Electronic Supplementary Material (ESI) for Dalton Transactions

Isolated Cationic Crown Ether Complexes of Gallium(I) and Indium(I)

Electronic supplementary information

Alexander Higelin, Christoph Haber, Stefan Meier and Ingo Krossing*

Prof. Dr. Ingo Krossing
Albert-Ludwigs-Universität Freiburg
Institut für Anorganische und Analytische Chemie,
Freiburger Materialforschungszentrum FMF
and Freiburg Institute for Advanced Studies FRIAS,
Section Soft Matter Science
Albertstr. 21
79104 Freiburg (Germany)
E-mail: krossing@uni-freiburg.de

Table of Contents

1. Quantum-chemical Data

1.1.Summary of the quantum chemical calculations:

(all values are given in hartrees)

	BP86/SV(P)		B3LYP/def2-TZVPP	
	E_{SCF}	E_{vib}	E_{SCF}	E_{vib}
C_6H_5F	-331.2468254861	0.0899754	-331.4366174934	0.0921416
[18]crown-6	-922.2902973818	0.3579634	-921.7179252771	0.3696215
$Ga(C_6H_5F)_2^+$	-2587.180000953	0.1817305	-2587.452007032	0.1863278
$In(C_6H_5F)_2^+$	-664.2152353733	0.1816597	-852.8230095832	0.1861753
$Ga([18]crown-6)^+$	-2847.049937786	0.3598534	-2847.476032561	0.3690519
$In([18]crown-6)^+$	-924.0891462864	0.3598441	-1112.845322211	

1.2.Fluorobenzene

Optimized atomic coordinates from the DFT (BP86/SV(P)) calculations (Bohr Units):

1.36139080546022	2.27246909180221	0.00000000000000	C
-1.28730257706180	2.23049810184745	0.00000000000000	C
2.67471686252994	-0.03565663632939	0.00000000000000	C
-2.64759748495706	-0.04236067117896	0.00000000000000	C
1.35082383061929	-2.34002939349849	0.00000000000000	C
-1.30674391785547	-2.33410653791926	0.00000000000000	C
2.35493041129814	4.10113475177969	0.00000000000000	H
-2.56501321153211	4.43674255753021	0.00000000000000	F
4.75820839919794	-0.02653944675203	0.00000000000000	H
-4.72774879052731	0.01444660646626	0.00000000000000	H
2.39207326137873	-4.14344734808886	0.00000000000000	H
-2.35773758855049	-4.13315107565886	0.00000000000000	H

List of calculated frequencies (BP86/SV(P)):

mode	symmetry	wave number	IR intensity	selection rules	
		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a"	234.29	0.03373	YES	YES
8	a'	399.20	1.70770	YES	YES
9	a"	412.85	0.00011	YES	YES
10	a"	500.90	7.65925	YES	YES
11	a'	509.35	3.65119	YES	YES
12	a'	605.85	0.12545	YES	YES
13	a"	682.06	16.63510	YES	YES

14	a"	747.79	56.87969	YES	YES
15	a"	807.32	0.00024	YES	YES
16	a'	808.11	19.99457	YES	YES
17	a"	884.40	7.60111	YES	YES
18	a"	943.52	0.00046	YES	YES
19	a"	969.12	0.17721	YES	YES
20	a'	987.54	0.12498	YES	YES
21	a'	1015.49	3.19233	YES	YES
22	a'	1059.76	8.61591	YES	YES
23	a'	1135.87	6.85271	YES	YES
24	a'	1137.59	0.13099	YES	YES
25	a'	1247.45	83.12963	YES	YES
26	a'	1283.36	0.47471	YES	YES
27	a'	1375.22	0.17022	YES	YES
28	a'	1450.35	0.60525	YES	YES
29	a'	1494.35	81.28575	YES	YES
30	a'	1613.50	9.67932	YES	YES
31	a'	1618.79	50.66334	YES	YES
32	a'	3095.76	0.26766	YES	YES
33	a'	3104.32	9.20949	YES	YES
34	a'	3116.60	16.95441	YES	YES
35	a'	3126.03	5.39480	YES	YES
36	a'	3127.88	0.13977	YES	YES

Optimized atomic coordinates from the DFT (B3LYP/TZVPP) calculations (Bohr Units):

1.34891272142885	2.24901509406438	0.00000000000000	c
-1.26612382354869	2.19374048938239	0.00000000000000	c
2.64807902096738	-0.03663469255952	0.00000000000000	c
-2.62135496338878	-0.04330323291186	0.00000000000000	c
1.33657386628921	-2.31539034733319	0.00000000000000	c
-1.29267231547853	-2.31163056676294	0.00000000000000	c
2.32580853650981	4.04329113564889	0.00000000000000	h
-2.54514761027895	4.40482899998468	0.00000000000000	f
4.69265372380221	-0.02987351914260	0.00000000000000	h
-4.66351135988107	0.00979493295404	0.00000000000000	h
2.35855189743209	-4.08539782057987	0.00000000000000	h
-2.32176969385355	-4.07844047274443	0.00000000000000	h

List of calculated frequencies (B3LYP/TZVPP):

# mode	symmetry	wave number	IR intensity	selection rules	
#		cm**(-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a"	238.93	0.06176	YES	YES
8	a'	406.52	1.96582	YES	YES
9	a"	424.94	0.00005	YES	YES

10	a''	512.16	10.44414	YES	YES
11	a'	526.34	5.41804	YES	YES
12	a'	629.06	0.18756	YES	YES
13	a''	697.78	18.17457	YES	YES
14	a''	770.59	70.05373	YES	YES
15	a'	825.15	26.41801	YES	YES
16	a''	836.87	0.00011	YES	YES
17	a''	915.73	7.48859	YES	YES
18	a''	979.19	0.00026	YES	YES
19	a''	993.12	0.02928	YES	YES
20	a'	1023.26	0.23169	YES	YES
21	a'	1041.04	3.73447	YES	YES
22	a'	1091.85	7.03309	YES	YES
23	a'	1177.95	13.24004	YES	YES
24	a'	1180.65	0.24210	YES	YES
25	a'	1248.34	102.18213	YES	YES
26	a'	1326.49	0.27367	YES	YES
27	a'	1347.61	0.48805	YES	YES
28	a'	1491.96	1.21664	YES	YES
29	a'	1529.52	77.84539	YES	YES
30	a'	1636.52	48.03987	YES	YES
31	a'	1643.40	9.16900	YES	YES
32	a'	3171.97	0.10580	YES	YES
33	a'	3180.79	8.47061	YES	YES
34	a'	3192.67	15.83117	YES	YES
35	a'	3201.44	5.03671	YES	YES
36	a'	3203.60	0.27007	YES	YES

1.3.[18]crown-6 ether

Optimized atomic coordinates from the DFT (BP86/SV(P)) calculations (Bohr Units):

-6.26950248544884	0.86624585292064	0.30878970339939	c
-6.64971094660926	2.91880869812319	1.99942154294734	o
-4.62348493109295	4.61114529255000	2.42043023708800	c
-3.71156241752441	6.09434114368993	0.09274127660432	c
-2.10072689823947	4.71149141772246	-1.55768343913436	o
0.48009940286282	4.72980392463661	-0.84464898640626	c
1.88577172360356	2.87389345607649	-2.54577543375388	c
4.47199374135619	2.91165182244835	-1.81495019947330	o
6.04916652404824	1.21601458716156	-3.14663622883675	c
5.82192977820737	-1.54838691615863	-2.32286981498192	c
3.58340626680267	-2.60214743121371	-3.34626451018610	o
3.09631784293247	-5.15619243250002	-2.73979433816795	c
2.55020202165807	-5.69187583294799	0.05368073831888	c
0.66246431917625	-4.02574803692820	0.92551588348127	o
-0.22287472127408	-4.57697963703803	3.39225273544356	c
-1.74666828965933	-2.34930799610661	4.42649973449229	c
-4.09142207752732	-1.89983257700581	3.24848263102890	o
-3.96320683464899	-0.79248125787073	0.80189104076257	c
-6.13383691830456	1.52763205151261	-1.69519853233766	h

-8.01368858882626	-0.29146535517934	0.48932845900623	h
-2.97988282263418	3.64898690376952	3.34292160277854	h
-5.37479325760959	5.99139248597881	3.81867315575616	h
-5.39011834575377	6.65786597107458	-1.04287569718508	h
-2.74665757471015	7.86613961631486	0.73467391895244	h
1.30278443110376	6.67177888830975	-1.04112912466316	h
0.75273867429166	4.13719953647470	1.16700925521720	h
1.66601480157402	3.44941073495936	-4.57066995312830	h
1.06588876804427	0.94831604433701	-2.33624174627122	h
8.01788374650409	1.84819760205278	-2.76532173537982	h
5.71109595675944	1.33631664289560	-5.23283000576841	h
5.82440176138105	-1.61071256964237	-0.21175945352576	h
7.52210936205013	-2.62122638732016	-3.00637477768495	h
4.70126924566109	-6.40539052183775	-3.34336695237832	h
1.40807912297498	-5.67178641830319	-3.87717638576007	h
4.30137966709301	-5.49850702502949	1.23263096279999	h
1.94047573039363	-7.71683393674935	0.21000088591440	h
1.40650560662952	-4.92545806658521	4.70501290651165	h
-1.41662483471744	-6.32636806801331	3.38139450394472	h
-2.17808950586860	-2.74902239422303	6.44649662449173	h
-0.52226808481944	-0.62109358912244	4.35207421332770	h
-2.20040974538892	0.33610137968016	0.59495580524367	h
-3.88644921445109	-2.27191760291401	-0.70331050248821	h

List of calculated frequencies (BP86/SV(P)):

# mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	34.54	0.34198	YES	YES
8	a	42.03	0.09582	YES	YES
9	a	49.76	0.52077	YES	YES
10	a	67.51	0.83788	YES	YES
11	a	75.89	1.12223	YES	YES
12	a	81.86	0.49931	YES	YES
13	a	96.75	2.22959	YES	YES
14	a	112.10	3.61223	YES	YES
15	a	123.74	4.93874	YES	YES
16	a	149.99	1.88105	YES	YES
17	a	162.95	5.01268	YES	YES
18	a	174.93	8.80121	YES	YES
19	a	176.71	2.84479	YES	YES
20	a	207.61	1.86576	YES	YES
21	a	238.27	6.60101	YES	YES
22	a	261.71	4.04602	YES	YES
23	a	274.11	1.47660	YES	YES
24	a	298.56	2.32595	YES	YES

25	a	306.91	0.13757	YES	YES
26	a	348.50	3.41290	YES	YES
27	a	357.36	1.07557	YES	YES
28	a	362.25	0.97076	YES	YES
29	a	383.25	2.41355	YES	YES
30	a	411.07	0.07676	YES	YES
31	a	472.17	0.98854	YES	YES
32	a	497.24	15.97549	YES	YES
33	a	513.37	2.35206	YES	YES
34	a	519.55	5.72072	YES	YES
35	a	570.30	8.93985	YES	YES
36	a	580.17	10.74387	YES	YES
37	a	782.18	5.97870	YES	YES
38	a	793.21	0.42214	YES	YES
39	a	808.90	2.79263	YES	YES
40	a	813.74	7.51873	YES	YES
41	a	828.47	12.87138	YES	YES
42	a	859.33	25.62243	YES	YES
43	a	872.50	7.92006	YES	YES
44	a	892.93	11.65044	YES	YES
45	a	901.29	19.62515	YES	YES
46	a	920.84	28.63128	YES	YES
47	a	934.45	36.91442	YES	YES
48	a	989.61	45.50145	YES	YES
49	a	998.53	1.39806	YES	YES
50	a	1016.48	17.49877	YES	YES
51	a	1031.23	23.00334	YES	YES
52	a	1040.89	17.37027	YES	YES
53	a	1055.34	32.84177	YES	YES
54	a	1057.59	20.14842	YES	YES
55	a	1082.48	1.51550	YES	YES
56	a	1088.11	26.31246	YES	YES
57	a	1100.31	7.81868	YES	YES
58	a	1117.09	11.95382	YES	YES
59	a	1117.46	45.31711	YES	YES
60	a	1127.49	2.80856	YES	YES
61	a	1130.88	137.83971	YES	YES
62	a	1139.26	43.88292	YES	YES
63	a	1154.82	192.81568	YES	YES
64	a	1156.07	247.29901	YES	YES
65	a	1159.70	78.94670	YES	YES
66	a	1174.82	97.64256	YES	YES
67	a	1197.25	8.86761	YES	YES
68	a	1225.96	23.04408	YES	YES
69	a	1229.55	2.60312	YES	YES
70	a	1238.51	8.74697	YES	YES
71	a	1246.19	30.84934	YES	YES
72	a	1247.80	43.15672	YES	YES
73	a	1257.69	26.02519	YES	YES
74	a	1272.22	4.54934	YES	YES
75	a	1280.96	28.64111	YES	YES
76	a	1290.35	27.41823	YES	YES
77	a	1298.99	34.60730	YES	YES

78	a	1303.29	7.72116	YES	YES
79	a	1328.10	6.82133	YES	YES
80	a	1336.11	46.42053	YES	YES
81	a	1344.26	18.72455	YES	YES
82	a	1354.25	23.43831	YES	YES
83	a	1357.56	13.47612	YES	YES
84	a	1368.07	20.90548	YES	YES
85	a	1374.71	6.70172	YES	YES
86	a	1377.34	6.08614	YES	YES
87	a	1383.09	4.89355	YES	YES
88	a	1385.69	9.49288	YES	YES
89	a	1397.76	3.53014	YES	YES
90	a	1404.14	2.78370	YES	YES
91	a	1412.11	12.14339	YES	YES
92	a	1419.04	1.47795	YES	YES
93	a	1420.38	6.82785	YES	YES
94	a	1422.19	3.68634	YES	YES
95	a	1427.08	5.66506	YES	YES
96	a	1431.07	7.77009	YES	YES
97	a	1440.51	13.92669	YES	YES
98	a	1451.37	4.76367	YES	YES
99	a	1456.53	14.11985	YES	YES
100	a	1470.26	1.80000	YES	YES
101	a	1473.53	1.56698	YES	YES
102	a	1480.00	4.87732	YES	YES
103	a	2852.99	18.16933	YES	YES
104	a	2854.32	36.06683	YES	YES
105	a	2862.70	52.53706	YES	YES
106	a	2872.34	155.22682	YES	YES
107	a	2873.65	4.97102	YES	YES
108	a	2874.35	65.19424	YES	YES
109	a	2884.96	65.52497	YES	YES
110	a	2890.08	27.11976	YES	YES
111	a	2891.86	110.24014	YES	YES
112	a	2892.02	75.63505	YES	YES
113	a	2893.86	53.87535	YES	YES
114	a	2904.04	11.64879	YES	YES
115	a	2912.21	56.59625	YES	YES
116	a	2920.09	59.78632	YES	YES
117	a	2923.77	55.83973	YES	YES
118	a	2936.97	57.93441	YES	YES
119	a	2986.85	14.49728	YES	YES
120	a	2988.64	29.03319	YES	YES
121	a	2993.52	50.71366	YES	YES
122	a	2994.94	24.75717	YES	YES
123	a	2996.28	32.36437	YES	YES
124	a	3000.63	36.37844	YES	YES
125	a	3010.56	46.17818	YES	YES
126	a	3015.02	24.39113	YES	YES

Optimized atomic coordinates from the DFT (B3LYP/TZVPP) calculations (Bohr Units):

-6.20512996928068	0.85722369842209	0.27101107973335	c
-6.58526068606560	2.88617703948955	1.96837161713849	o

-4.59638173291854	4.59103791715467	2.42689460751557	c
-3.69081746326448	6.10415839471114	0.12660197636102	c
-2.09045216411129	4.74660587634801	-1.53101633280916	o
0.48974517084656	4.74975472236744	-0.86807132989011	c
1.86621952489711	2.92737440309165	-2.61509654791317	c
4.43592409941199	2.90121493957963	-1.87629987417869	o
6.01255349967661	1.21093613409059	-3.18905433716719	c
5.80169176790235	-1.53279326866586	-2.32263691475969	c
3.55565349525208	-2.59748869878272	-3.27770308560770	o
3.07750952710504	-5.14140827584311	-2.68356743103353	c
2.56071413115203	-5.68461230396698	0.10602050449248	c
0.68366608325710	-4.03799785002905	0.99700673025812	o
-0.24232526035890	-4.60413928692528	3.42990855176109	c
-1.78891553058106	-2.39237620395508	4.44170860950115	c
-4.08192539919431	-1.93914962465036	3.19489493845689	o
-3.91754759504736	-0.81274354734019	0.77412345071947	c
-6.05180008808239	1.53625592903091	-1.70675019575462	h
-7.93887058852754	-0.29150719414711	0.42482810941412	h
-2.96358644895515	3.64364174953938	3.34229525308578	h
-5.36641438410685	5.94072998639868	3.82128745495115	h
-5.35866814463908	6.68258963557193	-0.98725976585797	h
-2.72861170849400	7.84837664152156	0.78974630473216	h
1.30277394651351	6.67800538700979	-1.04487683989524	h
0.79048160195050	4.12669732941114	1.11107359643467	h
1.66936035174230	3.56204865151765	-4.60637428970833	h
1.01932838241441	1.02819160623462	-2.46432075097520	h
7.96656450149873	1.85286400693683	-2.83309228415618	h
5.66205617937818	1.30038789180751	-5.25641510939993	h
5.84379594935035	-1.56660158224135	-0.22826020506783	h
7.47235786476113	-2.60633137399758	-3.02225183638878	h
4.66603403240663	-6.37213841949582	-3.30637546184520	h
1.38947500237140	-5.65507115928027	-3.79313361583266	h
4.30653507093791	-5.48707184621599	1.25940102598387	h
1.95908301415183	-7.69343420215305	0.26129830435456	h
1.34908482006099	-4.95489334468274	4.75972338041465	h
-1.42442736942779	-6.33982929658766	3.38019330645793	h
-2.27796085812915	-2.80789814072878	6.42871448209734	h
-0.57571882601590	-0.67688784443128	4.42156062398378	h
-2.15834741702532	0.29148215632719	0.60279697106174	h
-3.83744638281353	-2.27138063244160	-0.72690467066841	h

List of calculated frequencies (B3LYP/TZVPP):

# mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	35.78	0.33149	YES	YES
8	a	47.34	0.06481	YES	YES

9	a	52.28	0.41477	YES	YES
10	a	69.91	0.92235	YES	YES
11	a	78.12	1.32664	YES	YES
12	a	86.84	0.62972	YES	YES
13	a	97.09	3.02059	YES	YES
14	a	115.84	3.38509	YES	YES
15	a	127.67	5.24421	YES	YES
16	a	156.02	2.02774	YES	YES
17	a	168.88	5.75403	YES	YES
18	a	180.55	9.82884	YES	YES
19	a	181.28	2.19762	YES	YES
20	a	213.29	2.18389	YES	YES
21	a	246.63	7.88050	YES	YES
22	a	269.96	4.30651	YES	YES
23	a	281.45	1.75651	YES	YES
24	a	306.59	2.36811	YES	YES
25	a	316.68	0.05494	YES	YES
26	a	359.15	3.50239	YES	YES
27	a	368.99	1.04542	YES	YES
28	a	374.79	1.34766	YES	YES
29	a	394.58	2.72691	YES	YES
30	a	422.83	0.14745	YES	YES
31	a	488.21	0.85263	YES	YES
32	a	515.28	17.08768	YES	YES
33	a	529.95	3.19580	YES	YES
34	a	534.70	6.14580	YES	YES
35	a	586.44	9.36506	YES	YES
36	a	597.50	12.10547	YES	YES
37	a	805.65	6.37070	YES	YES
38	a	818.90	0.56151	YES	YES
39	a	836.80	4.26156	YES	YES
40	a	839.48	8.16001	YES	YES
41	a	855.81	13.80410	YES	YES
42	a	885.99	27.94921	YES	YES
43	a	899.41	9.62925	YES	YES
44	a	923.43	15.86034	YES	YES
45	a	929.87	19.34832	YES	YES
46	a	953.78	31.96730	YES	YES
47	a	963.62	38.82066	YES	YES
48	a	1020.96	50.84890	YES	YES
49	a	1031.16	0.84920	YES	YES
50	a	1051.11	21.39657	YES	YES
51	a	1062.91	19.25609	YES	YES
52	a	1074.61	18.95457	YES	YES
53	a	1089.07	22.54802	YES	YES
54	a	1093.18	34.58191	YES	YES
55	a	1119.77	1.65627	YES	YES
56	a	1126.23	30.90919	YES	YES
57	a	1137.71	6.72522	YES	YES
58	a	1156.19	9.63024	YES	YES
59	a	1159.74	33.70442	YES	YES

60	a	1168.02	2.67611	YES	YES
61	a	1173.10	125.20093	YES	YES
62	a	1179.79	54.77810	YES	YES
63	a	1198.16	290.50333	YES	YES
64	a	1201.61	177.68758	YES	YES
65	a	1204.68	91.58495	YES	YES
66	a	1219.53	91.17060	YES	YES
67	a	1241.41	8.31287	YES	YES
68	a	1271.02	22.84402	YES	YES
69	a	1274.00	3.47085	YES	YES
70	a	1285.22	11.26834	YES	YES
71	a	1293.19	34.76247	YES	YES
72	a	1296.71	47.09419	YES	YES
73	a	1304.72	29.16991	YES	YES
74	a	1317.38	7.04941	YES	YES
75	a	1326.15	26.52728	YES	YES
76	a	1336.27	42.74520	YES	YES
77	a	1344.50	37.80384	YES	YES
78	a	1347.65	10.82561	YES	YES
79	a	1376.33	10.78246	YES	YES
80	a	1389.13	54.74222	YES	YES
81	a	1396.21	31.65167	YES	YES
82	a	1406.46	34.47195	YES	YES
83	a	1409.21	10.26782	YES	YES
84	a	1420.46	23.05627	YES	YES
85	a	1425.48	11.02768	YES	YES
86	a	1429.16	3.16059	YES	YES
87	a	1436.34	5.00476	YES	YES
88	a	1438.05	8.22595	YES	YES
89	a	1452.59	3.90378	YES	YES
90	a	1455.99	2.46823	YES	YES
91	a	1466.00	12.60196	YES	YES
92	a	1469.61	5.48814	YES	YES
93	a	1470.60	1.43649	YES	YES
94	a	1475.28	3.95863	YES	YES
95	a	1480.01	4.83929	YES	YES
96	a	1481.64	5.19303	YES	YES
97	a	1490.32	13.11846	YES	YES
98	a	1499.69	4.78221	YES	YES
99	a	1509.00	11.83774	YES	YES
100	a	1517.77	1.55518	YES	YES
101	a	1520.44	1.24754	YES	YES
102	a	1527.31	4.64750	YES	YES
103	a	2940.70	13.02609	YES	YES
104	a	2941.61	29.89065	YES	YES
105	a	2949.90	46.05800	YES	YES
106	a	2960.36	171.06594	YES	YES
107	a	2962.44	7.53883	YES	YES
108	a	2963.50	26.08794	YES	YES
109	a	2972.86	58.84622	YES	YES
110	a	2975.75	27.61233	YES	YES

111	a	2981.02	76.89981	YES	YES
112	a	2982.13	53.03169	YES	YES
113	a	2983.25	76.93931	YES	YES
114	a	2992.16	8.80885	YES	YES
115	a	2997.64	63.00054	YES	YES
116	a	3010.70	49.05224	YES	YES
117	a	3011.11	67.48237	YES	YES
118	a	3021.18	62.71819	YES	YES
119	a	3064.62	41.08379	YES	YES
120	a	3069.72	44.45686	YES	YES
121	a	3073.78	64.71315	YES	YES
122	a	3074.02	12.63052	YES	YES
123	a	3077.55	2.02161	YES	YES
124	a	3088.08	48.74935	YES	YES
125	a	3090.19	25.79885	YES	YES
126	a	3094.63	36.87228	YES	YES

1.4. $Ga(C_6H_5F)_2^+$

Optimized atomic coordinates from the DFT (BP86/SV(P)) calculations (Bohr Units):

5.01464239860959	-1.29613313024807	-1.81898898344002	c
3.96222673426974	0.71401883039194	-3.21873656450225	c
3.66333396322131	3.12336701489755	-2.11016054496734	c
4.43995297663052	3.52207066577138	0.41228868691652	c
5.50687503173257	1.53815665350423	1.82929563473376	c
5.80231888481137	-0.84618782395606	0.68498119772346	c
2.88028929062839	4.69839816514591	-3.22290241665645	h
3.40692635847744	0.39690355525456	-5.20105439676464	h
5.30345480550166	-3.18048047305963	-2.65472188933574	h
4.23635259998424	5.40361816996947	1.28183503391135	h
6.15356598934639	1.81686492946910	3.78770676670408	h
6.84750871445013	-2.72302026441370	1.99645826120718	f
-3.86220464746969	-3.27060152173032	-1.91413800152780	c
-4.02480512841833	-0.91709779057988	-3.16071028436385	c
-4.93158760936907	1.23443943934049	-1.87318517943338	c
-5.71168065286452	0.98416271769010	0.66109526605340	c
-5.55802135757568	-1.34478454565691	1.93839651367488	c
-4.63493772275672	-3.47150115076779	0.63270576947711	c
-6.19842555405484	-1.46777219752173	3.91473416368250	h
-4.54036004084843	-5.30839152394765	1.60956795852829	h
-3.18875996946631	-4.95349838153622	-2.93706472347070	h
-3.47191080039997	-0.75327799398317	-5.16213715794069	h
-5.11338230119785	3.08003304454484	-2.81815314663615	h
-6.60732616764953	3.00046882752307	1.87349028688092	f
-0.00023270301180	-0.06655077560782	0.47769093424378	ga

List of calculated frequencies (BP86/SV(P)):

# mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-

2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	5.99	0.71031	YES	YES
8	a	11.29	0.77824	YES	YES
9	a	20.67	0.19781	YES	YES
10	a	58.17	0.15841	YES	YES
11	a	77.87	3.04076	YES	YES
12	a	95.31	0.47229	YES	YES
13	a	103.24	5.93315	YES	YES
14	a	122.03	53.47025	YES	YES
15	a	124.63	22.58805	YES	YES
16	a	232.47	0.68788	YES	YES
17	a	234.19	0.01547	YES	YES
18	a	385.71	0.11593	YES	YES
19	a	386.95	0.27010	YES	YES
20	a	403.80	1.92233	YES	YES
21	a	404.08	2.32719	YES	YES
22	a	492.07	17.53766	YES	YES
23	a	492.79	1.94194	YES	YES
24	a	508.18	4.25488	YES	YES
25	a	508.55	3.78657	YES	YES
26	a	597.64	0.05921	YES	YES
27	a	598.07	0.20611	YES	YES
28	a	659.27	8.65224	YES	YES
29	a	659.65	8.74641	YES	YES
30	a	774.85	190.01939	YES	YES
31	a	778.76	19.83890	YES	YES
32	a	809.67	19.06265	YES	YES
33	a	809.94	8.51291	YES	YES
34	a	843.01	1.20227	YES	YES
35	a	843.31	0.97259	YES	YES
36	a	902.48	0.51811	YES	YES
37	a	904.02	9.61933	YES	YES
38	a	963.17	0.00172	YES	YES
39	a	965.46	0.16974	YES	YES
40	a	978.41	2.83327	YES	YES
41	a	979.42	1.47511	YES	YES
42	a	984.59	1.59291	YES	YES
43	a	986.01	0.33823	YES	YES
44	a	1008.10	7.17340	YES	YES
45	a	1008.79	1.42062	YES	YES
46	a	1058.02	4.07383	YES	YES
47	a	1058.35	5.18765	YES	YES
48	a	1138.78	1.51237	YES	YES
49	a	1140.50	9.12239	YES	YES
50	a	1143.24	1.55596	YES	YES
51	a	1143.58	0.47024	YES	YES
52	a	1268.52	147.46302	YES	YES
53	a	1270.66	24.27741	YES	YES
54	a	1284.20	0.13922	YES	YES

55	a	1284.51	0.30668	YES	YES
56	a	1374.01	0.27196	YES	YES
57	a	1374.78	0.32105	YES	YES
58	a	1440.27	8.40962	YES	YES
59	a	1440.63	5.57881	YES	YES
60	a	1488.77	147.09070	YES	YES
61	a	1489.11	83.54668	YES	YES
62	a	1583.36	4.93938	YES	YES
63	a	1584.42	8.98799	YES	YES
64	a	1600.18	38.08057	YES	YES
65	a	1600.98	98.72419	YES	YES
66	a	3114.19	0.01181	YES	YES
67	a	3114.69	0.04675	YES	YES
68	a	3120.95	0.09676	YES	YES
69	a	3121.51	0.13109	YES	YES
70	a	3130.97	0.36971	YES	YES
71	a	3131.31	0.87564	YES	YES
72	a	3135.30	3.65319	YES	YES
73	a	3135.66	5.62580	YES	YES
74	a	3138.09	1.60526	YES	YES
75	a	3138.28	1.93123	YES	YES

