113.1(4)	C45-C40-B2	127.1(4)
C41-C40-B2	119.6(4)	F11-C33-C28	119.7(3)
F11-C33-C32	116.3(4)	C32-C33-C28	124.0(4)
C65-C64-H64	120.1	C65-C64-C63	119.9(4)
C63-C64-H64	120.1	C5-C4-C3	120.3(3)
C9-C4-C3	120.4(3)	C9-C4-C5	119.3(4)
C39-C34-C35	113.7(4)	C39-C34-B2	127.8(3)
C35-C34-B2	117.9(3)	C4-C5-H5	120.0
C6-C5-C4	120.0(4)	C6-C5-H5	120.0

F5-C45-C40	122.1(4)	F5-C45-C44	114.8(4)
C40-C45-C44	123.1(4)	C5-C6-H6	119.8
C7-C6-C5	120.3(4)	C7-C6-H6	119.8
N1-C1-H1	125.6	C2-C1-N1	108.7(4)
C2-C1-H1	125.6	C73-C74-Au1	73.8(3)
C73-C74-C81	161.7(5)	C81-C74-Au1	124.5(3)
C64-C65-H65	119.4	C64-C65-C66	121.3(4)
C66-C65-H65	119.4	C11-C10-B1	125.(2)
C11-C10-C15	121.(2)	C15-C10-B1	113.(2)
F15-C29-C28	121.6(4)	F15-C29-C30	114.9(4)
C30-C29-C28	123.5(4)	N2-C2-H2	125.8
C1-C2-N2	108.4(4)	C1-C2-H2	125.8
F12-C32-C33	120.8(4)	F12-C32-C31	119.1(4)
C31-C32-C33	120.1(4)	C64-C63-H63	119.5
C62-C63-C64	121.0(4)	C62-C63-H63	119.5
C49-C54-C58	122.3(4)	C49-C54-C53	116.6(4)
C53-C54-C58	121.1(4)	C63-C62-C67	120.0(4)
C61-C62-C63	117.1(4)	C61-C62-C67	123.0(4)
C74-C73-Au1	74.4(3)	C74-C73-C75	165.3(5)
C75-C73-Au1	120.1(3)	N4-C46-Au1	128.4(3)
N3-C46-Au1	126.7(3)	N3-C46-N4	104.9(4)
F10-C39-C34	121.4(3)	F10-C39-C38	114.5(4)
C34-C39-C38	124.1(4)	C54-C49-N4	117.7(4)
C54-C49-C50	124.0(4)	C50-C49-N4	118.3(4)
N3-C48-H48	126.5	C47-C48-N3	106.9(4)
C47-C48-H48	126.5	C62-C61-N3	117.9(4)
C66-C61-N3	118.4(4)	C66-C61-C62	123.6(4)
F14-C30-C29	119.7(4)	F14-C30-C31	120.0(4)
C31-C30-C29	120.3(4)	F29-C17-C16	120.3(5)
F29-C17-C18	119.9(4)	C18-C17-C16	119.8(4)
F6-C35-C34	119.3(3)	F6-C35-C36	116.6(4)
C36-C35-C34	124.1(4)	C86-C81-C74	122.9(4)
C86-C81-C82	119.9(4)	C82-C81-C74	117.3(4)
F1-C41-C40	119.4(4)	F1-C41-C42	115.8(4)
C42-C41-C40	124.8(4)	C20-C21-C16	112.9(4)
C20-C21-B1	126.2(4)	C16-C21-B1	120.2(4)
C62-C67-H67	107.6	C62-C67-C69	111.7(5)
C68-C67-C62	110.9(4)	C68-C67-H67	107.6
C68-C67-C69	111.2(5)	C69-C67-H67	107.6
N4-C47-H47	126.7	C48-C47-N4	106.7(4)
C48-C47-H47	126.7	F26-C20-C21	121.2(4)
F26-C20-C19	114.5(4)	C21-C20-C19	124.4(4)

C4-C9-H9	119.8	C4-C9-C8	120.5(4)
C8-C9-H9	119.8	C81-C86-H86	120.0
C81-C86-C85	120.0(4)	C85-C86-H86	120.0
C65-C66-C70	120.1(4)	C61-C66-C65	117.1(4)
C61-C66-C70	122.7(4)	F16-C11-C12	114.(2)
C10-C11-F16	123.(2)	C10-C11-C12	122.(2)
C49-C50-C55	122.5(4)	C51-C50-C49	116.8(4)
C51-C50-C55	120.7(4)	C9-C8-H8	120.2
C7-C8-C9	119.6(4)	C7-C8-H8	120.2
C6-C7-C8	120.3(4)	C6-C7-H7	119.9
C8-C7-H7	119.9	F30-C16-C17	115.6(4)
F30-C16-C21	120.4(4)	C17-C16-C21	124.1(5)
C50-C51-H51	119.7	C52-C51-C50	120.6(4)
C52-C51-H51	119.7	C80-C75-C73	118.2(5)
C76-C75-C73	124.5(5)	C76-C75-C80	117.3(6)
F13-C31-C32	120.8(4)	F13-C31-C30	120.8(4)
C32-C31-C30	118.4(4)	C22-C23-F25	117.0(19)
C24-C23-F25	115.0(19)	C24-C23-C22	128.(2)
F3-C43-C42	120.2(5)	F3-C43-C44	120.9(5)
C44-C43-C42	118.9(4)	F28-C18-C17	120.8(4)
F28-C18-C19	120.1(5)	C17-C18-C19	119.1(4)
F2-C42-C41	120.5(5)	F2-C42-C43	119.7(5)
C41-C42-C43	119.7(5)	C23-C22-B1	125.(2)
C23-C22-C27	110.(2)	C27-C22-B1	124.6(16)
F9-C38-C39	121.0(4)	F9-C38-C37	119.5(4)
C37-C38-C39	119.5(4)	C86-C85-H85	119.9
C86-C85-C84	120.1(5)	C84-C85-H85	119.9
F8-C37-C38	120.7(4)	F8-C37-C36	120.4(4)
C38-C37-C36	119.0(4)	F27-C19-C20	119.8(5)
F27-C19-C18	120.5(4)	C18-C19-C20	119.6(5)
N1-B1-C10	113.0(11)	N1-B1-C21	110.3(4)
N1-B1-C22	100.4(10)	N1-B1-C22A	106.4(8)
N1-B1-C10A	108.3(9)	C10-B1-C21	102.1(11)
C10-B1-C22	119.9(13)	C21-B1-C22	111.3(10)
C21-B1-C10A	104.2(10)	C22A-B1-C21	116.5(10)
C22A-B1-C10A	110.9(13)	C81-C82-H82	120.3
C83-C82-C81	119.4(5)	C83-C82-H82	120.3
C51-C52-H52	119.6	C53-C52-C51	120.8(4)
C53-C52-H52	119.6	C66-C70-H70	107.9
C66-C70-C71	111.5(5)	C71-C70-H70	107.9
C72-C70-C66	109.6(4)	C72-C70-H70	107.9
C72-C70-C71	112.0(5)	C54-C58-H58	107.5

C54-C58-C59	109.1(5)	C59-C58-H58	107.5
C60-C58-C54	112.6(5)	C60-C58-H58	107.5
C60-C58-C59	112.3(6)	F24-C24-C25	115.5(19)
C23-C24-F24	123.8(18)	C23-C24-C25	120.4(19)
N2-B2-C28	105.4(3)	N2-B2-C40	107.9(3)
N2-B2-C34	112.4(3)	C28-B2-C40	114.4(3)
C28-B2-C34	114.1(3)	C34-B2-C40	102.7(3)
C75-C80-H80	119.9	C79-C80-C75	120.3(7)
C79-C80-H80	119.9	F7-C36-C35	120.9(4)
F7-C36-C37	119.5(4)	C35-C36-C37	119.5(4)
F4-C44-C45	119.2(5)	F4-C44-C43	120.5(4)
C43-C44-C45	120.3(4)	C85-C84-H84	120.0
C83-C84-C85	120.0(4)	C83-C84-H84	120.0
F23-C25-C24	124.3(17)	F23-C25-C26	117.2(18)
C26-C25-C24	118.3(18)	C50-C55-H55	111.8
C50-C55-C57	106.2(5)	C56-C55-C50	113.8(5)
C56-C55-H55	111.8	C56-C55-C57	100.8(6)
C57-C55-H55	111.8	C57A-C55-C50	116.3(9)
C57A-C55-C56	127.1(9)	F21-C27-C22	118.7(19)
F21-C27-C26	117.(2)	C26-C27-C22	123.8(18)
C54-C53-H53	119.4	C52-C53-C54	121.3(4)
C52-C53-H53	119.4	C82-C83-H83	119.7
C84-C83-C82	120.6(5)	C84-C83-H83	119.7
F20-C15-C14	113.6(15)	C10-C15-F20	126.8(15)
C10-C15-C14	119.5(19)	C67-C68-H68A	109.5
C67-C68-H68B	109.5	C67-C68-H68C	109.5
H68A-C68-H68B	109.5	H68A-C68-H68C	109.5
H68B-C68-H68C	109.5	C70-C71-H71A	109.5
C70-C71-H71B	109.5	C70-C71-H71C	109.5
H71A-C71-H71B	109.5	H71A-C71-H71C	109.5
H71B-C71-H71C	109.5	F22-C26-C25	123.(2)
F22-C26-C27	117.6(18)	C27-C26-C25	118.9(19)
C67-C69-H69A	109.5	C67-C69-H69B	109.5
C67-C69-H69C	109.5	H69A-C69-H69B	109.5
H69A-C69-H69C	109.5	H69B-C69-H69C	109.5
F17-C12-C11	119.3(14)	F17-C12-C13	124.0(14)
C13-C12-C11	116.6(15)	C58-C59-H59A	109.5
C58-C59-H59B	109.5	C58-C59-H59C	109.5
H59A-C59-H59B	109.5	H59A-C59-H59C	109.5
H59B-C59-H59C	109.5	F18-C13-C12	115.7(16)
F18-C13-C14	125.9(15)	C14-C13-C12	118.3(13)
C70-C72-H72A	109.5	C70-C72-H72B	109.5

C70-C72-H72C	109.5	H72A-C72-H72B	109.5
H72A-C72-H72C	109.5	H72B-C72-H72C	109.5
C15-C14-F19	121.8(13)	C13-C14-F19	116.3(12)
C13-C14-C15	121.9(14)	C80-C79-H79	119.6
C78-C79-C80	120.9(7)	C78-C79-H79	119.6
C55-C56-H56A	109.5	C55-C56-H56B	109.5
C55-C56-H56C	109.5	H56A-C56-H56B	109.5
H56A-C56-H56C	109.5	H56B-C56-H56C	109.5
C79-C78-H78	119.9	C77-C78-C79	120.1(6)
C77-C78-H78	119.9	Cl2-C88-H88A	109.6
Cl2-C88-H88B	109.6	Cl1-C88-Cl2	110.1(6)
Cl1-C88-H88A	109.6	Cl1-C88-H88B	109.6
H88A-C88-H88B	108.2	H88C-C88-H88D	107.9
Cl1A-C88-H88C	109.1	Cl1A-C88-H88D	109.1
Cl1A-C88-Cl2A	112.3(12)	Cl2A-C88-H88C	109.1
Cl2A-C88-H88D	109.1	C75-C76-H76	119.7
C75-C76-C77	120.5(7)	C77-C76-H76	119.7
C78-C77-C76	120.6(7)	C78-C77-H77	119.7
C76-C77-H77	119.7	C58-C60-H60A	109.5
C58-C60-H60B	109.5	C58-C60-H60C	109.5
H60A-C60-H60B	109.5	H60A-C60-H60C	109.5
H60B-C60-H60C	109.5	Cl3-C87-H87A	110.0
Cl3-C87-H87B	110.0	Cl4-C87-Cl3	108.5(7)
Cl4-C87-H87A	110.0	Cl4-C87-H87B	110.0
H87A-C87-H87B	108.4	C55-C57-H57A	109.5
C55-C57-H57B	109.5	C55-C57-H57C	109.5
H57A-C57-H57B	109.5	H57A-C57-H57C	109.5
H57B-C57-H57C	109.5	F21A-C27A-C26A	113.(2)
F21A-C27A-C22A	123.3(18)	C22A-C27A-C26A	123.3(18)
F22A-C26A-C27A	125.(2)	C25A-C26A-C27A	121.(2)
C25A-C26A-F22A	114.6(19)	C26A-C25A-F23A	126.(2)
C26A-C25A-C24A	122.1(18)	F23A-C25A-C24A	112.(2)
C25A-C24A-C23A	117.(2)	F24A-C24A-C25A	127.(2)
F24A-C24A-C23A	116.(2)	F25A-C23A-C24A	119.(2)
F25A-C23A-C22A	122.5(18)	C22A-C23A-C24A	119.(2)
C27A-C22A-B1	130.9(14)	C27A-C22A-C23A	118.(2)
C23A-C22A-B1	110.1(17)	C55-C57A-H57D	109.5
C55-C57A-H57E	109.5	C55-C57A-H57F	109.5
H57D-C57A-H57E	109.5	H57D-C57A-H57F	109.5
H57E-C57A-H57F	109.5	F20A-C15A-C10A	114.7(16)
F20A-C15A-C14A	118.5(13)	C14A-C15A-C10A	126.6(17)
C15A-C10A-B1	125.(2)	C15A-C10A-C11A	106.(2)

C11A-C10A-B1	128.6(17)	F16A-C11A-C10A	121.(2)
C12A-C11A-C10A	128.7(17)	C12A-C11A-F16A	110.1(19)
C11A-C12A-F17A	125.4(12)	C11A-C12A-C13A	119.6(16)
F17A-C12A-C13A	114.8(16)	F18A-C13A-C12A	120.3(16)
C14A-C13A-C12A	119.7(13)	C14A-C13A-F18A	120.0(12)
C13A-C14A-C15A	119.1(10)	F19A-C14A-C15A	119.3(15)
F19A-C14A-C13A	121.7(13)		