Optimized atomic coordinates from the DFT (B3LYP/TZVPP) calculations (Bohr Units):

5.57439200483829	-1.15272522462723	-1.30072144249219	c
5.01436994952501	1.01395204033279	-2.69672164448345	c
4.49017105913581	3.29202279253722	-1.47499880383740	c
4.53494939654797	3.40687226421203	1.16142606963569	c
5.08912127922777	1.25793340913663	2.58459153404926	c
5.61418903234836	-0.98520087314422	1.32073367495384	c
4.10188803979544	4.97475521005855	-2.56674447126687	h
5.02388239575065	0.92345807382995	-4.73877379175574	h
6.03164236454423	-2.92648935818574	-2.20654557162319	h
4.16776171678011	5.17633770149379	2.11645840423910	h
5.17600082913778	1.31268899175084	4.62545976632580	h
6.17705816944795	-3.04476349084190	2.66826966562119	f
-4.50732499883107	-3.37564955653209	-1.25784697251961	c
-5.02328641669513	-1.17162977873119	-2.61241145894318	c
-5.56545131854156	1.07838419126483	-1.34869475410350	c
-5.59954109465365	1.06692443842058	1.27866585078926	c
-5.08213542578344	-1.09979343129552	2.67399552746728	c
-4.54216031528304	-3.33400220204120	1.38067221939585	c
-5.16320121306604	-1.03160596974980	4.71471491075434	h
-4.18048843129604	-5.04520089841011	2.43846725597606	h
-4.13159466533986	-5.12217884919888	-2.24917690917753	h
-5.03864928328782	-1.20429715798718	-4.65617456894496	h
-6.01518169148936	2.79731099625861	-2.35804223511050	h
-6.14757677080957	3.20627578203210	2.50210436553179	f
0.00116538799718	-0.01337910058240	0.00129337951864	ga

1.5.In$(C_6H_5F)_2^+$

Optimized atomic coordinates from the DFT (BP86/SV(P)) calculations (Bohr Units):

0.00133114733740	-1.22788062670430	-0.00105039965019	in
-1.87683389269028	-1.26589210016344	-5.92636457456360	c
1.87555845498718	-1.26603650827099	5.92533605647056	c
-1.25048398449920	1.26529809686779	-5.38868062092112	c
1.24943852103799	1.26513821708566	5.38746732674127	c
-2.72140345421286	2.60644202475120	-3.61516937729770	c
2.72152927207539	2.60652481375626	3.61514224518978	c
-4.76223156987490	1.41745431963728	-2.37338093993388	c
4.76327856905097	1.41772630683965	2.37461389524395	c
-5.33794573208917	-1.13006592314497	-2.92143037390217	c
5.33878898397449	-1.12983666158273	2.92285646650611	c
-3.89131070216040	-2.49225296752521	-4.69362144928719	c
3.89095011130293	-2.49222618744919	4.69394065924856	c
-0.52780131890206	-2.52954776804405	-7.64031823405375	f
0.52543334310009	-2.52989937655723	7.63820073517072	f
0.31441496576922	2.17007145252573	-6.42065651567320	h
-0.31616663570019	2.16973040174559	6.41842249586315	h
-2.29107990886740	4.60953502536123	-3.23824887012744	h
2.29154158366326	4.60963458244502	3.23793125757472	h
-5.93762236242687	2.48910298890425	-1.03046022845991	h
5.93957799720096	2.48955067939730	1.03254450484814	h
-6.95089538905645	-2.06081438994654	-1.98901267860604	h
6.95249421890777	-2.06040300666511	1.99144892934437	h
-4.33666380155743	-4.46568923116156	-5.18345581894387	h
4.33610158362965	-4.46566416210136	5.18394550921864	h

List of calculated frequencies (BP86/SV(P)):

# mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	5.53	0.45669	YES	YES
8	a	10.98	0.13456	YES	YES
9	a	15.85	0.58710	YES	YES
10	a	56.49	0.19270	YES	YES
11	a	69.62	2.07597	YES	YES
12	a	89.81	0.03258	YES	YES
13	a	93.55	3.13209	YES	YES
14	a	103.72	48.18639	YES	YES
15	a	105.06	0.27559	YES	YES
16	a	233.07	0.66312	YES	YES
17	a	234.62	0.00116	YES	YES
18	a	392.85	0.19540	YES	YES
19	a	393.27	0.31868	YES	YES
20	a	404.76	1.32676	YES	YES

21	a	404.82	2.61197	YES	YES
22	a	496.39	20.64424	YES	YES
23	a	496.98	0.36730	YES	YES
24	a	509.79	4.95523	YES	YES
25	a	509.79	3.38183	YES	YES
26	a	600.00	0.03200	YES	YES
27	a	600.19	0.21468	YES	YES
28	a	669.83	19.47051	YES	YES
29	a	670.23	2.18669	YES	YES
30	a	772.92	203.78073	YES	YES
31	a	776.68	15.92802	YES	YES
32	a	810.69	20.07348	YES	YES
33	a	810.91	8.03582	YES	YES
34	a	841.81	1.05660	YES	YES
35	a	841.91	0.65446	YES	YES
36	a	904.03	0.49663	YES	YES
37	a	904.46	12.65333	YES	YES
38	a	963.29	0.03042	YES	YES
39	a	964.99	0.23189	YES	YES
40	a	979.66	4.78606	YES	YES
41	a	979.96	0.05048	YES	YES
42	a	986.93	3.06761	YES	YES
43	a	987.67	0.00226	YES	YES
44	a	1008.52	8.63363	YES	YES
45	a	1008.99	0.27724	YES	YES
46	a	1057.81	3.55469	YES	YES
47	a	1057.97	4.96796	YES	YES
48	a	1139.14	1.30062	YES	YES
49	a	1140.23	9.15892	YES	YES
50	a	1142.54	1.47007	YES	YES
51	a	1142.68	0.17252	YES	YES
52	a	1267.26	148.29547	YES	YES
53	a	1269.21	21.90086	YES	YES
54	a	1284.07	0.00280	YES	YES
55	a	1284.10	0.36586	YES	YES
56	a	1372.41	0.21910	YES	YES
57	a	1372.72	0.29812	YES	YES
58	a	1440.07	9.61712	YES	YES
59	a	1440.33	4.97418	YES	YES
60	a	1489.14	178.29117	YES	YES
61	a	1489.41	49.50566	YES	YES
62	a	1586.13	4.56137	YES	YES
63	a	1586.71	9.93135	YES	YES
64	a	1601.26	24.64887	YES	YES
65	a	1601.49	106.37024	YES	YES
66	a	3112.43	0.00671	YES	YES
67	a	3112.60	0.06936	YES	YES
68	a	3119.88	0.16439	YES	YES
69	a	3120.06	0.28134	YES	YES
70	a	3129.07	0.19639	YES	YES
71	a	3129.19	0.41733	YES	YES
72	a	3134.08	4.01496	YES	YES
73	a	3134.25	5.03040	YES	YES

74	a	3136.21	0.37896	YES	YES
75	a	3136.31	1.00814	YES	YES

Optimized atomic coordinates from the DFT (B3LYP/TZVPP) calculations (Bohr Units):

0.00000000000000	0.00000000000000	-1.15708661177660	in
-1.96827134371198	5.95110560607800	-1.28216801499114	c
1.96827134371198	-5.95110560607800	-1.28216801499114	c
-1.39339606817042	5.51464854741643	1.24418624465522	c
1.39339606817042	-5.51464854741643	1.24418624465522	c
-2.88370110397541	3.81246378045122	2.59969837110466	c
2.88370110397541	-3.81246378045122	2.59969837110466	c
-4.89175681012189	2.56595402277705	1.42779483119425	c
4.89175681012189	-2.56595402277705	1.42779483119425	c
-5.42211734261196	3.03535676891120	-1.11357228244301	c
5.42211734261196	-3.03535676891120	-1.11357228244301	c
-3.95433530523120	4.73284362606027	-2.49418497449862	c
3.95433530523120	-4.73284362606027	-2.49418497449862	c
-0.56788404938921	7.60319197722172	-2.58459989887564	f
0.56788404938921	-7.60319197722172	-2.58459989887564	f
0.13666930153441	6.54377639878920	2.12503195269899	h
-0.13666930153441	-6.54377639878920	2.12503195269899	h
-2.50012014363908	3.50012105953534	4.58327364567543	h
2.50012014363908	-3.50012105953534	4.58327364567543	h
-6.07235343376358	1.28957144851043	2.50123180598889	h
6.07235343376358	-1.28957144851043	2.50123180598889	h
-7.00464558299461	2.10975726565654	-2.01772296929303	h
7.00464558299461	-2.10975726565654	-2.01772296929303	h
-4.35900402853487	5.15986939353423	-4.45113894078494	h
4.35900402853487	-5.15986939353423	-4.45113894078494	h

List of calculated frequencies (B3LYP/TZVPP):

# mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	b	1.23	0.68953	YES	YES
8	a	2.93	0.90361	YES	YES
9	a	9.57	0.10350	YES	YES
10	a	50.91	0.15140	YES	YES
11	b	60.87	2.75328	YES	YES
12	a	81.74	0.08280	YES	YES
13	b	83.38	29.67043	YES	YES
14	b	88.98	17.13578	YES	YES
15	a	89.95	0.20166	YES	YES
16	b	241.55	0.54370	YES	YES

17	a	242.96	0.00039	YES	YES
18	b	408.60	1.47869	YES	YES
19	a	408.66	2.93524	YES	YES
20	b	417.83	0.17420	YES	YES
21	a	418.18	0.34405	YES	YES
22	b	516.48	24.64610	YES	YES
23	a	517.04	0.22590	YES	YES
24	a	526.21	3.75095	YES	YES
25	b	526.24	7.04314	YES	YES
26	b	624.35	0.03654	YES	YES
27	a	624.54	0.19772	YES	YES
28	b	704.32	31.20296	YES	YES
29	a	704.73	2.35690	YES	YES
30	b	800.32	195.63767	YES	YES
31	a	802.98	9.69148	YES	YES
32	b	828.57	27.00220	YES	YES
33	a	828.70	11.62661	YES	YES
34	b	871.29	0.34552	YES	YES
35	a	871.33	0.35413	YES	YES
36	a	940.23	0.56770	YES	YES
37	b	940.89	13.55192	YES	YES
38	b	1006.23	0.07552	YES	YES
39	a	1007.46	0.09440	YES	YES
40	b	1015.90	11.42633	YES	YES
41	a	1016.50	0.04392	YES	YES
42	b	1027.03	3.05621	YES	YES
43	a	1027.55	0.12388	YES	YES
44	b	1037.43	2.75893	YES	YES
45	a	1037.64	0.17196	YES	YES
46	b	1090.23	2.48775	YES	YES
47	a	1090.33	3.54487	YES	YES
48	a	1181.61	3.31669	YES	YES
49	b	1182.14	15.77961	YES	YES
50	a	1186.40	1.42062	YES	YES
51	b	1186.47	0.16886	YES	YES
52	b	1268.02	185.44600	YES	YES
53	a	1269.80	37.41031	YES	YES
54	a	1328.08	0.04979	YES	YES
55	b	1328.25	0.02857	YES	YES
56	a	1351.27	0.06718	YES	YES
57	b	1351.42	0.16345	YES	YES
58	a	1486.08	9.55330	YES	YES
59	b	1486.29	5.06872	YES	YES
60	b	1526.46	154.94215	YES	YES
61	a	1526.66	49.07439	YES	YES
62	b	1620.91	5.13833	YES	YES
63	a	1621.63	8.77453	YES	YES
64	a	1622.42	23.53698	YES	YES
65	b	1622.97	84.45056	YES	YES
66	b	3184.71	0.00249	YES	YES
67	a	3184.77	0.05468	YES	YES

68	b	3191.65	0.47769	YES	YES
69	a	3191.74	1.13061	YES	YES
70	a	3200.81	0.01536	YES	YES
71	b	3200.86	0.05472	YES	YES
72	b	3205.68	2.10837	YES	YES
73	a	3205.72	3.37840	YES	YES
74	b	3208.40	0.15473	YES	YES
75	a	3208.46	0.62825	YES	YES

1.6.Ga([18]crown-6)$^+$

Optimized atomic coordinates from the DFT (BP86/SV(P)) calculations (Bohr Units):

0.00594834834875	0.00051630388377	0.00013968123174	ga
1.54629315469180	4.59585764109766	2.13426407810250	o
-1.94001615493059	4.55426030116082	-1.88116157386683	o
-2.80164817863485	0.00374485668448	-4.49017353778977	o
-1.53680399469164	-4.59275796228938	-2.14203806526230	o
1.92691452194817	-4.55573292203132	1.89056078591198	o
2.81226737515188	-0.00111646126165	4.47887455468939	o
-0.01854817676776	6.71767078828502	1.59241596417776	c
2.31570465908852	4.48549123053717	4.71059375335450	c
-0.57253989860100	6.77359670550077	-1.21377066094883	c
-2.70499156734475	4.52362822525831	-4.46096659969114	c
-4.30026208457533	2.19546683364269	-4.93102338651091	c
-4.08753992213218	-2.28662492987184	-5.07489068454783	c
-2.28551931031300	-4.48114550080819	-4.72445781703473	c
0.01209627711264	-6.72183091778170	-1.58425151945660	c
0.55031631094925	-6.77021878516364	1.22520197433960	c
2.68457135748808	-4.51995867422031	4.47240627941313	c
4.29462281933205	-2.20060718007053	4.93602170457631	c
4.11215864514511	2.28481818392259	5.05079788514196	c
0.96375747338708	8.50880935136497	2.12846003947553	h
-1.81972024033448	6.60959451147581	2.68999351816884	h
0.63911115527042	4.26175652286442	5.97649494727178	h
3.31002764221608	6.26704695325896	5.25645641399596	h
-1.71457060766635	8.49637879241027	-1.64730477613340	h
1.22852860190076	6.89229838715010	-2.31065766617462	h
-1.01926921013756	4.52229647440141	-5.73398475161537	h
-3.85548903749560	6.23803518474223	-4.90555176059723	h
-5.99286560739545	2.20269093512284	-3.66753117601572	h
-4.97981562027794	2.22859902888880	-6.93012752911175	h
-4.75112577567434	-2.26348394939208	-7.07944955690131	h
-5.77868411450315	-2.52565205435641	-3.83144758902911	h
-3.26959476510472	-6.26505099476035	-5.28089569986265	h
-0.59960539296672	-4.25019725418435	-5.97656141526967	h
1.82006903518098	-6.62858614083965	-2.67183461067997	h
-0.97803988386224	-8.50903227170811	-2.11920336029148	h
-1.25715192388752	-6.87413478169915	2.31292560276615	h
1.68037940381318	-8.49747925238080	1.67194139753420	h

3.82205374765494	-6.24029278899994	4.92736706775076 h
0.99540455507063	-4.50169310191696	5.74074585056752 h
4.96751430384723	-2.22768498550958	6.93746455121683 h
5.99100935682537	-2.22619588111109	3.67793601325279 h
5.79573568352863	2.51479402604317	3.79547990201056 h
4.78931703934524	2.26212555266057	7.05074177184142 h

List of calculated frequencies (BP86/SV(P)):

# mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	26.68	0.31448	YES	YES
8	a	28.36	0.19850	YES	YES
9	a	30.57	0.08059	YES	YES
10	a	60.38	47.58874	YES	YES
11	a	60.49	47.56666	YES	YES
12	a	61.06	0.10527	YES	YES
13	a	89.14	0.00219	YES	YES
14	a	89.58	0.00227	YES	YES
15	a	127.55	18.77882	YES	YES
16	a	130.66	0.00574	YES	YES
17	a	138.49	4.92999	YES	YES
18	a	141.30	4.99913	YES	YES
19	a	144.66	0.00403	YES	YES
20	a	145.86	0.00398	YES	YES
21	a	175.10	0.00303	YES	YES
22	a	216.13	1.13234	YES	YES
23	a	242.57	0.00678	YES	YES
24	a	245.98	19.06953	YES	YES
25	a	248.10	19.48330	YES	YES
26	a	250.44	0.01968	YES	YES
27	a	252.23	0.00184	YES	YES
28	a	270.26	0.00063	YES	YES
29	a	308.98	2.96369	YES	YES
30	a	309.41	2.74892	YES	YES
31	a	342.08	0.00565	YES	YES
32	a	354.07	0.00045	YES	YES
33	a	354.50	0.00030	YES	YES
34	a	524.50	0.83612	YES	YES
35	a	525.02	0.79926	YES	YES
36	a	532.50	0.00009	YES	YES
37	a	539.43	0.00011	YES	YES
38	a	540.11	0.00041	YES	YES
39	a	573.07	0.18583	YES	YES
40	a	816.79	0.00268	YES	YES
41	a	817.45	0.01887	YES	YES
42	a	824.04	22.69698	YES	YES

43	a	830.21	47.03997	YES	YES
44	a	832.12	48.22000	YES	YES
45	a	874.75	0.00108	YES	YES
46	a	918.84	0.00042	YES	YES
47	a	924.63	0.02385	YES	YES
48	a	951.89	0.00210	YES	YES
49	a	952.47	0.00480	YES	YES
50	a	960.79	91.58917	YES	YES
51	a	962.03	93.27298	YES	YES
52	a	1047.88	19.41300	YES	YES
53	a	1048.20	19.39747	YES	YES
54	a	1065.67	0.00062	YES	YES
55	a	1073.32	0.00103	YES	YES
56	a	1074.12	0.00431	YES	YES
57	a	1080.14	0.01292	YES	YES
58	a	1086.57	0.00548	YES	YES
59	a	1096.46	0.00204	YES	YES
60	a	1097.13	0.04146	YES	YES
61	a	1104.10	29.53078	YES	YES
62	a	1117.23	558.33789	YES	YES
63	a	1117.52	570.54891	YES	YES
64	a	1119.12	7.25960	YES	YES
65	a	1119.77	10.16923	YES	YES
66	a	1133.75	0.05974	YES	YES
67	a	1144.11	0.00571	YES	YES
68	a	1144.38	0.00259	YES	YES
69	a	1152.89	0.01205	YES	YES
70	a	1218.19	0.00369	YES	YES
71	a	1223.92	8.96010	YES	YES
72	a	1225.28	8.74231	YES	YES
73	a	1232.58	0.01052	YES	YES
74	a	1233.63	0.00057	YES	YES
75	a	1236.11	52.07636	YES	YES
76	a	1256.71	0.06937	YES	YES
77	a	1263.93	0.00061	YES	YES
78	a	1264.92	0.00176	YES	YES
79	a	1275.49	28.97997	YES	YES
80	a	1276.60	27.67748	YES	YES
81	a	1281.02	0.00472	YES	YES
82	a	1326.68	0.00116	YES	YES
83	a	1337.19	75.17550	YES	YES
84	a	1338.59	74.46901	YES	YES
85	a	1355.85	0.00200	YES	YES
86	a	1355.98	0.00077	YES	YES
87	a	1372.48	0.03948	YES	YES
88	a	1377.70	0.23040	YES	YES
89	a	1398.99	0.00064	YES	YES
90	a	1399.98	0.00017	YES	YES
91	a	1422.01	34.38127	YES	YES
92	a	1424.31	33.59971	YES	YES
93	a	1433.92	0.00595	YES	YES

94	a	1437.30	0.00104	YES	YES
95	a	1439.13	26.06833	YES	YES
96	a	1439.85	25.43483	YES	YES
97	a	1441.64	0.05176	YES	YES
98	a	1442.47	0.04315	YES	YES
99	a	1443.23	0.65645	YES	YES
100	a	1464.43	29.84550	YES	YES
101	a	1464.98	0.25564	YES	YES
102	a	1465.65	0.04479	YES	YES
103	a	1467.81	1.40044	YES	YES
104	a	1468.27	1.51161	YES	YES
105	a	1472.55	0.01521	YES	YES
106	a	2905.12	0.74402	YES	YES
107	a	2905.46	19.06284	YES	YES
108	a	2905.76	8.01563	YES	YES
109	a	2906.36	0.10536	YES	YES
110	a	2906.91	0.12263	YES	YES
111	a	2907.46	4.71925	YES	YES
112	a	2909.45	78.50375	YES	YES
113	a	2909.98	1.24174	YES	YES
114	a	2910.83	2.56375	YES	YES
115	a	2911.70	134.81754	YES	YES
116	a	2911.90	146.67088	YES	YES
117	a	2913.58	0.44514	YES	YES
118	a	2950.18	1.23344	YES	YES
119	a	2950.64	98.08167	YES	YES
120	a	2950.96	100.80377	YES	YES
121	a	2953.71	0.05455	YES	YES
122	a	2954.37	0.13230	YES	YES
123	a	2957.63	0.07546	YES	YES
124	a	2960.41	212.30857	YES	YES
125	a	2962.99	0.02078	YES	YES
126	a	2964.04	0.00704	YES	YES
127	a	2966.50	3.88614	YES	YES
128	a	2966.73	2.11374	YES	YES
129	a	2967.74	0.01263	YES	YES

Optimized atomic coordinates from the DFT (B3LYP/TZVPP) calculations (Bohr Units):

0.00000000000000	0.00000000000000	0.00000000000000	ga
-4.59272246682356	-2.65160955253382	0.29685364361132	o
-4.59272246682356	2.65160955253382	-0.29685364361132	o
0.00000000000000	5.30321910506763	0.29685364361132	o
4.59272246682357	2.65160955253381	-0.29685364361132	o
4.59272246682357	-2.65160955253381	0.29685364361132	o
0.00000000000000	-5.30321910506763	-0.29685364361132	o
-6.75278503021363	-1.30262155748788	-0.57497050047079	c
-4.50449587540856	-5.19677260371632	-0.57497050047079	c
-6.75278503021363	1.30262155748788	0.57497050047079	c
-4.50449587540856	5.19677260371632	0.57497050047079	c
-2.24828915480508	6.49939416120419	-0.57497050047079	c
2.24828915480508	6.49939416120419	-0.57497050047079	c

4.50449587540856	5.19677260371632	0.57497050047079	c
6.75278503021363	1.30262155748788	0.57497050047079	c
6.75278503021363	-1.30262155748788	-0.57497050047079	c
4.50449587540856	-5.19677260371632	-0.57497050047079	c
2.24828915480508	-6.49939416120419	0.57497050047079	c
-2.24828915480508	-6.49939416120419	0.57497050047079	c
-8.48180860084764	-2.28810555018092	-0.00449987872975	h
-6.72894564697350	-1.17632306398192	-2.64178111216970	h
-4.38319847995264	-5.23927633897279	-2.64178111216970	h
-6.22246183342068	-6.20140894328094	-0.00449987872975	h
-8.48180860084764	2.28810555018092	0.00449987872975	h
-6.72894564697350	1.17632306398192	2.64178111216970	h
-4.38319847995264	5.23927633897279	2.64178111216970	h
-6.22246183342068	6.20140894328094	0.00449987872975	h
-2.34574716702087	6.41559940295469	-2.64178111216970	h
-2.25934676742697	8.48951449346190	-0.00449987872975	h
2.25934676742697	8.48951449346190	-0.00449987872975	h
2.34574716702087	6.41559940295469	-2.64178111216970	h
6.22246183342068	6.20140894328094	0.00449987872975	h
4.38319847995264	5.23927633897279	2.64178111216970	h
6.72894564697350	1.17632306398192	2.64178111216970	h
8.48180860084764	2.28810555018092	0.00449987872975	h
6.72894564697350	-1.17632306398192	-2.64178111216970	h
8.48180860084764	-2.28810555018092	-0.00449987872975	h
6.22246183342068	-6.20140894328094	-0.00449987872975	h
4.38319847995264	-5.23927633897279	-2.64178111216970	h
2.25934676742697	-8.48951449346190	0.00449987872975	h
2.34574716702087	-6.41559940295469	2.64178111216970	h
-2.34574716702087	-6.41559940295469	2.64178111216970	h
-2.25934676742697	-8.48951449346190	0.00449987872975	h

List of calculated frequencies (B3LYP/TZVPP):

# mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a2u	14.83	0.13791	YES	NO
8	eu	38.81	0.10504	YES	NO
9	eu	38.81	0.10504	YES	NO
10	eu	69.31	43.81147	YES	NO
11	eu	69.31	43.81147	YES	NO
12	a2g	70.83	0.00000	NO	NO
13	eg	90.12	0.00000	NO	YES
14	eg	90.12	0.00000	NO	YES
15	a2u	122.66	20.74993	YES	NO
16	a1g	136.49	0.00000	NO	YES
17	eu	141.20	7.05186	YES	NO

18	eu	141.20	7.05186	YES	NO
19	eg	143.07	0.00000	NO	YES
20	eg	143.07	0.00000	NO	YES
21	a1u	172.30	0.00000	NO	NO
22	a2u	217.74	1.57211	YES	NO
23	a1g	239.87	0.00000	NO	YES
24	eu	242.75	17.98718	YES	NO
25	eu	242.75	17.98718	YES	NO
26	eg	249.91	0.00000	NO	YES
27	eg	249.91	0.00000	NO	YES
28	a1g	268.44	0.00000	NO	YES
29	eu	310.82	2.97963	YES	NO
30	eu	310.82	2.97963	YES	NO
31	a1u	348.05	0.00000	NO	NO
32	eg	357.46	0.00000	NO	YES
33	eg	357.46	0.00000	NO	YES
34	eu	531.12	1.24099	YES	NO
35	eu	531.12	1.24099	YES	NO
36	a2g	540.12	0.00000	NO	NO
37	eg	546.19	0.00000	NO	YES
38	eg	546.19	0.00000	NO	YES
39	a2u	580.41	0.09178	YES	NO
40	eg	831.84	0.00000	NO	YES
41	eg	831.84	0.00000	NO	YES
42	a2u	837.85	24.80769	YES	NO
43	eu	843.37	47.67553	YES	NO
44	eu	843.37	47.67553	YES	NO
45	a1g	878.07	0.00000	NO	YES
46	a1u	931.21	0.00000	NO	NO
47	a2g	943.75	0.00000	NO	NO
48	eg	959.58	0.00000	NO	YES
49	eg	959.58	0.00000	NO	YES
50	eu	976.85	99.15220	YES	NO
51	eu	976.85	99.15220	YES	NO
52	eu	1059.74	14.57832	YES	NO
53	eu	1059.74	14.57832	YES	NO
54	a1g	1075.24	0.00000	NO	YES
55	a2g	1086.55	0.00000	NO	NO
56	eg	1093.96	0.00000	NO	YES
57	eg	1093.96	0.00000	NO	YES
58	a1u	1106.40	0.00000	NO	NO
59	eu	1118.87	560.70530	YES	NO
60	eu	1118.87	560.70530	YES	NO
61	eg	1123.40	0.00000	NO	YES
62	eg	1123.40	0.00000	NO	YES
63	a2u	1127.14	31.53988	YES	NO
64	eg	1146.04	0.00000	NO	YES
65	eg	1146.04	0.00000	NO	YES
66	eu	1147.77	0.08606	YES	NO
67	eu	1147.77	0.08606	YES	NO
68	a1u	1153.22	0.00000	NO	NO

69	a1g	1161.31	0.00000	NO	YES
70	a2g	1253.32	0.00000	NO	NO
71	eu	1259.00	5.51824	YES	NO
72	eu	1259.00	5.51824	YES	NO
73	eg	1266.82	0.00000	NO	YES
74	eg	1266.82	0.00000	NO	YES
75	a2u	1269.68	49.81741	YES	NO
76	a1u	1290.15	0.00000	NO	NO
77	eg	1298.33	0.00000	NO	YES
78	eg	1298.33	0.00000	NO	YES
79	eu	1310.65	28.54679	YES	NO
80	eu	1310.65	28.54679	YES	NO
81	a1g	1315.95	0.00000	NO	YES
82	a2g	1373.55	0.00000	NO	NO
83	eu	1383.21	59.45324	YES	NO
84	eu	1383.21	59.45324	YES	NO
85	eg	1397.55	0.00000	NO	YES
86	eg	1397.55	0.00000	NO	YES
87	a1u	1405.70	0.00000	NO	NO
88	a2u	1426.52	0.44658	YES	NO
89	eg	1439.69	0.00000	NO	YES
90	eg	1439.69	0.00000	NO	YES
91	eu	1460.77	7.56752	YES	NO
92	eu	1460.77	7.56752	YES	NO
93	a1g	1471.62	0.00000	NO	YES
94	a2g	1496.41	0.00000	NO	NO
95	eu	1497.40	23.25032	YES	NO
96	eu	1497.40	23.25032	YES	NO
97	eg	1498.38	0.00000	NO	YES
98	eg	1498.38	0.00000	NO	YES
99	a1u	1498.70	0.00000	NO	NO
100	eg	1514.22	0.00000	NO	YES
101	eg	1514.22	0.00000	NO	YES
102	a2u	1514.23	28.15940	YES	NO
103	eu	1514.62	1.30397	YES	NO
104	eu	1514.62	1.30397	YES	NO
105	a1g	1515.96	0.00000	NO	YES
106	a2g	2993.58	0.00000	NO	NO
107	eu	2994.08	10.90568	YES	NO
108	eu	2994.08	10.90568	YES	NO
109	eg	2995.14	0.00000	NO	YES
110	eg	2995.14	0.00000	NO	YES
111	a1u	2995.84	0.00000	NO	NO
112	a2u	2998.95	70.55978	YES	NO
113	eg	2999.71	0.00000	NO	YES
114	eg	2999.71	0.00000	NO	YES
115	eu	3001.07	107.92800	YES	NO
116	eu	3001.07	107.92800	YES	NO
117	a1g	3002.54	0.00000	NO	YES
118	a1g	3031.42	0.00000	NO	YES
119	eu	3031.52	102.56802	YES	NO