Table 6. Anisotropic atomic displacement parameters (Å^2) for 5504.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au1	0.02619(9)	0.01850(8)	0.02281(8)	0.00721(6)	0.00802(6)	0.00406(6)
F15	0.0398(14)	0.0228(12)	0.0217(12)	0.0061(10)	0.0106(10)	0.0117(11)
F11	0.0338(13)	0.0178(11)	0.0268(12)	0.0046(10)	0.0150(10)	0.0053(10)
Cl2	0.0431(16)	0.061(3)	0.111(4)	0.050(2)	-0.0050(18)	0.0072(12)
Cl1	0.043(4)	0.056(7)	0.048(5)	0.030(5)	0.003(3)	0.017(3)
F10	0.0317(13)	0.0326(13)	0.0262(12)	0.0179(11)	0.0078(10)	0.0111(11)
F5	0.0411(16)	0.0488(17)	0.0263(13)	0.0222(13)	0.0004(11)	0.0068(13)
F6	0.0366(14)	0.0432(15)	0.0244(12)	0.0164(12)	0.0076(11)	0.0238(12)
F1	0.0296(13)	0.0375(15)	0.0264(13)	0.0129(12)	0.0056(10)	-0.0063(11)
F25	0.032(6)	0.024(4)	0.023(5)	0.006(4)	0.014(4)	0.004(4)
F12	0.0595(19)	0.0351(15)	0.0408(16)	0.0129(13)	0.0356(15)	0.0050(14)
F30	0.0376(15)	0.0223(12)	0.0322(14)	0.0024(11)	-0.0016(11)	0.0113(11)
F16	0.033(11)	0.037(5)	0.019(6)	0.011(4)	0.003(6)	0.012(6)
F29	0.0341(14)	0.0185(12)	0.0467(16)	0.0006(12)	0.0056(12)	0.0098(11)
F26	0.072(2)	0.0339(15)	0.0291(15)	0.0036(13)	-0.0098(14)	0.0257(15)
F14	0.068(2)	0.0162(12)	0.0379(16)	0.0093(12)	0.0148(14)	0.0037(12)
F28	0.0439(17)	0.0251(14)	0.068(2)	0.0214(14)	0.0114(15)	0.0150(12)
F7	0.0434(17)	0.062(2)	0.0434(17)	0.0202(16)	0.0173(14)	0.0393(16)
F9	0.065(2)	0.0565(19)	0.0299(14)	0.0256(14)	0.0252(14)	0.0223(16)
F8	0.0550(19)	0.068(2)	0.0454(18)	0.0200(17)	0.0372(16)	0.0335(17)
F4	0.0398(16)	0.079(2)	0.0243(14)	0.0209(16)	-0.0041(12)	0.0147(16)
F13	0.066(2)	0.0317(15)	0.0518(19)	0.0217(14)	0.0282(16)	-0.0034(14)
F21	0.027(7)	0.027(5)	0.034(6)	0.004(4)	0.005(4)	0.006(4)
N2	0.0176(15)	0.0159(15)	0.0177(15)	0.0049(13)	0.0038(12)	0.0031(12)
F27	0.067(2)	0.0470(19)	0.0486(19)	0.0255(16)	0.0038(16)	0.0267(17)
F3	0.0326(16)	0.092(3)	0.0339(17)	0.0100(18)	-0.0093(13)	-0.0195(17)
Cl3	0.180(4)	0.098(2)	0.126(3)	0.041(3)	0.018(2)	-0.007(2)
N1	0.0212(16)	0.0152(15)	0.0216(16)	0.0032(13)	0.0023(13)	0.0077(12)
Cl4	0.135(3)	0.175(4)	0.212(4)	0.122(4)	0.062(3)	0.051(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F2	0.053(2)	0.090(3)	0.0440(19)	0.023(2)	-0.0042(15)	-0.047(2)
N4	0.0229(17)	0.0220(17)	0.0254(17)	0.0052(14)	0.0092(14)	0.0069(14)
F22	0.043(6)	0.027(5)	0.041(5)	0.000(4)	-0.006(5)	-0.006(4)
F17	0.067(9)	0.031(4)	0.048(8)	0.012(5)	0.032(6)	0.006(5)
F24	0.043(5)	0.039(4)	0.028(5)	0.004(4)	0.018(3)	0.011(4)
F23	0.062(7)	0.034(5)	0.021(6)	-0.002(4)	0.005(4)	0.020(4)
N3	0.0271(17)	0.0170(16)	0.0251(17)	0.0043(14)	0.0108(14)	0.0057(13)
F20	0.019(4)	0.036(3)	0.048(6)	0.017(4)	-0.002(3)	0.008(3)
C28	0.0203(18)	0.0185(18)	0.0187(18)	0.0072(15)	0.0017(14)	0.0054(14)
C3	0.0197(18)	0.0167(17)	0.0170(17)	0.0046(15)	0.0051(14)	0.0060(14)
C40	0.0179(18)	0.028(2)	0.0200(18)	0.0067(16)	0.0058(14)	0.0102(16)
C33	0.027(2)	0.0165(18)	0.0214(19)	0.0060(16)	0.0058(15)	0.0037(15)
C64	0.032(2)	0.031(2)	0.022(2)	0.0020(18)	0.0086(17)	0.0084(19)
C4	0.0169(17)	0.0176(17)	0.0211(18)	0.0063(15)	0.0025(14)	0.0050(14)
C34	0.0177(17)	0.0210(18)	0.0196(18)	0.0075(16)	0.0046(14)	0.0047(14)
C5	0.0198(18)	0.0220(19)	0.0238(19)	0.0097(16)	0.0028(15)	0.0067(15)
C45	0.024(2)	0.035(2)	0.022(2)	0.0104(18)	0.0084(16)	0.0110(18)
C6	0.024(2)	0.0203(19)	0.027(2)	0.0025(17)	0.0004(16)	0.0064(16)
C1	0.030(2)	0.0144(17)	0.025(2)	0.0044(16)	-0.0006(16)	0.0051(16)
C74	0.029(2)	0.026(2)	0.034(2)	0.0165(19)	0.0112(18)	0.0075(17)
C65	0.035(2)	0.034(2)	0.024(2)	0.0046(19)	0.0057(18)	0.010(2)
C10	0.025(3)	0.025(2)	0.062(5)	0.016(3)	0.017(3)	0.008(2)
C29	0.032(2)	0.0219(19)	0.0188(18)	0.0100(16)	0.0069(16)	0.0098(16)
C2	0.025(2)	0.0153(17)	0.0226(19)	0.0033(16)	0.0016(15)	0.0010(15)
C32	0.034(2)	0.030(2)	0.024(2)	0.0113(18)	0.0142(18)	0.0046(18)
C63	0.029(2)	0.025(2)	0.031(2)	0.0072(18)	0.0126(18)	0.0102(17)
C54	0.033(2)	0.032(2)	0.024(2)	0.0124(18)	0.0099(17)	0.0157(19)
C62	0.029(2)	0.0226(19)	0.025(2)	0.0072(17)	0.0107(17)	0.0058(16)
C73	0.036(2)	0.026(2)	0.028(2)	0.0116(19)	0.0095(18)	-0.0013(18)
C46	0.026(2)	0.0191(18)	0.0206(19)	0.0038(16)	0.0050(16)	0.0066(16)
C39	0.0218(19)	0.026(2)	0.0201(19)	0.0079(16)	0.0061(15)	0.0050(16)
C49	0.029(2)	0.0201(19)	0.0170(18)	0.0043(16)	0.0077(15)	0.0091(16)
C48	0.029(2)	0.021(2)	0.039(2)	0.0068(19)	0.0169(19)	0.0012(17)
C61	0.028(2)	0.0171(18)	0.024(2)	0.0021(16)	0.0108(16)	0.0039(16)
C30	0.047(3)	0.0188(19)	0.024(2)	0.0091(17)	0.0073(19)	0.0064(18)
C17	0.023(2)	0.0196(19)	0.043(3)	0.0042(19)	0.0050(18)	0.0081(16)
C35	0.023(2)	0.031(2)	0.0184(18)	0.0076(17)	0.0040(15)	0.0077(17)
C81	0.031(2)	0.027(2)	0.029(2)	0.0123(18)	0.0076(17)	0.0127(18)
C41	0.0198(19)	0.033(2)	0.024(2)	0.0082(18)	0.0044(16)	0.0024(17)
F19	0.016(3)	0.043(4)	0.104(9)	0.031(5)	0.005(4)	0.007(3)
C21	0.028(2)	0.021(2)	0.033(2)	0.0042(18)	-0.0055(18)	0.0125(17)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C67	0.048(3)	0.041(3)	0.030(2)	0.017(2)	0.019(2)	0.024(2)
C47	0.026(2)	0.028(2)	0.037(2)	0.0116(19)	0.0167(18)	0.0055(17)
C20	0.036(2)	0.026(2)	0.032(2)	0.002(2)	-0.0063(19)	0.0143(19)
C9	0.023(2)	0.025(2)	0.028(2)	0.0086(18)	0.0076(16)	0.0054(16)
C86	0.036(2)	0.028(2)	0.028(2)	0.0133(19)	0.0079(18)	0.0101(19)
C66	0.030(2)	0.024(2)	0.029(2)	0.0049(18)	0.0081(18)	0.0095(17)
C11	0.025(3)	0.025(2)	0.062(5)	0.016(3)	0.018(3)	0.008(2)
C50	0.031(2)	0.026(2)	0.025(2)	0.0109(18)	0.0052(17)	0.0061(17)
C8	0.022(2)	0.031(2)	0.045(3)	0.017(2)	0.0105(19)	0.0016(18)
C7	0.031(2)	0.0182(19)	0.038(3)	0.0051(19)	0.0032(19)	-0.0004(17)
C16	0.025(2)	0.023(2)	0.032(2)	0.0042(18)	-0.0016(17)	0.0104(17)
C51	0.042(3)	0.034(2)	0.018(2)	0.0064(19)	0.0034(18)	0.001(2)
C75	0.036(3)	0.027(2)	0.038(3)	0.001(2)	0.014(2)	-0.0004(19)
F18	0.045(5)	0.043(5)	0.122(11)	0.044(6)	0.060(6)	0.020(4)
C31	0.042(3)	0.027(2)	0.031(2)	0.017(2)	0.010(2)	-0.0016(19)
C23	0.028(4)	0.022(3)	0.022(3)	0.004(2)	-0.001(3)	0.006(3)
C43	0.020(2)	0.059(3)	0.026(2)	0.003(2)	-0.0007(17)	0.000(2)
C18	0.026(2)	0.020(2)	0.051(3)	0.013(2)	0.003(2)	0.0083(17)
C42	0.028(2)	0.050(3)	0.032(2)	0.009(2)	0.0087(19)	-0.009(2)
C22	0.028(4)	0.022(3)	0.022(3)	0.004(2)	-0.001(3)	0.006(3)
C38	0.037(2)	0.033(2)	0.022(2)	0.0126(19)	0.0128(18)	0.0073(19)
C85	0.045(3)	0.031(2)	0.035(2)	0.012(2)	0.011(2)	0.018(2)
C37	0.036(2)	0.038(2)	0.030(2)	0.010(2)	0.021(2)	0.014(2)
C19	0.033(2)	0.033(2)	0.044(3)	0.019(2)	0.002(2)	0.015(2)
B1	0.027(2)	0.022(2)	0.029(2)	0.001(2)	-0.0066(19)	0.0128(19)
C82	0.030(2)	0.034(2)	0.037(2)	0.015(2)	0.0105(19)	0.0090(19)
C52	0.058(3)	0.020(2)	0.030(2)	0.0028(19)	0.017(2)	0.007(2)
C70	0.038(3)	0.035(2)	0.030(2)	0.007(2)	0.007(2)	0.017(2)
C58	0.042(3)	0.048(3)	0.032(2)	0.015(2)	0.004(2)	0.023(2)
C24	0.028(4)	0.022(3)	0.022(3)	0.004(2)	-0.001(3)	0.006(3)
B2	0.0190(19)	0.0180(19)	0.0174(19)	0.0077(16)	0.0050(15)	0.0066(16)
C80	0.043(3)	0.029(3)	0.057(3)	0.014(3)	-0.005(3)	0.002(2)
C36	0.028(2)	0.033(2)	0.030(2)	0.008(2)	0.0074(18)	0.0142(18)
C44	0.027(2)	0.057(3)	0.018(2)	0.013(2)	0.0028(16)	0.016(2)
C84	0.040(3)	0.049(3)	0.030(2)	0.015(2)	0.012(2)	0.024(2)
C25	0.028(4)	0.022(3)	0.022(3)	0.004(2)	-0.001(3)	0.006(3)
C55	0.032(3)	0.042(3)	0.066(4)	0.032(3)	0.001(2)	0.010(2)
C27	0.028(4)	0.022(3)	0.022(3)	0.004(2)	-0.001(3)	0.006(3)
C53	0.053(3)	0.030(2)	0.037(3)	0.016(2)	0.018(2)	0.025(2)
C83	0.034(3)	0.053(3)	0.037(3)	0.024(2)	0.014(2)	0.013(2)
C15	0.025(3)	0.025(2)	0.062(5)	0.016(3)	0.017(3)	0.008(2)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C68	0.058(4)	0.067(4)	0.038(3)	0.022(3)	-0.004(3)	0.014(3)
C71	0.083(5)	0.052(4)	0.068(4)	0.033(3)	0.026(4)	0.036(4)
C26	0.028(4)	0.022(3)	0.022(3)	0.004(2)	-0.001(3)	0.006(3)
C69	0.087(5)	0.056(4)	0.070(4)	0.045(3)	0.048(4)	0.043(4)
C12	0.025(3)	0.025(2)	0.062(5)	0.015(3)	0.018(3)	0.008(2)
C59	0.087(5)	0.059(4)	0.034(3)	0.023(3)	0.000(3)	0.027(4)
C13	0.025(3)	0.025(2)	0.063(5)	0.016(3)	0.018(3)	0.008(2)
C72	0.037(3)	0.060(4)	0.109(6)	0.025(4)	0.004(4)	0.023(3)
C14	0.025(3)	0.025(2)	0.063(5)	0.016(3)	0.017(3)	0.008(2)
C79	0.046(3)	0.029(3)	0.087(5)	0.007(3)	-0.004(3)	0.010(2)
C56	0.037(3)	0.069(5)	0.120(7)	0.032(5)	0.009(4)	0.022(3)
C78	0.055(4)	0.050(4)	0.099(6)	-0.032(4)	0.034(4)	-0.008(3)
C88	0.093(6)	0.077(5)	0.068(5)	0.035(4)	0.020(4)	0.031(5)
C76	0.143(8)	0.063(4)	0.045(4)	-0.012(3)	0.052(5)	-0.050(5)
C77	0.160(9)	0.080(6)	0.064(5)	-0.030(4)	0.078(6)	-0.053(6)
C60	0.069(5)	0.258(14)	0.045(4)	0.024(6)	0.002(4)	0.101(8)
C87	0.105(8)	0.142(11)	0.109(8)	0.044(8)	0.029(7)	0.045(8)
C57	0.056(6)	0.062(7)	0.063(6)	0.047(6)	0.010(5)	0.020(5)
Cl1A	0.082(7)	0.34(3)	0.31(3)	0.28(3)	-0.068(12)	-0.053(12)
Cl2A	0.081(4)	0.258(10)	0.178(9)	0.171(8)	0.054(5)	0.076(6)
F21A	0.033(10)	0.025(5)	0.068(15)	-0.009(9)	-0.014(8)	0.005(6)
C27A	0.050(12)	0.036(7)	0.016(8)	-0.009(6)	-0.009(7)	0.035(8)
C26A	0.075(16)	0.038(9)	0.026(10)	-0.005(7)	-0.016(8)	0.034(10)
F22A	0.091(17)	0.025(7)	0.081(16)	-0.018(8)	-0.058(11)	0.011(10)
F23A	0.18(2)	0.066(14)	0.022(6)	-0.008(7)	-0.001(12)	0.077(16)
C25A	0.09(2)	0.042(10)	0.015(7)	-0.003(6)	-0.007(10)	0.031(13)
C24A	0.078(17)	0.058(16)	0.025(7)	0.007(10)	-0.010(11)	0.048(15)
F24A	0.14(2)	0.078(13)	0.042(7)	0.034(8)	0.042(12)	0.077(13)
C23A	0.104(19)	0.050(9)	0.010(5)	0.009(5)	0.018(7)	0.068(13)
F25A	0.052(12)	0.046(8)	0.034(5)	0.027(5)	0.025(6)	0.030(8)
C22A	0.032(10)	0.024(7)	0.032(8)	0.004(5)	-0.007(7)	0.023(8)
C57A	0.036(10)	0.071(17)	0.13(3)	0.086(19)	0.015(12)	0.010(10)
F20A	0.024(5)	0.034(4)	0.051(8)	0.011(5)	0.003(4)	0.007(3)
C15A	0.005(5)	0.022(5)	0.057(9)	0.016(6)	0.008(5)	0.004(4)
C10A	0.021(6)	0.013(5)	0.037(9)	-0.018(5)	-0.020(5)	0.010(4)
C11A	0.025(7)	0.010(5)	0.028(7)	0.001(5)	0.006(6)	0.015(4)
F16A	0.016(6)	0.037(7)	0.022(9)	0.009(5)	0.001(6)	0.013(4)
C12A	0.017(7)	0.019(5)	0.069(12)	0.019(7)	0.003(6)	0.015(5)
F17A	0.051(7)	0.036(6)	0.041(8)	0.014(6)	0.019(5)	0.020(5)
C13A	0.022(7)	0.017(6)	0.076(12)	0.024(7)	0.009(7)	0.007(4)
F18A	0.051(6)	0.052(7)	0.101(11)	0.052(8)	0.045(7)	0.026(5)

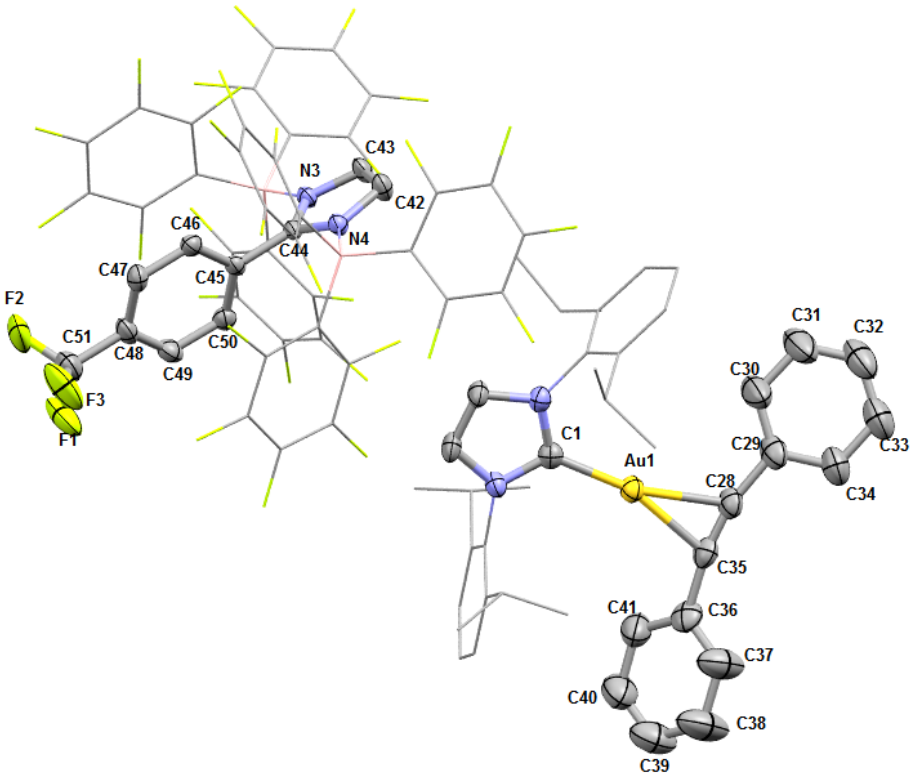
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F19A	0.021(4)	0.051(6)	0.102(12)	0.040(7)	0.002(5)	0.009(3)
C14A	0.014(5)	0.025(6)	0.067(12)	0.028(7)	0.018(7)	0.014(4)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 5504.

	x/a	y/b	z/c	U(eq)
H64	0.6394	0.0562	0.7741	0.037
H5	0.2567	0.0667	1.2618	0.026
H6	0.1643	-0.0716	1.1956	0.032
H1	0.2668	0.3818	1.4469	0.031
H65	0.5178	0.1301	0.7685	0.04
H2	0.4141	0.3428	1.4982	0.028
H63	0.7112	0.0588	0.8972	0.035
H48	0.4151	0.1462	1.0470	0.037
H67	0.6451	0.1663	1.0880	0.044
H47	0.4091	0.2689	1.1695	0.036
H9	0.0784	0.1130	1.4248	0.032
H86	0.7360	0.2608	0.9021	0.036
H8	-0.0112	-0.0265	1.3599	0.04
H7	0.0320	-0.1182	1.2448	0.039
H51	0.6998	0.5504	1.3693	0.041
H85	0.7785	0.1862	0.7797	0.044
H82	0.9136	0.4729	0.9202	0.04
H52	0.6039	0.6373	1.3480	0.046
H70	0.4210	0.2531	0.9377	0.043
H58	0.3814	0.3729	1.0896	0.049
H80	0.8519	0.6251	1.0591	0.057
H84	0.8888	0.2544	0.7281	0.046
H55	0.6604	0.3307	1.2393	0.054
H53	0.4703	0.5868	1.2369	0.044
H83	0.9549	0.3970	0.7975	0.047
H68A	0.8296	0.1581	1.0335	0.085
H68B	0.8215	0.1880	1.1261	0.085
H68C	0.7950	0.2420	1.0791	0.085
H71A	0.5248	0.3191	0.8763	0.092
H71B	0.4072	0.3149	0.8496	0.092
H71C	0.4599	0.2514	0.7890	0.092
H69A	0.6012	0.0194	1.0236	0.088
H69B	0.7011	0.0534	1.0945	0.088
H69C	0.7103	0.0194	1.0019	0.088

	x/a	y/b	z/c	U(eq)
H59A	0.4489	0.5216	1.0715	0.089
H59B	0.3766	0.4374	1.0010	0.089
H59C	0.4914	0.4402	1.0353	0.089
H72A	0.3383	0.1210	0.7794	0.109
H72B	0.2770	0.1860	0.8268	0.109
H72C	0.3100	0.1238	0.8614	0.109
H79	0.8889	0.7568	1.1628	0.074
H56A	0.8116	0.4238	1.2420	0.118
H56B	0.8332	0.3781	1.2986	0.118
H56C	0.8244	0.4725	1.3380	0.118
H78	0.8742	0.7767	1.2909	0.109
H88A	1.0518	0.1673	1.0210	0.092
H88B	1.0857	0.2649	1.0793	0.092
H88C	1.0557	0.2228	1.0723	0.092
H88D	1.0688	0.1644	0.9842	0.092
H76	0.7706	0.5325	1.2116	0.123
H77	0.8059	0.6681	1.3136	0.153
H60A	0.2837	0.4427	1.1754	0.197
H60B	0.2481	0.4361	1.0866	0.197
H60C	0.3161	0.5218	1.1580	0.197
H87A	0.4880	0.4358	1.3391	0.144
H87B	0.4231	0.3673	1.3595	0.144
H57A	0.7092	0.4568	1.4110	0.08
H57B	0.7247	0.3648	1.3853	0.08
H57C	0.6127	0.3793	1.3736	0.08
H57D	0.6219	0.3621	1.3588	0.101
H57E	0.6839	0.2972	1.3123	0.101
H57F	0.5762	0.2968	1.2661	0.101

Crystal Structure Report for 3[IMP-CF_3]



Thermal ellipsoid plot of 5517. Ellipsoids shown at 50% probability, $B(C_6F_5)_3$ and diisopropylphenyl substituents shown in wireframe, hydrogen atoms hidden for clarity.

A specimen of $C_{87}H_{52}AuB_2F_{33}N_4$ was used for the X-ray crystallographic analysis. The X-ray intensity data were measured (λ = 0.71073 Å). The total exposure time was 7.35 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 75190 reflections to a maximum θ angle of28.22° (0.75 Å resolution), of which 13363 were independent (average redundancy 5.627, completeness = 97.0%, R_{int} =6.60%, R_{sig} = 6.18%) and 11016 (82.44%) were greater than $2\sigma(F^2)$. The final cell constants of a = 15.283(12) Å, b =18.375(14) Å, c = 19.561(15) Å, α = 63.006(14)°, β = 67.128(14)°, γ = 89.768(15)°, volume = 4410.(10) $Å^3$, are based upon the refinement of the XYZ-centroids of 9860 reflections above 20 σ(I) with 4.52° < 2θ < 46.58°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.807. The structure was solved and refined using the Bruker SHELXTL Software Package, with Z = 44 for the formula unit,$C_{87}H_{52}AuB_2F_{33}N_4$. The final anisotropic full-matrix least-squares refinement on F^2 with 1152 variables converged at R1 =6.77%, for the observed data and wR2 = 21.70% for all data. The goodness-of-fit was 1.074. The largest peak in the final difference electron density synthesis was 6.534 $e^-/Å^3$ and the largest hole was -1.124 $e^-/Å^3$ with an RMS deviation of 0.205$e^-/Å^3$. On the basis of the final model, the calculated density

was 1.500 g/cm^3 and F(000), 1976 e$^-$. PLATON SQUEEZE was used to account for disordered solvent within the crystal.

Table 1. Sample and crystal data for 5517.

Identification code	5517	
Chemical formula	$C_{87}H_{52}AuB_2F_{33}N_4$	
Formula weight	1998.91 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Unit cell dimensions	a = 15.283(12) Å	α = 63.006(14)°
	b = 18.375(14) Å	β = 67.128(14)°
	c = 19.561(15) Å	γ = 89.768(15)°
Volume	4410.(10) Å^3	
Z	44	
Density (calculated)	1.500 g/cm^3	
Absorption coefficient	1.777 mm^{-1}	
F(000)	1976	

Table 2. Data collection and structure refinement for 5517.

Theta range for data collection	1.30 to 28.22°	
Index ranges	-17<=h<=17, -20<=k<=20, -22<=l<=22	
Reflections collected	75190	
Independent reflections	13363 [R(int) = 0.0660]	
Coverage of independent reflections	97.0%	
Absorption correction	Multi-Scan	
Structure solution technique	direct methods	
Structure solution program	XT, VERSION 2014/5	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	13363 / 0 / 1152	
Goodness-of-fit on F^2	1.074	
Δ/σ_{max}	0.001	
Final R indices	11016 data; I>2σ(I)	R1 = 0.0677, wR2 = 0.2066
	all data	R1 = 0.0819, wR2 = 0.2170

Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.1369P)^2+22.5530P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	6.534 and -1.124 eÅ^{-3}
R.M.S. deviation from mean	0.205 eÅ^{-3}

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 5517.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij}tensor.

	x/a	y/b	z/c	U(eq)
Au1	0.57295(3)	0.34865(2)	0.43924(2)	0.03087(16)
F5	0.4774(4)	0.2557(3)	0.9537(3)	0.0381(13)
F26	0.9667(4)	0.4001(3)	0.1171(4)	0.0386(13)
F16	0.2230(4)	0.2781(3)	0.2915(3)	0.0342(12)
F6	0.4210(4)	0.9934(3)	0.1251(3)	0.0317(12)
F21	0.1277(4)	0.3233(3)	0.0370(3)	0.0358(13)
F11	0.2384(4)	0.9567(3)	0.2375(3)	0.0335(12)
F30	0.2334(4)	0.4469(3)	0.1642(4)	0.0411(14)
F1	0.5103(4)	0.0763(4)	0.2052(4)	0.0404(14)
F20	0.9203(4)	0.3315(3)	0.2968(3)	0.0372(13)
F25	0.9159(4)	0.1769(3)	0.3305(3)	0.0412(14)
F10	0.2673(4)	0.2097(3)	0.0098(3)	0.0335(12)
F15	0.3842(4)	0.1671(3)	0.2554(4)	0.0383(13)
F18	0.9993(5)	0.3136(4)	0.5095(4)	0.0569(18)
F17	0.1771(4)	0.2915(4)	0.4283(4)	0.0427(14)
F7	0.4008(5)	0.9313(4)	0.0333(4)	0.0485(16)
F12	0.1691(4)	0.8616(3)	0.4036(4)	0.0490(15)
F2	0.6967(4)	0.1171(4)	0.1175(5)	0.0505(16)
F9	0.2528(5)	0.1498(4)	0.9163(4)	0.0509(16)
F4	0.6656(4)	0.2928(4)	0.8672(4)	0.0550(17)
F22	0.0284(5)	0.2286(4)	0.0120(4)	0.0563(18)
F19	0.8704(5)	0.3294(4)	0.4431(4)	0.0541(17)
F14	0.3138(5)	0.0682(4)	0.4226(4)	0.0586(18)
F27	0.9682(5)	0.5593(4)	0.0489(4)	0.0512(16)
F8	0.3190(5)	0.0088(5)	0.9256(5)	0.0616(19)
F29	0.2409(5)	0.6089(4)	0.0845(6)	0.073(2)
F3	0.7803(4)	0.2249(4)	0.9462(5)	0.0568(18)
F13	0.2042(5)	0.9155(5)	0.4994(4)	0.0639(19)

	x/a	y/b	z/c	U(eq)
N3	0.3108(5)	0.2132(4)	0.1308(5)	0.0217(15)
F24	0.8164(4)	0.0885(4)	0.3021(5)	0.0604(19)
F28	0.1077(6)	0.6687(4)	0.0253(5)	0.067(2)
N4	0.2027(5)	0.2887(4)	0.1551(4)	0.0225(16)
F33	0.8885(6)	0.8961(4)	0.4929(4)	0.073(2)
F23	0.8691(5)	0.1109(5)	0.1447(6)	0.073(2)
F32	0.9544(6)	0.8481(4)	0.4092(5)	0.083(3)
N1	0.3988(6)	0.2402(5)	0.4747(5)	0.0299(17)
C44	0.2184(6)	0.2107(5)	0.1748(5)	0.0211(18)
C45	0.1418(6)	0.1333(5)	0.2367(5)	0.0213(18)
N2	0.4814(5)	0.3220(5)	0.3409(5)	0.0280(17)
C70	0.0731(6)	0.3009(5)	0.2875(6)	0.0249(19)
C64	0.4805(6)	0.1666(5)	0.0862(6)	0.0249(19)
C52	0.3193(6)	0.0678(5)	0.2346(6)	0.0242(19)
F31	0.8483(6)	0.9150(5)	0.3954(6)	0.110(4)
C63	0.3009(7)	0.1386(5)	0.0201(6)	0.029(2)
C69	0.5431(7)	0.1337(6)	0.1217(6)	0.031(2)
C71	0.1343(6)	0.2918(5)	0.3248(6)	0.0257(19)
C65	0.5287(7)	0.2209(6)	0.9991(6)	0.032(2)
C76	0.1070(7)	0.4142(6)	0.1375(6)	0.028(2)
C17	0.3545(7)	0.2219(6)	0.4337(6)	0.032(2)
C77	0.1711(7)	0.4721(6)	0.1302(7)	0.034(2)
C82	0.0273(6)	0.2565(5)	0.1844(6)	0.0254(19)
C75	0.9851(7)	0.3156(6)	0.3308(6)	0.031(2)
C81	0.0399(7)	0.4488(6)	0.1080(6)	0.028(2)
C43	0.3568(7)	0.2965(5)	0.0797(6)	0.032(2)
C58	0.3415(6)	0.1017(5)	0.0763(5)	0.0227(18)
C59	0.3769(6)	0.0338(6)	0.0752(6)	0.027(2)
C46	0.1006(6)	0.1074(6)	0.3229(6)	0.028(2)
C47	0.0289(7)	0.0368(6)	0.3791(6)	0.032(2)
C50	0.1114(6)	0.0875(5)	0.2077(6)	0.0247(19)
C16	0.4061(7)	0.2721(6)	0.3510(6)	0.034(2)
C83	0.0494(7)	0.2654(6)	0.1060(6)	0.029(2)
C73	0.0230(8)	0.3086(6)	0.4383(6)	0.038(2)
C57	0.3323(7)	0.0917(6)	0.2885(6)	0.030(2)
C62	0.2936(7)	0.1098(7)	0.9696(6)	0.037(2)
C53	0.2627(6)	0.9881(6)	0.2785(6)	0.028(2)

	x/a	y/b	z/c	U(eq)
C87	0.9464(7)	0.1951(6)	0.2490(6)	0.032(2)
C30	0.3623(7)	0.2020(6)	0.5664(6)	0.036(2)
C48	0.9992(7)	0.9922(6)	0.3505(6)	0.033(2)
C23	0.6406(7)	0.3651(6)	0.2217(6)	0.035(2)
C74	0.9586(7)	0.3173(6)	0.4045(6)	0.036(2)
C61	0.3269(7)	0.0396(7)	0.9732(6)	0.037(2)
C8	0.6537(7)	0.3670(6)	0.5023(7)	0.037(2)
C54	0.2237(7)	0.9364(6)	0.3663(7)	0.036(2)
C84	0.9992(8)	0.2185(7)	0.0905(7)	0.041(3)
C49	0.0405(7)	0.0172(6)	0.2647(6)	0.031(2)
C66	0.6267(7)	0.2412(6)	0.9520(7)	0.037(2)
C55	0.2403(8)	0.9641(7)	0.4153(6)	0.044(3)
C35	0.3893(7)	0.1290(7)	0.6099(6)	0.040(2)
C15	0.4774(6)	0.3017(5)	0.4172(6)	0.027(2)
C42	0.2901(6)	0.3414(6)	0.0952(6)	0.031(2)
C80	0.0400(8)	0.5329(7)	0.0709(6)	0.040(2)
C72	0.1112(8)	0.2974(6)	0.3982(6)	0.033(2)
C60	0.3685(7)	0.0008(6)	0.0270(7)	0.036(2)
C86	0.8930(7)	0.1471(6)	0.2373(7)	0.040(3)
C7	0.6977(8)	0.4191(7)	0.4273(7)	0.040(2)
C78	0.1738(8)	0.5574(6)	0.0906(8)	0.046(3)
C85	0.9201(8)	0.1592(7)	0.1571(9)	0.049(3)
C19	0.5400(9)	0.4677(7)	0.2288(7)	0.045(3)
C67	0.6832(7)	0.2051(7)	0.9929(8)	0.044(3)
B2	0.1018(7)	0.3131(6)	0.1918(7)	0.025(2)
C79	0.1063(9)	0.5868(6)	0.0618(7)	0.045(3)
C18	0.5563(7)	0.3876(6)	0.2603(6)	0.031(2)
C68	0.6420(7)	0.1531(6)	0.0772(7)	0.036(2)
C9	0.6169(8)	0.3088(7)	0.5931(7)	0.042(3)
C31	0.3000(8)	0.2404(8)	0.6059(7)	0.047(3)
C51	0.9213(8)	0.9145(6)	0.4135(7)	0.045(3)
C1	0.7627(8)	0.4877(7)	0.3459(7)	0.047(3)
C22	0.7123(9)	0.4276(8)	0.1471(7)	0.053(3)
C20	0.6167(12)	0.5292(7)	0.1516(8)	0.062(4)
C56	0.2961(8)	0.0424(7)	0.3759(7)	0.038(2)
B1	0.3617(7)	0.1360(6)	0.1344(6)	0.023(2)
C34	0.3504(9)	0.0938(8)	0.6980(8)	0.057(3)

	x/a	y/b	z/c	U(eq)
C21	0.6996(11)	0.5073(10)	0.1131(9)	0.068(4)
C24	0.6541(8)	0.2762(7)	0.2583(8)	0.046(3)
C36	0.4589(8)	0.0889(7)	0.5664(8)	0.047(3)
C6	0.8513(8)	0.5151(7)	0.3385(8)	0.054(3)
C39	0.2723(9)	0.3211(8)	0.5548(8)	0.059(3)
C32	0.2631(9)	0.2015(9)	0.6950(8)	0.061(4)
C26	0.7278(10)	0.2665(9)	0.2961(9)	0.065(4)
C5	0.9169(10)	0.5858(9)	0.2605(11)	0.075(4)
C27	0.4463(11)	0.4883(8)	0.2724(10)	0.069(4)
C33	0.2892(10)	0.1299(9)	0.7388(8)	0.064(4)
C37	0.4274(11)	0.9972(8)	0.6083(10)	0.076(4)
C41	0.1637(9)	0.3156(9)	0.5968(9)	0.066(4)
C40	0.3268(10)	0.3940(9)	0.5458(11)	0.078(5)
C14	0.6800(12)	0.2725(11)	0.6251(9)	0.089(6)
C10	0.5209(9)	0.2895(10)	0.6469(8)	0.066(4)
C2	0.7390(12)	0.5260(9)	0.2811(9)	0.083(5)
C4	0.8930(12)	0.6251(9)	0.1940(9)	0.074(4)
C11	0.4898(12)	0.2368(11)	0.7322(9)	0.079(5)
C38	0.5593(9)	0.1087(9)	0.5600(10)	0.071(4)
C25	0.6872(13)	0.2451(11)	0.1935(11)	0.088(5)
C3	0.8093(16)	0.5949(12)	0.2037(10)	0.107(7)
C12	0.5531(15)	0.2032(9)	0.7638(10)	0.084(5)
C13	0.6398(14)	0.2152(13)	0.7158(10)	0.116(8)
C29	0.4677(19)	0.5676(13)	0.2778(17)	0.141(10)
C28	0.3859(17)	0.5033(15)	0.2218(17)	0.138(9)

Table 4. Bond lengths (Å) for 5517.