120	eu	3031.52	102.56802	YES	NO
121	eg	3033.16	0.00000	NO	YES
122	eg	3033.16	0.00000	NO	YES
123	a1u	3034.47	0.00000	NO	NO
124	a2u	3041.25	192.99234	YES	NO
125	eg	3042.30	0.00000	NO	YES
126	eg	3042.30	0.00000	NO	YES
127	eu	3044.10	3.54828	YES	NO
128	eu	3044.10	3.54828	YES	NO
129	a2g	3044.81	0.00000	NO	NO

1.7.In([18]crown-6)$^{+}$

Optimized atomic coordinates from the DFT (BP86/SV(P)) calculations (Bohr Units):

0.78803952453644	0.05056041318796	-0.55221034001176	in
1.61360373228930	4.64513256739690	2.12092932317478	o
-1.88684517002701	4.54033199529324	-1.90240843601521	o
-2.79883169057338	0.00402384553155	-4.55264771607899	o
-1.49324681505820	-4.57671519048653	-2.15888361602512	o
1.99769691252603	-4.59521337316104	1.87368020731239	o
2.82151124111859	0.00012627207745	4.44924354214843	o
-0.00523338890573	6.72849575172018	1.58260966619717	c
2.29366590819877	4.48561822810606	4.72113862933757	c
-0.56529522837686	6.78764483737982	-1.22420136765107	c
-2.72998206723530	4.53308183878710	-4.46097575142180	c
-4.32153075388524	2.19604779367511	-4.91073486973443	c
-4.11870044647903	-2.29024511012393	-5.04700303639891	c
-2.32532615516595	-4.49788286350002	-4.71951305197196	c
0.02210702389565	-6.73231864861806	-1.59797890852870	c
0.57032486209032	-6.77970726585143	1.21156302433186	c
2.66841510542151	-4.52219866302731	4.47990648974939	c
4.27634028289743	-2.20567991578241	4.97463719229040	c
4.08989564218567	2.28761517923833	5.09323835523744	c
0.92748133134654	8.54236986204205	2.13043398713276	h
-1.80422697314045	6.56453753904713	2.67650943897533	h
0.57282698695601	4.22716775382288	5.91866314438019	h
3.25507127091256	6.26208227183196	5.33730776275692	h
-1.75010230485926	8.48460517308231	-1.64065089718696	h
1.22713816967254	6.95828326767236	-2.32890974621442	h
-1.08474052134942	4.56786252807318	-5.78587617460206	h
-3.91115505779747	6.24017134390407	-4.84590946744782	h
-5.96782412613472	2.17386376397794	-3.58775427434059	h
-5.07118967968461	2.25265671439557	-6.88399633723553	h
-4.85601462797896	-2.29941029624975	-7.02567545808246	h
-5.76289033517392	-2.49107161106380	-3.73638150889249	h
-3.34773353973344	-6.27866276971606	-5.21107946229652	h
-0.67973246027592	-4.30943766986964	-6.03118168867437	h
1.82397622887277	-6.68197430857598	-2.69860169970657	h
-1.00642037186141	-8.50200688125872	-2.11580844401838	h
-1.23770488901688	-6.83529600684968	2.30101912926113	h
1.65948127530253	-8.53180525446362	1.66376994478118	h

3.77661524291391	-6.24308729528837	5.00041003180027	h
0.93522910612160	-4.47352372622960	5.68552819357149	h
4.87670347195838	-2.21869687580135	6.99862340424156	h
6.01712057703581	-2.25016489190619	3.77939008457579	h
5.81787604766204	2.53987822650018	3.90417090075313	h
4.69360665879852	2.24294145108013	7.11560980052700	h

List of calculated frequencies (BP86/SV(P)):

# mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	30.63	0.11931	YES	YES
8	a	33.13	0.06899	YES	YES
9	a	36.52	1.28216	YES	YES
10	a	62.67	0.26771	YES	YES
11	a	66.17	28.07729	YES	YES
12	a	66.52	28.54174	YES	YES
13	a	94.69	0.02161	YES	YES
14	a	95.20	0.02852	YES	YES
15	a	130.42	14.14921	YES	YES
16	a	133.59	1.97433	YES	YES
17	a	136.48	6.29995	YES	YES
18	a	138.27	7.33903	YES	YES
19	a	148.69	0.97071	YES	YES
20	a	149.69	1.61762	YES	YES
21	a	175.45	0.00661	YES	YES
22	a	216.85	0.53670	YES	YES
23	a	243.75	10.53234	YES	YES
24	a	244.85	13.52389	YES	YES
25	a	245.49	15.27782	YES	YES
26	a	253.37	4.99933	YES	YES
27	a	254.37	4.67565	YES	YES
28	a	271.18	0.06985	YES	YES
29	a	308.78	2.96090	YES	YES
30	a	309.23	2.74087	YES	YES
31	a	341.54	0.00400	YES	YES
32	a	353.24	0.02745	YES	YES
33	a	353.71	0.01555	YES	YES
34	a	523.02	0.42831	YES	YES
35	a	523.58	0.41620	YES	YES
36	a	531.36	0.00146	YES	YES
37	a	538.67	0.08116	YES	YES
38	a	539.24	0.10291	YES	YES
39	a	571.90	0.12130	YES	YES
40	a	815.46	0.40579	YES	YES
41	a	816.12	0.06546	YES	YES
42	a	822.55	20.80967	YES	YES

43	a	828.68	49.31510	YES	YES
44	a	830.02	50.69298	YES	YES
45	a	872.06	1.54026	YES	YES
46	a	917.67	0.01895	YES	YES
47	a	922.38	0.01833	YES	YES
48	a	949.39	0.87258	YES	YES
49	a	949.89	0.83507	YES	YES
50	a	958.96	90.88336	YES	YES
51	a	959.97	92.30039	YES	YES
52	a	1045.59	20.64081	YES	YES
53	a	1045.81	20.73802	YES	YES
54	a	1063.03	0.38225	YES	YES
55	a	1072.13	0.02210	YES	YES
56	a	1072.65	0.01673	YES	YES
57	a	1078.18	0.01401	YES	YES
58	a	1084.20	0.04178	YES	YES
59	a	1094.91	3.70674	YES	YES
60	a	1095.20	3.34818	YES	YES
61	a	1102.67	29.21110	YES	YES
62	a	1114.28	550.81223	YES	YES
63	a	1114.34	552.71686	YES	YES
64	a	1118.36	2.04482	YES	YES
65	a	1118.70	3.75126	YES	YES
66	a	1132.68	0.53349	YES	YES
67	a	1141.18	0.98588	YES	YES
68	a	1141.42	1.17962	YES	YES
69	a	1149.61	0.00717	YES	YES
70	a	1216.72	0.23299	YES	YES
71	a	1222.96	7.23853	YES	YES
72	a	1224.01	7.15199	YES	YES
73	a	1231.81	2.13662	YES	YES
74	a	1232.80	0.35905	YES	YES
75	a	1235.73	48.94961	YES	YES
76	a	1256.00	0.08385	YES	YES
77	a	1263.37	0.13646	YES	YES
78	a	1264.25	0.01780	YES	YES
79	a	1274.72	30.58923	YES	YES
80	a	1276.00	29.90025	YES	YES
81	a	1280.56	0.36529	YES	YES
82	a	1325.91	0.16669	YES	YES
83	a	1336.22	69.02594	YES	YES
84	a	1337.66	68.76286	YES	YES
85	a	1355.00	0.10386	YES	YES
86	a	1355.09	0.02178	YES	YES
87	a	1370.85	0.03970	YES	YES
88	a	1377.64	0.19512	YES	YES
89	a	1397.99	0.04492	YES	YES
90	a	1399.05	0.01064	YES	YES
91	a	1420.79	33.55776	YES	YES
92	a	1422.91	32.67911	YES	YES
93	a	1432.63	0.15270	YES	YES

94	a	1436.83	3.21947	YES	YES
95	a	1438.93	17.20924	YES	YES
96	a	1439.22	22.97410	YES	YES
97	a	1441.28	3.08585	YES	YES
98	a	1442.08	0.22042	YES	YES
99	a	1442.97	0.11305	YES	YES
100	a	1463.03	26.22284	YES	YES
101	a	1464.62	8.25195	YES	YES
102	a	1465.21	0.67814	YES	YES
103	a	1467.50	1.12412	YES	YES
104	a	1467.81	0.65388	YES	YES
105	a	1471.51	0.21573	YES	YES
106	a	2906.71	0.37936	YES	YES
107	a	2907.00	18.25365	YES	YES
108	a	2907.35	8.93365	YES	YES
109	a	2907.89	0.53436	YES	YES
110	a	2908.32	1.94056	YES	YES
111	a	2908.87	3.10010	YES	YES
112	a	2910.95	74.61095	YES	YES
113	a	2911.38	1.15660	YES	YES
114	a	2912.12	17.46774	YES	YES
115	a	2913.01	124.15699	YES	YES
116	a	2913.18	109.06526	YES	YES
117	a	2914.72	12.26040	YES	YES
118	a	2952.29	4.43461	YES	YES
119	a	2952.75	97.32990	YES	YES
120	a	2953.03	102.31843	YES	YES
121	a	2955.83	0.83282	YES	YES
122	a	2956.46	1.20050	YES	YES
123	a	2959.75	0.07969	YES	YES
124	a	2962.13	187.82077	YES	YES
125	a	2964.96	1.05167	YES	YES
126	a	2965.81	1.49339	YES	YES
127	a	2968.41	3.21773	YES	YES
128	a	2968.63	1.32163	YES	YES
129	a	2969.74	0.28783	YES	YES

Optimized atomic coordinates from the DFT (B3LYP/TZVPP) calculations (Bohr Units):

0.00000000000000	0.00000000000000	0.00000000000000	in
-4.65846957903170	-2.68956866546562	0.35576015464098	o
-4.65846957903170	2.68956866546562	-0.35576015464098	o
0.00000000000000	5.37913733093126	0.35576015464098	o
4.65846957903170	2.68956866546562	-0.35576015464098	o
4.65846957903170	-2.68956866546562	0.35576015464098	o
0.00000000000000	-5.37913733093126	-0.35576015464098	o
-6.78715598561840	-1.31310859421022	-0.55906432064151	c
-4.53076339332291	-5.22129520588805	-0.55906432064151	c
-6.78715598561840	1.31310859421022	0.55906432064151	c
-4.53076339332291	5.22129520588805	0.55906432064151	c
-2.25639259229549	6.53440380009821	-0.55906432064151	c
2.25639259229549	6.53440380009821	-0.55906432064151	c

4.53076339332291	5.22129520588804	0.55906432064151	c
6.78715598561840	1.31310859421022	0.55906432064151	c
6.78715598561840	-1.31310859421022	-0.55906432064151	c
4.53076339332291	-5.22129520588804	-0.55906432064151	c
2.25639259229549	-6.53440380009821	0.55906432064151	c
-2.25639259229549	-6.53440380009821	0.55906432064151	c
-8.53720080320252	-2.26982433573497	-0.00310290748019	h
-6.73488241381639	-1.20963878252725	-2.62659370156978	h
-4.41501912197967	-5.22775987060242	-2.62659370156978	h
-6.23432593847588	-6.25852060491482	-0.00310290748019	h
-8.53720080320252	2.26982433573497	0.00310290748019	h
-6.73488241381639	1.20963878252725	2.62659370156978	h
-4.41501912197967	5.22775987060242	2.62659370156978	h
-6.23432593847588	6.25852060491482	0.00310290748019	h
-2.31986329183673	6.43739865312969	-2.62659370156978	h
-2.30287486472661	8.52834494064981	-0.00310290748019	h
2.30287486472662	8.52834494064981	-0.00310290748019	h
2.31986329183673	6.43739865312969	-2.62659370156978	h
6.23432593847588	6.25852060491481	0.00310290748019	h
4.41501912197967	5.22775987060242	2.62659370156978	h
6.73488241381639	1.20963878252725	2.62659370156978	h
8.53720080320252	2.26982433573497	0.00310290748019	h
6.73488241381639	-1.20963878252725	-2.62659370156978	h
8.53720080320252	-2.26982433573497	-0.00310290748019	h
6.23432593847588	-6.25852060491481	-0.00310290748019	h
4.41501912197967	-5.22775987060242	-2.62659370156978	h
2.30287486472662	-8.52834494064981	0.00310290748019	h
2.31986329183673	-6.43739865312969	2.62659370156978	h
-2.31986329183673	-6.43739865312969	2.62659370156978	h
-2.30287486472661	-8.52834494064981	0.00310290748019	h

List of calculated frequencies (B3LYP/TZVPP):

The B3LYP/TZVPP calculation was performed on the basis of BP86/SV(P) optimized coordinates. It shows one imaginary frequency, probably because of symmetry restraints. Due to the low frequency and flat potential energy surface, the impact on the reported reaction enthalpies may be neglected. Further calculations to find the minimum were futile.

# mode #	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1	a2u	-36.50	0.00000	YES	NO
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7		0.00	0.00000	-	-
8	eu	44.79	0.00837	YES	NO
9	eu	44.79	0.00837	YES	NO
10	a2g	76.21	0.00000	NO	NO
11	eu	77.84	23.93524	YES	NO
12	eu	77.84	23.93524	YES	NO

13	eg	100.32	0.00000	NO	YES
14	eg	100.32	0.00000	NO	YES
15	a2u	128.34	19.31148	YES	NO
16	eg	146.78	0.00000	NO	YES
17	eg	146.78	0.00000	NO	YES
18	a1g	148.36	0.00000	NO	YES
19	eu	148.46	14.96863	YES	NO
20	eu	148.46	14.96863	YES	NO
21	a1u	169.17	0.00000	NO	NO
22	a2u	221.38	0.90470	YES	NO
23	eu	238.20	22.81456	YES	NO
24	eu	238.20	22.81456	YES	NO
25	a1g	239.18	0.00000	NO	YES
26	eg	249.81	0.00000	NO	YES
27	eg	249.81	0.00000	NO	YES
28	a1g	266.51	0.00000	NO	YES
29	eu	309.53	3.54561	YES	NO
30	eu	309.53	3.54561	YES	NO
31	a1u	348.76	0.00000	NO	NO
32	eg	356.13	0.00000	NO	YES
33	eg	356.13	0.00000	NO	YES
34	eu	525.43	1.07548	YES	NO
35	eu	525.43	1.07548	YES	NO
36	a2g	533.25	0.00000	NO	NO
37	eg	542.99	0.00000	NO	YES
38	eg	542.99	0.00000	NO	YES
39	a2u	577.52	0.00442	YES	NO
40	eg	829.92	0.00000	NO	YES
41	eg	829.92	0.00000	NO	YES
42	a2u	835.86	25.56906	YES	NO
43	eu	839.71	49.61404	YES	NO
44	eu	839.71	49.61404	YES	NO
45	a1g	871.81	0.00000	NO	YES
46	a1u	923.29	0.00000	NO	NO
47	a2g	942.14	0.00000	NO	NO
48	eg	951.50	0.00000	NO	YES
49	eg	951.50	0.00000	NO	YES
50	eu	970.65	99.68656	YES	NO
51	eu	970.65	99.68656	YES	NO
52	eu	1055.79	22.14738	YES	NO
53	eu	1055.79	22.14738	YES	NO
54	a1g	1068.78	0.00000	NO	YES
55	a2g	1083.11	0.00000	NO	NO
56	eg	1089.91	0.00000	NO	YES
57	eg	1089.91	0.00000	NO	YES
58	a1u	1101.40	0.00000	NO	NO
59	eu	1113.40	553.81575	YES	NO
60	eu	1113.40	553.81575	YES	NO
61	eg	1119.35	0.00000	NO	YES
62	eg	1119.35	0.00000	NO	YES
63	a2u	1123.28	31.61281	YES	NO

64	eg	1141.25	0.00000	NO	YES
65	eg	1141.25	0.00000	NO	YES
66	a1u	1146.17	0.00000	NO	NO
67	eu	1147.21	0.36410	YES	NO
68	eu	1147.21	0.36410	YES	NO
69	a1g	1161.11	0.00000	NO	YES
70	a2g	1253.06	0.00000	NO	NO
71	eu	1259.42	3.35599	YES	NO
72	eu	1259.42	3.35599	YES	NO
73	eg	1268.60	0.00000	NO	YES
74	eg	1268.60	0.00000	NO	YES
75	a2u	1272.17	48.77803	YES	NO
76	a1u	1294.00	0.00000	NO	NO
77	eg	1301.82	0.00000	NO	YES
78	eg	1301.82	0.00000	NO	YES
79	eu	1314.04	31.44749	YES	NO
80	eu	1314.04	31.44749	YES	NO
81	a1g	1319.48	0.00000	NO	YES
82	a2g	1374.70	0.00000	NO	NO
83	eu	1384.06	57.92388	YES	NO
84	eu	1384.06	57.92388	YES	NO
85	eg	1397.59	0.00000	NO	YES
86	eg	1397.59	0.00000	NO	YES
87	a1u	1404.03	0.00000	NO	NO
88	a2u	1428.63	0.32421	YES	NO
89	eg	1439.84	0.00000	NO	YES
90	eg	1439.84	0.00000	NO	YES
91	eu	1459.31	7.06768	YES	NO
92	eu	1459.31	7.06768	YES	NO
93	a1g	1469.56	0.00000	NO	YES
94	a2g	1495.77	0.00000	NO	NO
95	eu	1496.54	23.74312	YES	NO
96	eu	1496.54	23.74312	YES	NO
97	eg	1497.31	0.00000	NO	YES
98	eg	1497.31	0.00000	NO	YES
99	a1u	1497.53	0.00000	NO	NO
100	a2u	1513.83	31.46685	YES	NO
101	eg	1513.95	0.00000	NO	YES
102	eg	1513.95	0.00000	NO	YES
103	eu	1514.29	1.39265	YES	NO
104	eu	1514.29	1.39265	YES	NO
105	a1g	1515.58	0.00000	NO	YES
106	a2g	2994.39	0.00000	NO	NO
107	eu	2994.86	9.83643	YES	NO
108	eu	2994.86	9.83643	YES	NO
109	eg	2995.91	0.00000	NO	YES
110	eg	2995.91	0.00000	NO	YES
111	a1u	2996.71	0.00000	NO	NO
112	a2u	2999.15	65.90505	YES	NO
113	eg	3000.10	0.00000	NO	YES
114	eg	3000.10	0.00000	NO	YES

115	eu	3001.56	105.61880	YES	NO
116	eu	3001.56	105.61880	YES	NO
117	a1g	3002.95	0.00000	NO	YES
118	a1g	3032.10	0.00000	NO	YES
119	eu	3032.25	107.14525	YES	NO
120	eu	3032.25	107.14525	YES	NO
121	eg	3034.10	0.00000	NO	YES
122	eg	3034.10	0.00000	NO	YES
123	a1u	3035.69	0.00000	NO	NO
124	a2u	3041.05	181.99006	YES	NO
125	eg	3042.43	0.00000	NO	YES
126	eg	3042.43	0.00000	NO	YES
127	eu	3044.43	1.96090	YES	NO
128	eu	3044.43	1.96090	YES	NO
129	a2g	3045.21	0.00000	NO	NO

1.8.Ga([18]crown-6)(PhF)$_2^+$

Atomic coordinates from the DFT (BP86/SV(P)) calculations (Bohr Units):

-0.29979856261071	0.44990740608186	-0.29158304879446	ga
2.53887243330966	-0.75615360141155	-4.66197155532837	o
4.47814717730059	2.09130462099004	-0.67404471923190	o
1.49969313991444	3.27361177109228	3.46908532351028	o
-2.86655686640575	0.44542875516562	4.25413424761638	o
2.00228470011773	-2.96091596870282	-6.03606700985621	c
5.07987377002105	-0.08811651896507	-4.54919270018876	c
5.47754773576470	2.23853318338828	-3.16307858750596	c
5.03334871282370	4.19218874319041	0.88828635460654	c
4.13792088575674	3.74921804223067	3.43129080101041	c
0.45561945585548	2.97405238575830	5.88313485914460	c
-2.25572179376282	2.53416193838229	5.76759700386250	c
-5.42855306036581	-0.18120442788225	4.16932333912666	c
-0.74305272248920	-3.39740490905384	-6.22706162930931	c
2.80579624846501	-4.42624740054535	-5.19504439792782	h
2.72720253892652	-2.81215672814334	-7.75428159174538	h
5.73991731095881	0.11255349824799	-6.28817537219160	h
6.04102627171529	-1.46563237777914	-3.72540439052032	h
7.31113009758473	2.59867718828957	-3.07273078147002	h
4.65687747420248	3.65015859875849	-4.07628873740912	h
4.21460597190898	5.72405743189396	0.19328288035639	h
6.88138747949993	4.48194044993567	0.91587635603145	h
5.04274065166492	2.28311182267689	4.16063059895170	h
4.51350395309922	5.24503075646934	4.49029332145683	h
0.78991200736685	4.51089105417057	6.89623593201492	h
1.28042821763143	1.52894102345320	6.73836821153296	h
-2.90639229312061	2.25006051275075	7.49849164805037	h
-3.09661212486247	4.05762134582962	5.08058707112107	h
-6.38208996577632	1.22734073390422	3.39041602492681	h
-6.06472936034490	-0.41180770691522	5.91352165523450	h

-5.87845905620428	-2.50246841077939	2.71790029156409	c
-1.53883529098525	-1.97549938356368	-7.14620551924495	h
-1.05992199912813	-4.96531067496102	-7.19722812461978	h
-1.83608921044675	-3.61385413941061	-3.80407368910378	o
-5.03528215649339	-3.93548552588452	3.57547690434743	h
-7.71515946613055	-2.85630073042319	2.68023804989296	h
-4.98214305785857	-2.32559004547998	0.24789596536871	o
-4.45313312642787	-4.10644904841270	-3.84268079383740	c
-5.41853751190334	-4.46150969003773	-1.24438296101622	c
-4.78566823264299	-5.64719944990371	-4.85045283903524	h
-5.34757829590983	-2.67719248829628	-4.65337330145965	h
-7.25589932597336	-4.80799097505531	-1.30802893690601	h
-4.57832748220869	-5.94186444457397	-0.46808346886885	h
5.85537957719591	-4.04505184661165	4.98908653214889	c
5.74921476349378	-4.45060597029653	2.39607993247768	c
3.64585510006966	-4.04284086704540	6.40959366030656	c
7.97113584399999	-3.54657988936085	6.16721738751489	f
7.25933270449865	-4.45211775119651	1.42523313576221	h
3.43360106171038	-4.85393021715391	1.22348597465792	c
1.33024139828626	-4.44614621664154	5.23705639427055	c
3.71838278874691	-3.76565583903135	8.18183551210931	h
1.22415217362912	-4.85171923758766	2.64397420555434	c
-0.17983874819611	-4.44465333300279	6.20790319098599	h
-0.35847455879176	-5.12737358744048	1.84256025320582	h
3.36107337303313	-5.13111524516797	-0.54869918536109	h
-3.38279224923150	3.46451190423912	-5.22677289956646	c
-5.18345558195414	3.63948164615228	-3.32236360258167	c
-4.75736013529058	5.19771201429949	-1.25112928328245	c
-2.53062025316564	6.58093484601105	-1.08422867192301	c
-0.72995692044300	6.40596510409789	-2.98858127712406	c
-1.15595788080030	4.84777253047319	-5.05981559642328	c
-3.98298816379071	1.98213514274915	-7.08450596126391	f
-6.70532761945648	2.69412725486299	-3.43642747148628	h
-5.98808206871516	5.31729388348909	0.05036289352314	h
-2.23945125182662	7.64589000375119	0.33138406557092	h
0.79193401432059	7.35135728990970	-2.87451740821945	h
0.07470736084052	4.72817176402233	-6.36136446501261	h

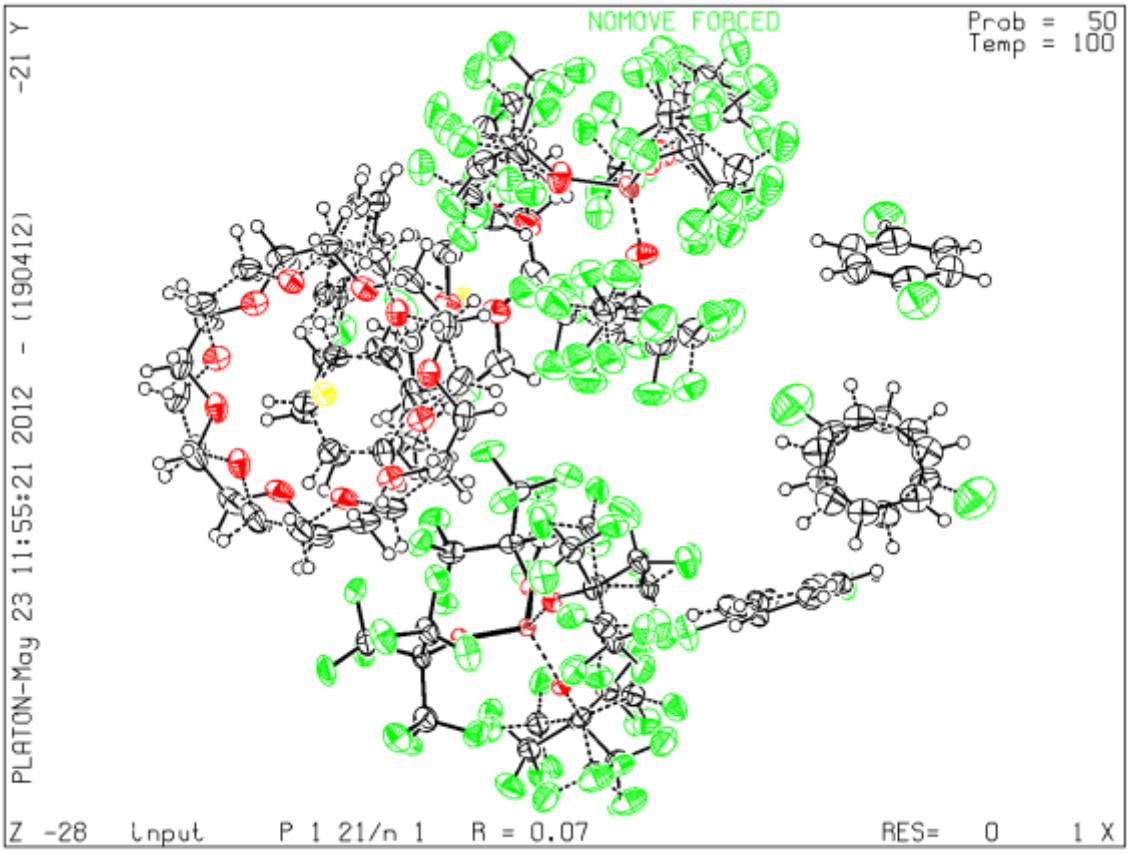
2. Crystal Structure Data

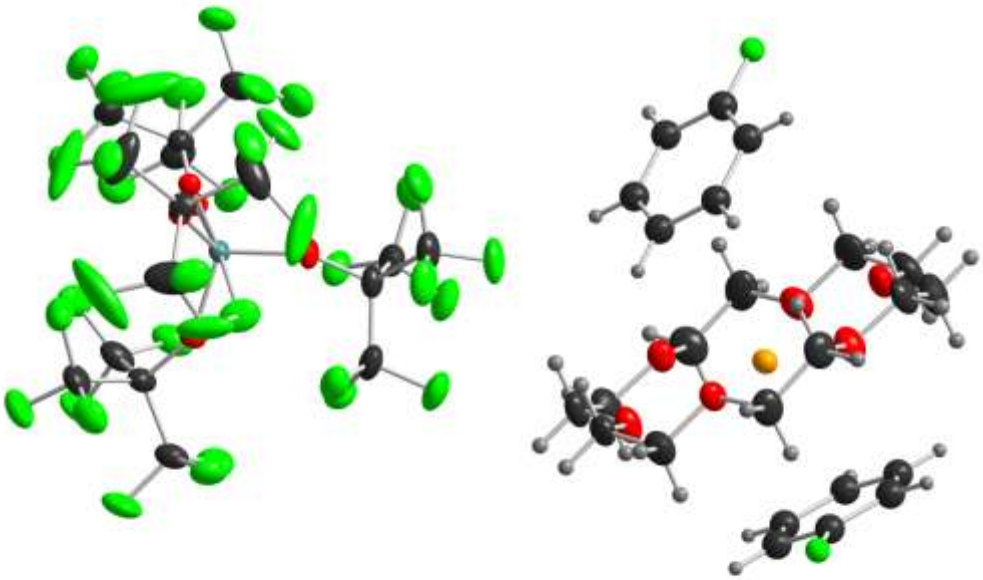
Crystal structures containing the $[Al(OC(CF_3)_3)_4]^-$ anion are commonly severly disordered.[1, 2] As a consequence, the crystals do not scatter well and only sparse high angle data can be recorded. This results in poor data qualitity, which however in most cases does not affect the cationic part of the structures.