Au1-C15	1.980(9)	Au1-C8	2.178(9)
Au1-C7	2.188(10)	F5-C65	1.356(11)
F26-C81	1.344(11)	F16-C71	1.340(10)
F6-C59	1.346(10)	F21-C83	1.357(11)
F11-C53	1.334(10)	F30-C77	1.334(11)
F1-C69	1.354(11)	F20-C75	1.360(10)
F25-C87	1.346(11)	F10-C63	1.361(10)
F15-C57	1.330(11)	F18-C73	1.343(11)
F17-C72	1.335(11)	F7-C60	1.339(11)

F12-C54	1.322(11)	F2-C68	1.341(11)
F9-C62	1.351(11)	F4-C66	1.346(12)
F22-C84	1.343(12)	F19-C74	1.342(11)
F14-C56	1.314(11)	F27-C80	1.344(12)
F8-C61	1.332(11)	F29-C78	1.336(12)
F3-C67	1.351(12)	F13-C55	1.330(12)
N3-C44	1.327(11)	N3-C43	1.384(11)
N3-B1	1.602(11)	F24-C86	1.326(12)
F28-C79	1.338(12)	N4-C44	1.355(11)
N4-C42	1.364(12)	N4-B2	1.590(12)
F33-C51	1.302(13)	F23-C85	1.345(12)
F32-C51	1.347(13)	N1-C15	1.340(12)
N1-C17	1.377(12)	N1-C30	1.450(13)
C44-C45	1.487(12)	C45-C50	1.379(12)
C45-C46	1.382(12)	N2-C15	1.340(12)
N2-C16	1.373(12)	N2-C18	1.460(12)
C70-C71	1.364(12)	C70-C75	1.387(13)
C70-B2	1.653(13)	C64-C69	1.380(13)
C64-C65	1.388(13)	C64-B1	1.646(13)
C52-C53	1.387(13)	C52-C57	1.392(13)
C52-B1	1.618(13)	F31-C51	1.297(13)
C63-C62	1.355(13)	C63-C58	1.383(13)
C69-C68	1.369(14)	C71-C72	1.393(13)
C65-C66	1.361(14)	C76-C77	1.374(13)
C76-C81	1.385(12)	C76-B2	1.653(13)
C17-C16	1.323(14)	C17-H17	0.95
C77-C78	1.390(14)	C82-C83	1.365(13)
C82-C87	1.380(13)	C82-B2	1.641(13)
C75-C74	1.354(14)	C81-C80	1.378(13)
C43-C42	1.341(13)	C43-H43	0.95
C58-C59	1.366(12)	C58-B1	1.650(13)
C59-C60	1.377(13)	C46-C47	1.370(13)
C46-H46	0.95	C47-C48	1.349(14)
C47-H47	0.95	C50-C49	1.361(13)
C50-H50	0.95	C16-H16	0.95
C83-C84	1.364(14)	C73-C72	1.343(14)
C73-C74	1.359(14)	C57-C56	1.383(14)
C62-C61	1.368(14)	C53-C54	1.389(14)

C87-C86	1.357(14)	C30-C31	1.388(15)
C30-C35	1.389(15)	C48-C49	1.379(14)
C48-C51	1.502(14)	C23-C22	1.377(16)
C23-C18	1.389(14)	C23-C24	1.510(15)
C61-C60	1.364(14)	C8-C7	1.218(15)
C8-C9	1.455(15)	C54-C55	1.374(15)
C84-C85	1.358(17)	C49-H49	0.95
C66-C67	1.372(15)	C55-C56	1.374(16)
C35-C34	1.392(16)	C35-C36	1.505(15)
C42-H42	0.95	C80-C79	1.326(16)
C86-C85	1.365(17)	C7-C1	1.440(16)
C78-C79	1.360(15)	C19-C18	1.381(14)
C19-C20	1.420(18)	C19-C27	1.506(18)
C67-C68	1.340(16)	C9-C10	1.361(17)
C9-C14	1.363(18)	C31-C32	1.404(17)
C31-C39	1.535(17)	C1-C2	1.334(18)
C1-C6	1.381(16)	C22-C21	1.36(2)
C22-H22	0.95	C20-C21	1.37(2)
C20-H20	0.95	C34-C33	1.360(19)
C34-H34	0.95	C21-H21	0.95
C24-C25	1.533(16)	C24-C26	1.544(16)
C24-H24	1.0	C36-C37	1.481(16)
C36-C38	1.526(17)	C36-H36	1.0
C6-C5	1.429(19)	C6-H6	0.95
C39-C40	1.488(18)	C39-C41	1.522(18)
C39-H39	1.0	C32-C33	1.367(19)
C32-H32	0.95	C26-H26A	0.98
C26-H26B	0.98	C26-H26C	0.98
C5-C4	1.37(2)	C5-H5	0.95
C27-C28	1.54(2)	C27-C29	1.56(2)
C27-H27	1.0	C33-H33	0.95
C37-H37A	0.98	C37-H37B	0.98
C37-H37C	0.98	C41-H41A	0.98
C41-H41B	0.98	C41-H41C	0.98
C40-H40A	0.98	C40-H40B	0.98
C40-H40C	0.98	C14-C13	1.45(2)
C14-H14	0.95	C10-C11	1.366(19)
C10-H10	0.95	C2-C3	1.43(2)

C2-H2	0.95	C4-C3	1.31(2)
C4-H4	0.95	C11-C12	1.35(2)
C11-H11	0.95	C38-H38A	0.98
C38-H38B	0.98	C38-H38C	0.98
C25-H25A	0.98	C25-H25B	0.98
C25-H25C	0.98	C3-H3	0.95
C12-C13	1.24(2)	C12-H12	0.95
C13-H13	0.95	C29-H29A	0.98
C29-H29B	0.98	C29-H29C	0.98
C28-H28A	0.98	C28-H28B	0.98
C28-H28C	0.98		

Table 5. Bond angles (°) for 5517.

C15-Au1-C8	162.3(4)	C15-Au1-C7	165.1(4)
C8-Au1-C7	32.4(4)	C44-N3-C43	106.8(7)
C44-N3-B1	127.7(7)	C43-N3-B1	125.5(7)
C44-N4-C42	105.8(7)	C44-N4-B2	126.6(7)
C42-N4-B2	127.6(7)	C15-N1-C17	109.7(8)
C15-N1-C30	125.4(8)	C17-N1-C30	124.8(8)
N3-C44-N4	110.7(7)	N3-C44-C45	125.1(7)
N4-C44-C45	124.2(7)	C50-C45-C46	119.9(8)
C50-C45-C44	119.5(7)	C46-C45-C44	120.6(8)
C15-N2-C16	109.9(8)	C15-N2-C18	123.8(7)
C16-N2-C18	126.3(8)	C71-C70-C75	112.9(8)
C71-C70-B2	126.4(8)	C75-C70-B2	119.7(7)
C69-C64-C65	112.4(8)	C69-C64-B1	125.7(8)
C65-C64-B1	121.2(8)	C53-C52-C57	112.5(8)
C53-C52-B1	129.2(8)	C57-C52-B1	118.1(8)
C62-C63-F10	114.7(8)	C62-C63-C58	124.1(8)
F10-C63-C58	121.2(8)	F1-C69-C68	113.9(8)
F1-C69-C64	121.7(8)	C68-C69-C64	124.3(9)
F16-C71-C70	121.4(8)	F16-C71-C72	114.9(8)
C70-C71-C72	123.7(8)	F5-C65-C66	114.9(9)
F5-C65-C64	119.8(8)	C66-C65-C64	125.3(9)
C77-C76-C81	112.7(8)	C77-C76-B2	121.2(8)
C81-C76-B2	125.2(8)	C16-C17-N1	107.3(8)
C16-C17-H17	126.4	N1-C17-H17	126.4

F30-C77-C76	119.6(8)	F30-C77-C78	116.8(9)
C76-C77-C78	123.6(9)	C83-C82-C87	113.7(8)
C83-C82-B2	117.8(8)	C87-C82-B2	128.3(8)
C74-C75-F20	116.5(8)	C74-C75-C70	124.9(9)
F20-C75-C70	118.6(8)	F26-C81-C80	115.3(8)
F26-C81-C76	120.6(8)	C80-C81-C76	124.1(9)
C42-C43-N3	107.5(8)	C42-C43-H43	126.3
N3-C43-H43	126.3	C59-C58-C63	113.8(8)
C59-C58-B1	118.2(7)	C63-C58-B1	127.6(7)
F6-C59-C58	120.0(8)	F6-C59-C60	115.8(8)
C58-C59-C60	124.1(8)	C47-C46-C45	120.0(9)
C47-C46-H46	120.0	C45-C46-H46	120.0
C48-C47-C46	119.9(9)	C48-C47-H47	120.0
C46-C47-H47	120.0	C49-C50-C45	119.1(8)
C49-C50-H50	120.4	C45-C50-H50	120.4
C17-C16-N2	107.3(8)	C17-C16-H16	126.4
N2-C16-H16	126.4	F21-C83-C84	115.4(9)
F21-C83-C82	119.7(8)	C84-C83-C82	124.9(9)
C72-C73-F18	120.7(9)	C72-C73-C74	119.0(9)
F18-C73-C74	120.3(9)	F15-C57-C56	115.7(8)
F15-C57-C52	119.2(8)	C56-C57-C52	125.1(9)
F9-C62-C63	120.1(9)	F9-C62-C61	120.0(8)
C63-C62-C61	119.9(9)	F11-C53-C52	120.7(8)
F11-C53-C54	114.5(8)	C52-C53-C54	124.8(9)
F25-C87-C86	114.6(9)	F25-C87-C82	121.3(9)
C86-C87-C82	124.0(10)	C31-C30-C35	123.7(10)
C31-C30-N1	117.2(9)	C35-C30-N1	119.0(9)
C47-C48-C49	120.4(9)	C47-C48-C51	118.9(9)
C49-C48-C51	120.7(9)	C22-C23-C18	117.2(10)
C22-C23-C24	120.5(10)	C18-C23-C24	122.3(9)
F19-C74-C75	120.5(9)	F19-C74-C73	120.0(9)
C75-C74-C73	119.5(9)	F8-C61-C60	120.0(9)
F8-C61-C62	121.2(9)	C60-C61-C62	118.8(9)
C7-C8-C9	169.5(10)	C7-C8-Au1	74.3(7)
C9-C8-Au1	116.0(7)	F12-C54-C55	119.3(9)
F12-C54-C53	121.2(9)	C55-C54-C53	119.4(9)
F22-C84-C85	120.5(10)	F22-C84-C83	121.2(10)
C85-C84-C83	118.3(10)	C50-C49-C48	120.6(9)

C50-C49-H49	119.7	C48-C49-H49	119.7
F4-C66-C65	120.2(9)	F4-C66-C67	121.6(9)
C65-C66-C67	118.2(10)	F13-C55-C54	120.6(11)
F13-C55-C56	120.5(10)	C54-C55-C56	118.9(9)
C30-C35-C34	116.7(10)	C30-C35-C36	123.4(9)
C34-C35-C36	119.9(10)	N1-C15-N2	105.9(7)
N1-C15-Au1	127.3(7)	N2-C15-Au1	126.7(7)
C43-C42-N4	109.3(8)	C43-C42-H42	125.4
N4-C42-H42	125.4	C79-C80-F27	120.0(9)
C79-C80-C81	120.8(9)	F27-C80-C81	119.1(10)
F17-C72-C73	120.4(8)	F17-C72-C71	119.7(8)
C73-C72-C71	119.9(8)	F7-C60-C61	120.6(9)
F7-C60-C59	120.1(9)	C61-C60-C59	119.2(8)
F24-C86-C87	121.2(10)	F24-C86-C85	119.9(10)
C87-C86-C85	118.9(10)	C8-C7-C1	166.5(10)
C8-C7-Au1	73.3(7)	C1-C7-Au1	120.1(8)
F29-C78-C79	121.0(9)	F29-C78-C77	119.0(10)
C79-C78-C77	120.0(10)	F23-C85-C84	120.2(11)
F23-C85-C86	119.5(11)	C84-C85-C86	120.2(9)
C18-C19-C20	115.6(11)	C18-C19-C27	122.2(11)
C20-C19-C27	122.1(11)	C68-C67-F3	121.7(10)
C68-C67-C66	120.1(9)	F3-C67-C66	118.2(11)
N4-B2-C82	103.2(7)	N4-B2-C70	112.0(7)
C82-B2-C70	116.7(8)	N4-B2-C76	112.1(7)
C82-B2-C76	112.4(7)	C70-B2-C76	100.8(7)
C80-C79-F28	121.3(10)	C80-C79-C78	118.7(9)
F28-C79-C78	120.0(11)	C19-C18-C23	124.4(10)
C19-C18-N2	118.2(9)	C23-C18-N2	117.3(8)
C67-C68-F2	120.4(9)	C67-C68-C69	119.7(9)
F2-C68-C69	119.8(10)	C10-C9-C14	119.1(12)
C10-C9-C8	121.6(11)	C14-C9-C8	119.2(11)
C30-C31-C32	116.7(11)	C30-C31-C39	121.6(10)
C32-C31-C39	121.7(11)	F31-C51-F33	108.6(11)
F31-C51-F32	102.5(10)	F33-C51-F32	106.5(9)
F31-C51-C48	112.8(9)	F33-C51-C48	115.5(9)
F32-C51-C48	110.1(9)	C2-C1-C6	120.7(12)
C2-C1-C7	122.9(11)	C6-C1-C7	116.3(11)
C21-C22-C23	120.7(13)	C21-C22-H22	119.7

C23-C22-H22	119.7	C21-C20-C19	120.2(12)
C21-C20-H20	119.9	C19-C20-H20	119.9
F14-C56-C55	118.9(9)	F14-C56-C57	121.8(10)
C55-C56-C57	119.3(9)	N3-B1-C52	105.4(7)
N3-B1-C64	110.7(7)	C52-B1-C64	113.9(7)
N3-B1-C58	110.8(7)	C52-B1-C58	114.2(7)
C64-B1-C58	102.0(7)	C33-C34-C35	121.2(12)
C33-C34-H34	119.4	C35-C34-H34	119.4
C22-C21-C20	121.9(13)	C22-C21-H21	119.0
C20-C21-H21	119.0	C23-C24-C25	113.6(11)
C23-C24-C26	110.3(10)	C25-C24-C26	109.0(10)
C23-C24-H24	107.9	C25-C24-H24	107.9
C26-C24-H24	107.9	C37-C36-C35	114.0(10)
C37-C36-C38	108.8(11)	C35-C36-C38	110.6(10)
C37-C36-H36	107.7	C35-C36-H36	107.7
C38-C36-H36	107.7	C1-C6-C5	118.8(13)
C1-C6-H6	120.6	C5-C6-H6	120.6
C40-C39-C41	110.4(10)	C40-C39-C31	110.3(11)
C41-C39-C31	111.0(11)	C40-C39-H39	108.4
C41-C39-H39	108.4	C31-C39-H39	108.4
C33-C32-C31	120.5(12)	C33-C32-H32	119.8
C31-C32-H32	119.8	C24-C26-H26A	109.5
C24-C26-H26B	109.5	H26A-C26-H26B	109.5
C24-C26-H26C	109.5	H26A-C26-H26C	109.5
H26B-C26-H26C	109.5	C4-C5-C6	120.8(13)
C4-C5-H5	119.6	C6-C5-H5	119.6
C19-C27-C28	109.2(13)	C19-C27-C29	110.0(14)
C28-C27-C29	110.0(14)	C19-C27-H27	109.2
C28-C27-H27	109.2	C29-C27-H27	109.2
C34-C33-C32	121.3(11)	C34-C33-H33	119.4
C32-C33-H33	119.4	C36-C37-H37A	109.5
C36-C37-H37B	109.5	H37A-C37-H37B	109.5
C36-C37-H37C	109.5	H37A-C37-H37C	109.5
H37B-C37-H37C	109.5	C39-C41-H41A	109.5
C39-C41-H41B	109.5	H41A-C41-H41B	109.5
C39-C41-H41C	109.5	H41A-C41-H41C	109.5
H41B-C41-H41C	109.5	C39-C40-H40A	109.5
C39-C40-H40B	109.5	H40A-C40-H40B	109.5