Both structures presented herein are highly disordered. Disorder in the anions, solvent molecules and one of two independent crown ether ligands was resolved in each case. While we were able to refine the structure containing the indium crown ether complex (**2**) to R1(wR2) (I>2σ(I))/(all reflections) of 5.39(13.64)/7.61(15.19), the homologous gallium structure (**1**) was impossible to refine further than 7.19(18.61)/9.49(20.49). We do however note that both structures are perfectly isostructural and deduce the credibility of the gallium structure from the homologous indium structure. Both substances crystallized in the same space group and similar parameters, with a slightly larger cell volume for the indium structure. The following table gives the crystallographic positions of all metal atoms: aluminium at the centre of the anions, as well as gallium and indium. The positions can be translated from **1** to **2** a via simple mathematical relationship.

1				**2**			
a	19.7737			a	19.7449		
b	15.9218			b	15.9218		
c	35.5352			c	35.6744		
Al1	0.4096	0.2749	0.8201	Al1	0.4086	0.7274	0.3193
	0.0904	0.7749	0.6799		0.0914	0.2274	0.1807
	0.5904	0.7251	0.1799		0.5914	0.2726	0.6807
	0.9096	0.2251	0.3201		0.9086	0.7726	0.8193
Al2	0.7556	0.8061	0.9352	Al2	0.7556	0.195	0.435
	0.7444	0.3061	0.5648		0.7444	0.695	0.065
	0.2444	0.1939	0.0648		0.2444	0.805	0.565
	0.2556	0.6939	0.4352		0.2556	0.305	0.935
Ga1	0.617	0.7873	0.6779	In1	0.6117	0.2119	0.1763
	0.883	0.2873	0.8221		0.8883	0.7119	0.3237
	0.383	0.2127	0.3221		0.3883	0.7881	0.8237
	0.117	0.7127	0.1779		0.1117	0.2881	0.6763
Ga2	0.2253	0.2449	0.5934	In2	0.2181	0.7548	0.0945
	0.2747	0.7449	0.9066		0.2819	0.2548	0.4055
	0.7747	0.7551	0.4066		0.7819	0.2452	0.9055
	0.7253	0.2551	0.0934		0.7181	0.7452	0.5945

2.1.[Ga([18]crown-6)(PhF)$_2$]$_4$[Al(OC(CF$_3$)$_3$)$_4$]$_4$•PhF (1)





2.1.1. Crystal data and structure refinement for CCDC 864619

Identification code	CCDC 864619
Empirical formula	$C_{166}H_{141}Al_4F_{153}Ga_4O_{40}$
Formula weight	6069.88
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	19.7737(7)
b/Å	15.8400(6)
c/Å	35.5352(12)
α/°	90.00
β/°	96.0003(17)
γ/°	90.00
Volume/Å^3	11069.2(7)
Z	2
ρ_{calc}mg/mm^3	1.821
m/mm^{-1}	0.695
F(000)	640.0
Crystal size/mm^3	0.2 × 0.15 × 0.1
2Θ range for data collection	3.3 to 52.8°
Index ranges	$-24 \le h \le 24$, $-19 \le k \le 19$, $-42 \le l \le 44$
Reflections collected	99060
Independent reflections	22436[R(int) = 0.0364]
Data/restraints/parameters	22436/7127/1980
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0719, wR_2 = 0.1861
Final R indexes [all data]	R_1 = 0.0949, wR_2 = 0.2049
Largest diff. peak/hole / e Å^{-3}	1.15/-1.49

2.1.2. Fractional Atomic Coordinates and Equivalent Isotropic Displacement Parameters

Atom	*x*	*y*	*z*	U(eq)
Ga1	6170.2(2)	7872.6(3)	6779.23(14)	26.17(12)
Ga2	2746.6(3)	7448.5(3)	9065.85(14)	30.94(13)
Al1	4096.1(6)	2749.0(7)	8201.4(3)	17.9(2)
O1	3263.6(13)	3085.7(18)	8111.4(8)	24.0(6)
C1	2635(2)	3111(3)	8230.8(11)	27.4(9)
C2	2197(2)	3738(3)	7974.3(13)	36.2(11)
C3	2301(2)	2221(3)	8195.5(14)	38.9(11)
C4	2664(2)	3405(3)	8650.6(13)	38.2(11)
F1	2295.0(15)	3639(2)	7613.0(8)	42.3(7)
F2	1529.0(14)	3644(2)	8001.2(9)	48.1(8)
F3	2357.7(15)	4534.9(18)	8069.6(9)	45.2(7)
F4	1751.6(15)	2162(2)	8383.4(10)	51.5(8)

F5	2742.6(15)	1636.2(18)	8337(1)	46.7(8)
F6	2117.4(15)	2028.8(19)	7838.0(9)	44.7(7)
F7	2052.4(15)	3650(2)	8739.3(9)	53.2(9)
F8	2878.1(16)	2791(2)	8885.1(8)	48.8(8)
F9	3082.7(14)	4058(2)	8710.5(8)	44.2(7)
O2	4573.5(15)	3297.8(17)	7900.9(8)	26.3(6)
C5	4686(2)	4049(3)	7739.3(11)	28.7(9)
C6	4033(3)	4380(3)	7507.8(13)	36.9(11)
C7	5252(3)	3918(3)	7472.2(13)	38.7(11)
C8	4935(2)	4708(3)	8048.6(12)	32.7(10)
F10	3609.8(15)	4735.9(18)	7727.7(9)	42.9(7)
F11	4164.7(17)	4964.5(19)	7249.1(8)	48.4(8)
F12	3700.9(16)	3753.3(18)	7318.0(8)	42.6(7)
F13	4998.9(17)	3536.7(19)	7151.7(8)	47.4(8)
F14	5526.7(17)	4645.2(19)	7375.7(9)	50.0(8)
F15	5748.1(15)	3435(2)	7631.8(9)	45.2(7)
F16	4902.9(17)	5501.4(17)	7917.6(8)	45.2(7)
F17	5576.9(15)	4556.9(19)	8185.3(8)	42.8(7)
F18	4559.1(15)	4666.3(17)	8335.8(7)	36.0(6)
O3	4349(4)	2941(5)	8668.1(16)	22.8(7)
C9	4728(4)	2756(5)	8997(2)	26.2(10)
C10	4577(4)	3439(5)	9294.9(19)	37.5(15)
C11	4567(4)	1871(4)	9153.5(19)	31.0(14)
C12	5485(3)	2798(5)	8931.3(19)	34.9(14)
F19	4537(3)	4199(3)	9137.2(15)	40.3(11)
F20	3994(3)	3265(4)	9441.1(13)	50.2(12)
F21	5078(3)	3457(4)	9580.3(14)	46.7(13)
F22	3908(3)	1734(3)	9126.4(15)	44(1)
F23	4811(3)	1788(4)	9524.3(13)	39.9(13)
F24	4833(3)	1273(3)	8951.4(14)	45.5(11)
F25	5591(2)	2419(3)	8603.1(15)	40.6(10)
F26	5672(3)	3620(4)	8908.0(15)	52.5(13)
F27	5896(3)	2426(4)	9210.3(14)	43.8(14)
O3B	4316(8)	2896(9)	8684(3)	22.8(7)
C9B	4820(6)	2773(7)	8974(3)	26.2(10)
C10B	4514(6)	2143(7)	9245(3)	37.5(15)
C11B	5484(5)	2387(7)	8848(3)	31.0(14)
C12B	4992(5)	3612(6)	9184(3)	34.9(14)
F19B	4073(4)	2516(5)	9443(2)	40.3(11)
F20B	5011(6)	1748(9)	9470(3)	50.2(12)
F21B	4195(6)	1512(6)	9040(2)	46.7(13)
F22B	5410(4)	1579(5)	8759(2)	44(1)

F23B	6013(5)	2459(8)	9103(3)	39.9(13)
F24B	5662(5)	2819(6)	8551(3)	45.5(11)
F25B	5402(4)	4092(5)	9006(2)	40.6(10)
F26B	5307(5)	3533(9)	9534(3)	52.5(13)
F27B	4417(5)	4056(8)	9219(3)	43.8(14)
O4	4215(3)	1692(3)	8106.9(17)	21.7(6)
C13	4294(3)	1106(4)	7836.6(18)	25.0(9)
C14	4388(3)	233(4)	8033.2(18)	32.4(14)
C15	3675(3)	1066(4)	7528.5(18)	33.6(14)
C16	4942(3)	1305(4)	7638.0(18)	31.9(13)
F28	4981(3)	151(3)	8220.4(14)	55.2(11)
F29	3911(3)	138(3)	8275.0(14)	53.6(13)
F30	4274(3)	-400(3)	7772.7(16)	32(1)
F31	3505(3)	1869(3)	7423.4(14)	45.9(12)
F32	3150(2)	691(3)	7658.9(14)	51.2(12)
F33	3793(2)	647(3)	7221.4(14)	36.1(12)
F34	5435(2)	1591(3)	7899.7(14)	44.9(11)
F35	4828(2)	1872(3)	7374.3(12)	42.5(10)
F36	5176(4)	634(5)	7468(2)	44.8(11)
O4B	4181(8)	1686(7)	8105(3)	21.7(6)
C13B	4341(6)	1111(8)	7848(3)	25.0(9)
C14B	4072(6)	245(7)	7973(3)	32.4(14)
C15B	3982(6)	1362(8)	7453(3)	33.6(14)
C16B	5117(6)	1035(7)	7818(3)	31.9(13)
F28B	3384(5)	264(7)	7897(3)	55.2(11)
F29B	4389(9)	-408(10)	7823(5)	53.6(13)
F30B	4270(5)	127(6)	8344(2)	32(1)
F31B	4384(6)	1932(6)	7290(3)	45.9(12)
F32B	3949(8)	715(10)	7214(5)	51.2(12)
F33B	3360(5)	1642(7)	7493(3)	36.1(12)
F34B	5383(5)	552(6)	8110(3)	44.9(11)
F35B	5391(7)	1792(6)	7787(3)	42.5(10)
F36B	5260(10)	591(12)	7518(5)	44.8(11)
Al1A	7555.6(6)	8060.8(9)	9351.9(4)	25.5(3)
O1A	8284(4)	8298(6)	9141(2)	32.9(8)
C1A	8659(4)	8218(5)	8849(2)	28.2(11)
C2A	8254(4)	8533(5)	8478(2)	38.0(16)
C3A	9309(4)	8773(5)	8927(2)	38.9(17)
C4A	8861(5)	7288(5)	8798(2)	36.4(13)
F1A	7606(3)	8273(4)	8455.3(18)	50.2(13)
F2A	8240(4)	9382(4)	8472.6(17)	55.8(14)
F3A	8508(3)	8289(4)	8162.5(15)	45.4(13)

F4A	9155(3)	9512(4)	9079.5(18)	51.4(13)
F5A	9625(3)	8918(4)	8619.1(17)	52.0(14)
F6A	9747(3)	8388(4)	9171.4(18)	55.9(14)
F7A	9362(3)	7189(4)	8582.9(19)	48.9(16)
F8A	8330(3)	6835(4)	8651.8(18)	37.6(13)
F9A	9039(4)	6924(5)	9129(2)	57.9(17)
O1C	8249(5)	8282(10)	9116(3)	32.9(8)
C1C	8562(5)	8246(7)	8799(3)	28.2(11)
C2C	8035(6)	8428(7)	8453(3)	38.0(16)
C3C	9110(6)	8947(7)	8830(3)	38.9(17)
C4C	8885(6)	7374(7)	8746(3)	36.4(13)
F1C	7875(5)	9239(5)	8429(2)	50.2(13)
F2C	8247(6)	8216(7)	8125(3)	55.8(14)
F3C	7479(5)	7973(6)	8476(3)	45.4(13)
F4C	9660(5)	8726(6)	9068(3)	51.4(13)
F5C	9340(5)	9114(6)	8500(3)	52.0(14)
F6C	8877(5)	9651(6)	8958(3)	55.9(14)
F7C	8439(6)	6811(8)	8587(3)	48.9(16)
F8C	9343(5)	7393(6)	8496(3)	37.6(13)
F9C	9196(7)	7107(8)	9079(3)	57.9(17)
O2A	7319(5)	7044(5)	9229(3)	43.8(12)
C5A	6778(4)	6507(5)	9169(2)	42.0(19)
C6A	6238(4)	6834(6)	8844(3)	48(2)
C7A	6426(5)	6389(6)	9536(3)	53(2)
C8A	7074(5)	5657(5)	9052(3)	51.6(18)
F10A	6543(4)	7135(6)	8555(2)	72.6(17)
F11A	5840(4)	6176(5)	8708(2)	76.5(17)
F12A	5829(3)	7393(4)	8967(2)	64.3(14)
F13A	5798(3)	6046(4)	9464(2)	62.6(14)
F14A	6326(4)	7147(4)	9694(2)	55.6(13)
F15A	6812(4)	5941(5)	9784(2)	80(2)
F16A	7226(5)	5715(8)	8692(2)	68(2)
F17A	6638(4)	5027(4)	9088(3)	80.2(19)
F18A	7661(4)	5481(5)	9269(3)	64(2)
O2C	7321(7)	7040(5)	9277(4)	43.8(12)
C5C	6931(5)	6333(6)	9284(3)	42.0(19)
C6C	6376(6)	6526(8)	9553(3)	48(2)
C7C	7354(5)	5554(6)	9432(3)	53(2)
C8C	6618(5)	6164(6)	8874(3)	51.6(18)
F10C	5902(4)	7018(6)	9373(3)	72.6(17)
F11C	6647(5)	6879(6)	9870(3)	76.5(17)
F12C	6082(4)	5808(5)	9655(3)	64.3(14)

F13C	7516(4)	5617(5)	9804(2)	62.6(14)
F14C	6997(4)	4841(4)	9358(2)	55.6(13)
F15C	7915(6)	5539(9)	9268(4)	80(2)
F16C	6404(5)	6870(7)	8694(3)	68(2)
F17C	6066(5)	5674(6)	8875(3)	80.2(19)
F18C	7053(6)	5781(8)	8664(4)	64(2)
O3A	6880(6)	8687(8)	9181(4)	46.5(10)
C9A	6447(5)	9310(7)	9244(3)	36.6(18)
C10A	6830(5)	10108(6)	9122(3)	52(3)
C11A	6283(5)	9405(7)	9657(3)	54(4)
C12A	5790(5)	9181(7)	8972(3)	45(3)
F19A	7495(5)	10043(7)	9241(3)	62.0(15)
F20A	6562(6)	10798(6)	9241(3)	71.3(18)
F21A	6810(7)	10195(8)	8746(3)	65.6(16)
F22A	5720(5)	9904(6)	9677(2)	54.7(13)
F23A	6779(5)	9695(6)	9900(3)	57.7(13)
F24A	6130(5)	8680(5)	9800(2)	48.1(12)
F25A	5438(4)	9893(6)	8916(3)	60.3(14)
F26A	5377(4)	8620(7)	9111(3)	61.2(16)
F27A	5925(5)	8876(6)	8644(2)	52.9(12)
O3C	6870(4)	8712(5)	9206(3)	46.5(10)
C9C	6614(4)	9513(5)	9211(2)	36.6(18)
C10C	6460(5)	9918(6)	8810(2)	55(3)
C11C	7078(4)	10163(5)	9453(2)	46(2)
C12C	5928(4)	9454(5)	9385(2)	52(2)
F19C	6203(3)	9336(4)	8565.3(16)	62.0(15)
F20C	7055(3)	10145(5)	8689(2)	71.3(18)
F21C	6044(3)	10574(4)	8789.9(17)	65.6(16)
F22C	7014(4)	10010(4)	9817.6(14)	54.7(13)
F23C	6920(3)	10961(3)	9386.5(18)	57.7(13)
F24C	7698(3)	10047(4)	9399.5(16)	48.1(12)
F25C	5985(3)	8961(5)	9685.5(19)	60.3(14)
F26C	5447(3)	9152(5)	9127.3(19)	61.2(16)
F27C	5706(3)	10191(4)	9504.4(17)	52.9(12)
O4A	7721(4)	8258(6)	9825.2(17)	38.4(9)
C13A	8157(4)	8119(5)	10138(2)	38.7(15)
C14A	8875(4)	8406(6)	10077(2)	52.2(19)
C15A	7903(5)	8677(6)	10462(3)	45.9(13)
C16A	8161(4)	7181(5)	10255(2)	50.8(19)
F28A	9178(3)	7809(4)	9876.3(17)	65.6(14)
F29A	9275(3)	8493(5)	10402.4(17)	72.6(15)
F30A	8886(3)	9131(4)	9886.1(18)	64.1(14)

F31A	8192(3)	8414(4)	10800.7(16)	51.1(14)
F32A	8073(4)	9498(5)	10416(2)	64.1(19)
F33A	7239(3)	8648(4)	10460.4(19)	51.5(14)
F34A	8205(3)	6696(4)	9953.0(17)	65.9(14)
F35A	8641(4)	6991(5)	10520.5(19)	81.7(17)
F36A	7564(3)	7000(4)	10393.5(16)	61.1(14)
O4C	7778(7)	8311(11)	9826(2)	38.4(9)
C13C	8257(5)	8352(7)	10127(3)	38.7(15)
C14C	8846(6)	8929(8)	10051(3)	52.2(19)
C15C	7942(7)	8708(9)	10479(4)	45.9(13)
C16C	8534(6)	7461(7)	10222(3)	50.8(19)
F28C	9211(5)	9163(8)	10362(3)	65.6(14)
F29C	8595(6)	9619(7)	9857(3)	72.6(15)
F30C	9259(5)	8567(7)	9823(3)	64.1(14)
F31C	7855(6)	9541(7)	10435(3)	51.1(14)
F32C	8357(7)	8642(8)	10798(3)	64.1(19)
F33C	7358(5)	8346(7)	10503(3)	51.5(14)
F34C	8664(6)	7072(6)	9904(3)	65.9(14)
F35C	9151(6)	7495(8)	10426(3)	81.7(17)
F36C	8066(6)	7027(6)	10408(3)	61.1(14)
C101	5886(3)	6589(3)	5890.9(13)	40.0(12)
C102	6622(3)	6735(4)	5917.5(14)	42.0(12)
O103	6807.7(17)	7469(2)	6126.5(10)	40.5(8)
C104	7494(3)	7688(4)	6144.8(16)	46.3(13)
C105	7635(3)	8471(4)	6347.4(17)	53.0(15)
O106	7440.0(17)	8421(2)	6722.4(10)	38.5(8)
C107	7632(3)	9117(4)	6955.1(17)	51.8(15)
C108	7460(3)	8972(4)	7336.4(16)	49.5(14)
O109	6758.9(17)	8815(2)	7344.1(10)	38.5(8)
C110	6547(3)	8719(4)	7703.4(14)	47.1(14)
C111	5816(3)	8569(4)	7686.0(16)	45.5(13)
O112	5611.4(17)	7872(2)	7459.6(9)	32.5(7)
C113	4925(3)	7660(4)	7448.3(15)	41.7(12)
C114	4763(3)	6886(3)	7229.7(13)	39.9(12)
O115	4930.2(17)	6946(2)	6860.1(9)	36.8(8)
C116	4771(2)	6234(3)	6635.5(13)	32.6(10)
C117	4963(3)	6351(4)	6247.7(15)	41.5(12)
O118	5661.0(16)	6516(2)	6253.4(8)	31.1(7)
C201	3393(3)	5563(4)	9603.6(19)	42.7(16)
C202	4020(3)	6077(4)	9563.8(17)	40.5(14)
O203	3858(2)	6938(3)	9608.0(12)	36.9(9)
C204	4428(3)	7478(4)	9600(2)	41.7(16)

C205	4217(3)	8366(4)	9650.3(18)	43.1(15)
O206	3772(2)	8598(3)	9325.6(12)	37.9(10)
C207	3618(4)	9475(4)	9313(2)	44.5(19)
C208	3170(3)	9665(4)	8966.2(19)	45.3(15)
O209	2542(2)	9228(3)	8980.4(12)	38.3(10)
C210	2056(4)	9410(5)	8668.5(18)	45.8(16)
C211	1420(3)	8938(4)	8702.5(19)	44.5(15)
O212	1570(2)	8070(3)	8680.5(12)	40(1)
C213	981(3)	7568(5)	8714(2)	48.0(16)
C214	1156(3)	6658(5)	8677(2)	46.5(16)
O215	1634(2)	6430(3)	8982.7(12)	39.6(10)
C216	1787(4)	5548(4)	8986.6(19)	43.9(15)
C217	2267(3)	5347(4)	9329.9(18)	41.1(14)
O218	2887(2)	5778(3)	9301.2(11)	35.7(9)
C401	4197(10)	6597(12)	9557(8)	42.7(16)
C402	4288(15)	7461(12)	9713(7)	40.5(14)
O403	3956(9)	8018(10)	9437(5)	36.9(9)
C404	3992(13)	8864(12)	9567(7)	41.7(16)
C405	3731(11)	9430(20)	9262(10)	43.1(15)
O406	3024(8)	9252(11)	9170(5)	37.9(10)
C407	2726(10)	9762(15)	8872(7)	44.5(19)
C408	1988(10)	9621(12)	8815(9)	45.3(15)
O409	1888(9)	8758(10)	8691(5)	38.3(10)
C410	1201(11)	8517(12)	8635(8)	45.8(16)
C411	1107(14)	7636(12)	8525(7)	44.5(15)
O412	1410(9)	7122(10)	8820(5)	40(1)
C413	1272(14)	6258(12)	8765(7)	48.0(16)
C414	1578(9)	5750(18)	9087(8)	46.5(16)
O415	2293(7)	5834(11)	9113(5)	39.6(10)
C416	2634(10)	5350(16)	9405(7)	43.9(15)
C417	3380(11)	5507(12)	9440(9)	41.1(14)
O418	3502(8)	6364(10)	9539(5)	35.7(9)
F501	6436(2)	1540(4)	7253.9(14)	55.4(12)
C501	7047(2)	1385(4)	7426.3(14)	33.1(15)
C502	7109(2)	1239(4)	7814.1(14)	34.0(16)
C503	7745(3)	1082(5)	8006.9(12)	37.5(16)
C504	8319(2)	1070(5)	7811.9(17)	35.8(16)
C505	8256(2)	1216(5)	7424.1(17)	33.8(15)
C506	7621(2)	1373(4)	7231.3(12)	32.7(15)
F511	8671(5)	1083(8)	7192(3)	55.4(12)
C511	8152(6)	1232(12)	7370(4)	33.1(15)
C512	7493(7)	1474(11)	7238(3)	34.0(16)

C513	7007(5)	1569(11)	7491(4)	37.5(16)
C514	7179(7)	1423(11)	7875(4)	35.8(16)
C515	7837(7)	1181(13)	8006(3)	33.8(15)
C516	8324(6)	1086(13)	7754(4)	32.7(15)
F601	4995(4)	8385(4)	5761.1(17)	67.8(15)
C601	5206(3)	8878(5)	6040.6(17)	30.4(17)
C602	4778(4)	8939(6)	6326(2)	31.4(17)
C603	4952(5)	9458(7)	6636(2)	34.3(17)
C604	5555(5)	9915(6)	6661.8(19)	35.5(17)
C605	5983(4)	9855(6)	6377(2)	30.8(16)
C606	5809(3)	9336(5)	6066.1(17)	29.1(16)
F611	5980(5)	9181(6)	5746(2)	67.8(15)
C611	5617(5)	9264(8)	6030(3)	30.4(17)
C612	5029(5)	8829(7)	6092(3)	31.4(17)
C613	4724(6)	8968(9)	6422(3)	34.3(17)
C614	5008(7)	9542(10)	6689(3)	35.5(17)
C615	5596(7)	9977(9)	6626(3)	30.8(16)
C616	5901(6)	9838(9)	6297(3)	29.1(16)
F701	4536(2)	8152(3)	8474.2(13)	63.2(13)
C701	3998(2)	7685(3)	8395.6(14)	34.2(15)
C702	3389(2)	7952(3)	8200.5(17)	30.5(14)
C703	2861(2)	7381(3)	8118(2)	32.0(14)
C704	2940(2)	6544(3)	8230(2)	34.9(15)
C705	3548(3)	6277(3)	8426(2)	35.9(14)
C706	4077(2)	6847(3)	8508.2(16)	36.0(15)
F711	4645(7)	6553(12)	8698(4)	63.2(13)
C711	4014(8)	6636(14)	8528(6)	34.2(15)
C712	4080(9)	7490(14)	8449(6)	30.5(14)
C713	3542(13)	7926(12)	8255(8)	32.0(14)
C714	2938(11)	7508(16)	8139(9)	34.9(15)
C715	2871(9)	6654(16)	8218(10)	35.9(14)
C716	3409(11)	6219(12)	8413(9)	36.0(15)
F801	7914(4)	3812(4)	9726(2)	107(2)
C801	8130(3)	3104(3)	9894.7(15)	45.7(16)
C802	7646(2)	2538(4)	9998.4(17)	49.3(16)
C803	7848(3)	1773(3)	10165.6(17)	46.5(16)
C804	8535(3)	1574(3)	10229.0(17)	54.6(18)
C805	9020(2)	2140(4)	10125.4(18)	55.3(18)
C806	8817(2)	2905(3)	9958.2(17)	50.5(17)
F811	9167(9)	1139(10)	10360(5)	107(2)
C811	8763(6)	1752(7)	10219(4)	45.7(16)
C812	8988(6)	2522(8)	10092(5)	49.3(16)

C813	8521(8)	3123(7)	9945(4)	46.5(16)
C814	7828(7)	2954(9)	9925(4)	54.6(18)
C815	7603(5)	2183(10)	10051(5)	55.3(18)
C816	8070(7)	1582(8)	10198(5)	50.5(17)
C901	9814(4)	4660(4)	10298.0(18)	62.2(17)
F901	9634(5)	4286(6)	10616(2)	87(3)
C902	9358(3)	5210(4)	10122(2)	61.6(17)
C903	9573(4)	5514(4)	9836(2)	66.1(18)

2.1.3. Anisotropic Displacement Parameters

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ga1	23.3(2)	26.9(2)	28.2(2)	0.72(19)	1.93(19)	-0.14(18)
Ga2	30.1(3)	36.2(3)	27.0(3)	-2.4(2)	5.3(2)	0.5(2)
Al1	17.4(6)	19.5(5)	17.3(5)	-1.1(4)	4.5(4)	0.6(4)
O1	19.3(14)	29.0(15)	23.9(14)	-1.3(12)	3.4(11)	4.2(11)
C1	20(2)	36(2)	26(2)	-3.7(17)	3.0(17)	4.4(17)
C2	25(2)	44(3)	38(3)	-4(2)	-3(2)	8(2)
C3	29(2)	43(3)	46(3)	3(2)	12(2)	-1(2)
C4	25(2)	54(3)	37(3)	-11(2)	8(2)	3(2)
F1	39.1(16)	52.6(18)	32.9(15)	3.0(13)	-6.5(12)	10.6(13)
F2	20.8(14)	60(2)	62(2)	-4.6(16)	-2.1(13)	10.5(13)
F3	40.2(16)	30.9(15)	64(2)	-4.9(14)	0.5(14)	12.0(12)
F4	33.4(16)	61(2)	63(2)	3.3(16)	21.8(15)	-6.8(14)
F5	40.8(17)	37.2(16)	64(2)	13.0(14)	15.6(15)	2.2(13)
F6	39.0(16)	44.6(17)	50.8(18)	-17.2(14)	6.0(14)	-8.6(13)
F7	32.6(16)	85(2)	44.0(17)	-21.9(16)	12.3(13)	12.3(16)
F8	40.8(17)	79(2)	28.0(15)	8.2(15)	11.4(13)	7.8(16)
F9	33.7(15)	55.6(18)	42.6(16)	-23.4(14)	0.3(13)	7.1(13)
O2	30.7(16)	23.1(14)	27.1(15)	0.9(12)	12.8(13)	-3.2(12)
C5	36(2)	27(2)	25(2)	0.9(17)	11.2(18)	-5.6(18)
C6	48(3)	32(2)	31(2)	7.5(19)	7(2)	-8(2)
C7	49(3)	36(3)	34(3)	-2(2)	22(2)	-10(2)
C8	42(3)	26(2)	31(2)	0.5(18)	8(2)	-4.0(19)
F10	45.6(17)	35.0(15)	48.5(17)	7.4(13)	7.1(14)	8.0(13)
F11	67(2)	40.5(16)	36.9(16)	15.6(13)	2.4(15)	-10.7(15)
F12	50.8(18)	40.6(16)	34.7(15)	5.0(12)	-3.1(13)	-11.8(13)
F13	68(2)	47.4(17)	30.8(15)	-7.7(13)	23.7(14)	-15.8(15)
F14	64(2)	43.4(17)	48.0(18)	0.5(14)	31.0(15)	-22.2(15)
F15	37.2(16)	48.3(17)	54.1(18)	-2.7(14)	23.7(14)	-4.0(13)
F16	74(2)	25.8(14)	37.4(16)	1.1(12)	13.4(15)	-10.5(14)
F17	40.5(17)	47.0(17)	40.9(16)	-6.3(13)	3.5(13)	-10.7(13)
F18	52.1(17)	30.2(14)	27.8(13)	-0.9(11)	14.0(12)	3.1(12)

O3	24.8(16)	25.2(16)	18.3(14)	-1.1(12)	1.5(12)	1.7(13)
C9	25(3)	33(2)	20(2)	-1.3(17)	0.9(19)	2.4(19)
C10	43(4)	42(4)	27(3)	0(3)	-1(3)	2(3)
C11	30(3)	39(3)	23(3)	-1(3)	-5(3)	7(3)
C12	28(3)	45(4)	30(3)	-6(3)	-4(3)	-2(3)
F19	56(3)	36(2)	29(2)	-5.9(17)	8.7(19)	-1.0(19)
F20	51(3)	69(3)	33(2)	-3(2)	15(2)	7(2)
F21	68(4)	42(2)	26(2)	-3.1(17)	-17(2)	-12(2)
F22	44(2)	36(2)	52(3)	2.3(19)	4(2)	4.2(18)
F23	48(3)	52(3)	20(2)	11.6(19)	1.9(19)	11(2)
F24	50(3)	38(2)	47(2)	0.2(19)	-1(2)	12.3(19)
F25	31(2)	46(2)	45(2)	-7(2)	4.1(18)	6.9(19)
F26	36(2)	71(3)	49(3)	8(2)	-3(2)	-27(2)
F27	33(2)	69(3)	27(3)	-1(2)	-2.7(19)	10(2)
O3B	24.8(16)	25.2(16)	18.3(14)	-1.1(12)	1.5(12)	1.7(13)
C9B	25(3)	33(2)	20(2)	-1.3(17)	0.9(19)	2.4(19)
C10B	43(4)	42(4)	27(3)	0(3)	-1(3)	2(3)
C11B	30(3)	39(3)	23(3)	-1(3)	-5(3)	7(3)
C12B	28(3)	45(4)	30(3)	-6(3)	-4(3)	-2(3)
F19B	56(3)	36(2)	29(2)	-5.9(17)	8.7(19)	-1.0(19)
F20B	51(3)	69(3)	33(2)	-3(2)	15(2)	7(2)
F21B	68(4)	42(2)	26(2)	-3.1(17)	-17(2)	-12(2)
F22B	44(2)	36(2)	52(3)	2.3(19)	4(2)	4.2(18)
F23B	48(3)	52(3)	20(2)	11.6(19)	1.9(19)	11(2)
F24B	50(3)	38(2)	47(2)	0.2(19)	-1(2)	12.3(19)
F25B	31(2)	46(2)	45(2)	-7(2)	4.1(18)	6.9(19)
F26B	36(2)	71(3)	49(3)	8(2)	-3(2)	-27(2)
F27B	33(2)	69(3)	27(3)	-1(2)	-2.7(19)	10(2)
O4	23.7(14)	20.7(12)	21.2(12)	-1.9(10)	5.1(11)	1(1)
C13	26.4(19)	23.0(17)	26.0(18)	-4.2(15)	4.9(16)	3.1(15)
C14	39(3)	28(2)	30(2)	-4.3(18)	5(2)	3(2)
C15	32(3)	35(3)	33(2)	-10(2)	1(2)	2(2)
C16	31(2)	31(3)	35(3)	-8(2)	10(2)	-1(2)
F28	67(2)	43(2)	53(2)	-5.5(17)	-8.3(19)	14.2(19)
F29	80(3)	37(2)	48(2)	2.2(17)	25(2)	-4(2)
F30	40(2)	21.7(16)	35(2)	-6.5(14)	6.1(16)	1.1(15)
F31	53(2)	41(2)	40(2)	-0.2(17)	-7.8(18)	12.1(18)
F32	37(2)	58(2)	59(2)	-26.6(19)	5.9(18)	-10.0(17)
F33	39(2)	42(2)	25.0(17)	-11.4(15)	-6.0(17)	4.2(18)
F34	28.0(18)	54(2)	53(2)	-15.9(18)	6.0(18)	2.4(17)
F35	55(2)	35.8(18)	40.9(19)	-2.3(15)	25.5(17)	-5.5(17)
F36	44(2)	41.4(16)	52(2)	-14.7(16)	20.9(17)	4.8(15)

O4B	23.7(14)	20.7(12)	21.2(12)	-1.9(10)	5.1(11)	1(1)
C13B	26.4(19)	23.0(17)	26.0(18)	-4.2(15)	4.9(16)	3.1(15)
C14B	39(3)	28(2)	30(2)	-4.3(18)	5(2)	3(2)
C15B	32(3)	35(3)	33(2)	-10(2)	1(2)	2(2)
C16B	31(2)	31(3)	35(3)	-8(2)	10(2)	-1(2)
F28B	67(2)	43(2)	53(2)	-5.5(17)	-8.3(19)	14.2(19)
F29B	80(3)	37(2)	48(2)	2.2(17)	25(2)	-4(2)
F30B	40(2)	21.7(16)	35(2)	-6.5(14)	6.1(16)	1.1(15)
F31B	53(2)	41(2)	40(2)	-0.2(17)	-7.8(18)	12.1(18)
F32B	37(2)	58(2)	59(2)	-26.6(19)	5.9(18)	-10.0(17)
F33B	39(2)	42(2)	25.0(17)	-11.4(15)	-6.0(17)	4.2(18)
F34B	28.0(18)	54(2)	53(2)	-15.9(18)	6.0(18)	2.4(17)
F35B	55(2)	35.8(18)	40.9(19)	-2.3(15)	25.5(17)	-5.5(17)
F36B	44(2)	41.4(16)	52(2)	-14.7(16)	20.9(17)	4.8(15)
Al1A	19.8(6)	35.9(7)	21.3(6)	-2.8(5)	5.4(5)	-2.6(5)
O1A	29.0(16)	46.8(18)	24.6(16)	0.9(14)	10.9(13)	-2.6(14)
C1A	27(2)	33(2)	26(2)	-1.8(17)	7.7(18)	-0.1(17)
C2A	41(3)	42(3)	32(2)	3(2)	7(2)	1(3)
C3A	41(3)	41(3)	36(3)	-4(2)	10(2)	-3(3)
C4A	33(2)	37(2)	39(3)	-4(2)	5(2)	1.7(19)
F1A	51(3)	54(2)	43(2)	2(2)	-8(2)	13(2)
F2A	62(3)	58(2)	50(2)	8(2)	13(2)	5(2)
F3A	50(2)	61(3)	26.0(19)	0.1(18)	9.2(18)	8(2)
F4A	48(2)	47(2)	61(3)	-17(2)	15(2)	-14.5(19)
F5A	48(3)	59(2)	53(3)	0(2)	25(2)	-12(2)
F6A	46(2)	63(3)	59(3)	-11(2)	6(2)	-6(2)
F7A	47(2)	46(3)	56(3)	0(2)	14(2)	2(2)
F8A	34(2)	36(2)	45(2)	-16.7(18)	18.8(18)	-2.7(17)
F9A	61(3)	56(3)	55(2)	11(2)	-1(2)	16(2)
O1C	29.0(16)	46.8(18)	24.6(16)	0.9(14)	10.9(13)	-2.6(14)
C1C	27(2)	33(2)	26(2)	-1.8(17)	7.7(18)	-0.1(17)
C2C	41(3)	42(3)	32(2)	3(2)	7(2)	1(3)
C3C	41(3)	41(3)	36(3)	-4(2)	10(2)	-3(3)
C4C	33(2)	37(2)	39(3)	-4(2)	5(2)	1.7(19)
F1C	51(3)	54(2)	43(2)	2(2)	-8(2)	13(2)
F2C	62(3)	58(2)	50(2)	8(2)	13(2)	5(2)
F3C	50(2)	61(3)	26.0(19)	0.1(18)	9.2(18)	8(2)
F4C	48(2)	47(2)	61(3)	-17(2)	15(2)	-14.5(19)
F5C	48(3)	59(2)	53(3)	0(2)	25(2)	-12(2)
F6C	46(2)	63(3)	59(3)	-11(2)	6(2)	-6(2)
F7C	47(2)	46(3)	56(3)	0(2)	14(2)	2(2)
F8C	34(2)	36(2)	45(2)	-16.7(18)	18.8(18)	-2.7(17)

F9C	61(3)	56(3)	55(2)	11(2)	-1(2)	16(2)
O2A	51(2)	34.2(19)	50(3)	-12.8(17)	23(2)	-10.9(16)
C5A	39(4)	42(4)	49(5)	-5(3)	21(3)	-11(3)
C6A	30(4)	48(5)	67(5)	-12(4)	5(4)	1(3)
C7A	54(5)	52(5)	58(4)	15(4)	32(4)	-5(4)
C8A	54(5)	39(4)	63(4)	1(3)	9(4)	-11(3)
F10A	50(3)	88(4)	81(4)	-14(3)	14(3)	-15(3)
F11A	69(4)	71(4)	92(4)	-29(3)	19(3)	-13(3)
F12A	38(3)	69(3)	87(4)	-5(3)	10(3)	-6(2)
F13A	50(3)	63(3)	78(4)	-1(3)	21(3)	-7(2)
F14A	65(3)	45(3)	63(3)	-4(2)	33(3)	-1(2)
F15A	96(5)	68(4)	82(4)	27(3)	38(4)	1(4)
F16A	58(4)	91(5)	58(4)	-24(3)	16(3)	-13(3)
F17A	64(4)	47(3)	132(6)	-14(3)	21(4)	-25(3)
F18A	80(5)	40(3)	75(4)	-1(3)	16(4)	-15(3)
O2C	51(2)	34.2(19)	50(3)	-12.8(17)	23(2)	-10.9(16)
C5C	39(4)	42(4)	49(5)	-5(3)	21(3)	-11(3)
C6C	30(4)	48(5)	67(5)	-12(4)	5(4)	1(3)
C7C	54(5)	52(5)	58(4)	15(4)	32(4)	-5(4)
C8C	54(5)	39(4)	63(4)	1(3)	9(4)	-11(3)
F10C	50(3)	88(4)	81(4)	-14(3)	14(3)	-15(3)
F11C	69(4)	71(4)	92(4)	-29(3)	19(3)	-13(3)
F12C	38(3)	69(3)	87(4)	-5(3)	10(3)	-6(2)
F13C	50(3)	63(3)	78(4)	-1(3)	21(3)	-7(2)
F14C	65(3)	45(3)	63(3)	-4(2)	33(3)	-1(2)
F15C	96(5)	68(4)	82(4)	27(3)	38(4)	1(4)
F16C	58(4)	91(5)	58(4)	-24(3)	16(3)	-13(3)
F17C	64(4)	47(3)	132(6)	-14(3)	21(4)	-25(3)
F18C	80(5)	40(3)	75(4)	-1(3)	16(4)	-15(3)
O3A	46(2)	53(2)	40(2)	-9.7(18)	5.1(17)	19.8(18)
C9A	22(4)	52(4)	36(3)	-8(3)	2(3)	11(3)
C10A	24(6)	34(6)	92(10)	0(6)	-18(6)	0(5)
C11A	15(6)	92(10)	57(6)	-57(7)	7(5)	-5(6)
C12A	36(7)	61(8)	40(6)	-12(6)	12(5)	-19(6)
F19A	76(4)	63(3)	43(3)	-10(2)	-9(3)	13(3)
F20A	62(4)	65(4)	87(4)	12(3)	8(3)	21(3)
F21A	69(4)	61(3)	63(3)	14(3)	-9(3)	29(3)
F22A	77(4)	53(3)	34(2)	-12(2)	4(2)	12(3)
F23A	60(3)	46(3)	66(3)	-8(2)	3(3)	10(2)
F24A	59(3)	48(3)	36(3)	-2(2)	0(2)	-8(2)
F25A	47(3)	74(4)	61(3)	21(3)	10(2)	9(3)
F26A	30(2)	83(5)	70(3)	-21(4)	-1(2)	-9(3)

F27A	56(3)	57(3)	48(3)	-3(2)	19(2)	12(2)
O3C	46(2)	53(2)	40(2)	-9.7(18)	5.1(17)	19.8(18)
C9C	22(4)	52(4)	36(3)	-8(3)	2(3)	11(3)
C10C	48(6)	64(7)	57(5)	3(5)	21(4)	10(5)
C11C	64(6)	33(4)	43(5)	-2(4)	8(4)	18(4)
C12C	54(5)	46(5)	60(6)	-1(4)	25(5)	5(4)
F19C	76(4)	63(3)	43(3)	-10(2)	-9(3)	13(3)
F20C	62(4)	65(4)	87(4)	12(3)	8(3)	21(3)
F21C	69(4)	61(3)	63(3)	14(3)	-9(3)	29(3)
F22C	77(4)	53(3)	34(2)	-12(2)	4(2)	12(3)
F23C	60(3)	46(3)	66(3)	-8(2)	3(3)	10(2)
F24C	59(3)	48(3)	36(3)	-2(2)	0(2)	-8(2)
F25C	47(3)	74(4)	61(3)	21(3)	10(2)	9(3)
F26C	30(2)	83(5)	70(3)	-21(4)	-1(2)	-9(3)
F27C	56(3)	57(3)	48(3)	-3(2)	19(2)	12(2)
O4A	37(2)	51(2)	26.7(15)	2.5(14)	2.9(14)	-0.3(16)
C13A	40(3)	46(3)	30(2)	1(2)	2(2)	1(2)
C14A	49(3)	64(4)	43(3)	1(3)	1(2)	-4(3)
C15A	47(3)	55(3)	36(2)	-3(2)	4(2)	6(2)
C16A	56(4)	56(3)	41(3)	0(3)	13(3)	4(3)
F28A	49(2)	93(3)	53(2)	-8(2)	1(2)	8(2)
F29A	62(3)	95(3)	58(3)	-4(2)	-9(2)	-5(2)
F30A	53(3)	86(3)	53(2)	-6(2)	5(2)	-19(2)
F31A	62(3)	60(3)	30(2)	-0.9(19)	1.6(19)	-1(2)
F32A	70(3)	67(3)	54(3)	-7(2)	-1(2)	-2(2)
F33A	56(2)	54(3)	46(2)	0(2)	15.3(18)	9(2)
F34A	75(3)	62(3)	60(2)	-3(2)	6(2)	22(2)
F35A	85(3)	84(3)	72(3)	9(2)	-13(2)	26(2)
F36A	73(3)	59(2)	54(2)	13.6(19)	20(3)	1(3)
O4C	37(2)	51(2)	26.7(15)	2.5(14)	2.9(14)	-0.3(16)
C13C	40(3)	46(3)	30(2)	1(2)	2(2)	1(2)
C14C	49(3)	64(4)	43(3)	1(3)	1(2)	-4(3)
C15C	47(3)	55(3)	36(2)	-3(2)	4(2)	6(2)
C16C	56(4)	56(3)	41(3)	0(3)	13(3)	4(3)
F28C	49(2)	93(3)	53(2)	-8(2)	1(2)	8(2)
F29C	62(3)	95(3)	58(3)	-4(2)	-9(2)	-5(2)
F30C	53(3)	86(3)	53(2)	-6(2)	5(2)	-19(2)
F31C	62(3)	60(3)	30(2)	-0.9(19)	1.6(19)	-1(2)
F32C	70(3)	67(3)	54(3)	-7(2)	-1(2)	-2(2)
F33C	56(2)	54(3)	46(2)	0(2)	15.3(18)	9(2)
F34C	75(3)	62(3)	60(2)	-3(2)	6(2)	22(2)
F35C	85(3)	84(3)	72(3)	9(2)	-13(2)	26(2)

F36C	73(3)	59(2)	54(2)	13.6(19)	20(3)	1(3)
C101	48(3)	46(3)	28(2)	-8(2)	9(2)	-8(2)
C102	48(3)	53(3)	26(2)	-3(2)	14(2)	1(2)
O103	34.2(19)	43(2)	47(2)	-11.5(16)	17.3(16)	-5.2(15)
C104	33(3)	66(4)	44(3)	1(3)	19(2)	-6(2)
C105	39(3)	64(4)	60(4)	-2(3)	22(3)	-12(3)
O106	30.5(18)	45(2)	40.5(19)	4.0(15)	5.1(15)	-10.7(15)
C107	34(3)	56(3)	65(4)	-13(3)	6(3)	-18(3)
C108	41(3)	55(3)	49(3)	-5(3)	-9(3)	-21(3)
O109	31.3(18)	46(2)	37.7(19)	-11.5(15)	0.4(15)	-7.3(15)
C110	58(3)	51(3)	31(3)	-11(2)	-1(2)	-20(3)
C111	47(3)	47(3)	43(3)	-20(2)	7(2)	-4(2)
O112	35.9(18)	37.9(18)	23.8(15)	-5.3(13)	4.2(13)	-6.8(14)
C113	33(3)	57(3)	37(3)	-11(2)	16(2)	-1(2)
C114	38(3)	54(3)	30(2)	0(2)	12(2)	-14(2)
O115	35.5(18)	43.2(19)	33.2(17)	-9.3(14)	10.7(14)	-13.7(15)
C116	28(2)	35(2)	35(2)	-3.2(19)	2.5(19)	-11.4(19)
C117	38(3)	44(3)	42(3)	-9(2)	2(2)	-12(2)
O118	30.0(17)	44.0(18)	19.5(15)	-0.6(13)	3.1(12)	-4.2(14)
C201	56(4)	41(3)	33(3)	7(3)	12(3)	12(3)
C202	43(3)	52(4)	27(3)	6(3)	4(3)	13(3)
O203	34(2)	43(2)	33(2)	1.5(18)	5.9(18)	5.6(19)
C204	28(3)	62(4)	34(3)	-1(3)	-3(3)	-2(3)
C205	31(3)	60(4)	38(3)	-4(3)	5(3)	-10(3)
O206	34(2)	44(2)	36(2)	-3.1(18)	5.6(18)	-6.4(18)
C207	45(4)	34(3)	58(4)	-6(3)	20(3)	-10(3)
C208	51(4)	36(3)	53(4)	3(3)	26(3)	-10(3)
O209	46(2)	37(2)	33(2)	1.3(17)	9.3(19)	-3.2(19)
C210	57(4)	50(4)	30(3)	5(3)	5(3)	16(3)
C211	46(4)	54(4)	33(3)	-2(3)	3(3)	19(3)
O212	33(2)	53(3)	34(2)	-4.7(19)	3.2(18)	10.1(19)
C213	26(3)	73(4)	45(4)	-12(3)	5(3)	-1(3)
C214	32(3)	64(4)	43(4)	-17(3)	4(3)	-8(3)
O215	35(2)	43(2)	41(2)	-17.1(19)	7.9(19)	-9.5(18)
C216	52(4)	37(3)	46(4)	-14(3)	19(3)	-14(3)
C217	55(4)	31(3)	42(3)	-7(3)	26(3)	-11(3)
O218	43(2)	34(2)	32(2)	1.3(17)	12.6(18)	-2.1(18)
C401	56(4)	41(3)	33(3)	7(3)	12(3)	12(3)
C402	43(3)	52(4)	27(3)	6(3)	4(3)	13(3)
O403	34(2)	43(2)	33(2)	1.5(18)	5.9(18)	5.6(19)
C404	28(3)	62(4)	34(3)	-1(3)	-3(3)	-2(3)
C405	31(3)	60(4)	38(3)	-4(3)	5(3)	-10(3)

O406	34(2)	44(2)	36(2)	-3.1(18)	5.6(18)	-6.4(18)
C407	45(4)	34(3)	58(4)	-6(3)	20(3)	-10(3)
C408	51(4)	36(3)	53(4)	3(3)	26(3)	-10(3)
O409	46(2)	37(2)	33(2)	1.3(17)	9.3(19)	-3.2(19)
C410	57(4)	50(4)	30(3)	5(3)	5(3)	16(3)
C411	46(4)	54(4)	33(3)	-2(3)	3(3)	19(3)
O412	33(2)	53(3)	34(2)	-4.7(19)	3.2(18)	10.1(19)
C413	26(3)	73(4)	45(4)	-12(3)	5(3)	-1(3)
C414	32(3)	64(4)	43(4)	-17(3)	4(3)	-8(3)
O415	35(2)	43(2)	41(2)	-17.1(19)	7.9(19)	-9.5(18)
C416	52(4)	37(3)	46(4)	-14(3)	19(3)	-14(3)
C417	55(4)	31(3)	42(3)	-7(3)	26(3)	-11(3)
O418	43(2)	34(2)	32(2)	1.3(17)	12.6(18)	-2.1(18)
F501	30(2)	81(3)	54(3)	13(2)	1.1(19)	7(2)
C501	25(3)	37(4)	37(3)	0(3)	-2(3)	5(3)
C502	25(3)	40(4)	37(3)	-2(3)	3(3)	-4(3)
C503	38(4)	41(4)	32(3)	-6(3)	-1(2)	-6(3)
C504	30(3)	35(3)	39(3)	-13(3)	-9(3)	-2(3)
C505	24(3)	33(3)	44(4)	-4(3)	1(3)	-3(3)
C506	30(3)	31(3)	38(3)	6(3)	7(2)	9(3)
F511	30(2)	81(3)	54(3)	13(2)	1.1(19)	7(2)
C511	25(3)	37(4)	37(3)	0(3)	-2(3)	5(3)
C512	25(3)	40(4)	37(3)	-2(3)	3(3)	-4(3)
C513	38(4)	41(4)	32(3)	-6(3)	-1(2)	-6(3)
C514	30(3)	35(3)	39(3)	-13(3)	-9(3)	-2(3)
C515	24(3)	33(3)	44(4)	-4(3)	1(3)	-3(3)
C516	30(3)	31(3)	38(3)	6(3)	7(2)	9(3)
F601	88(4)	64(3)	50(3)	-4(2)	4(3)	4(3)
C601	24(4)	38(4)	28(3)	2(3)	0(3)	4(3)
C602	24(4)	31(3)	39(4)	0(3)	2(3)	5(3)
C603	28(3)	35(4)	41(4)	1(3)	9(3)	6(3)
C604	41(4)	28(4)	39(4)	1(3)	9(3)	2(3)
C605	40(4)	27(3)	24(4)	6(3)	-3(3)	-2(3)
C606	24(4)	40(4)	23(3)	5(2)	-1(3)	-2(3)
F611	88(4)	64(3)	50(3)	-4(2)	4(3)	4(3)
C611	24(4)	38(4)	28(3)	2(3)	0(3)	4(3)
C612	24(4)	31(3)	39(4)	0(3)	2(3)	5(3)
C613	28(3)	35(4)	41(4)	1(3)	9(3)	6(3)
C614	41(4)	28(4)	39(4)	1(3)	9(3)	2(3)
C615	40(4)	27(3)	24(4)	6(3)	-3(3)	-2(3)
C616	24(4)	40(4)	23(3)	5(2)	-1(3)	-2(3)
F701	45(2)	90(3)	52(3)	3(2)	-2(2)	-25(2)

C701	30(3)	50(4)	22(3)	5(3)	3(2)	0(3)
C702	27(3)	42(3)	20(3)	-1(2)	-6(2)	-5(2)
C703	36(3)	36(3)	24(3)	-2(2)	2(2)	-9(2)
C704	39(3)	35(3)	31(3)	-6(3)	5(3)	-2(3)
C705	36(4)	34(3)	38(3)	-9(2)	8(3)	6(2)
C706	29(3)	50(4)	30(3)	2(3)	7(2)	7(2)
F711	45(2)	90(3)	52(3)	3(2)	-2(2)	-25(2)
C711	30(3)	50(4)	22(3)	5(3)	3(2)	0(3)
C712	27(3)	42(3)	20(3)	-1(2)	-6(2)	-5(2)
C713	36(3)	36(3)	24(3)	-2(2)	2(2)	-9(2)
C714	39(3)	35(3)	31(3)	-6(3)	5(3)	-2(3)
C715	36(4)	34(3)	38(3)	-9(2)	8(3)	6(2)
C716	29(3)	50(4)	30(3)	2(3)	7(2)	7(2)
F801	138(4)	88(3)	97(3)	-6(3)	15(3)	16(3)
C801	57(3)	41(3)	41(3)	-6(2)	12(2)	-2(2)
C802	54(3)	51(3)	46(3)	-10(2)	17(2)	0(2)
C803	55(3)	49(3)	38(3)	-3(2)	16(2)	-9(2)
C804	63(3)	53(3)	48(3)	0(3)	9(3)	-5(3)
C805	58(3)	61(3)	48(3)	-3(3)	8(3)	-3(2)
C806	53(3)	53(3)	46(3)	-2(2)	8(3)	-9(2)
F811	138(4)	88(3)	97(3)	-6(3)	15(3)	16(3)
C811	57(3)	41(3)	41(3)	-6(2)	12(2)	-2(2)
C812	54(3)	51(3)	46(3)	-10(2)	17(2)	0(2)
C813	55(3)	49(3)	38(3)	-3(2)	16(2)	-9(2)
C814	63(3)	53(3)	48(3)	0(3)	9(3)	-5(3)
C815	58(3)	61(3)	48(3)	-3(3)	8(3)	-3(2)
C816	53(3)	53(3)	46(3)	-2(2)	8(3)	-9(2)
C901	77(5)	53(4)	58(4)	-7(3)	9(3)	-7(3)
F901	101(7)	86(6)	81(6)	17(5)	33(5)	-10(5)
C902	56(4)	57(4)	74(4)	-2(3)	19(3)	5(3)
C903	55(4)	59(4)	84(5)	-2(3)	5(4)	9(3)

2.1.4. Bond Lengths

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Al1	O1	1.728(3)	C12A	F27A	1.314(11)
Al1	O2	1.731(3)	O3C	C9C	1.367(9)
Al1	O3	1.709(5)	C9C	C10C	1.564(10)
Al1	O3B	1.741(9)	C9C	C11C	1.573(10)
Al1	O4	1.729(5)	C9C	C12C	1.551(9)
Al1	O4B	1.730(10)	C10C	F19C	1.332(10)
O1	C1	1.355(5)	C10C	F20C	1.343(10)
C1	C2	1.549(6)	C10C	F21C	1.323(9)

C1	C3	1.556(6)	C11C	F22C	1.337(9)
C1	C4	1.558(6)	C11C	F23C	1.317(8)
C2	F1	1.328(5)	C11C	F24C	1.273(9)
C2	F2	1.343(5)	C12C	F25C	1.319(9)
C2	F3	1.337(5)	C12C	F26C	1.337(9)
C3	F4	1.337(5)	C12C	F27C	1.332(9)
C3	F5	1.335(6)	O4A	C13A	1.353(9)
C3	F6	1.320(6)	C13A	C14A	1.528(10)
C4	F7	1.338(5)	C13A	C15A	1.573(10)
C4	F8	1.322(6)	C13A	C16A	1.542(10)
C4	F9	1.328(6)	C14A	F28A	1.361(9)
O2	C5	1.350(5)	C14A	F29A	1.338(9)
C5	C6	1.549(6)	C14A	F30A	1.334(9)
C5	C7	1.556(6)	C15A	F31A	1.343(10)
C5	C8	1.559(6)	C15A	F32A	1.359(10)
C6	F10	1.328(6)	C15A	F33A	1.313(9)
C6	F11	1.349(5)	C16A	F34A	1.329(9)
C6	F12	1.334(5)	C16A	F35A	1.303(9)
C7	F13	1.339(5)	C16A	F36A	1.357(10)
C7	F14	1.334(5)	O4C	C13C	1.355(11)
C7	F15	1.324(6)	C13C	C14C	1.527(12)
C8	F16	1.339(5)	C13C	C15C	1.558(12)
C8	F17	1.332(5)	C13C	C16C	1.538(12)
C8	F18	1.326(5)	C14C	F28C	1.308(12)
O3	C9	1.353(8)	C14C	F29C	1.359(13)
C9	C10	1.564(9)	C14C	F30C	1.337(12)
C9	C11	1.552(9)	C15C	F31C	1.337(13)
C9	C12	1.540(9)	C15C	F32C	1.334(13)
C10	F19	1.327(8)	C15C	F33C	1.300(13)
C10	F20	1.341(8)	C16C	F34C	1.338(11)
C10	F21	1.343(8)	C16C	F35C	1.354(12)
C11	F22	1.315(8)	C16C	F36C	1.376(12)
C11	F23	1.362(8)	C101	C102	1.468(7)
C11	F24	1.330(8)	C101	O118	1.411(5)
C12	F25	1.348(8)	C102	O103	1.408(6)
C12	F26	1.359(8)	O103	C104	1.395(6)
C12	F27	1.350(8)	C104	C105	1.447(8)
O3B	C9B	1.369(12)	C105	O106	1.428(6)
C9B	C10B	1.555(12)	O106	C107	1.407(6)
C9B	C11B	1.556(12)	C107	C108	1.449(8)
C9B	C12B	1.545(12)	C108	O109	1.412(6)
C10B	F19B	1.315(12)	O109	C110	1.394(6)