C39-C40-H40C	109.5	H40A-C40-H40C	109.5
H40B-C40-H40C	109.5	C9-C14-C13	117.1(14)
C9-C14-H14	121.5	C13-C14-H14	121.5
C9-C10-C11	119.8(13)	C9-C10-H10	120.1
C11-C10-H10	120.1	C1-C2-C3	117.7(14)
C1-C2-H2	121.1	C3-C2-H2	121.1
C3-C4-C5	117.8(14)	C3-C4-H4	121.1
C5-C4-H4	121.1	C12-C11-C10	120.7(15)
C12-C11-H11	119.7	C10-C11-H11	119.7
C36-C38-H38A	109.5	C36-C38-H38B	109.5
H38A-C38-H38B	109.5	C36-C38-H38C	109.5
H38A-C38-H38C	109.5	H38B-C38-H38C	109.5
C24-C25-H25A	109.5	C24-C25-H25B	109.5
H25A-C25-H25B	109.5	C24-C25-H25C	109.5
H25A-C25-H25C	109.5	H25B-C25-H25C	109.5
C4-C3-C2	124.2(16)	C4-C3-H3	117.9
C2-C3-H3	117.9	C13-C12-C11	120.9(15)
C13-C12-H12	119.6	C11-C12-H12	119.6
C12-C13-C14	122.1(15)	C12-C13-H13	119.0
C14-C13-H13	119.0	C27-C29-H29A	109.5
C27-C29-H29B	109.5	H29A-C29-H29B	109.5
C27-C29-H29C	109.5	H29A-C29-H29C	109.5
H29B-C29-H29C	109.5	C27-C28-H28A	109.5
C27-C28-H28B	109.5	H28A-C28-H28B	109.5
C27-C28-H28C	109.5	H28A-C28-H28C	109.5
H28B-C28-H28C	109.5		

Table 6. Anisotropic atomic displacement parameters (Å^2) for 5517.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au1	0.0307(2)	0.0300(2)	0.0324(2)	-0.01642(18)	-0.01277(18)	0.00158(16)
F5	0.031(3)	0.036(3)	0.031(3)	-0.007(3)	-0.011(3)	0.007(2)
F26	0.039(3)	0.043(3)	0.043(3)	-0.021(3)	-0.027(3)	0.021(3)
F16	0.029(3)	0.040(3)	0.042(3)	-0.022(3)	-0.020(3)	0.014(2)
F6	0.028(3)	0.028(3)	0.039(3)	-0.015(3)	-0.015(3)	0.010(2)
F21	0.037(3)	0.036(3)	0.027(3)	-0.010(3)	-0.014(3)	0.009(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F11	0.032(3)	0.024(3)	0.036(3)	-0.012(2)	-0.010(3)	0.000(2)
F30	0.035(3)	0.032(3)	0.063(4)	-0.022(3)	-0.028(3)	0.010(3)
F1	0.035(3)	0.048(3)	0.044(4)	-0.020(3)	-0.025(3)	0.014(3)
F20	0.026(3)	0.047(3)	0.038(3)	-0.018(3)	-0.017(3)	0.017(3)
F25	0.028(3)	0.039(3)	0.030(3)	-0.006(3)	-0.003(3)	0.002(3)
F10	0.036(3)	0.034(3)	0.032(3)	-0.015(3)	-0.019(3)	0.019(3)
F15	0.047(3)	0.034(3)	0.045(3)	-0.025(3)	-0.024(3)	0.010(3)
F18	0.077(5)	0.074(5)	0.047(4)	-0.042(4)	-0.036(4)	0.037(4)
F17	0.050(4)	0.043(3)	0.048(4)	-0.022(3)	-0.035(3)	0.012(3)
F7	0.058(4)	0.045(4)	0.065(4)	-0.043(3)	-0.029(4)	0.024(3)
F12	0.045(4)	0.027(3)	0.035(3)	0.005(3)	-0.004(3)	-0.003(3)
F2	0.036(3)	0.058(4)	0.087(5)	-0.046(4)	-0.042(4)	0.024(3)
F9	0.065(4)	0.069(4)	0.045(4)	-0.035(3)	-0.040(3)	0.031(4)
F4	0.033(3)	0.049(4)	0.046(4)	-0.012(3)	0.004(3)	0.001(3)
F22	0.079(5)	0.065(4)	0.060(4)	-0.042(4)	-0.049(4)	0.032(4)
F19	0.046(4)	0.074(5)	0.040(4)	-0.031(4)	-0.014(3)	0.034(3)
F14	0.082(5)	0.072(5)	0.047(4)	-0.041(4)	-0.037(4)	0.031(4)
F27	0.063(4)	0.054(4)	0.052(4)	-0.026(3)	-0.040(4)	0.041(3)
F8	0.084(5)	0.078(5)	0.069(5)	-0.059(4)	-0.047(4)	0.033(4)
F29	0.072(5)	0.027(3)	0.122(7)	-0.030(4)	-0.053(5)	0.011(3)
F3	0.020(3)	0.061(4)	0.087(5)	-0.045(4)	-0.010(3)	0.011(3)
F13	0.067(5)	0.074(5)	0.024(3)	-0.009(3)	-0.012(3)	0.016(4)
N3	0.017(4)	0.017(4)	0.028(4)	-0.010(3)	-0.008(3)	0.003(3)
F24	0.025(3)	0.048(4)	0.085(5)	-0.023(4)	-0.014(4)	-0.002(3)
F28	0.085(5)	0.032(3)	0.080(5)	-0.019(4)	-0.043(4)	0.028(4)
N4	0.015(4)	0.016(4)	0.025(4)	-0.004(3)	-0.006(3)	-0.002(3)
F33	0.074(5)	0.050(4)	0.040(4)	-0.008(3)	0.007(4)	-0.025(4)
F23	0.063(5)	0.077(5)	0.125(7)	-0.065(5)	-0.065(5)	0.019(4)
F32	0.083(6)	0.031(4)	0.074(5)	-0.011(4)	0.005(5)	-0.017(4)
N1	0.028(4)	0.030(4)	0.031(5)	-0.017(4)	-0.010(4)	0.004(4)
C44	0.022(5)	0.022(4)	0.020(5)	-0.009(4)	-0.010(4)	0.001(4)
C45	0.014(4)	0.022(4)	0.021(5)	-0.005(4)	-0.007(4)	0.005(3)
N2	0.025(4)	0.029(4)	0.037(5)	-0.019(4)	-0.016(4)	0.008(3)
C70	0.027(5)	0.020(4)	0.028(5)	-0.009(4)	-0.015(4)	0.008(4)
C64	0.021(5)	0.024(5)	0.027(5)	-0.015(4)	-0.006(4)	0.002(4)
C52	0.023(5)	0.021(4)	0.031(5)	-0.013(4)	-0.014(4)	0.011(4)
F31	0.061(5)	0.079(6)	0.102(7)	0.030(5)	-0.043(5)	-0.047(5)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C63	0.025(5)	0.024(5)	0.027(5)	-0.009(4)	-0.006(4)	0.006(4)
C69	0.028(5)	0.030(5)	0.040(6)	-0.020(5)	-0.018(5)	0.011(4)
C71	0.020(5)	0.021(4)	0.031(5)	-0.011(4)	-0.008(4)	0.005(4)
C65	0.029(5)	0.026(5)	0.043(6)	-0.018(5)	-0.015(5)	0.010(4)
C76	0.026(5)	0.028(5)	0.022(5)	-0.009(4)	-0.008(4)	0.007(4)
C17	0.022(5)	0.040(6)	0.035(6)	-0.022(5)	-0.009(5)	0.002(4)
C77	0.034(6)	0.022(5)	0.042(6)	-0.011(5)	-0.017(5)	0.007(4)
C82	0.020(5)	0.020(4)	0.028(5)	-0.006(4)	-0.010(4)	0.006(4)
C75	0.030(5)	0.030(5)	0.032(6)	-0.012(4)	-0.017(5)	0.011(4)
C81	0.030(5)	0.031(5)	0.027(5)	-0.014(4)	-0.016(4)	0.011(4)
C43	0.023(5)	0.021(5)	0.045(6)	-0.014(5)	-0.011(5)	0.005(4)
C58	0.016(4)	0.022(4)	0.020(5)	-0.008(4)	-0.001(4)	-0.002(4)
C59	0.020(5)	0.030(5)	0.026(5)	-0.011(4)	-0.007(4)	0.002(4)
C46	0.024(5)	0.028(5)	0.032(5)	-0.014(4)	-0.013(4)	0.009(4)
C47	0.025(5)	0.027(5)	0.022(5)	-0.004(4)	0.000(4)	-0.001(4)
C50	0.019(5)	0.025(5)	0.024(5)	-0.008(4)	-0.009(4)	0.004(4)
C16	0.026(5)	0.044(6)	0.037(6)	-0.025(5)	-0.012(5)	0.004(4)
C83	0.028(5)	0.027(5)	0.031(6)	-0.011(4)	-0.015(5)	0.011(4)
C73	0.055(7)	0.034(5)	0.026(5)	-0.014(5)	-0.020(5)	0.019(5)
C57	0.031(5)	0.030(5)	0.031(6)	-0.015(4)	-0.017(5)	0.013(4)
C62	0.036(6)	0.046(6)	0.026(5)	-0.017(5)	-0.014(5)	0.008(5)
C53	0.023(5)	0.028(5)	0.032(5)	-0.013(4)	-0.014(4)	0.010(4)
C87	0.022(5)	0.031(5)	0.034(6)	-0.009(5)	-0.012(5)	0.009(4)
C30	0.028(5)	0.041(6)	0.034(6)	-0.021(5)	-0.007(5)	-0.004(5)
C48	0.026(5)	0.023(5)	0.037(6)	-0.009(4)	-0.008(5)	0.001(4)
C23	0.023(5)	0.049(6)	0.028(5)	-0.019(5)	-0.008(5)	-0.005(5)
C74	0.035(6)	0.038(6)	0.033(6)	-0.017(5)	-0.014(5)	0.019(5)
C61	0.039(6)	0.045(6)	0.033(6)	-0.024(5)	-0.014(5)	0.005(5)
C8	0.034(6)	0.038(6)	0.042(7)	-0.022(6)	-0.016(5)	-0.003(5)
C54	0.034(6)	0.025(5)	0.040(6)	-0.009(5)	-0.016(5)	0.011(4)
C84	0.053(7)	0.039(6)	0.048(7)	-0.021(6)	-0.038(6)	0.020(6)
C49	0.028(5)	0.027(5)	0.040(6)	-0.017(5)	-0.016(5)	0.005(4)
C66	0.031(6)	0.030(5)	0.038(6)	-0.017(5)	-0.002(5)	-0.001(4)
C55	0.044(7)	0.048(7)	0.026(6)	-0.013(5)	-0.009(5)	0.019(5)
C35	0.030(6)	0.047(6)	0.026(6)	-0.012(5)	-0.004(5)	-0.005(5)
C15	0.020(5)	0.023(5)	0.035(6)	-0.015(4)	-0.008(4)	0.002(4)
C42	0.022(5)	0.021(5)	0.038(6)	-0.008(4)	-0.010(5)	0.001(4)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C80	0.051(7)	0.039(6)	0.029(6)	-0.014(5)	-0.021(5)	0.024(5)
C72	0.047(6)	0.026(5)	0.035(6)	-0.014(5)	-0.028(5)	0.015(4)
C60	0.034(6)	0.034(5)	0.045(6)	-0.026(5)	-0.013(5)	0.014(5)
C86	0.021(5)	0.033(6)	0.056(7)	-0.015(5)	-0.017(5)	0.003(5)
C7	0.040(6)	0.037(6)	0.047(7)	-0.024(6)	-0.020(6)	0.003(5)
C78	0.041(6)	0.032(6)	0.064(8)	-0.025(6)	-0.020(6)	0.007(5)
C85	0.049(7)	0.042(6)	0.091(10)	-0.040(7)	-0.053(7)	0.023(6)
C19	0.058(7)	0.036(6)	0.046(7)	-0.015(5)	-0.031(6)	0.008(5)
C67	0.021(5)	0.039(6)	0.083(9)	-0.041(7)	-0.020(6)	0.012(5)
B2	0.021(5)	0.024(5)	0.032(6)	-0.013(5)	-0.014(5)	0.009(4)
C79	0.056(7)	0.027(6)	0.046(7)	-0.011(5)	-0.023(6)	0.022(5)
C18	0.039(6)	0.026(5)	0.024(5)	-0.006(4)	-0.017(5)	-0.003(4)
C68	0.030(6)	0.033(5)	0.052(7)	-0.024(5)	-0.020(5)	0.011(5)
C9	0.056(7)	0.041(6)	0.035(6)	-0.022(5)	-0.021(6)	0.005(5)
C31	0.040(6)	0.062(7)	0.045(7)	-0.035(6)	-0.014(6)	0.005(6)
C51	0.045(7)	0.031(6)	0.046(7)	-0.009(5)	-0.019(6)	0.001(5)
C1	0.048(7)	0.047(7)	0.036(6)	-0.022(6)	-0.006(6)	-0.011(5)
C22	0.042(7)	0.066(9)	0.040(7)	-0.023(7)	-0.011(6)	-0.015(6)
C20	0.093(11)	0.026(6)	0.050(8)	0.004(6)	-0.045(8)	-0.017(7)
C56	0.046(6)	0.044(6)	0.040(6)	-0.028(5)	-0.026(5)	0.025(5)
B1	0.020(5)	0.021(5)	0.027(6)	-0.012(5)	-0.009(5)	0.009(4)
C34	0.057(8)	0.057(8)	0.039(7)	-0.011(6)	-0.018(6)	0.000(6)
C21	0.065(10)	0.074(10)	0.041(8)	-0.009(7)	-0.022(7)	-0.030(8)
C24	0.033(6)	0.058(7)	0.053(7)	-0.034(6)	-0.017(6)	0.016(5)
C36	0.040(6)	0.044(6)	0.048(7)	-0.018(6)	-0.015(6)	0.007(5)
C6	0.031(6)	0.049(7)	0.058(8)	-0.023(6)	-0.002(6)	-0.005(5)
C39	0.061(8)	0.068(8)	0.059(8)	-0.047(7)	-0.019(7)	0.020(7)
C32	0.044(7)	0.087(10)	0.049(8)	-0.046(8)	0.000(6)	-0.003(7)
C26	0.055(8)	0.094(10)	0.079(10)	-0.059(9)	-0.040(8)	0.038(8)
C5	0.042(8)	0.063(9)	0.104(13)	-0.051(9)	-0.006(8)	-0.008(7)
C27	0.088(10)	0.039(7)	0.091(11)	-0.029(7)	-0.053(9)	0.030(7)
C33	0.066(9)	0.084(10)	0.031(7)	-0.022(7)	-0.017(7)	-0.001(8)
C37	0.071(10)	0.044(7)	0.085(11)	-0.027(8)	-0.015(8)	-0.003(7)
C41	0.050(8)	0.092(10)	0.088(10)	-0.068(9)	-0.032(8)	0.026(7)
C40	0.052(8)	0.067(9)	0.115(13)	-0.059(10)	-0.020(9)	0.021(7)
C14	0.075(10)	0.113(13)	0.047(9)	-0.024(9)	-0.016(8)	0.055(10)
C10	0.040(7)	0.104(11)	0.042(8)	-0.030(8)	-0.013(6)	-0.009(7)

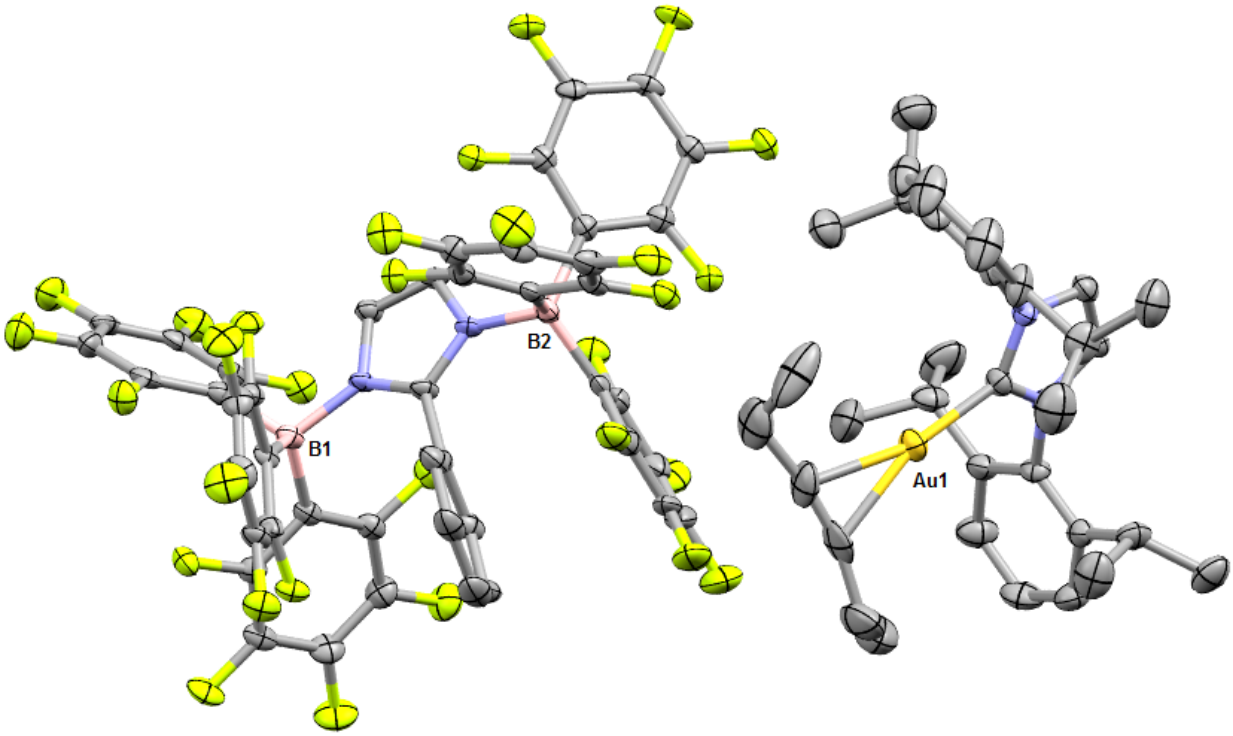
	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C2	0.097(12)	0.079(10)	0.047(8)	-0.009(8)	-0.034(9)	-0.036(9)
C4	0.080(11)	0.068(9)	0.049(8)	-0.029(8)	-0.005(8)	-0.019(8)
C11	0.063(9)	0.101(12)	0.046(9)	-0.032(9)	-0.004(8)	-0.020(9)
C38	0.044(8)	0.065(9)	0.091(11)	-0.031(8)	-0.028(8)	0.014(7)
C25	0.113(13)	0.111(13)	0.113(13)	-0.093(12)	-0.073(12)	0.056(11)
C3	0.141(18)	0.099(13)	0.041(9)	-0.009(9)	-0.033(10)	-0.043(12)
C12	0.116(15)	0.060(9)	0.050(9)	-0.016(8)	-0.024(10)	0.026(9)
C13	0.104(14)	0.145(17)	0.046(9)	-0.015(10)	-0.022(10)	0.088(14)
C29	0.20(3)	0.126(17)	0.22(3)	-0.14(2)	-0.14(2)	0.098(18)
C28	0.134(19)	0.16(2)	0.20(2)	-0.11(2)	-0.128(19)	0.107(17)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 5517.

	x/a	y/b	z/c	U(eq)
H17	0.2975	0.1808	0.4599	0.038
H43	0.4234	0.3180	0.0407	0.038
H46	0.1221	0.1385	0.3430	0.034
H47	0.0002	0.0192	0.4383	0.038
H50	0.1394	0.1048	0.1486	0.03
H16	0.3935	0.2734	0.3067	0.041
H49	0.0194	-0.0149	0.2453	0.037
H42	0.3018	0.4006	0.0687	0.037
H22	0.7713	0.4148	0.1190	0.064
H20	0.6104	0.5857	0.1266	0.074
H34	0.3667	0.0437	0.7302	0.069
H21	0.7499	0.5491	0.0611	0.082
H24	0.5904	0.2396	0.3056	0.055
H36	0.4649	0.1134	0.5071	0.057
H6	0.8684	0.4874	0.3845	0.065
H39	0.2905	0.3290	0.4966	0.07
H32	0.2196	0.2252	0.7249	0.074
H26A	0.7912	0.3015	0.2507	0.098
H26B	0.7334	0.2080	0.3222	0.098
H26C	0.7055	0.2839	0.3395	0.098
H5	0.9778	0.6056	0.2549	0.09
H27	0.4091	0.4404	0.3313	0.083

	x/a	y/b	z/c	U(eq)
H33	0.2642	0.1048	0.7990	0.077
H37A	0.4159	-0.0281	0.6680	0.113
H37B	0.4780	-0.0250	0.5791	0.113
H37C	0.3674	-0.0159	0.6055	0.113
H41A	0.1287	0.2660	0.6044	0.099
H41B	0.1470	0.3656	0.5605	0.099
H41C	0.1453	0.3116	0.6524	0.099
H40A	0.3108	0.3868	0.6024	0.117
H40B	0.3089	0.4451	0.5127	0.117
H40C	0.3966	0.3982	0.5165	0.117
H14	0.7474	0.2844	0.5895	0.107
H10	0.4758	0.3125	0.6252	0.08
H2	0.6777	0.5081	0.2860	0.099
H4	0.9357	0.6729	0.1425	0.088
H11	0.4229	0.2237	0.7697	0.095
H38A	0.5871	0.1685	0.5214	0.106
H38B	0.6015	0.0768	0.5379	0.106
H38C	0.5539	0.0936	0.6166	0.106
H25A	0.6415	0.2521	0.1684	0.132
H25B	0.6895	0.1859	0.2223	0.132
H25C	0.7519	0.2774	0.1485	0.132
H3	0.7940	0.6203	0.1565	0.128
H12	0.5310	0.1700	0.8237	0.101
H13	0.6811	0.1857	0.7393	0.14
H29A	0.5169	0.5622	0.2992	0.212
H29B	0.4080	0.5738	0.3165	0.212
H29C	0.4917	0.6169	0.2210	0.212
H28A	0.4127	0.5586	0.1708	0.208
H28B	0.3186	0.5004	0.2576	0.208
H28C	0.3882	0.4606	0.2049	0.208

Crystal Structure Report for 4[IMP-H]



Thermal ellipsoid plot of 5614. Ellipsoids shown at 50% probability, hydrogens omitted for clarity.

A specimen of $C_{79}H_{55}AuB_2Cl_2F_{30}N_4$, approximate dimensions 0.021 mm x 0.066 mm x 0.179 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The integration of the data using a monoclinic unit cell yielded a total of 68338 reflections to a maximum θ angle of 28.09° (0.75 Å resolution), of which 18569 were independent (average redundancy 3.680, completeness = 97.1%, R_{int} = 10.00%, R_{sig} = 12.77%) and 10701 (57.63%) were greater than $2\sigma(F^2)$. The final cell constants of a = 12.184(6) Å, b = 19.349(10) Å, c = 33.546(17) Å, β = 96.835(9)°, volume = 7852.(7) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.5286 and 0.7456. The final anisotropic full-matrix least-squares refinement on F^2 with 1073 variables converged at R1 = 6.62%, for the observed data and wR2 = 15.35% for all data. The goodness-of-fit was 1.013. The largest peak in the final difference electron density synthesis was 1.882 $e^-/Å^3$ and the largest hole was -1.467 $e^-/Å^3$ with an RMS deviation of 0.132 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.624 g/cm^3 and F(000), 3800 e^-.

Table 1. Sample and crystal data for 5614.

Identification code	5614
Chemical formula	$C_{79}H_{55}AuB_2Cl_2F_{30}N_4$
Formula weight	1919.75 g/mol
Wavelength	0.71073 Å

Crystal size	0.021 x 0.066 x 0.179 mm	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 12.184(6) Å	α = 90°
	b = 19.349(10) Å	β = 96.835(9)°
	c = 33.546(17) Å	γ = 90°
Volume	7852.(7) $Å^3$	
Z	4	
Density (calculated)	1.624 g/cm^3	
Absorption coefficient	2.060 mm^{-1}	
F(000)	3800	

Table 2. Data collection and structure refinement for 5614.

Theta range for data collection	1.61 to 28.09°	
Index ranges	-16<=h<=11, -21<=k<=25, -43<=l<=44	
Reflections collected	68338	
Independent reflections	18569 [R(int) = 0.1000]	
Max. and min. transmission	0.7456 and 0.5286	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	XL (Sheldrick, 2008)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	18569 / 0 / 1073	
Goodness-of-fit on F^2	1.013	
Δ/σ_{max}	0.002	
Final R indices	10701 data; I>2σ(I)	R1 = 0.0662, wR2 = 0.1297
	all data	R1 = 0.1380, wR2 = 0.1535
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0554P)^2+17.5424P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	1.882 and -1.467 $eÅ^{-3}$	
R.M.S. deviation from mean	0.132 $eÅ^{-3}$	

Table 3. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for 5614.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Au1	0.78446(2)	0.72233(2)	0.54641(2)	0.03186(9)
Cl2	0.2978(2)	0.94930(13)	0.84754(9)	0.0784(8)
Cl1	0.1982(2)	0.85198(16)	0.89789(9)	0.0829(8)
F11	0.2804(3)	0.48430(17)	0.78158(10)	0.0254(8)
F15	0.2407(3)	0.71400(18)	0.82589(10)	0.0288(8)

	x/a	y/b	z/c	U(eq)
F30	0.3562(3)	0.82464(18)	0.59858(10)	0.0271(8)
F10	0.0656(3)	0.59896(19)	0.68132(10)	0.0311(9)
F6	0.0803(3)	0.48669(18)	0.80743(10)	0.0268(8)
F20	0.5665(3)	0.81208(18)	0.65811(10)	0.0278(8)
F1	0.9181(3)	0.65176(19)	0.73340(10)	0.0286(9)
F12	0.4654(3)	0.47307(19)	0.82930(11)	0.0336(9)
F27	0.2377(3)	0.01788(18)	0.70231(11)	0.0320(9)
F16	0.3996(3)	0.7836(2)	0.77781(10)	0.0300(8)
F26	0.3040(3)	0.89599(18)	0.73089(10)	0.0267(8)
F29	0.3032(3)	0.95009(18)	0.57258(10)	0.0296(9)
F28	0.2340(3)	0.04687(18)	0.62243(11)	0.0339(9)
F19	0.7540(3)	0.8482(2)	0.70159(12)	0.0364(10)
F5	0.1115(3)	0.62500(19)	0.86343(10)	0.0312(9)
F7	0.0072(3)	0.37085(19)	0.77051(11)	0.0339(9)
F25	0.1898(3)	0.73584(19)	0.62606(11)	0.0339(9)
F2	0.7388(3)	0.6854(2)	0.76632(12)	0.0406(10)
F21	0.5602(3)	0.67824(19)	0.67114(12)	0.0363(10)
F9	0.9897(3)	0.4842(2)	0.64561(11)	0.0416(11)
F17	0.5816(3)	0.8270(2)	0.81991(11)	0.0409(10)
F4	0.9332(3)	0.6617(2)	0.89496(11)	0.0423(10)
F3	0.7433(3)	0.6923(2)	0.84762(12)	0.0426(11)
F14	0.4341(3)	0.7031(2)	0.87150(12)	0.0421(11)
F8	0.9619(3)	0.3670(2)	0.68926(12)	0.0430(11)
F13	0.5464(3)	0.5809(2)	0.87520(12)	0.0448(11)
F24	0.1853(4)	0.6359(2)	0.57112(13)	0.0512(12)
F22	0.5539(4)	0.5817(2)	0.61513(13)	0.0536(13)
F18	0.7637(3)	0.8585(2)	0.78290(13)	0.0471(11)
F23	0.3676(5)	0.5585(2)	0.56427(14)	0.0612(14)
N2	0.1691(4)	0.6751(2)	0.74453(14)	0.0192(11)
N1	0.2679(4)	0.7433(2)	0.70932(14)	0.0204(11)
N3	0.7021(4)	0.7767(3)	0.46478(13)	0.0212(11)
N4	0.7891(4)	0.8559(3)	0.49959(14)	0.0225(12)
C43	0.2659(5)	0.9837(3)	0.6365(2)	0.0243(15)
C4	0.3441(5)	0.6247(3)	0.72413(17)	0.0206(13)
C46	0.7575(5)	0.7896(3)	0.50115(17)	0.0238(14)
C61	0.6468(5)	0.7120(3)	0.45310(17)	0.0227(14)
C42	0.2673(5)	0.9695(3)	0.67675(19)	0.0238(14)
C3	0.2624(5)	0.6810(3)	0.72652(18)	0.0199(13)
C16	0.0846(5)	0.5475(3)	0.74649(18)	0.0202(13)
C66	0.7018(6)	0.6646(3)	0.43166(18)	0.0267(15)
C41	0.2991(5)	0.9048(3)	0.69080(18)	0.0208(13)

	x/a	y/b	z/c	U(eq)
C2	0.1738(5)	0.7783(3)	0.71633(17)	0.0225(13)
C30	0.5783(5)	0.8219(3)	0.77988(19)	0.0275(15)
C10	0.2457(5)	0.5987(3)	0.80291(17)	0.0181(13)
C47	0.7530(5)	0.8852(3)	0.46266(18)	0.0265(15)
C1	0.1147(5)	0.7370(3)	0.73828(18)	0.0224(14)
C21	0.0546(5)	0.5432(3)	0.70532(18)	0.0229(14)
C40	0.3256(5)	0.8505(3)	0.66620(17)	0.0213(13)
C5	0.4481(5)	0.6271(4)	0.7470(2)	0.0300(16)
C17	0.0614(5)	0.4880(3)	0.76679(18)	0.0233(14)
C12	0.3928(6)	0.6485(4)	0.84998(19)	0.0290(16)
C22	0.0288(5)	0.6393(3)	0.79585(18)	0.0215(14)
C44	0.2991(5)	0.9346(3)	0.61167(18)	0.0235(14)
C24	0.9272(5)	0.6546(3)	0.77396(18)	0.0216(14)
C25	0.8333(5)	0.6726(3)	0.7906(2)	0.0266(15)
C67	0.8205(6)	0.6744(4)	0.4234(2)	0.0323(16)
C18	0.0214(5)	0.4277(3)	0.74867(19)	0.0242(14)
C48	0.6994(5)	0.8349(3)	0.44080(17)	0.0214(14)
C45	0.3274(5)	0.8694(3)	0.62614(18)	0.0229(14)
C29	0.4848(5)	0.7985(3)	0.75675(19)	0.0255(15)
C11	0.2928(5)	0.6526(3)	0.82621(18)	0.0242(14)
C28	0.4753(5)	0.7919(3)	0.71561(18)	0.0223(14)
C14	0.4078(5)	0.5320(3)	0.82901(19)	0.0241(14)
C8	0.3952(6)	0.5153(4)	0.6969(2)	0.0362(18)
C13	0.4498(5)	0.5874(4)	0.85159(19)	0.0312(16)
C34	0.3759(5)	0.7144(3)	0.65105(18)	0.0246(14)
C15	0.3092(5)	0.5394(3)	0.80511(17)	0.0232(14)
C20	0.0136(6)	0.4846(4)	0.68575(19)	0.0301(16)
C9	0.3210(6)	0.5682(3)	0.6990(2)	0.0287(15)
C19	0.9997(5)	0.4257(4)	0.7075(2)	0.0304(16)
C33	0.5669(5)	0.8118(3)	0.69883(19)	0.0245(14)
C32	0.6669(5)	0.8335(3)	0.7206(2)	0.0282(15)
C38	0.4634(6)	0.6203(3)	0.6178(2)	0.0336(17)
C31	0.6710(5)	0.8380(4)	0.7614(2)	0.0334(17)
C55	0.6691(5)	0.9371(3)	0.5532(2)	0.0288(15)
C70	0.4852(6)	0.7547(4)	0.4890(2)	0.0342(17)
C39	0.4657(6)	0.6721(4)	0.6466(2)	0.0301(16)
C27	0.9310(6)	0.6602(3)	0.8548(2)	0.0295(16)
C49	0.8510(5)	0.8926(3)	0.53250(18)	0.0255(15)
C54	0.7930(6)	0.9309(4)	0.55839(19)	0.0335(17)
C62	0.5394(6)	0.7029(3)	0.46324(19)	0.0289(16)
C35	0.2830(6)	0.6988(3)	0.62459(19)	0.0284(15)

	x/a	y/b	z/c	U(eq)
C26	0.8344(6)	0.6759(3)	0.8312(2)	0.0289(16)
C23	0.0227(5)	0.6419(3)	0.83720(19)	0.0256(15)
C50	0.9655(6)	0.8866(4)	0.5366(2)	0.0361(18)
C64	0.5375(7)	0.5944(4)	0.4284(2)	0.043(2)
C7	0.4954(6)	0.5180(4)	0.7198(2)	0.0397(19)
C6	0.5218(6)	0.5739(4)	0.7449(2)	0.0352(18)
B1	0.1339(6)	0.6144(4)	0.7725(2)	0.0218(16)
C65	0.6441(6)	0.6049(4)	0.4197(2)	0.0363(18)
C36	0.2799(7)	0.6469(4)	0.5962(2)	0.0380(18)
C59	0.0266(6)	0.8470(4)	0.5072(2)	0.0405(19)
C37	0.3681(7)	0.6078(4)	0.5926(2)	0.041(2)
C68	0.8404(7)	0.6519(4)	0.3813(2)	0.046(2)
C75	0.8134(7)	0.6733(5)	0.6067(2)	0.048(2)
C63	0.4862(6)	0.6427(4)	0.4503(2)	0.0425(19)
C76	0.8111(7)	0.6261(5)	0.5823(2)	0.049(2)
B2	0.3639(6)	0.7728(4)	0.6855(2)	0.0242(15)
C52	0.9661(7)	0.9578(5)	0.5958(2)	0.057(3)
C53	0.8550(7)	0.9634(4)	0.5903(2)	0.046(2)
C71	0.4604(9)	0.7216(5)	0.5276(2)	0.065(3)
C51	0.0218(7)	0.9202(5)	0.5696(2)	0.055(2)
C72	0.3803(7)	0.7842(5)	0.4671(3)	0.065(3)
C69	0.8995(6)	0.6369(5)	0.4552(2)	0.052(2)
C58	0.0942(7)	0.7875(5)	0.5273(3)	0.065(3)
C57	0.6199(7)	0.8961(4)	0.5857(2)	0.052(2)
C60	0.0996(7)	0.8952(5)	0.4857(2)	0.055(2)
C56	0.6312(8)	0.0116(4)	0.5519(3)	0.061(3)
C78	0.7078(10)	0.5453(5)	0.5341(3)	0.075(3)
C77	0.8120(10)	0.5591(5)	0.5614(3)	0.072(3)
C79	0.2843(8)	0.8619(4)	0.8590(3)	0.061(3)
C74	0.8212(8)	0.7206(5)	0.6410(2)	0.064(3)
C73	0.9123(7)	0.7730(6)	0.6398(3)	0.083(4)

Table 4. Bond lengths (Å) for 5614.