C10B	F20B	1.352(12)	C110	C111	1.460(7)
C10B	F21B	1.353(12)	C111	O112	1.400(6)
C11B	F22B	1.323(11)	O112	C113	1.395(6)
C11B	F23B	1.315(12)	C113	C114	1.468(7)
C11B	F24B	1.337(12)	C114	O115	1.391(6)
C12B	F25B	1.320(11)	O115	C116	1.398(5)
C12B	F26B	1.338(11)	C116	C117	1.479(7)
C12B	F27B	1.353(11)	C117	O118	1.403(6)
O4	C13	1.356(7)	C201	C202	1.503(9)
C13	C14	1.552(8)	C201	O218	1.430(8)
C13	C15	1.554(8)	C202	O203	1.413(7)
C13	C16	1.559(8)	O203	C204	1.418(8)
C14	F28	1.292(8)	C204	C205	1.483(9)
C14	F29	1.350(8)	C205	O206	1.425(8)
C14	F30	1.367(7)	O206	C207	1.421(8)
C15	F31	1.357(7)	C207	C208	1.471(10)
C15	F32	1.322(8)	C208	O209	1.427(7)
C15	F33	1.319(7)	O209	C210	1.418(7)
C16	F34	1.352(7)	C210	C211	1.479(9)
C16	F35	1.300(7)	C211	O212	1.411(8)
C16	F36	1.329(8)	O212	C213	1.426(8)
O4B	C13B	1.352(12)	C213	C214	1.492(9)
C13B	C14B	1.554(12)	C214	O215	1.412(8)
C13B	C15B	1.556(12)	O215	C216	1.429(8)
C13B	C16B	1.553(12)	C216	C217	1.500(9)
C14B	F28B	1.360(12)	C217	O218	1.417(7)
C14B	F29B	1.348(13)	C401	C402	1.481(18)
C14B	F30B	1.348(12)	C401	O418	1.418(17)
C15B	F31B	1.371(12)	C402	O403	1.428(17)
C15B	F32B	1.328(13)	O403	C404	1.417(17)
C15B	F33B	1.329(12)	C404	C405	1.463(18)
C16B	F34B	1.352(12)	C405	O406	1.430(18)
C16B	F35B	1.325(12)	O406	C407	1.410(17)
C16B	F36B	1.330(13)	C407	C408	1.469(18)
Al1A	O1A	1.732(6)	C408	O409	1.444(17)
Al1A	O1C	1.715(8)	O409	C410	1.405(17)
Al1A	O2A	1.722(7)	C410	C411	1.455(17)
Al1A	O2C	1.696(8)	C411	O412	1.410(17)
Al1A	O3A	1.723(8)	O412	C413	1.406(18)
Al1A	O3C	1.739(6)	C413	C414	1.477(18)
Al1A	O4A	1.708(6)	C414	O415	1.415(17)
Al1A	O4C	1.742(8)	O415	C416	1.404(18)

O1A	C1A	1.344(8)	C416	C417	1.489(17)
C1A	C2A	1.553(9)	C417	O418	1.416(17)
C1A	C3A	1.557(9)	F501	C501	1.320(6)
C1A	C4A	1.541(9)	C501	C502	1.3900
C2A	F1A	1.339(9)	C501	C506	1.3900
C2A	F2A	1.344(9)	C502	C503	1.3900
C2A	F3A	1.334(9)	C503	C504	1.3900
C3A	F4A	1.339(9)	C504	C505	1.3900
C3A	F5A	1.335(9)	C505	C506	1.3900
C3A	F6A	1.313(10)	F511	C511	1.283(12)
C4A	F7A	1.324(9)	C511	C512	1.3900
C4A	F8A	1.332(9)	C511	C516	1.3900
C4A	F9A	1.323(9)	C512	C513	1.3900
O1C	C1C	1.343(11)	C513	C514	1.3900
C1C	C2C	1.553(12)	C514	C515	1.3900
C1C	C3C	1.546(11)	C515	C516	1.3900
C1C	C4C	1.542(12)	F601	C601	1.298(8)
C2C	F1C	1.325(12)	C601	C602	1.3900
C2C	F2C	1.321(12)	C601	C606	1.3900
C2C	F3C	1.324(12)	C602	C603	1.3900
C3C	F4C	1.352(12)	C603	C604	1.3900
C3C	F5C	1.329(11)	C604	C605	1.3900
C3C	F6C	1.306(12)	C605	C606	1.3900
C4C	F7C	1.339(12)	F611	C611	1.304(10)
C4C	F8C	1.334(12)	C611	C612	1.3900
C4C	F9C	1.343(12)	C611	C616	1.3900
O2A	C5A	1.366(10)	C612	C613	1.3900
C5A	C6A	1.576(11)	C613	C614	1.3900
C5A	C7A	1.554(10)	C614	C615	1.3900
C5A	C8A	1.541(10)	C615	C616	1.3900
C6A	F10A	1.332(11)	F701	C701	1.302(5)
C6A	F11A	1.364(10)	C701	C702	1.3900
C6A	F12A	1.305(10)	C701	C706	1.3900
C7A	F13A	1.355(11)	C702	C703	1.3900
C7A	F14A	1.350(11)	C703	C704	1.3900
C7A	F15A	1.311(11)	C704	C705	1.3900
C8A	F16A	1.345(11)	C705	C706	1.3900
C8A	F17A	1.334(9)	F711	C711	1.335(14)
C8A	F18A	1.354(10)	C711	C712	1.3900
O2C	C5C	1.360(11)	C711	C716	1.3900
C5C	C6C	1.559(12)	C712	C713	1.3900
C5C	C7C	1.551(12)	C713	C714	1.3900

C5C	C8C	1.548(11)	C714	C715	1.3900
C6C	F10C	1.331(12)	C715	C716	1.3900
C6C	F11C	1.319(12)	F801	C801	1.322(7)
C6C	F12C	1.344(12)	C801	C802	1.3900
C7C	F13C	1.330(11)	C801	C806	1.3900
C7C	F14C	1.343(11)	C802	C803	1.3900
C7C	F15C	1.306(12)	C803	C804	1.3900
C8C	F16C	1.335(11)	C804	C805	1.3900
C8C	F17C	1.339(11)	C805	C806	1.3900
C8C	F18C	1.341(12)	F811	C811	1.322(11)
O3A	C9A	1.341(11)	C811	C812	1.3900
C9A	C10A	1.558(12)	C811	C816	1.3900
C9A	C11A	1.545(11)	C812	C813	1.3900
C9A	C12A	1.550(11)	C813	C814	1.3900
C10A	F19A	1.343(11)	C814	C815	1.3900
C10A	F20A	1.304(12)	C815	C816	1.3900
C10A	F21A	1.340(13)	C901	F901	1.356(9)
C11A	F22A	1.374(11)	C901	C902	1.359(9)
C11A	F23A	1.319(11)	C901	C903[1]	1.375(10)
C11A	F24A	1.303(12)	C902	C903	1.240(10)
C12A	F25A	1.328(11)	C903	C901[1]	1.376(10)
C12A	F26A	1.336(11)			

2.1.5. Bond Angles

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Al1	O2	107.53(15)	F14A	C7A	F13A	105.3(8)
O1	Al1	O3B	106.0(5)	F15A	C7A	C5A	110.4(8)
O1	Al1	O4	114.2(3)	F15A	C7A	F13A	111.6(8)
O1	Al1	O4B	112.0(5)	F15A	C7A	F14A	107.7(9)
O2	Al1	O3B	116.3(6)	F16A	C8A	C5A	109.0(8)
O3	Al1	O1	107.5(3)	F16A	C8A	F18A	106.9(8)
O3	Al1	O2	112.7(3)	F17A	C8A	C5A	111.1(7)
O3	Al1	O3B	3.7(9)	F17A	C8A	F16A	110.6(9)
O3	Al1	O4	109.2(3)	F17A	C8A	F18A	108.4(8)
O3	Al1	O4B	109.9(5)	F18A	C8A	C5A	110.7(8)
O4	Al1	O2	105.8(2)	C5C	O2C	Al1A	158.1(11)
O4	Al1	O3B	107.2(5)	O2C	C5C	C6C	106.7(10)
O4	Al1	O4B	2.2(7)	O2C	C5C	C7C	112.0(9)
O4B	Al1	O2	107.2(5)	O2C	C5C	C8C	107.2(9)
O4B	Al1	O3B	107.8(6)	C7C	C5C	C6C	109.8(8)
C1	O1	Al1	147.0(3)	C8C	C5C	C6C	111.9(8)
O1	C1	C2	108.0(3)	C8C	C5C	C7C	109.3(8)

O1	C1	C3	110.1(3)	F10C	C6C	C5C	109.1(9)
O1	C1	C4	111.5(3)	F10C	C6C	F12C	108.8(10)
C2	C1	C3	109.0(4)	F11C	C6C	C5C	110.9(9)
C2	C1	C4	109.5(4)	F11C	C6C	F10C	111.3(10)
C3	C1	C4	108.7(4)	F11C	C6C	F12C	106.1(10)
F1	C2	C1	111.4(4)	F12C	C6C	C5C	110.6(9)
F1	C2	F2	107.5(4)	F13C	C7C	C5C	110.0(9)
F1	C2	F3	107.6(4)	F13C	C7C	F14C	108.8(8)
F2	C2	C1	112.4(4)	F14C	C7C	C5C	110.4(9)
F3	C2	C1	110.6(4)	F15C	C7C	C5C	108.5(9)
F3	C2	F2	107.2(4)	F15C	C7C	F13C	108.5(10)
F4	C3	C1	112.6(4)	F15C	C7C	F14C	110.6(11)
F5	C3	C1	110.1(4)	F16C	C8C	C5C	112.5(9)
F5	C3	F4	107.2(4)	F16C	C8C	F17C	105.7(10)
F6	C3	C1	111.0(4)	F16C	C8C	F18C	107.6(10)
F6	C3	F4	108.0(4)	F17C	C8C	C5C	110.1(9)
F6	C3	F5	107.8(4)	F17C	C8C	F18C	108.0(10)
F7	C4	C1	111.6(4)	F18C	C8C	C5C	112.6(10)
F8	C4	C1	111.1(4)	C9A	O3A	Al1A	148.2(11)
F8	C4	F7	107.6(4)	O3A	C9A	C10A	102.3(10)
F8	C4	F9	108.6(4)	O3A	C9A	C11A	115.6(10)
F9	C4	C1	110.2(4)	O3A	C9A	C12A	107.9(9)
F9	C4	F7	107.5(4)	C11A	C9A	C10A	110.0(9)
C5	O2	Al1	146.0(3)	C11A	C9A	C12A	111.2(8)
O2	C5	C6	111.1(3)	C12A	C9A	C10A	109.5(8)
O2	C5	C7	107.6(3)	F19A	C10A	C9A	109.8(9)
O2	C5	C8	110.2(3)	F20A	C10A	C9A	111.4(10)
C6	C5	C7	109.6(4)	F20A	C10A	F19A	112.3(10)
C6	C5	C8	109.4(4)	F20A	C10A	F21A	105.4(10)
C7	C5	C8	108.9(3)	F21A	C10A	C9A	113.3(10)
F10	C6	C5	111.9(4)	F21A	C10A	F19A	104.3(10)
F10	C6	F11	106.8(4)	F22A	C11A	C9A	110.8(9)
F10	C6	F12	107.9(4)	F23A	C11A	C9A	116.1(9)
F11	C6	C5	112.6(4)	F23A	C11A	F22A	108.5(9)
F12	C6	C5	110.8(4)	F24A	C11A	C9A	111.4(9)
F12	C6	F11	106.7(4)	F24A	C11A	F22A	105.4(9)
F13	C7	C5	110.5(4)	F24A	C11A	F23A	104.0(10)
F14	C7	C5	112.3(4)	F25A	C12A	C9A	111.9(9)
F14	C7	F13	107.3(4)	F25A	C12A	F26A	106.8(9)
F15	C7	C5	111.4(4)	F26A	C12A	C9A	111.1(9)
F15	C7	F13	107.3(4)	F27A	C12A	C9A	111.6(9)
F15	C7	F14	107.8(4)	F27A	C12A	F25A	109.4(9)

F16	C8	C5	112.6(4)	F27A	C12A	F26A	105.7(9)
F17	C8	C5	110.8(4)	C9C	O3C	Al1A	145.6(8)
F17	C8	F16	107.7(4)	O3C	C9C	C10C	113.9(7)
F18	C8	C5	110.3(3)	O3C	C9C	C11C	114.8(7)
F18	C8	F16	107.7(4)	O3C	C9C	C12C	106.9(7)
F18	C8	F17	107.4(4)	C10C	C9C	C11C	106.0(7)
C9	O3	Al1	151.5(6)	C12C	C9C	C10C	107.0(6)
O3	C9	C10	107.9(6)	C12C	C9C	C11C	107.8(6)
O3	C9	C11	112.9(6)	F19C	C10C	C9C	109.6(7)
O3	C9	C12	108.6(7)	F19C	C10C	F20C	105.3(7)
C11	C9	C10	108.7(6)	F20C	C10C	C9C	108.0(7)
C12	C9	C10	109.3(6)	F21C	C10C	C9C	115.6(7)
C12	C9	C11	109.4(6)	F21C	C10C	F19C	108.4(7)
F19	C10	C9	110.4(6)	F21C	C10C	F20C	109.5(8)
F19	C10	F20	109.5(6)	F22C	C11C	C9C	107.6(7)
F19	C10	F21	107.8(6)	F23C	C11C	C9C	114.6(7)
F20	C10	C9	110.6(6)	F23C	C11C	F22C	107.7(6)
F20	C10	F21	108.0(6)	F24C	C11C	C9C	109.9(6)
F21	C10	C9	110.3(6)	F24C	C11C	F22C	107.9(7)
F22	C11	C9	111.2(6)	F24C	C11C	F23C	108.9(7)
F22	C11	F23	107.7(6)	F25C	C12C	C9C	110.7(7)
F22	C11	F24	106.7(6)	F25C	C12C	F26C	109.7(8)
F23	C11	C9	111.6(6)	F25C	C12C	F27C	105.3(7)
F24	C11	C9	110.0(6)	F26C	C12C	C9C	109.7(7)
F24	C11	F23	109.5(6)	F27C	C12C	C9C	113.9(7)
F25	C12	C9	110.8(6)	F27C	C12C	F26C	107.3(7)
F25	C12	F26	107.8(6)	C13A	O4A	Al1A	145.1(7)
F25	C12	F27	107.7(6)	O4A	C13A	C14A	110.9(7)
F26	C12	C9	109.1(6)	O4A	C13A	C15A	106.6(7)
F27	C12	C9	112.9(6)	O4A	C13A	C16A	111.2(7)
F27	C12	F26	108.4(6)	C14A	C13A	C15A	108.1(6)
C9B	O3B	Al1	144.0(11)	C14A	C13A	C16A	110.2(7)
O3B	C9B	C10B	105.1(10)	C16A	C13A	C15A	109.7(6)
O3B	C9B	C11B	114.2(10)	F28A	C14A	C13A	109.5(7)
O3B	C9B	C12B	110.3(9)	F29A	C14A	C13A	112.4(7)
C10B	C9B	C11B	108.7(9)	F29A	C14A	F28A	105.8(7)
C12B	C9B	C10B	109.5(9)	F30A	C14A	C13A	113.2(7)
C12B	C9B	C11B	109.1(8)	F30A	C14A	F28A	107.5(7)
F19B	C10B	C9B	111.4(9)	F30A	C14A	F29A	108.1(7)
F19B	C10B	F20B	111.9(10)	F31A	C15A	C13A	110.1(7)
F19B	C10B	F21B	108.8(10)	F31A	C15A	F32A	108.6(8)
F20B	C10B	C9B	111.0(10)	F32A	C15A	C13A	110.3(7)

F20B	C10B	F21B	104.3(10)	F33A	C15A	C13A	111.9(7)
F21B	C10B	C9B	109.2(9)	F33A	C15A	F31A	108.9(8)
F22B	C11B	C9B	111.9(9)	F33A	C15A	F32A	107.0(8)
F22B	C11B	F24B	109.7(10)	F34A	C16A	C13A	109.9(7)
F23B	C11B	C9B	113.8(10)	F34A	C16A	F36A	107.7(7)
F23B	C11B	F22B	108.1(9)	F35A	C16A	C13A	113.5(7)
F23B	C11B	F24B	104.0(9)	F35A	C16A	F34A	110.3(7)
F24B	C11B	C9B	108.9(9)	F35A	C16A	F36A	106.5(8)
F25B	C12B	C9B	112.3(9)	F36A	C16A	C13A	108.7(6)
F25B	C12B	F26B	104.5(9)	C13C	O4C	Al1A	149.3(11)
F25B	C12B	F27B	108.0(9)	O4C	C13C	C14C	111.9(10)
F26B	C12B	C9B	115.2(10)	O4C	C13C	C15C	110.2(10)
F26B	C12B	F27B	106.0(10)	O4C	C13C	C16C	109.4(10)
F27B	C12B	C9B	110.3(9)	C14C	C13C	C15C	107.6(9)
C13	O4	Al1	145.9(5)	C14C	C13C	C16C	109.1(9)
O4	C13	C14	107.9(5)	C16C	C13C	C15C	108.6(9)
O4	C13	C15	112.8(5)	F28C	C14C	C13C	112.6(10)
O4	C13	C16	110.1(6)	F28C	C14C	F29C	110.0(11)
C14	C13	C15	109.2(5)	F28C	C14C	F30C	108.4(10)
C14	C13	C16	108.5(5)	F29C	C14C	C13C	109.0(10)
C15	C13	C16	108.2(5)	F30C	C14C	C13C	112.1(10)
F28	C14	C13	112.4(5)	F30C	C14C	F29C	104.5(11)
F28	C14	F29	108.6(6)	F31C	C15C	C13C	108.8(11)
F28	C14	F30	110.6(5)	F32C	C15C	C13C	113.1(11)
F29	C14	C13	109.0(5)	F32C	C15C	F31C	103.6(11)
F29	C14	F30	105.8(6)	F33C	C15C	C13C	109.1(10)
F30	C14	C13	110.2(5)	F33C	C15C	F31C	109.8(12)
F31	C15	C13	108.0(5)	F33C	C15C	F32C	112.3(12)
F32	C15	C13	111.1(5)	F34C	C16C	C13C	109.4(9)
F32	C15	F31	109.6(6)	F34C	C16C	F35C	103.3(10)
F33	C15	C13	114.2(5)	F34C	C16C	F36C	112.0(11)
F33	C15	F31	107.7(6)	F35C	C16C	C13C	111.2(10)
F33	C15	F32	106.1(5)	F35C	C16C	F36C	112.1(10)
F34	C16	C13	108.9(5)	F36C	C16C	C13C	108.8(9)
F35	C16	C13	112.1(5)	O118	C101	C102	111.1(4)
F35	C16	F34	108.8(5)	O103	C102	C101	111.5(4)
F35	C16	F36	105.5(6)	C104	O103	C102	115.3(4)
F36	C16	C13	112.7(6)	O103	C104	C105	111.9(5)
F36	C16	F34	108.7(6)	O106	C105	C104	111.1(5)
C13B	O4B	Al1	145.4(11)	C107	O106	C105	115.0(4)
O4B	C13B	C14B	106.7(10)	O106	C107	C108	110.5(5)
O4B	C13B	C15B	108.8(10)	O109	C108	C107	111.9(4)

O4B	C13B	C16B	113.6(11)	C110	O109	C108	115.3(4)
C14B	C13B	C15B	110.2(9)	O109	C110	C111	111.8(4)
C16B	C13B	C14B	108.7(9)	O112	C111	C110	112.2(4)
C16B	C13B	C15B	108.7(9)	C113	O112	C111	115.3(4)
F28B	C14B	C13B	106.8(9)	O112	C113	C114	111.9(4)
F29B	C14B	C13B	112.1(12)	O115	C114	C113	112.5(4)
F29B	C14B	F28B	115.8(12)	C114	O115	C116	115.0(4)
F30B	C14B	C13B	109.3(9)	O115	C116	C117	111.5(4)
F30B	C14B	F28B	112.2(10)	O118	C117	C116	110.9(4)
F30B	C14B	F29B	100.5(11)	C117	O118	C101	113.9(4)
F31B	C15B	C13B	108.6(9)	O218	C201	C202	108.6(5)
F32B	C15B	C13B	111.5(12)	O203	C202	C201	108.3(5)
F32B	C15B	F31B	103.3(11)	C202	O203	C204	113.0(5)
F32B	C15B	F33B	110.0(11)	O203	C204	C205	109.6(5)
F33B	C15B	C13B	109.2(9)	O206	C205	C204	107.7(5)
F33B	C15B	F31B	114.2(11)	C207	O206	C205	113.0(5)
F34B	C16B	C13B	107.5(9)	O206	C207	C208	109.6(6)
F35B	C16B	C13B	110.5(10)	O209	C208	C207	108.7(5)
F35B	C16B	F34B	116.5(11)	C210	O209	C208	113.2(5)
F35B	C16B	F36B	106.8(12)	O209	C210	C211	110.3(5)
F36B	C16B	C13B	112.9(12)	O212	C211	C210	107.6(5)
F36B	C16B	F34B	102.6(12)	C211	O212	C213	111.1(5)
O1A	Al1A	O3C	113.5(5)	O212	C213	C214	109.3(5)
O1A	Al1A	O4C	103.4(6)	O215	C214	C213	108.8(5)
O1C	Al1A	O1A	3.6(7)	C214	O215	C216	112.5(5)
O1C	Al1A	O2A	106.0(7)	O215	C216	C217	109.3(5)
O1C	Al1A	O3A	109.8(8)	O218	C217	C216	108.6(5)
O1C	Al1A	O3C	111.8(5)	C217	O218	C201	111.9(5)
O1C	Al1A	O4C	107.0(6)	O418	C401	C402	109.7(19)
O2A	Al1A	O1A	108.0(4)	O403	C402	C401	106.6(17)
O2A	Al1A	O3A	105.6(5)	C404	O403	C402	110.8(16)
O2A	Al1A	O3C	107.3(6)	O403	C404	C405	110(2)
O2A	Al1A	O4C	119.6(8)	O406	C405	C404	107.9(19)
O2C	Al1A	O1A	111.4(7)	C407	O406	C405	112.3(16)
O2C	Al1A	O1C	109.7(6)	O406	C407	C408	110.4(18)
O2C	Al1A	O2A	5.7(9)	O409	C408	C407	106.7(17)
O2C	Al1A	O3A	107.7(8)	C410	O409	C408	113.6(16)
O2C	Al1A	O3C	109.1(5)	O409	C410	C411	113.2(19)
O2C	Al1A	O4A	110.5(7)	O412	C411	C410	108.8(18)
O2C	Al1A	O4C	114.0(6)	C413	O412	C411	113.5(16)
O3A	Al1A	O1A	111.8(5)	O412	C413	C414	111.4(19)
O3A	Al1A	O3C	3.3(8)	O415	C414	C413	108.9(18)

O3A	Al1A	O4C	108.6(8)	C416	O415	C414	113.3(16)
O3C	Al1A	O4C	105.3(5)	O415	C416	C417	111.4(19)
O4A	Al1A	O1A	107.7(4)	O418	C417	C416	108.8(17)
O4A	Al1A	O1C	111.3(6)	C417	O418	C401	113.6(15)
O4A	Al1A	O2A	116.1(5)	F501	C501	C502	118.2(4)
O4A	Al1A	O3A	107.7(5)	F501	C501	C506	121.8(4)
O4A	Al1A	O3C	104.4(5)	C502	C501	C506	120.0
O4A	Al1A	O4C	4.5(8)	C501	C502	C503	120.0
C1A	O1A	Al1A	149.9(7)	C504	C503	C502	120.0
O1A	C1A	C2A	110.3(7)	C503	C504	C505	120.0
O1A	C1A	C3A	108.8(6)	C506	C505	C504	120.0
O1A	C1A	C4A	110.6(7)	C505	C506	C501	120.0
C2A	C1A	C3A	108.1(6)	F511	C511	C512	130.9(11)
C4A	C1A	C2A	109.0(6)	F511	C511	C516	109.0(11)
C4A	C1A	C3A	110.0(6)	C512	C511	C516	120.0
F1A	C2A	C1A	111.0(6)	C511	C512	C513	120.0
F1A	C2A	F2A	106.8(7)	C514	C513	C512	120.0
F2A	C2A	C1A	110.0(7)	C513	C514	C515	120.0
F3A	C2A	C1A	114.4(7)	C516	C515	C514	120.0
F3A	C2A	F1A	107.6(7)	C515	C516	C511	120.0
F3A	C2A	F2A	106.7(7)	F601	C601	C602	115.3(5)
F4A	C3A	C1A	110.4(7)	F601	C601	C606	124.7(5)
F5A	C3A	C1A	113.7(7)	C602	C601	C606	120.0
F5A	C3A	F4A	109.1(7)	C603	C602	C601	120.0
F6A	C3A	C1A	109.3(6)	C602	C603	C604	120.0
F6A	C3A	F4A	107.4(7)	C605	C604	C603	120.0
F6A	C3A	F5A	106.8(7)	C604	C605	C606	120.0
F7A	C4A	C1A	113.6(7)	C605	C606	C601	120.0
F7A	C4A	F8A	108.6(7)	F611	C611	C612	127.7(8)
F8A	C4A	C1A	111.0(7)	F611	C611	C616	112.2(8)
F9A	C4A	C1A	111.1(7)	C612	C611	C616	120.0
F9A	C4A	F7A	108.3(7)	C611	C612	C613	120.0
F9A	C4A	F8A	103.8(7)	C614	C613	C612	120.0
C1C	O1C	Al1A	149.7(10)	C613	C614	C615	120.0
O1C	C1C	C2C	109.1(10)	C616	C615	C614	120.0
O1C	C1C	C3C	107.0(9)	C615	C616	C611	120.0
O1C	C1C	C4C	111.9(10)	F701	C701	C702	125.4(4)
C3C	C1C	C2C	109.3(8)	F701	C701	C706	114.5(4)
C4C	C1C	C2C	108.8(8)	C702	C701	C706	120.0
C4C	C1C	C3C	110.8(9)	C701	C702	C703	120.0
F1C	C2C	C1C	111.5(9)	C702	C703	C704	120.0
F2C	C2C	C1C	113.7(10)	C705	C704	C703	120.0

F2C	C2C	F1C	106.6(10)	C704	C705	C706	120.0
F2C	C2C	F3C	105.0(10)	C705	C706	C701	120.0
F3C	C2C	C1C	110.0(9)	F711	C711	C712	94.8(17)
F3C	C2C	F1C	109.7(10)	F711	C711	C716	145.1(17)
F4C	C3C	C1C	111.7(9)	C712	C711	C716	120.0
F5C	C3C	C1C	112.5(9)	C711	C712	C713	120.0
F5C	C3C	F4C	106.1(9)	C714	C713	C712	120.0
F6C	C3C	C1C	111.6(9)	C713	C714	C715	120.0
F6C	C3C	F4C	107.1(9)	C714	C715	C716	120.0
F6C	C3C	F5C	107.6(10)	C715	C716	C711	120.0
F7C	C4C	C1C	112.6(10)	F801	C801	C802	117.9(5)
F7C	C4C	F9C	112.5(11)	F801	C801	C806	122.0(5)
F8C	C4C	C1C	112.3(10)	C802	C801	C806	120.0
F8C	C4C	F7C	101.4(10)	C801	C802	C803	120.0
F8C	C4C	F9C	108.3(11)	C804	C803	C802	120.0
F9C	C4C	C1C	109.4(10)	C805	C804	C803	120.0
C5A	O2A	Al1A	144.1(8)	C806	C805	C804	120.0
O2A	C5A	C6A	111.6(8)	C805	C806	C801	120.0
O2A	C5A	C7A	110.9(8)	F811	C811	C812	124.5(8)
O2A	C5A	C8A	105.8(7)	F811	C811	C816	115.5(8)
C7A	C5A	C6A	109.0(7)	C812	C811	C816	120.0
C8A	C5A	C6A	109.7(7)	C811	C812	C813	120.0
C8A	C5A	C7A	109.7(7)	C812	C813	C814	120.0
F10A	C6A	C5A	110.8(8)	C815	C814	C813	120.0
F10A	C6A	F11A	106.9(8)	C814	C815	C816	120.0
F11A	C6A	C5A	109.3(8)	C815	C816	C811	120.0
F12A	C6A	C5A	112.0(8)	F901	C901	C902	116.4(8)
F12A	C6A	F10A	111.2(8)	F901	C901	C903[1]	121.2(8)
F12A	C6A	F11A	106.4(7)	C902	C901	C903[1]	122.4(7)
F13A	C7A	C5A	111.8(8)	C903	C902	C901	111.0(6)
F14A	C7A	C5A	109.9(7)	C902	C903	C901[1]	126.7(7)