Au1-C46	1.997(6)	Au1-C75	2.224(7)
Au1-C76	2.220(7)	Cl2-C79	1.746(9)
Cl1-C79	1.780(10)	F11-C15	1.348(7)
F15-C11	1.346(7)	F30-C45	1.344(7)
F10-C21	1.363(7)	F6-C17	1.356(7)
F20-C33	1.366(7)	F1-C24	1.353(7)
F12-C14	1.338(7)	F27-C42	1.347(7)

F16-C29	1.354(7)	F26-C41	1.350(7)
F29-C44	1.352(7)	F28-C43	1.350(7)
F19-C32	1.332(7)	F5-C23	1.351(7)
F7-C18	1.344(7)	F25-C35	1.349(8)
F2-C25	1.352(7)	F21-C39	1.338(8)
F9-C20	1.343(7)	F17-C30	1.342(7)
F4-C27	1.344(7)	F3-C26	1.335(7)
F14-C12	1.342(7)	F8-C19	1.345(7)
F13-C13	1.344(7)	F24-C36	1.361(8)
F22-C38	1.345(8)	F18-C31	1.327(7)
F23-C37	1.345(8)	N2-C3	1.354(8)
N2-C1	1.372(7)	N2-B1	1.595(9)
N1-C3	1.342(7)	N1-C2	1.376(8)
N1-B2	1.598(9)	N3-C46	1.345(7)
N3-C61	1.453(8)	N3-C48	1.383(7)
N4-C46	1.342(8)	N4-C47	1.386(7)
N4-C49	1.448(7)	C43-C42	1.377(9)
C43-C44	1.356(9)	C4-C3	1.484(8)
C4-C5	1.401(9)	C4-C9	1.389(9)
C61-C66	1.386(9)	C61-C62	1.402(9)
C42-C41	1.377(8)	C16-C21	1.388(8)
C16-C17	1.384(8)	C16-B1	1.636(9)
C66-C67	1.516(10)	C66-C65	1.387(9)
C41-C40	1.397(8)	C2-H2	0.95
C2-C1	1.350(8)	C30-C29	1.377(9)
C30-C31	1.388(10)	C10-C11	1.385(8)
C10-C15	1.382(8)	C10-B1	1.629(9)
C47-H47	0.95	C47-C48	1.339(9)
C1-H1	0.95	C21-C20	1.374(9)
C40-C45	1.395(8)	C40-B2	1.681(9)
C5-H5	0.95	C5-C6	1.373(9)
C17-C18	1.378(9)	C12-C11	1.377(9)
C12-C13	1.370(10)	C22-C24	1.393(8)
C22-C23	1.399(9)	C22-B1	1.650(10)
C44-C45	1.381(8)	C24-C25	1.377(9)
C25-C26	1.361(9)	C67-H67	1.0
C67-C68	1.525(9)	C67-C69	1.531(9)
C18-C19	1.374(9)	C48-H48	0.95
C29-C28	1.377(8)	C28-C33	1.363(9)
C28-B2	1.635(9)	C14-C13	1.375(9)
C14-C15	1.370(8)	C8-H8	0.95
C8-C9	1.373(9)	C8-C7	1.363(10)

C34-C39	1.389(9)	C34-C35	1.386(9)
C34-B2	1.635(10)	C20-C19	1.375(9)
C9-H9	0.95	C33-C32	1.407(9)
C32-C31	1.365(9)	C38-C39	1.390(9)
C38-C37	1.375(11)	C55-H55	1.0
C55-C54	1.504(10)	C55-C57	1.527(10)
C55-C56	1.513(11)	C70-H70	1.0
C70-C62	1.526(10)	C70-C71	1.506(10)
C70-C72	1.508(11)	C27-C26	1.372(9)
C27-C23	1.371(9)	C49-C54	1.395(9)
C49-C50	1.390(9)	C54-C53	1.386(9)
C62-C63	1.377(10)	C35-C36	1.380(9)
C50-C59	1.514(10)	C50-C51	1.392(10)
C64-H64	0.95	C64-C65	1.380(10)
C64-C63	1.384(10)	C7-H7	0.95
C7-C6	1.385(11)	C6-H6	0.95
C65-H65	0.95	C36-C37	1.332(11)
C59-H59	1.0	C59-C58	1.525(11)
C59-C60	1.529(11)	C68-H68A	0.98
C68-H68B	0.98	C68-H68C	0.98
C75-C76	1.224(11)	C75-C74	1.464(12)
C63-H63	0.95	C76-C77	1.475(13)
C52-H52	0.95	C52-C53	1.348(11)
C52-C51	1.379(11)	C53-H53	0.95
C71-H71A	0.98	C71-H71B	0.98
C71-H71C	0.98	C51-H51	0.95
C72-H72A	0.98	C72-H72B	0.98
C72-H72C	0.98	C69-H69A	0.98
C69-H69B	0.98	C69-H69C	0.98
C58-H58A	0.98	C58-H58B	0.98
C58-H58C	0.98	C57-H57A	0.98
C57-H57B	0.98	C57-H57C	0.98
C60-H60A	0.98	C60-H60B	0.98
C60-H60C	0.98	C56-H56A	0.98
C56-H56B	0.98	C56-H56C	0.98
C78-H78A	0.98	C78-H78B	0.98
C78-H78C	0.98	C78-C77	1.499(14)
C77-H77A	0.99	C77-H77B	0.99
C79-H79A	0.99	C79-H79B	0.99
C74-H74A	0.99	C74-H74B	0.99
C74-C73	1.507(13)	C73-H73A	0.98
C73-H73B	0.98	C73-H73C	0.98

Table 5. Bond angles (°) for 5614.

C46-Au1-C75	164.5(3)	C46-Au1-C76	163.6(3)
C76-Au1-C75	32.0(3)	C3-N2-C1	106.0(5)
C3-N2-B1	128.5(5)	C1-N2-B1	125.1(5)
C3-N1-C2	106.4(5)	C3-N1-B2	127.8(5)
C2-N1-B2	125.8(5)	C46-N3-C61	124.8(5)
C46-N3-C48	110.6(5)	C48-N3-C61	124.5(5)
C46-N4-C47	111.3(5)	C46-N4-C49	124.5(5)
C47-N4-C49	124.2(5)	F28-C43-C42	119.5(6)
F28-C43-C44	121.0(6)	C44-C43-C42	119.5(6)
C5-C4-C3	121.0(6)	C9-C4-C3	121.4(6)
C9-C4-C5	117.6(6)	N3-C46-Au1	126.0(5)
N4-C46-Au1	129.1(4)	N4-C46-N3	104.9(5)
C66-C61-N3	118.2(6)	C66-C61-C62	124.4(6)
C62-C61-N3	117.4(5)	F27-C42-C43	120.9(6)
F27-C42-C41	119.9(6)	C41-C42-C43	119.2(6)
N2-C3-C4	124.6(5)	N1-C3-N2	110.8(5)
N1-C3-C4	124.6(5)	C21-C16-B1	128.0(5)
C17-C16-C21	113.2(5)	C17-C16-B1	118.6(5)
C61-C66-C67	122.9(6)	C61-C66-C65	116.2(6)
C65-C66-C67	120.8(6)	F26-C41-C42	115.7(5)
F26-C41-C40	120.5(5)	C42-C41-C40	123.8(6)
N1-C2-H2	125.9	C1-C2-N1	108.2(5)
C1-C2-H2	125.9	F17-C30-C29	120.8(6)
F17-C30-C31	120.2(6)	C29-C30-C31	119.0(6)
C11-C10-B1	118.2(5)	C15-C10-C11	113.8(5)
C15-C10-B1	127.5(5)	N4-C47-H47	127.0
C48-C47-N4	105.9(6)	C48-C47-H47	127.0
N2-C1-H1	125.7	C2-C1-N2	108.7(6)
C2-C1-H1	125.7	F10-C21-C16	120.5(5)
F10-C21-C20	115.3(5)	C20-C21-C16	124.2(6)
C41-C40-B2	121.2(5)	C45-C40-C41	113.8(6)
C45-C40-B2	124.8(6)	C4-C5-H5	119.9
C6-C5-C4	120.1(7)	C6-C5-H5	119.9
F6-C17-C16	119.3(5)	F6-C17-C18	115.9(5)
C18-C17-C16	124.7(6)	F14-C12-C11	121.1(6)
F14-C12-C13	120.1(6)	C11-C12-C13	118.8(6)
C24-C22-C23	111.5(6)	C24-C22-B1	120.2(5)
C23-C22-B1	128.0(5)	F29-C44-C43	119.2(5)
F29-C44-C45	120.5(6)	C43-C44-C45	120.3(6)

F1-C24-C22	118.8(5)	F1-C24-C25	116.5(5)
C25-C24-C22	124.6(6)	F2-C25-C24	119.3(6)
F2-C25-C26	120.1(6)	C26-C25-C24	120.5(6)
C66-C67-H67	107.4	C66-C67-C68	113.3(6)
C66-C67-C69	110.4(6)	C68-C67-H67	107.4
C68-C67-C69	110.7(6)	C69-C67-H67	107.4
F7-C18-C17	120.9(6)	F7-C18-C19	120.2(6)
C19-C18-C17	118.8(6)	N3-C48-H48	126.4
C47-C48-N3	107.2(5)	C47-C48-H48	126.4
F30-C45-C40	121.9(6)	F30-C45-C44	115.0(5)
C44-C45-C40	123.1(6)	F16-C29-C30	114.2(6)
F16-C29-C28	121.7(6)	C30-C29-C28	124.0(6)
F15-C11-C10	119.7(5)	F15-C11-C12	116.0(6)
C12-C11-C10	124.2(6)	C29-C28-B2	127.1(6)
C33-C28-C29	114.4(6)	C33-C28-B2	118.0(5)
F12-C14-C13	120.0(6)	F12-C14-C15	121.1(6)
C15-C14-C13	118.9(6)	C9-C8-H8	120.2
C7-C8-H8	120.2	C7-C8-C9	119.6(7)
F13-C13-C12	120.5(6)	F13-C13-C14	119.6(6)
C12-C13-C14	119.9(6)	C39-C34-B2	128.4(6)
C35-C34-C39	113.4(6)	C35-C34-B2	118.0(6)
F11-C15-C10	121.4(5)	F11-C15-C14	114.1(6)
C14-C15-C10	124.4(6)	F9-C20-C21	120.4(6)
F9-C20-C19	120.2(6)	C19-C20-C21	119.4(6)
C4-C9-H9	119.0	C8-C9-C4	122.1(6)
C8-C9-H9	119.0	F8-C19-C18	119.7(6)
F8-C19-C20	121.0(6)	C18-C19-C20	119.3(6)
F20-C33-C32	114.7(6)	C28-C33-F20	120.6(6)
C28-C33-C32	124.8(6)	F19-C32-C33	120.4(6)
F19-C32-C31	121.9(6)	C31-C32-C33	117.7(6)
F22-C38-C39	119.9(7)	F22-C38-C37	120.0(6)
C37-C38-C39	120.1(7)	F18-C31-C30	120.6(6)
F18-C31-C32	119.5(6)	C32-C31-C30	119.9(6)
C54-C55-H55	107.3	C54-C55-C57	110.6(6)
C54-C55-C56	112.2(6)	C57-C55-H55	107.3
C56-C55-H55	107.3	C56-C55-C57	111.8(6)
C62-C70-H70	108.3	C71-C70-H70	108.3
C71-C70-C62	110.6(6)	C71-C70-C72	109.5(7)
C72-C70-H70	108.3	C72-C70-C62	111.8(6)
F21-C39-C34	120.9(6)	F21-C39-C38	115.9(6)
C38-C39-C34	123.2(7)	F4-C27-C26	119.1(6)
F4-C27-C23	121.2(6)	C26-C27-C23	119.7(6)

C54-C49-N4	118.6(6)	C50-C49-N4	117.4(6)
C50-C49-C54	124.0(6)	C49-C54-C55	123.1(6)
C53-C54-C55	120.0(7)	C53-C54-C49	116.9(7)
C61-C62-C70	122.3(6)	C63-C62-C61	116.6(6)
C63-C62-C70	121.1(7)	F25-C35-C34	119.2(6)
F25-C35-C36	117.2(6)	C36-C35-C34	123.6(7)
F3-C26-C25	120.9(6)	F3-C26-C27	120.9(6)
C25-C26-C27	118.2(6)	F5-C23-C22	120.3(6)
F5-C23-C27	114.3(6)	C27-C23-C22	125.3(6)
C49-C50-C59	122.9(6)	C51-C50-C49	115.7(7)
C51-C50-C59	121.4(7)	C65-C64-H64	119.7
C63-C64-H64	119.7	C63-C64-C65	120.6(7)
C8-C7-H7	120.0	C8-C7-C6	120.0(7)
C6-C7-H7	120.0	C5-C6-C7	120.7(7)
C5-C6-H6	119.7	C7-C6-H6	119.7
N2-B1-C16	112.1(5)	N2-B1-C10	104.0(5)
N2-B1-C22	110.0(5)	C16-B1-C22	103.2(5)
C10-B1-C16	114.4(5)	C10-B1-C22	113.3(5)
C66-C65-C64	121.2(7)	C66-C65-H65	119.4
C64-C65-H65	119.4	F24-C36-C35	119.5(7)
C37-C36-F24	119.1(7)	C37-C36-C35	121.4(7)
C50-C59-H59	107.6	C50-C59-C58	112.0(7)
C50-C59-C60	111.0(7)	C58-C59-H59	107.6
C58-C59-C60	110.8(7)	C60-C59-H59	107.6
F23-C37-C38	119.4(7)	C36-C37-F23	122.2(8)
C36-C37-C38	118.3(7)	C67-C68-H68A	109.5
C67-C68-H68B	109.5	C67-C68-H68C	109.5
H68A-C68-H68B	109.5	H68A-C68-H68C	109.5
H68B-C68-H68C	109.5	C76-C75-Au1	73.9(5)
C76-C75-C74	170.2(8)	C74-C75-Au1	115.9(6)
C62-C63-C64	120.9(7)	C62-C63-H63	119.5
C64-C63-H63	119.5	C75-C76-Au1	74.2(5)
C75-C76-C77	166.6(8)	C77-C76-Au1	119.2(5)
N1-B2-C40	109.0(5)	N1-B2-C28	112.0(5)
N1-B2-C34	103.8(5)	C28-B2-C40	102.0(5)
C28-B2-C34	117.1(5)	C34-B2-C40	112.9(5)
C53-C52-H52	119.4	C53-C52-C51	121.2(7)
C51-C52-H52	119.4	C54-C53-H53	119.5
C52-C53-C54	121.0(8)	C52-C53-H53	119.5
C70-C71-H71A	109.5	C70-C71-H71B	109.5
C70-C71-H71C	109.5	H71A-C71-H71B	109.5
H71A-C71-H71C	109.5	H71B-C71-H71C	109.5

C50-C51-H51	119.4	C52-C51-C50	121.3(7)
C52-C51-H51	119.4	C70-C72-H72A	109.5
C70-C72-H72B	109.5	C70-C72-H72C	109.5
H72A-C72-H72B	109.5	H72A-C72-H72C	109.5
H72B-C72-H72C	109.5	C67-C69-H69A	109.5
C67-C69-H69B	109.5	C67-C69-H69C	109.5
H69A-C69-H69B	109.5	H69A-C69-H69C	109.5
H69B-C69-H69C	109.5	C59-C58-H58A	109.5
C59-C58-H58B	109.5	C59-C58-H58C	109.5
H58A-C58-H58B	109.5	H58A-C58-H58C	109.5
H58B-C58-H58C	109.5	C55-C57-H57A	109.5
C55-C57-H57B	109.5	C55-C57-H57C	109.5
H57A-C57-H57B	109.5	H57A-C57-H57C	109.5
H57B-C57-H57C	109.5	C59-C60-H60A	109.5
C59-C60-H60B	109.5	C59-C60-H60C	109.5
H60A-C60-H60B	109.5	H60A-C60-H60C	109.5
H60B-C60-H60C	109.5	C55-C56-H56A	109.5
C55-C56-H56B	109.5	C55-C56-H56C	109.5
H56A-C56-H56B	109.5	H56A-C56-H56C	109.5
H56B-C56-H56C	109.5	H78A-C78-H78B	109.5
H78A-C78-H78C	109.5	H78B-C78-H78C	109.5
C77-C78-H78A	109.5	C77-C78-H78B	109.5
C77-C78-H78C	109.5	C76-C77-C78	113.2(9)
C76-C77-H77A	108.9	C76-C77-H77B	108.9
C78-C77-H77A	108.9	C78-C77-H77B	108.9
H77A-C77-H77B	107.7	Cl2-C79-Cl1	110.2(5)
Cl2-C79-H79A	109.6	Cl2-C79-H79B	109.6
Cl1-C79-H79A	109.6	Cl1-C79-H79B	109.6
H79A-C79-H79B	108.1	C75-C74-H74A	109.1
C75-C74-H74B	109.1	C75-C74-C73	112.3(8)
H74A-C74-H74B	107.9	C73-C74-H74A	109.1
C73-C74-H74B	109.1	C74-C73-H73A	109.5
C74-C73-H73B	109.5	C74-C73-H73C	109.5
H73A-C73-H73B	109.5	H73A-C73-H73C	109.5
H73B-C73-H73C	109.5		

Table 6. Anisotropic atomic displacement parameters (Å^2) for 5614.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au1	0.03828(16)	0.03220(15)	0.02398(13)	0.00651(12)	-0.00089(10)	0.00374(15)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl2	0.0753(18)	0.0498(16)	0.111(2)	-0.0038(14)	0.0148(15)	-0.0143(13)
Cl1	0.0524(15)	0.099(2)	0.094(2)	0.0320(16)	-0.0073(14)	0.0017(15)
F11	0.0205(19)	0.018(2)	0.036(2)	0.0004(15)	-0.0023(15)	-0.0008(15)
F15	0.031(2)	0.019(2)	0.036(2)	-0.0048(15)	0.0052(16)	-0.0051(17)
F30	0.034(2)	0.023(2)	0.0259(19)	0.0015(15)	0.0089(16)	0.0029(17)
F10	0.037(2)	0.030(2)	0.026(2)	0.0076(16)	0.0010(17)	0.0039(18)
F6	0.030(2)	0.025(2)	0.0251(19)	0.0055(15)	0.0026(16)	-0.0054(17)
F20	0.023(2)	0.026(2)	0.036(2)	0.0072(16)	0.0082(16)	0.0021(16)
F1	0.0187(19)	0.034(2)	0.032(2)	0.0038(16)	-0.0008(16)	0.0023(17)
F12	0.024(2)	0.032(2)	0.042(2)	0.0028(17)	-0.0049(17)	0.0044(18)
F27	0.034(2)	0.022(2)	0.040(2)	-0.0021(16)	0.0033(18)	0.0055(18)
F16	0.027(2)	0.036(2)	0.0274(18)	0.0021(17)	0.0058(15)	-0.0022(19)
F26	0.032(2)	0.021(2)	0.0265(19)	0.0008(15)	0.0039(16)	-0.0002(17)
F29	0.030(2)	0.030(2)	0.029(2)	0.0114(16)	0.0049(16)	0.0015(18)
F28	0.037(2)	0.018(2)	0.045(2)	0.0113(16)	-0.0020(18)	0.0075(18)
F19	0.023(2)	0.028(2)	0.060(3)	0.0021(19)	0.0120(19)	-0.0059(18)
F5	0.027(2)	0.039(2)	0.027(2)	0.0048(16)	0.0011(16)	0.0039(18)
F7	0.029(2)	0.022(2)	0.050(2)	0.0049(17)	0.0021(18)	-0.0109(17)
F25	0.031(2)	0.030(2)	0.039(2)	0.0003(16)	-0.0010(17)	0.0010(18)
F2	0.024(2)	0.038(3)	0.059(3)	0.010(2)	0.0036(19)	0.0045(19)
F21	0.034(2)	0.027(2)	0.050(2)	0.0093(18)	0.0136(19)	0.0109(18)
F9	0.050(3)	0.047(3)	0.025(2)	-0.0053(18)	-0.0063(18)	0.001(2)
F17	0.031(2)	0.054(3)	0.035(2)	0.0011(19)	-0.0021(18)	-0.008(2)
F4	0.047(3)	0.049(3)	0.034(2)	0.0009(19)	0.0173(19)	0.005(2)
F3	0.034(2)	0.038(2)	0.061(3)	0.002(2)	0.028(2)	0.006(2)
F14	0.039(2)	0.039(3)	0.046(2)	-0.0135(18)	-0.0042(19)	-0.015(2)
F8	0.041(3)	0.034(3)	0.051(3)	-0.0139(19)	-0.006(2)	-0.010(2)
F13	0.029(2)	0.054(3)	0.047(3)	-0.006(2)	-0.0140(19)	-0.003(2)
F24	0.063(3)	0.039(3)	0.048(3)	-0.010(2)	-0.009(2)	-0.015(2)
F22	0.069(3)	0.029(3)	0.068(3)	0.003(2)	0.032(3)	0.020(2)
F18	0.029(2)	0.053(3)	0.056(3)	-0.001(2)	-0.008(2)	-0.012(2)
F23	0.099(4)	0.030(3)	0.057(3)	-0.014(2)	0.019(3)	0.006(3)
N2	0.018(3)	0.013(3)	0.026(3)	0.002(2)	0.003(2)	0.005(2)
N1	0.023(3)	0.014(3)	0.025(3)	0.002(2)	0.002(2)	0.005(2)
N3	0.027(3)	0.018(3)	0.019(2)	0.001(2)	0.000(2)	0.001(3)
N4	0.027(3)	0.021(3)	0.019(3)	0.000(2)	0.001(2)	-0.002(2)
C43	0.013(3)	0.016(3)	0.042(4)	0.008(3)	-0.007(3)	0.002(3)
C4	0.023(3)	0.016(3)	0.026(3)	0.008(2)	0.012(3)	0.003(3)
C46	0.024(3)	0.025(4)	0.022(3)	0.004(2)	-0.001(3)	0.002(3)
C61	0.022(3)	0.020(4)	0.025(3)	-0.003(2)	-0.003(2)	-0.003(3)
C42	0.020(3)	0.016(3)	0.034(4)	-0.004(3)	0.001(3)	-0.003(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C3	0.015(3)	0.014(3)	0.031(3)	0.002(2)	0.004(3)	0.004(3)
C16	0.013(3)	0.019(3)	0.029(3)	0.004(2)	0.002(2)	0.001(3)
C66	0.034(4)	0.024(4)	0.023(3)	0.000(3)	0.001(3)	0.001(3)
C41	0.013(3)	0.024(4)	0.025(3)	0.002(3)	0.002(2)	-0.001(3)
C2	0.023(3)	0.017(3)	0.028(3)	0.003(3)	0.004(2)	0.012(3)
C30	0.025(4)	0.028(4)	0.028(4)	0.004(3)	-0.003(3)	0.001(3)
C10	0.011(3)	0.017(3)	0.027(3)	0.003(2)	0.004(2)	-0.004(2)
C47	0.028(4)	0.024(4)	0.029(4)	0.005(3)	0.007(3)	-0.001(3)
C1	0.020(3)	0.017(4)	0.031(3)	0.002(2)	0.007(3)	0.003(3)
C21	0.017(3)	0.022(4)	0.030(3)	0.005(3)	0.002(3)	0.002(3)
C40	0.017(3)	0.023(4)	0.023(3)	0.002(2)	0.002(3)	0.001(3)
C5	0.028(4)	0.024(4)	0.038(4)	0.011(3)	0.008(3)	0.002(3)
C17	0.021(3)	0.023(4)	0.025(3)	0.000(3)	0.001(3)	0.001(3)
C12	0.027(4)	0.031(4)	0.028(4)	-0.005(3)	-0.002(3)	-0.009(3)
C22	0.015(3)	0.017(3)	0.034(4)	0.003(3)	0.005(3)	-0.001(3)
C44	0.020(3)	0.024(4)	0.026(3)	0.005(3)	-0.001(3)	-0.001(3)
C24	0.019(3)	0.018(3)	0.028(3)	0.006(2)	0.002(3)	0.000(3)
C25	0.024(4)	0.014(3)	0.043(4)	0.008(3)	0.008(3)	-0.003(3)
C67	0.030(4)	0.027(4)	0.041(4)	-0.003(3)	0.006(3)	0.007(3)
C18	0.010(3)	0.020(4)	0.042(4)	0.004(3)	0.001(3)	-0.002(3)
C48	0.024(3)	0.021(4)	0.018(3)	0.002(2)	0.001(2)	0.002(3)
C45	0.017(3)	0.024(4)	0.028(3)	0.001(3)	0.002(3)	0.000(3)
C29	0.027(4)	0.019(3)	0.031(4)	0.006(3)	0.008(3)	0.005(3)
C11	0.025(4)	0.017(3)	0.031(3)	0.001(3)	0.006(3)	0.000(3)
C28	0.024(3)	0.012(3)	0.032(3)	0.005(2)	0.008(3)	0.002(3)
C14	0.021(3)	0.018(3)	0.033(4)	0.006(3)	0.002(3)	0.005(3)
C8	0.044(5)	0.018(4)	0.049(4)	0.003(3)	0.017(4)	0.006(3)
C13	0.022(4)	0.039(4)	0.029(4)	0.004(3)	-0.009(3)	-0.003(3)
C34	0.029(4)	0.019(4)	0.027(3)	0.011(3)	0.012(3)	0.003(3)
C15	0.033(4)	0.014(3)	0.022(3)	0.001(2)	0.001(3)	-0.008(3)
C20	0.027(4)	0.034(4)	0.028(4)	-0.003(3)	-0.003(3)	-0.001(3)
C9	0.022(4)	0.023(4)	0.041(4)	0.007(3)	0.007(3)	0.000(3)
C19	0.023(4)	0.028(4)	0.040(4)	-0.006(3)	0.000(3)	-0.009(3)
C33	0.022(3)	0.016(3)	0.036(4)	0.007(3)	0.004(3)	0.003(3)
C32	0.016(3)	0.021(4)	0.049(4)	0.004(3)	0.011(3)	0.003(3)
C38	0.048(5)	0.014(4)	0.043(4)	0.005(3)	0.023(4)	0.009(3)
C31	0.020(4)	0.030(4)	0.049(4)	0.004(3)	-0.002(3)	-0.007(3)
C55	0.026(4)	0.029(4)	0.034(4)	-0.003(3)	0.011(3)	-0.004(3)
C70	0.031(4)	0.023(4)	0.048(4)	-0.003(3)	0.005(3)	-0.005(3)
C39	0.031(4)	0.026(4)	0.034(4)	0.006(3)	0.010(3)	-0.001(3)
C27	0.036(4)	0.021(4)	0.035(4)	0.001(3)	0.018(3)	0.002(3)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C49	0.024(4)	0.032(4)	0.020(3)	0.000(3)	-0.001(3)	-0.004(3)
C54	0.038(4)	0.033(4)	0.029(4)	-0.003(3)	0.003(3)	-0.012(3)
C62	0.032(4)	0.020(4)	0.035(4)	0.001(3)	0.004(3)	0.001(3)
C35	0.034(4)	0.025(4)	0.027(4)	0.002(3)	0.007(3)	0.003(3)
C26	0.025(4)	0.013(3)	0.052(4)	0.003(3)	0.019(3)	0.005(3)
C23	0.027(4)	0.011(3)	0.039(4)	0.006(3)	0.003(3)	0.000(3)
C50	0.024(4)	0.059(5)	0.026(4)	-0.006(3)	0.004(3)	-0.008(4)
C64	0.047(5)	0.025(4)	0.056(5)	-0.004(3)	-0.004(4)	-0.009(4)
C7	0.034(4)	0.034(5)	0.054(5)	0.015(4)	0.020(4)	0.018(4)
C6	0.026(4)	0.036(4)	0.045(4)	0.019(3)	0.012(3)	0.014(3)
B1	0.021(4)	0.018(4)	0.027(4)	0.003(3)	0.002(3)	0.003(3)
C65	0.038(5)	0.028(4)	0.043(4)	-0.010(3)	0.005(3)	0.000(3)
C36	0.057(5)	0.023(4)	0.034(4)	0.003(3)	0.006(4)	-0.008(4)
C59	0.018(4)	0.060(5)	0.043(4)	-0.004(4)	0.001(3)	0.002(4)
C37	0.068(6)	0.020(4)	0.039(4)	-0.004(3)	0.019(4)	-0.002(4)
C68	0.041(5)	0.052(5)	0.043(4)	-0.009(4)	0.005(4)	0.018(4)
C75	0.051(5)	0.070(6)	0.022(4)	0.011(4)	0.003(4)	0.014(5)
C63	0.034(4)	0.034(5)	0.060(5)	-0.005(4)	0.005(4)	-0.002(4)
C76	0.055(6)	0.055(6)	0.035(5)	0.031(4)	0.001(4)	0.009(5)
B2	0.027(4)	0.020(4)	0.026(4)	0.008(3)	0.005(3)	0.003(3)
C52	0.046(5)	0.087(7)	0.037(5)	-0.023(4)	0.004(4)	-0.027(5)
C53	0.048(5)	0.056(6)	0.036(4)	-0.014(4)	0.012(4)	-0.020(4)
C71	0.096(8)	0.063(6)	0.039(5)	-0.004(4)	0.023(5)	0.007(6)
C51	0.029(4)	0.092(7)	0.044(5)	-0.016(5)	0.002(4)	-0.022(5)
C72	0.061(6)	0.072(7)	0.060(6)	-0.008(5)	0.006(5)	0.035(5)
C69	0.035(5)	0.076(7)	0.044(5)	0.004(4)	-0.003(4)	0.015(4)
C58	0.044(5)	0.089(8)	0.061(6)	0.002(5)	0.008(4)	0.009(5)
C57	0.050(5)	0.045(5)	0.063(6)	0.004(4)	0.023(4)	-0.007(4)
C60	0.047(5)	0.076(7)	0.045(5)	-0.001(4)	0.015(4)	0.001(5)
C56	0.063(6)	0.046(6)	0.080(7)	-0.003(5)	0.024(5)	0.008(5)
C78	0.114(10)	0.048(6)	0.067(7)	0.000(5)	0.024(6)	-0.014(6)
C77	0.118(9)	0.039(6)	0.055(6)	0.016(4)	0.002(6)	0.008(6)
C79	0.055(6)	0.036(5)	0.090(7)	-0.010(5)	0.003(5)	-0.004(4)
C74	0.072(7)	0.086(7)	0.031(4)	0.016(5)	-0.001(4)	0.018(6)
C73	0.035(5)	0.156(11)	0.056(6)	-0.052(7)	0.000(4)	-0.007(7)

Table 7. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 5614.

	x/a	y/b	z/c	U(eq)
H2	0.1538	0.8236	0.7073	0.027

	x/a	y/b	z/c	U(eq)
H47	0.7639	0.9314	0.4545	0.032
H1	0.0468	0.7489	0.7478	0.027
H5	0.4676	0.6656	0.7639	0.036
H67	0.8375	0.7249	0.4258	0.039
H48	0.6659	0.8386	0.4138	0.026
H8	0.3768	0.4770	0.6796	0.043
H9	0.2516	0.5660	0.6828	0.034
H55	0.6414	0.9157	0.5268	0.035
H70	0.5381	0.7936	0.4959	0.041
H64	0.4991	0.5535	0.4193	0.052
H7	0.5472	0.4816	0.7184	0.048
H6	0.5916	0.5754	0.7609	0.042
H65	0.6787	0.5706	0.4052	0.044
H59	0.9701	0.8267	0.4864	0.049
H68A	0.8369	0.6014	0.3794	0.068
H68B	0.9135	0.6678	0.3758	0.068
H68C	0.7836	0.6722	0.3616	0.068
H63	0.4133	0.6343	0.4564	0.051
H52	1.0068	0.9803	0.6180	0.068
H53	0.8187	0.9900	0.6086	0.055
H71A	0.4034	0.6862	0.5217	0.097
H71B	0.4340	0.7569	0.5451	0.097
H71C	0.5278	0.7003	0.5411	0.097
H51	1.1001	0.9171	0.5742	0.066
H72A	0.3974	0.8089	0.4431	0.097
H72B	0.3468	0.8162	0.4848	0.097
H72C	0.3284	0.7465	0.4592	0.097
H69A	0.8855	0.6521	0.4820	0.078
H69B	0.9760	0.6477	0.4512	0.078
H69C	0.8875	0.5869	0.4527	0.078
H58A	1.1490	0.8058	0.5485	0.097
H58B	1.1321	0.7632	0.5073	0.097
H58C	1.0450	0.7554	0.5391	0.097
H57A	0.6342	0.8467	0.5824	0.078
H57B	0.5399	0.9041	0.5834	0.078
H57C	0.6538	0.9112	0.6122	0.078
H60A	1.0548	0.9332	0.4732	0.083
H60B	1.1324	0.8694	0.4649	0.083
H60C	1.1585	0.9140	0.5051	0.083
H56A	0.6545	1.0337	0.5778	0.092
H56B	0.5505	1.0133	0.5463	0.092

	x/a	y/b	z/c	U(eq)
H56C	0.6641	1.0361	0.5307	0.092
H78A	0.7000	0.5795	0.5124	0.113
H78B	0.6443	0.5484	0.5494	0.113
H78C	0.7111	0.4989	0.5226	0.113
H77A	0.8230	0.5217	0.5816	0.086
H77B	0.8754	0.5581	0.5455	0.086
H79A	0.3581	0.8420	0.8677	0.073
H79B	0.2518	0.8367	0.8347	0.073
H74A	0.8350	0.6935	0.6661	0.076
H74B	0.7499	0.7450	0.6412	0.076
H73A	0.8943	0.8038	0.6168	0.124
H73B	0.9820	0.7491	0.6372	0.124
H73C	0.9198	0.8002	0.6646	0.124