2.1.6. Hydrogen Atom Coordinates and Isotropic Displacement Parameters

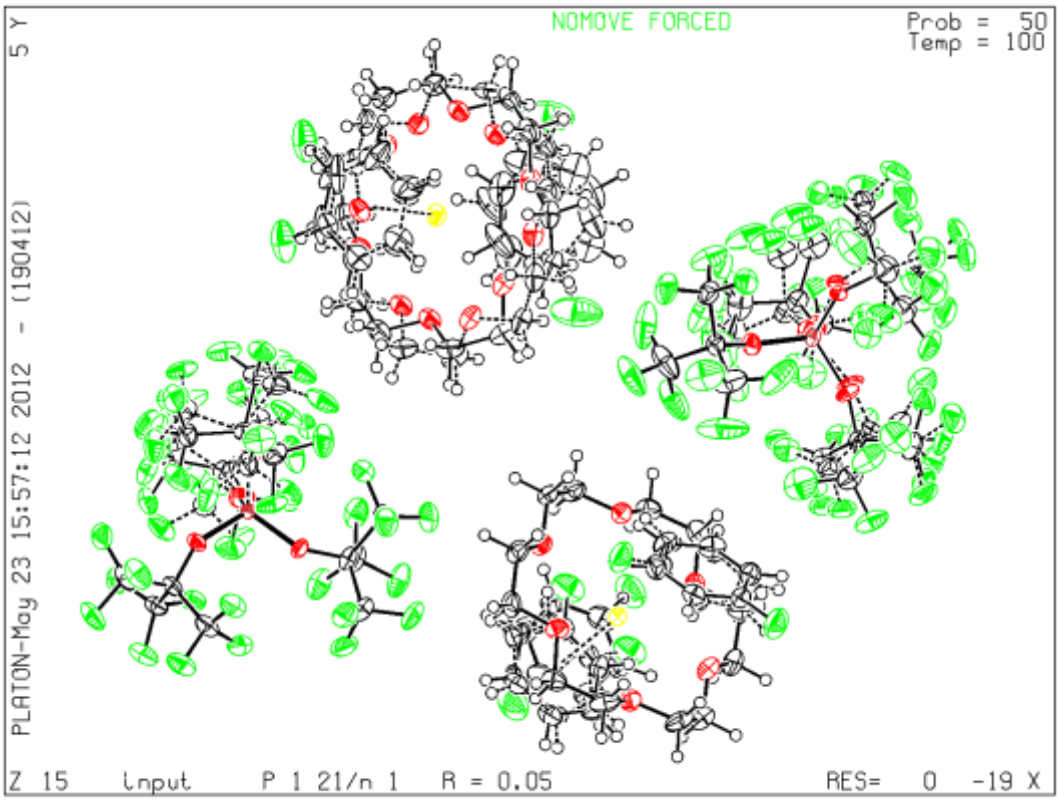
Atom	***x***	***y***	***z***	**U(eq)**
H10A	5646	7063	5753	48
H10B	5774	6065	5746	48
H10C	6862	6243	6040	50
H10D	6765	6790	5660	50
H10E	7626	7745	5885	56
H10F	7771	7231	6273	56
H10G	8127	8598	6359	64
H10H	7384	8937	6210	64

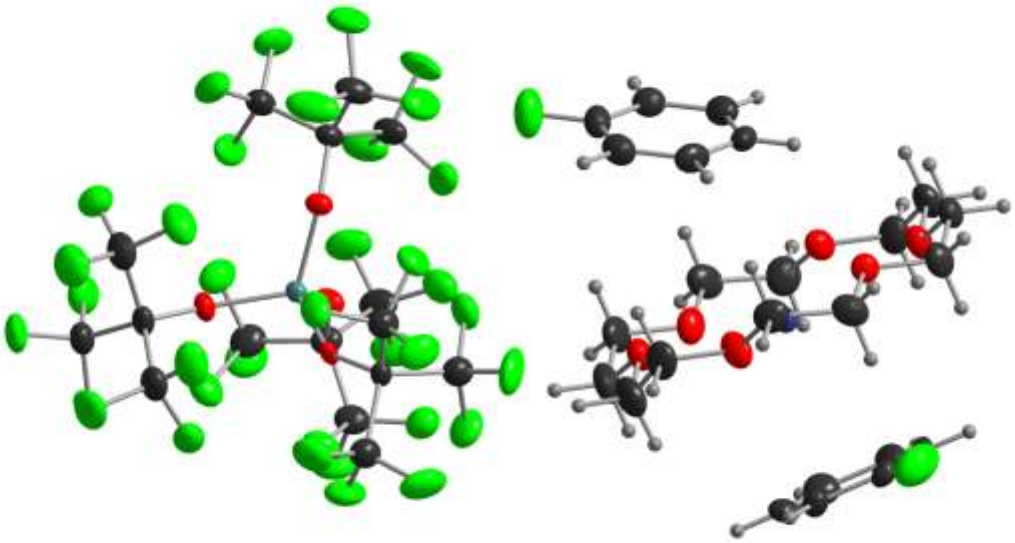
H10I	7397	9630	6850	62
H10J	8128	9211	6960	62
H10K	7723	8483	7447	59
H10L	7591	9473	7494	59
H11A	6663	9234	7854	57
H11B	6792	8238	7833	57
H11C	5690	8473	7945	55
H11D	5570	9077	7583	55
H11E	4646	8131	7333	50
H11F	4806	7580	7710	50
H11G	5014	6407	7357	48
H11H	4271	6767	7225	48
H11I	4277	6122	6624	39
H11J	5014	5738	6753	39
H11K	4847	5835	6097	50
H11L	4701	6827	6125	50
H20A	3501	4954	9593	51
H20B	3221	5683	9850	51
H20C	4389	5907	9759	49
H20D	4176	5982	9311	49
H20E	4620	7418	9355	50
H20F	4784	7321	9804	50
H20G	3980	8419	9881	52
H20H	4620	8740	9677	52
H20I	4043	9805	9316	53
H20J	3390	9635	9537	53
H20K	3086	10281	8947	54
H20L	3388	9484	8741	54
H21A	2242	9250	8430	55
H21B	1960	10023	8660	55
H21C	1245	9068	8947	53
H21D	1069	9099	8496	53
H21E	616	7727	8515	58
H21F	813	7669	8963	58
H21G	741	6308	8678	56
H21H	1350	6563	8434	56
H21I	1997	5394	8755	53
H21J	1363	5217	8991	53
H21K	2068	5528	9561	49
H21L	2349	4731	9346	49
H40A	4351	6576	9301	51
H40B	4476	6195	9721	51

H40C	4083	7508	9955	49
H40D	4778	7602	9760	49
H40E	4470	9011	9654	50
H40F	3720	8927	9784	50
H40G	3793	10027	9344	52
H40H	3980	9344	9037	52
H40I	2929	9626	8636	53
H40J	2819	10364	8932	53
H40K	1783	9715	9054	54
H40L	1773	10014	8621	54
H41A	963	8878	8436	55
H41B	990	8615	8872	55
H41C	616	7507	8478	53
H41D	1319	7527	8290	53
H41E	1455	6066	8530	58
H41F	774	6168	8733	58
H41G	1408	5949	9325	56
H41H	1449	5150	9050	56
H41I	2546	4743	9353	53
H41J	2454	5490	9647	53
H41K	3612	5135	9637	49
H41L	3563	5381	9197	49
H50A	6717	1247	7947	41
H50B	7787	982	8272	45
H50C	8753	963	7944	43
H50D	8649	1208	7291	41
H50E	7578	1473	6966	39
H51A	7376	1575	6976	41
H51B	6557	1735	7401	45
H51C	6847	1488	8047	43
H51D	7955	1080	8268	41
H51E	8774	920	7843	39
H60A	4366	8626	6308	38
H60B	4660	9499	6831	41
H60C	5674	10270	6874	43
H60D	6395	10168	6394	37
H60E	6102	9295	5871	35
H61A	4835	8437	5909	38
H61B	4322	8671	6465	41
H61C	4800	9637	6914	43
H61D	5790	10370	6809	37
H61E	6303	10136	6254	35

H70A	3335	8525	8124	37
H70B	2445	7564	7985	38
H70C	2579	6154	8174	42
H70D	3603	5704	8503	43
H70E	4493	6665	8642	43
H71A	4493	7775	8528	37
H71B	3588	8509	8201	38
H71C	2570	7806	8006	42
H71D	2458	6369	8139	43
H71E	3364	5635	8467	43
H80A	7176	2674	9955	59
H80B	7517	1386	10236	56
H80C	8674	1051	10343	65
H80D	9489	2004	10169	66
H80E	9148	3292	9887	61
H81A	9461	2637	10106	59
H81B	8675	3649	9858	56
H81C	7509	3364	9824	65
H81D	7129	2068	10038	66
H81E	7916	1056	10285	61
H901	9706	4385	10522	75
H902	8930	5343	10207	74
H903	9286	5908	9695	79

2.2.[In([18]crown-6)(PhF)$_2$]$_4$[Al(OC(CF$_3$)$_3$)$_4$]$_4$•PhF (2)





2.2.1. Crystal data and structure refinement of CCDC 861241

Identification code	CCDC 861241
Empirical formula	$C_{166}H_{141}Al_4F_{153}In_4O_{40}$
Formula weight	6249.82
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	19.7449(3)
b/Å	15.9218(2)
c/Å	35.6744(6)
α/°	90.00
β/°	95.9320(10)
γ/°	90.00
Volume/Å^3	11155.1(3)
Z	2
ρ_{calc}mg/mm^3	1.711
m/mm^{-1}	0.607
F(000)	5648.0
Crystal size/mm^3	0.2 × 0.2 × 0.1
2Θ range for data collection	3.3 to 54.96°
Index ranges	$-25 \le h \le 8$, $-20 \le k \le 20$, $-44 \le l \le 45$
Reflections collected	75318
Independent reflections	24937[R(int) = 0.0306]
Data/restraints/parameters	24937/3408/2111
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R_1 = 0.0539, wR_2 = 0.1364
Final R indexes [all data]	R_1 = 0.0761, wR_2 = 0.1519
Largest diff. peak/hole / e Å^{-3}	0.82/-0.60

2.2.2. Fractional Atomic Coordinates and Equivalent Isotropic Displacement Parameters

Atom	***x***	***y***	***z***	**U(eq)**
In1	6116.90(13)	2119.26(17)	1763.29(8)	25.09(7)
In2	2180.99(14)	7548.40(18)	945.43(8)	30.37(8)
Al1	914.1(5)	2273.7(6)	1807.1(3)	17.0(2)
Al1A	7444.5(5)	6950.4(7)	650.0(3)	22.3(2)
O1	824(8)	3346(7)	1900(3)	22.8(11)
C1	733(3)	3911(5)	2172.5(19)	25.3(8)
C2	1326(3)	3911(4)	2488.0(16)	36.3(12)
C3	64(3)	3736(4)	2359.5(17)	36.8(13)
C4	666(3)	4785(4)	1982.5(18)	38.6(16)
F1	1880.5(18)	4264(3)	2366.6(12)	55.1(11)
F2	1481(2)	3114(2)	2593.4(12)	44.9(10)
F3	1183(4)	4322(5)	2792.0(17)	45.9(12)
F4	154(2)	3166(2)	2624.4(11)	49.5(10)

F5	-427(3)	3462(4)	2097.2(14)	54.5(14)
F6	-177(4)	4423(5)	2517(2)	54.4(13)
F7	86(2)	4892(2)	1782.7(12)	54.4(11)
F8	1145(3)	4867(2)	1749.0(12)	56.9(11)
F9	744(7)	5415(8)	2233(4)	43.4(7)
O1B	780(20)	3290(20)	1912(9)	22.8(11)
C1B	680(6)	3904(11)	2164(4)	25.3(8)
C2B	-97(6)	4011(8)	2197(4)	36.3(12)
C3B	1023(6)	3664(8)	2559(3)	36.8(13)
C4B	964(7)	4745(10)	2032(4)	38.6(16)
F1B	-392(9)	3281(9)	2211(5)	55.1(11)
F2B	-369(5)	4470(6)	1908(2)	44.9(10)
F3B	-191(11)	4429(13)	2513(4)	45.9(12)
F4B	1640(6)	3333(8)	2518(4)	49.5(10)
F5B	654(5)	3086(6)	2724(3)	54.5(14)
F6B	1148(10)	4309(11)	2792(6)	54.4(13)
F7B	745(7)	4879(7)	1668(3)	54.4(11)
F8B	1657(6)	4737(6)	2105(3)	56.9(11)
F9B	760(18)	5399(19)	2225(10)	43.4(7)
O2	692(9)	2095(13)	1329(4)	17(2)
C5	291(4)	2263(5)	1011(3)	21.2(12)
C6	425(3)	1581(5)	716.0(19)	35.2(8)
C7	-481(3)	2235(5)	1075(2)	35.2(8)
C8	439(4)	3151(5)	860(2)	35.2(8)
F10	1005(2)	1737(3)	568.8(14)	48.2(13)
F11	-71(5)	1564(10)	431(3)	53(3)
F12	471(8)	829(8)	870(6)	53(4)
F13	-688(3)	1432(4)	1098.3(17)	49.0(14)
F14	-582(4)	2621(4)	1398(2)	44.0(17)
F15	-882(8)	2612(12)	809(4)	61(4)
F16	179(2)	3747(3)	1055.7(13)	40.9(12)
F17	1112(3)	3278(4)	891(2)	44.3(17)
F18	200(7)	3263(9)	500(3)	46(3)
O2B	595(12)	2111(18)	1355(5)	29(6)
C5B	169(6)	2257(6)	1043(4)	21.2(12)
C6B	-14(4)	1417(5)	835(2)	35.2(8)
C7B	-504(5)	2658(6)	1157(3)	35.2(8)
C8B	491(5)	2875(6)	775(3)	35.2(8)
F10B	-449(4)	976(5)	1022(2)	49.6(19)
F11B	-303(6)	1530(13)	487(3)	49(3)
F12B	535(8)	947(10)	824(6)	52(4)
F13B	-667(5)	2259(7)	1467(3)	51(3)

F14B	-1003(10)	2572(16)	879(5)	56(5)
F15B	-394(4)	3451(4)	1252(2)	64(2)
F16B	833(5)	3474(6)	965(3)	61(3)
F17B	15(8)	3223(13)	525(5)	64(6)
F18B	909(3)	2487(6)	564.2(18)	61(2)
O3	438.5(13)	1740.5(16)	2111.2(7)	27.2(6)
C9	309.9(18)	998(2)	2271.3(10)	28.4(8)
C10	48(2)	348(2)	1963.1(11)	34.3(9)
C11	968(2)	654(3)	2501.5(12)	38.2(10)
C12	-247(2)	1138(3)	2541.4(12)	38.8(10)
F19	78.4(15)	-443.7(15)	2093.0(7)	46.8(7)
F20	-588.0(13)	508.9(17)	1829.2(7)	43.5(6)
F21	424.5(13)	377.8(15)	1677.6(7)	37.4(5)
F22	833.6(15)	76.0(17)	2754.4(8)	50.9(7)
F23	1387.4(13)	295.0(16)	2275.5(8)	45.0(6)
F24	1309.6(14)	1269.7(16)	2687.0(7)	44.6(6)
F25	13.9(15)	1509.9(18)	2858.6(7)	50.3(7)
F26	-527.2(15)	407.2(17)	2637.9(8)	51.6(7)
F27	-742.2(13)	1619.8(17)	2384.7(8)	45.5(6)
O4	1741.8(12)	1929.5(16)	1888.3(7)	25.9(5)
C13	2368.5(17)	1888(2)	1764.5(10)	29.5(8)
C14	2328(2)	1595(3)	1350.6(13)	41.2(10)
C15	2811.4(19)	1278(3)	2023.1(12)	36.9(9)
C16	2703(2)	2785(3)	1793.0(14)	41.8(11)
F28	2111.3(14)	2197(2)	1112.0(8)	52.1(7)
F29	1905.4(13)	943.7(19)	1296.2(8)	49.3(7)
F30	2935.6(13)	1343(2)	1257.3(8)	55.7(8)
F31	2646.8(14)	488.5(16)	1930.1(9)	50.2(7)
F32	3477.7(12)	1372.9(19)	1989.5(9)	51.3(7)
F33	2719.7(13)	1386.0(18)	2380.4(7)	45.8(6)
F34	3247.8(14)	2832(2)	1600.7(9)	55.6(8)
F35	2260.8(13)	3364.0(17)	1650.3(9)	50.7(7)
F36	2893.7(13)	2980.1(17)	2146.0(8)	47.3(7)
O1A	8138(5)	6289(6)	827(3)	24(2)
C1A	8401(4)	5503(5)	795(2)	23(2)
C2A	7932(3)	4882(4)	561.6(17)	31.7(15)
C3A	9077(3)	5607(4)	613(2)	39.2(17)
C4A	8558(4)	5138(4)	1207(2)	43.6(18)
F1A	7950(3)	5001(4)	194.2(16)	43.3(12)
F2A	8099(3)	4078(3)	627.5(17)	51.2(11)
F3A	7302(3)	4983(3)	617.2(15)	42.5(11)
F4A	9557(3)	5953(4)	856.8(18)	52.2(16)

F5A	9304(4)	4866(5)	498(2)	48.6(19)
F6A	8996(4)	6091(6)	311(2)	48.4(19)
F7A	8988(3)	4495(3)	1214.2(13)	54.7(14)
F8A	7977(4)	4911(6)	1338(2)	81(3)
F9A	8829(3)	5731(4)	1432.9(14)	56.7(15)
O1C	8122(10)	6407(11)	758(6)	47(6)
C1C	8543(5)	5730(7)	764(3)	22(3)
C2C	8153(5)	4947(6)	886(3)	56(4)
C3C	8735(5)	5588(7)	358(3)	46(3)
C4C	9216(5)	5832(6)	1033(3)	43(3)
F1C	7486(4)	4974(5)	758(2)	43.3(12)
F2C	8405(4)	4225(4)	771(3)	51.2(11)
F3C	8135(5)	4860(6)	1256(3)	42.5(11)
F4C	8212(4)	5254(7)	142(3)	61(3)
F5C	9290(7)	5091(9)	341(4)	65(4)
F6C	8878(7)	6301(8)	200(4)	56(3)
F7C	9549(4)	5112(5)	1100(2)	60(2)
F8C	9096(5)	6160(6)	1358(2)	60(2)
F9C	9631(5)	6387(6)	893(3)	54(3)
O2A	6728.7(13)	6710.2(17)	866.0(7)	29.9(6)
C5A	6362.0(18)	6769(2)	1161.7(10)	28.8(8)
C6A	6794(3)	6492(3)	1526.7(14)	59.5(16)
C7A	5724(3)	6183(3)	1087.3(16)	64.7(19)
C8A	6121(2)	7673(3)	1216.1(13)	37.9(10)
F10A	6843(3)	5651(2)	1533.3(11)	112.4(19)
F11A	7418.4(17)	6799(3)	1536.6(8)	75.7(12)
F12A	6542(2)	6726(2)	1839.8(8)	76.2(11)
F13A	5906(2)	5456(2)	946.9(12)	90.4(14)
F14A	5429(2)	6033(2)	1399.9(11)	87.7(14)
F15A	5259.6(16)	6528(3)	841.4(12)	87.1(14)
F16A	5906.7(18)	8013(2)	888.9(9)	66.8(9)
F17A	6631.0(13)	8157.5(16)	1368.6(8)	45.5(6)
F18A	5626.9(14)	7726.5(19)	1442.2(9)	56.4(8)
O3A	7195(12)	6660(20)	194(7)	29.1(17)
C9A	6739(7)	6653(8)	-117(5)	32.5(15)
C10A	6484(7)	7547(8)	-217(3)	54(2)
C11A	7077(9)	6292(13)	-457(6)	44.2(12)
C12A	6141(6)	6075(9)	-45(4)	60(3)
F19A	5884(6)	7525(8)	-431(3)	84.6(18)
F20A	6362(6)	7942(7)	95(3)	65.6(14)
F21A	6942(8)	7957(7)	-400(3)	63.1(13)
F22A	6687(15)	6440(30)	-780(7)	64(3)

F23A	7140(16)	5459(12)	-422(11)	63(2)
F24A	7665(8)	6657(8)	-479(5)	50.3(13)
F25A	5797(6)	5804(11)	-351(3)	86(2)
F26A	5729(5)	6479(10)	173(3)	74.3(17)
F27A	6387(6)	5411(8)	153(3)	66.4(16)
O3C	7296(5)	6765(9)	172(3)	29.1(17)
C9C	6854(3)	6877(4)	-142(2)	32.5(15)
C10C	6852(4)	7817(5)	-258.6(19)	54(2)
C11C	7118(5)	6335(7)	-458(3)	44.2(12)
C12C	6125(3)	6616(6)	-81.1(19)	60(3)
F19C	6383(3)	8006(4)	-528.9(15)	84.6(18)
F20C	6802(3)	8316(3)	38.4(13)	65.6(14)
F21C	7457(3)	7999(3)	-386.5(13)	63.1(13)
F22C	6832(6)	6562(12)	-802(3)	64(3)
F23C	6963(6)	5520(6)	-407(5)	63(2)
F24C	7785(3)	6366(3)	-455(2)	50.3(13)
F25C	5732(3)	6521(5)	-402.0(14)	86(2)
F26C	5820(2)	7210(4)	120.3(14)	74.3(17)
F27C	6112(3)	5907(4)	112.7(15)	66.4(16)
O4A	7697(7)	7927(8)	792(4)	21(2)
C13A	8198(5)	8503(6)	838(3)	36(3)
C14A	7887(4)	9353(5)	943(3)	49(3)
C15A	8570(6)	8619(8)	479(3)	52(5)
C16A	8733(5)	8232(6)	1165(3)	51(2)
F28A	8309(3)	9996(4)	903(3)	69(2)
F29A	7734(8)	9338(10)	1297(4)	68(4)
F30A	7326(4)	9514(8)	717(4)	61(3)
F31A	8187(3)	9063(4)	224.2(18)	71(2)
F32A	9184(3)	8985(5)	554(3)	65(2)
F33A	8682(3)	7876(4)	322(2)	46.2(16)
F34A	9154(2)	7657(4)	1049.7(19)	56.5(17)
F35A	8432(4)	7892(5)	1450(2)	53.5(18)
F36A	9120(3)	8872(5)	1311(2)	72(2)
O4C	7616(9)	8030(10)	701(5)	28(3)
C13C	8068(5)	8672(6)	725(3)	31(3)
C14C	7669(5)	9459(5)	581(2)	39(2)
C15C	8641(6)	8483(8)	476(4)	62(7)
C16C	8369(5)	8823(6)	1136(3)	51(2)
F28C	8022(4)	10162(4)	654(2)	59(2)
F29C	7095(5)	9514(11)	739(4)	52(3)
F30C	7520(4)	9402(4)	210.1(17)	68(2)
F31C	8406(5)	8085(6)	161(3)	66(3)

F32C	8951(5)	9180(6)	372(3)	62(3)
F33C	9112(3)	7977(5)	651(3)	81(3)
F34C	8919(4)	9325(6)	1148(3)	70(2)
F35C	8552(6)	8109(6)	1309(3)	70(3)
F36C	7919(8)	9191(12)	1335(3)	62(4)
C101	7648(2)	1554(3)	1367.4(15)	50.6(13)
O102	7470.4(14)	1624.4(19)	1742.9(8)	37.5(7)
C103	7631(2)	917(3)	1971.3(15)	49.0(12)
C104	7459(2)	1067(3)	2352.0(14)	48.1(12)
O105	6750.8(14)	1203.0(19)	2356.1(8)	37.7(7)
C106	6538(2)	1328(3)	2712.2(13)	45.6(11)
C107	5796(2)	1463(3)	2686.2(14)	43.2(11)
O108	5600.9(14)	2186.2(18)	2473.3(8)	31.2(6)
C109	4907(2)	2382(3)	2448.4(13)	39.9(10)
C110	4752(2)	3148(3)	2231.8(12)	37.3(10)
O111	4918.3(14)	3082.8(18)	1861.3(8)	32.3(6)
C112	4772.2(19)	3795(3)	1638.1(11)	31.1(8)
C113	4967(2)	3671(3)	1251.1(12)	37.6(10)
O114	5671.2(13)	3522.9(17)	1260.6(7)	28.9(6)
C115	5898(2)	3431(3)	900.3(12)	37.8(10)
C116	6638(2)	3285(3)	931.0(12)	39.1(10)
O117	6819.3(15)	2543.4(19)	1132.2(9)	39.5(7)
C118	7517(2)	2340(3)	1158.8(14)	44.8(11)
C201	1558(3)	9426(3)	377.0(17)	37.2(12)
O202	2060.8(18)	9226(2)	674(1)	31.8(7)
C203	2688(3)	9645(3)	648.5(16)	37.1(12)
C204	3166(3)	9458(3)	985.7(17)	40.4(13)
O205	3341.6(17)	8587(2)	983.5(10)	35.3(8)
C206	3803(3)	8350(4)	1292.6(17)	41.0(13)
C207	3990(3)	7460(4)	1257(2)	45.1(14)
O208	3406.9(17)	6951(2)	1295.9(11)	36.9(8)
C209	3549(3)	6074(4)	1275.7(17)	41.7(13)
C210	2914(3)	5596(4)	1309.9(16)	41.2(14)
O211	2439.1(18)	5765(2)	992.2(10)	33.9(8)
C212	1812(3)	5336(4)	1006.4(16)	41.0(13)
C213	1353(4)	5519(5)	659(4)	43.8(18)
O214	1196.2(17)	6379(2)	645.1(10)	33.6(8)
C215	758(3)	6618(4)	320.4(16)	39.0(12)
C216	532(3)	7494(4)	370.3(17)	36.9(13)
O217	1101.6(17)	8046(2)	356(1)	33.9(8)
C218	943(3)	8900(4)	409.7(15)	38.3(12)
C401	2353(9)	9636(14)	582(6)	37.2(12)

O402	2687(6)	9146(9)	872(4)	31.8(7)
C403	3403(8)	9217(13)	917(6)	37.1(12)
C404	3715(12)	8712(10)	1226(7)	40.4(13)
O405	3597(7)	7838(8)	1162(4)	35.3(8)
C406	3858(11)	7331(11)	1466(6)	41.0(13)
C407	3784(9)	6441(12)	1354(8)	45.1(14)
O408	3081(7)	6225(10)	1311(4)	36.9(8)
C409	2962(10)	5383(12)	1194(8)	41.7(13)
C410	2226(9)	5235(13)	1114(6)	41.2(14)
O411	1953(7)	5723(9)	806(4)	33.9(8)
C412	1279(15)	5510(20)	677(15)	41.0(13)
C413	1009(11)	6127(10)	393(6)	43.8(18)
O414	1012(7)	6950(8)	528(4)	33.6(8)
C415	707(12)	7541(11)	263(6)	39.0(12)
C416	790(8)	8405(12)	410(7)	36.9(13)
O417	1488(6)	8632(8)	435(4)	33.9(8)
C418	1618(9)	9470(11)	551(7)	38.3(12)
F901	5018(2)	1579(3)	733.1(12)	65.1(12)
C901	5188(2)	1076(4)	1015.2(14)	29.8(14)
C902	4738(3)	1013(5)	1289.1(18)	33.9(16)
C903	4886(4)	482(7)	1596(2)	37.9(18)
C904	5484(5)	15(7)	1629(2)	39.8(17)
C905	5934(4)	78(5)	1355(2)	35.5(17)
C906	5786(2)	608(4)	1048.3(15)	30.6(14)
F971	6032(7)	797(8)	750(4)	65.1(12)
C971	5598(8)	721(14)	1013(5)	29.8(14)
C972	4997(9)	1140(13)	1065(6)	33.9(16)
C973	4672(11)	989(19)	1386(7)	37.9(18)
C974	4949(16)	420(20)	1655(7)	39.8(17)
C975	5549(16)	0(20)	1603(7)	35.5(17)
C976	5874(11)	151(17)	1282(7)	30.6(14)
F911	8573.0(18)	3503(3)	2750.5(12)	60.8(11)
C911	7966(3)	3647(2)	2575.2(17)	35.0(14)
C912	7878(3)	3795(3)	2189.2(17)	39.1(15)
C913	7230(4)	3946(4)	2010.3(15)	38.9(15)
C914	6671(3)	3948(4)	2217.3(19)	41.1(15)
C915	6760(3)	3800(4)	2603.2(19)	41.2(15)
C916	7407(3)	3649(3)	2782.1(15)	35.1(14)
F961	6330(6)	3971(9)	2802(4)	60.8(11)
C961	6828(9)	3846(8)	2589(5)	35.0(14)
C962	7457(10)	3560(11)	2749(5)	39.1(15)
C963	7981(10)	3428(13)	2524(7)	38.9(15)

C964	7876(12)	3583(13)	2139(6)	41.1(15)
C965	7247(13)	3869(16)	1979(5)	41.2(15)
C966	6723(11)	4001(13)	2204(5)	35.1(14)
F921	446(2)	6853(4)	1527.6(12)	79.3(15)
C921	922(3)	7363(4)	1599(2)	57(2)
C922	865(3)	8203(4)	1495(2)	53(2)
C923	1402(4)	8752(3)	1591(3)	55.6(19)
C924	1996(4)	8461(4)	1793(2)	44.8(17)
C925	2053(4)	7620(4)	1897.2(19)	35.6(15)
C926	1516(4)	7071(4)	1800(2)	33.2(14)
F981	333(7)	8488(12)	1294(4)	79.3(15)
C981	941(11)	8232(12)	1503(8)	57(2)
C982	1444(12)	8820(13)	1609(9)	53(2)
C983	2027(13)	8582(17)	1836(9)	55.6(19)
C984	2107(16)	7755(18)	1957(8)	44.8(17)
C985	1603(17)	7166(14)	1851(8)	35.6(15)
C986	1020(14)	7404(12)	1624(8)	33.2(14)
F931	2929(4)	8797(3)	-287.0(15)	116(2)
C931	3130(3)	8088(2)	-125.0(14)	57.7(19)
C932	2637(2)	7540(4)	-18.6(16)	59(2)
C933	2829(3)	6775(3)	147.6(18)	64(3)
C934	3513(4)	6558(3)	207.4(16)	70(2)
C935	4006(2)	7107(4)	101.0(16)	71(2)
C936	3815(3)	7872(3)	-65.3(15)	61(2)
F951	4137(19)	6064(17)	350(8)	116(2)
C951	3696(13)	6740(14)	193(9)	57.7(19)
C952	2995(13)	6617(17)	161(10)	59(2)
C953	2560(12)	7250(20)	15(11)	64(3)
C954	2826(17)	8007(18)	-98(9)	70(2)
C955	3527(18)	8129(15)	-66(10)	71(2)
C956	3961(13)	7496(17)	80(10)	61(2)
C942	5632(3)	-168(3)	-117.1(16)	51.5(12)
C943	5433(3)	-565(3)	193.6(15)	50.1(12)
C944	4798(3)	-398(3)	305.2(15)	49.9(12)
F941	4602(4)	-773(5)	590(2)	79(2)

2.2.3. Anisotropic Displacement Parameters

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
In1	23.26(12)	24.91(13)	27.12(14)	0.45(10)	2.73(10)	1.72(10)
In2	28.04(13)	31.92(15)	31.54(16)	-3.76(12)	4.95(11)	-0.65(11)
Al1	16.9(4)	17.6(5)	17.2(5)	0.2(4)	4.6(4)	0.5(4)
Al1A	17.8(5)	27.4(6)	22.3(5)	-1.5(4)	4.1(4)	1.4(4)

O1	27(2)	20.0(19)	22.5(15)	-2.3(14)	7.4(13)	-0.7(16)
C1	32(2)	21.5(17)	23.0(19)	-2.9(14)	3.4(15)	4.4(15)
C2	36(3)	34(3)	38(3)	-10(2)	1(2)	6(2)
C3	36(3)	32(3)	46(4)	-10(3)	19(3)	-3(2)
C4	57(5)	25(2)	34(3)	-1(2)	10(4)	6(3)
F1	35.8(18)	61(3)	70(3)	-29(2)	12.4(18)	-17.5(17)
F2	53(2)	36(2)	40(2)	1.5(15)	-20.7(17)	17.6(17)
F3	66(3)	49(3)	18.2(19)	-12.1(17)	-13.7(19)	5(2)
F4	70(3)	35.5(19)	49(2)	-6.3(16)	34.7(19)	-9.6(17)
F5	26.7(17)	68(3)	69(4)	-30(2)	10(2)	-0.9(19)
F6	51(3)	35(2)	84(3)	-20(2)	44(2)	-1.0(19)
F7	71(3)	35.4(19)	52(2)	0.4(16)	-18(2)	18.3(19)
F8	104(3)	30.6(18)	43(2)	3.6(17)	40(2)	-7(2)
F9	62.8(18)	21.9(12)	47.8(16)	-7.2(11)	16.3(13)	0.4(12)
O1B	27(2)	20.0(19)	22.5(15)	-2.3(14)	7.4(13)	-0.7(16)
C1B	32(2)	21.5(17)	23.0(19)	-2.9(14)	3.4(15)	4.4(15)
C2B	36(3)	34(3)	38(3)	-10(2)	1(2)	6(2)
C3B	36(3)	32(3)	46(4)	-10(3)	19(3)	-3(2)
C4B	57(5)	25(2)	34(3)	-1(2)	10(4)	6(3)
F1B	35.8(18)	61(3)	70(3)	-29(2)	12.4(18)	-17.5(17)
F2B	53(2)	36(2)	40(2)	1.5(15)	-20.7(17)	17.6(17)
F3B	66(3)	49(3)	18.2(19)	-12.1(17)	-13.7(19)	5(2)
F4B	70(3)	35.5(19)	49(2)	-6.3(16)	34.7(19)	-9.6(17)
F5B	26.7(17)	68(3)	69(4)	-30(2)	10(2)	-0.9(19)
F6B	51(3)	35(2)	84(3)	-20(2)	44(2)	-1.0(19)
F7B	71(3)	35.4(19)	52(2)	0.4(16)	-18(2)	18.3(19)
F8B	104(3)	30.6(18)	43(2)	3.6(17)	40(2)	-7(2)
F9B	62.8(18)	21.9(12)	47.8(16)	-7.2(11)	16.3(13)	0.4(12)
O2	16(4)	24(5)	12(4)	-2(3)	3(3)	7(3)
C5	17(3)	26.3(19)	20(2)	-2.0(15)	2(2)	2.2(18)
C6	37.3(16)	36(2)	31(2)	-1.4(17)	0.8(15)	1.5(18)
C7	37.3(16)	36(2)	31(2)	-1.4(17)	0.8(15)	1.5(18)
C8	37.3(16)	36(2)	31(2)	-1.4(17)	0.8(15)	1.5(18)
F10	54(3)	52(3)	42(3)	-10(2)	24(2)	5(2)
F11	83(7)	50(4)	25(3)	-9(3)	-7(4)	-10(6)
F12	67(6)	26(4)	64(8)	-11(4)	1(4)	-2(4)
F13	34(3)	48(3)	64(4)	4(3)	6(2)	-17(2)
F14	28(3)	53(4)	53(5)	-4(3)	13(3)	7(3)
F15	31(5)	70(6)	76(8)	15(5)	-23(6)	3(4)
F16	46(3)	27(2)	49(3)	3.0(19)	1(2)	12.3(19)
F17	29(3)	40(3)	65(4)	5(3)	12(3)	-5(2)
F18	67(6)	46(5)	23(3)	9(3)	-4(3)	-8(4)

O2B	26(8)	28(8)	33(9)	0(6)	-2(6)	-2(6)
C5B	17(3)	26.3(19)	20(2)	-2.0(15)	2(2)	2.2(18)
C6B	37.3(16)	36(2)	31(2)	-1.4(17)	0.8(15)	1.5(18)
C7B	37.3(16)	36(2)	31(2)	-1.4(17)	0.8(15)	1.5(18)
C8B	37.3(16)	36(2)	31(2)	-1.4(17)	0.8(15)	1.5(18)
F10B	55(4)	43(4)	47(4)	10(3)	-14(3)	-25(3)
F11B	60(7)	55(5)	28(5)	-3(5)	-16(5)	-16(6)
F12B	57(8)	54(10)	41(7)	-27(6)	-15(6)	27(7)
F13B	27(4)	84(8)	43(5)	2(5)	9(3)	13(5)
F14B	30(7)	71(9)	63(8)	-3(6)	-17(6)	7(5)
F15B	71(5)	55(4)	61(5)	-18(4)	-26(4)	39(4)
F16B	78(7)	48(6)	49(6)	28(4)	-30(5)	-36(5)
F17B	69(10)	51(6)	65(9)	36(6)	-31(7)	-15(6)
F18B	55(4)	100(7)	30(4)	2(4)	17(3)	-27(4)
O3	33.3(13)	21.4(12)	29.2(14)	4.1(11)	14.4(11)	-1.7(10)
C9	34.2(19)	26.1(19)	26(2)	5.1(15)	9.1(15)	-7.1(15)
C10	45(2)	24.5(19)	35(2)	5.8(17)	9.6(18)	-2.9(17)
C11	46(2)	32(2)	37(2)	9.1(18)	6.2(19)	-8.4(18)
C12	46(2)	37(2)	37(2)	-0.4(19)	20.0(19)	-13.3(19)
F19	74.3(19)	25.4(12)	42.3(15)	3.4(11)	13.0(13)	-9.3(12)
F20	40.1(13)	46.7(15)	43.9(15)	-7.5(12)	5.9(11)	-7.2(11)
F21	50.4(14)	28.8(12)	35.1(13)	0(1)	14.4(11)	4.8(10)
F22	68.2(18)	40.1(15)	43.7(16)	17.3(12)	2.4(13)	-8.7(13)
F23	46.8(14)	34.6(13)	54.3(17)	8.2(12)	8.2(12)	9.3(11)
F24	50.4(15)	39.3(14)	42.3(15)	6.3(12)	-4.2(12)	-8.7(12)
F25	70.9(18)	50.8(16)	33.0(14)	-9.7(12)	23.6(13)	-17.0(14)
F26	67.1(18)	40.8(15)	52.5(17)	1.4(13)	33.1(14)	-19.9(13)
F27	40.4(14)	44.7(15)	55.1(17)	-3.9(13)	22.2(12)	-1.6(12)
O4	17.7(11)	30.6(14)	29.8(14)	1.3(11)	3.5(10)	5.5(10)
C13	19.1(16)	42(2)	27(2)	-5.2(17)	3.1(14)	6.2(15)
C14	25.9(19)	54(3)	44(3)	-8(2)	9.0(18)	5.3(19)
C15	25.6(19)	44(2)	40(3)	-4.3(19)	-1.3(17)	7.4(17)
C16	28(2)	46(3)	54(3)	6(2)	14.3(19)	1.1(18)
F28	42.9(15)	82(2)	33.0(15)	9.0(14)	12.1(11)	8.3(14)
F29	37.0(13)	62.1(18)	48.4(16)	-27.3(14)	2.5(12)	4.7(12)
F30	36.4(14)	84(2)	49.5(17)	-21.7(16)	16.3(12)	10.3(14)
F31	45.1(15)	33.5(14)	71(2)	-3.6(13)	-0.3(13)	14.4(12)
F32	21.7(11)	63.4(18)	67.2(19)	-6.5(15)	-3.1(11)	11.0(12)
F33	42.7(14)	57.0(17)	35.5(15)	6.2(12)	-6.7(11)	8.8(12)
F34	38.7(14)	65.6(19)	67(2)	4.4(16)	26.1(14)	-4.5(13)
F35	43.1(14)	39.5(15)	72(2)	17.5(14)	18.5(13)	2.9(12)
F36	40.4(14)	48.8(16)	52.9(17)	-13.7(13)	6.1(12)	-10.0(12)

O1A	26(3)	29(4)	15(3)	-4(3)	-11(2)	12(3)
C1A	19(3)	25(5)	26(4)	0(3)	0(3)	2(4)
C2A	41(4)	26(3)	28(4)	2(3)	1(3)	11(3)
C3A	36(4)	35(4)	49(5)	-2(3)	15(4)	5(3)
C4A	42(4)	43(4)	46(5)	-5(4)	2(4)	8(4)
F1A	52(3)	38(2)	39(3)	-3.3(18)	-1(2)	-1(2)
F2A	51(3)	25(2)	74(4)	3(2)	-7(2)	7(2)
F3A	48(3)	37(2)	41(3)	3.7(19)	-6(2)	0.4(18)
F4A	19(2)	72(4)	65(4)	-22(4)	-1(2)	2(3)
F5A	42(3)	39(3)	68(5)	-12(3)	25(4)	13(2)
F6A	45(4)	59(4)	44(5)	9(3)	16(3)	-6(3)
F7A	64(3)	58(3)	40(3)	5(2)	-4(2)	33(2)
F8A	97(6)	101(5)	56(4)	20(4)	52(4)	30(4)
F9A	64(4)	72(4)	30(3)	-12(3)	-14(2)	27(3)
O1C	47(8)	38(7)	60(13)	21(6)	18(7)	30(5)
C1C	31(7)	15(6)	22(5)	2(4)	2(4)	-5(5)
C2C	29(6)	34(7)	101(13)	-6(7)	-15(7)	2(5)
C3C	38(6)	48(8)	49(8)	-25(6)	-9(6)	11(6)
C4C	31(6)	59(8)	39(7)	-6(6)	-2(5)	0(5)
F1C	52(3)	38(2)	39(3)	-3.3(18)	-1(2)	-1(2)
F2C	51(3)	25(2)	74(4)	3(2)	-7(2)	7(2)
F3C	48(3)	37(2)	41(3)	3.7(19)	-6(2)	0.4(18)
F4C	44(5)	80(8)	55(6)	-42(5)	-9(4)	12(4)
F5C	48(5)	77(9)	72(9)	-32(6)	14(6)	14(6)
F6C	59(6)	81(9)	29(6)	-2(5)	17(5)	19(6)
F7C	40(4)	54(5)	80(6)	13(4)	-18(4)	19(3)
F8C	74(6)	72(6)	33(4)	3(4)	-1(4)	-7(5)
F9C	44(4)	52(5)	65(6)	-13(5)	0(4)	-17(4)
O2A	31.0(13)	35.2(15)	26.0(14)	0.5(11)	14.2(11)	0.0(11)
C5A	31.4(19)	30(2)	27(2)	-4.8(16)	13.2(15)	-0.5(15)
C6A	80(4)	61(3)	40(3)	13(2)	20(3)	36(3)
C7A	91(4)	46(3)	67(4)	-27(3)	56(4)	-32(3)
C8A	31(2)	38(2)	45(3)	-8.7(19)	5.5(18)	4.7(17)
F10A	216(5)	63(2)	67(2)	34(2)	55(3)	70(3)
F11A	62(2)	129(3)	32.6(16)	-7.3(18)	-11.4(14)	50(2)
F12A	114(3)	89(3)	28.8(16)	7.0(16)	25.6(17)	31(2)
F13A	119(3)	50.1(19)	116(3)	-45(2)	80(3)	-45(2)
F14A	110(3)	66(2)	102(3)	-27(2)	82(2)	-42(2)
F15A	36.6(16)	137(4)	90(3)	-58(3)	14.8(17)	-24(2)
F16A	78(2)	65(2)	54.1(19)	1.1(16)	-9.5(16)	37.3(17)
F17A	43.2(14)	34.4(13)	59.4(18)	-16.3(12)	8.1(12)	-7.4(11)
F18A	41.0(14)	56.8(18)	75(2)	-27.2(16)	23.9(14)	0.4(13)

O3A	28(3)	39(4)	20.6(18)	4.1(18)	6(2)	-1(3)
C9A	31(3)	45(4)	22(2)	6(3)	4(2)	6(3)
C10A	72(6)	73(6)	22(3)	11(3)	22(4)	17(4)
C11A	48(3)	54(3)	31(2)	-2(2)	5(2)	6(2)
C12A	43(3)	108(8)	27(4)	10(5)	-6(3)	0(5)
F19A	100(4)	85(4)	64(3)	17(3)	-16(3)	53(3)
F20A	85(4)	58(3)	54(3)	-2(2)	9(3)	37(3)
F21A	94(4)	50(2)	51(2)	15.8(19)	34(3)	3(3)
F22A	86(6)	88(6)	19.5(19)	5(2)	6(3)	17(5)
F23A	79(7)	59(2)	49(2)	-8(2)	-6(5)	3(3)
F24A	54(3)	53(4)	47(2)	-7(3)	21(2)	17(2)
F25A	47(2)	162(7)	44(3)	-7(4)	-16.8(18)	-8(4)
F26A	34.5(19)	141(5)	47(2)	0(3)	6.4(17)	29(3)
F27A	62(4)	93(5)	42(2)	0(3)	-5(2)	-31(3)
O3C	28(3)	39(4)	20.6(18)	4.1(18)	6(2)	-1(3)
C9C	31(3)	45(4)	22(2)	6(3)	4(2)	6(3)
C10C	72(6)	73(6)	22(3)	11(3)	22(4)	17(4)
C11C	48(3)	54(3)	31(2)	-2(2)	5(2)	6(2)
C12C	43(3)	108(8)	27(4)	10(5)	-6(3)	0(5)
F19C	100(4)	85(4)	64(3)	17(3)	-16(3)	53(3)
F20C	85(4)	58(3)	54(3)	-2(2)	9(3)	37(3)
F21C	94(4)	50(2)	51(2)	15.8(19)	34(3)	3(3)
F22C	86(6)	88(6)	19.5(19)	5(2)	6(3)	17(5)
F23C	79(7)	59(2)	49(2)	-8(2)	-6(5)	3(3)
F24C	54(3)	53(4)	47(2)	-7(3)	21(2)	17(2)
F25C	47(2)	162(7)	44(3)	-7(4)	-16.8(18)	-8(4)
F26C	34.5(19)	141(5)	47(2)	0(3)	6.4(17)	29(3)
F27C	62(4)	93(5)	42(2)	0(3)	-5(2)	-31(3)
O4A	22(4)	20(4)	21(6)	7(3)	2(3)	2(3)
C13A	25(4)	29(5)	55(7)	0(5)	16(5)	0(4)
C14A	38(5)	30(4)	83(8)	-9(4)	22(5)	-7(4)
C15A	50(8)	45(7)	60(10)	9(6)	10(7)	3(6)
C16A	43(4)	47(5)	61(6)	-11(4)	-3(4)	-7(3)
F28A	58(4)	30(3)	126(7)	-14(4)	41(4)	-15(3)
F29A	67(7)	46(5)	100(10)	-36(6)	45(6)	-14(4)
F30A	43(6)	31(3)	114(8)	8(4)	28(5)	8(5)
F31A	75(4)	65(4)	77(4)	30(3)	32(3)	-2(3)
F32A	41(4)	58(5)	102(7)	-5(4)	36(4)	-13(3)
F33A	44(4)	50(4)	48(4)	-4(3)	17(3)	1(3)
F34A	25(2)	60(4)	83(5)	-18(3)	-3(2)	3(2)
F35A	53(4)	65(5)	41(5)	-4(3)	-5(3)	-2(3)
F36A	47(3)	66(5)	101(6)	-31(4)	-8(4)	-17(3)

O4C	33(5)	18(5)	32(9)	5(4)	2(5)	3(4)
C13C	32(6)	29(6)	35(6)	5(5)	10(5)	-3(4)
C14C	41(6)	35(5)	45(6)	9(4)	19(5)	2(5)
C15C	49(10)	31(7)	115(19)	-17(9)	55(11)	-16(7)
C16C	43(4)	47(5)	61(6)	-11(4)	-3(4)	-7(3)
F28C	83(6)	27(3)	71(5)	7(3)	31(4)	-4(3)
F29C	49(7)	42(4)	73(5)	7(4)	37(5)	14(6)
F30C	107(6)	55(4)	43(4)	19(3)	14(4)	5(4)
F31C	66(6)	80(6)	60(6)	-24(5)	39(4)	-10(5)
F32C	55(6)	55(5)	83(7)	8(4)	33(5)	-19(4)
F33C	40(4)	59(5)	150(10)	-11(5)	31(5)	7(3)
F34C	58(5)	64(5)	85(6)	-5(5)	-12(4)	-25(4)
F35C	88(8)	69(6)	47(7)	20(5)	-22(6)	-13(6)
F36C	89(11)	69(10)	28(5)	-12(4)	13(5)	-30(7)
C101	34(2)	57(3)	64(3)	1(3)	21(2)	10(2)
O102	29.5(14)	42.2(17)	40.3(17)	-2.9(14)	1.0(12)	10.2(12)
C103	33(2)	47(3)	67(3)	10(2)	5(2)	15(2)
C104	42(2)	47(3)	51(3)	2(2)	-15(2)	19(2)
O105	32.2(14)	41.5(17)	38.3(17)	13.0(13)	-1.7(12)	3.2(12)
C106	60(3)	42(3)	33(2)	6(2)	-8(2)	16(2)
C107	47(2)	44(3)	38(3)	19(2)	5(2)	-1(2)
O108	36.9(14)	34.1(15)	22.7(14)	5.2(11)	3.0(11)	6.1(12)
C109	32(2)	56(3)	33(2)	7(2)	13.0(17)	-1.3(19)
C110	35(2)	46(2)	33(2)	0.3(19)	11.4(17)	12.5(18)
O111	31.3(14)	38.4(16)	28.4(15)	7.1(12)	8.0(11)	9.5(12)
C112	27.0(18)	33(2)	33(2)	2.3(17)	0.7(16)	8.9(15)
C113	37(2)	42(2)	33(2)	8.1(19)	0.0(17)	11.9(18)
O114	30.9(13)	34.6(15)	21.4(13)	2.2(11)	3.5(10)	2.5(11)
C115	52(3)	36(2)	27(2)	5.2(17)	11.4(18)	4.4(19)
C116	47(2)	46(3)	26(2)	2.5(18)	11.3(18)	-4(2)
O117	34.2(15)	39.1(17)	48.5(19)	10.4(14)	20.4(13)	3.1(13)
C118	32(2)	65(3)	40(3)	-2(2)	15.5(19)	3(2)
C201	56(3)	26(2)	31(3)	6(2)	7(3)	9(2)
O202	38.5(18)	28.7(17)	29.4(18)	2.3(14)	10.3(14)	-4.1(15)
C203	49(3)	27(2)	39(3)	-8(2)	20(3)	-10(2)
C204	46(3)	31(3)	47(3)	-11(2)	16(3)	-10(2)
O205	31.2(17)	39(2)	36(2)	-15.6(16)	5.2(15)	-7.3(15)
C206	30(3)	53(4)	40(3)	-10(3)	6(2)	-7(3)
C207	23(2)	60(4)	51(4)	-6(3)	0(2)	3(2)
O208	27.4(17)	45(2)	38(2)	-3.4(16)	2.5(14)	7.9(15)
C209	43(3)	43(3)	38(3)	-2(2)	-1(2)	16(3)
C210	56(3)	36(3)	31(3)	3(2)	4(2)	15(3)

O211	41.7(19)	30.2(18)	31.1(19)	3.3(15)	9.7(14)	-3.1(15)
C212	52(3)	33(3)	41(3)	-1(2)	18(3)	-7(2)
C213	41(3)	35(3)	56(4)	-4(3)	12(3)	-13(3)
O214	35.1(18)	33.0(19)	32.5(19)	-1.2(15)	2.7(15)	-10.0(15)
C215	29(2)	50(3)	38(3)	-2(3)	1(2)	-13(2)
C216	22(2)	53(3)	35(3)	4(2)	-2.7(19)	-5(2)
O217	31.0(17)	36.4(19)	34.6(19)	2.2(15)	5.1(15)	3.5(14)
C218	41(3)	45(3)	28(3)	7(2)	3(2)	7(2)
C401	56(3)	26(2)	31(3)	6(2)	7(3)	9(2)
O402	38.5(18)	28.7(17)	29.4(18)	2.3(14)	10.3(14)	-4.1(15)
C403	49(3)	27(2)	39(3)	-8(2)	20(3)	-10(2)
C404	46(3)	31(3)	47(3)	-11(2)	16(3)	-10(2)
O405	31.2(17)	39(2)	36(2)	-15.6(16)	5.2(15)	-7.3(15)
C406	30(3)	53(4)	40(3)	-10(3)	6(2)	-7(3)
C407	23(2)	60(4)	51(4)	-6(3)	0(2)	3(2)
O408	27.4(17)	45(2)	38(2)	-3.4(16)	2.5(14)	7.9(15)
C409	43(3)	43(3)	38(3)	-2(2)	-1(2)	16(3)
C410	56(3)	36(3)	31(3)	3(2)	4(2)	15(3)
O411	41.7(19)	30.2(18)	31.1(19)	3.3(15)	9.7(14)	-3.1(15)
C412	52(3)	33(3)	41(3)	-1(2)	18(3)	-7(2)
C413	41(3)	35(3)	56(4)	-4(3)	12(3)	-13(3)
O414	35.1(18)	33.0(19)	32.5(19)	-1.2(15)	2.7(15)	-10.0(15)
C415	29(2)	50(3)	38(3)	-2(3)	1(2)	-13(2)
C416	22(2)	53(3)	35(3)	4(2)	-2.7(19)	-5(2)
O417	31.0(17)	36.4(19)	34.6(19)	2.2(15)	5.1(15)	3.5(14)
C418	41(3)	45(3)	28(3)	7(2)	3(2)	7(2)
F901	75(3)	62(3)	54(2)	12(2)	-16(2)	-15(2)
C901	25(3)	35(3)	29(3)	-4(2)	-5(2)	-5(3)
C902	17(3)	33(3)	51(5)	-4(3)	1(2)	-3(2)
C903	31(3)	34(4)	50(5)	0(4)	14(3)	-11(2)
C904	48(5)	29(3)	44(4)	5(3)	8(3)	-5(3)
C905	41(3)	24(3)	41(5)	-8(3)	0(3)	3(2)
C906	24(3)	39(4)	28(3)	-6(2)	2(2)	0(3)
F971	75(3)	62(3)	54(2)	12(2)	-16(2)	-15(2)
C971	25(3)	35(3)	29(3)	-4(2)	-5(2)	-5(3)
C972	17(3)	33(3)	51(5)	-4(3)	1(2)	-3(2)
C973	31(3)	34(4)	50(5)	0(4)	14(3)	-11(2)
C974	48(5)	29(3)	44(4)	5(3)	8(3)	-5(3)
C975	41(3)	24(3)	41(5)	-8(3)	0(3)	3(2)
C976	24(3)	39(4)	28(3)	-6(2)	2(2)	0(3)
F911	34.0(17)	88(3)	59(2)	15(2)	-0.7(16)	7.9(18)
C911	27(2)	32(3)	46(4)	5(3)	1(2)	1(2)

C912	40(3)	37(4)	42(4)	-1(3)	13(3)	1(3)
C913	51(3)	37(4)	26(3)	-1(2)	-8(3)	4(3)
C914	29(3)	33(3)	58(4)	-17(3)	-11(3)	3(2)
C915	35(3)	35(3)	55(4)	-8(3)	11(3)	-6(2)
C916	41(3)	29(3)	36(3)	2(2)	5(2)	-2(2)
F961	34.0(17)	88(3)	59(2)	15(2)	-0.7(16)	7.9(18)
C961	27(2)	32(3)	46(4)	5(3)	1(2)	1(2)
C962	40(3)	37(4)	42(4)	-1(3)	13(3)	1(3)
C963	51(3)	37(4)	26(3)	-1(2)	-8(3)	4(3)
C964	29(3)	33(3)	58(4)	-17(3)	-11(3)	3(2)
C965	35(3)	35(3)	55(4)	-8(3)	11(3)	-6(2)
C966	41(3)	29(3)	36(3)	2(2)	5(2)	-2(2)
F921	53(2)	132(4)	52(2)	0(3)	2.0(19)	-34(3)
C921	26(3)	111(7)	34(4)	-11(4)	13(3)	-25(4)
C922	37(3)	92(6)	31(3)	4(3)	9(3)	33(4)
C923	72(5)	32(3)	64(5)	-16(3)	14(4)	10(3)
C924	63(4)	36(4)	35(4)	-18(3)	1(3)	-9(3)
C925	47(3)	43(4)	14(3)	-5(2)	-9(2)	-11(3)
C926	36(3)	42(3)	21(3)	-4(2)	1(2)	-13(2)
F981	53(2)	132(4)	52(2)	0(3)	2.0(19)	-34(3)
C981	26(3)	111(7)	34(4)	-11(4)	13(3)	-25(4)
C982	37(3)	92(6)	31(3)	4(3)	9(3)	33(4)
C983	72(5)	32(3)	64(5)	-16(3)	14(4)	10(3)
C984	63(4)	36(4)	35(4)	-18(3)	1(3)	-9(3)
C985	47(3)	43(4)	14(3)	-5(2)	-9(2)	-11(3)
C986	36(3)	42(3)	21(3)	-4(2)	1(2)	-13(2)
F931	207(5)	62(3)	83(3)	-3(2)	31(3)	31(3)
C931	111(6)	30(3)	36(4)	-9(2)	26(4)	5(3)
C932	59(4)	77(6)	45(4)	-25(4)	27(3)	2(4)
C933	101(6)	55(4)	45(4)	-17(3)	46(4)	-37(5)
C934	127(8)	54(5)	30(3)	6(3)	16(4)	1(4)
C935	64(4)	114(7)	34(4)	-10(5)	0(3)	2(5)
C936	76(5)	72(5)	38(4)	-18(4)	19(4)	-41(4)
F951	207(5)	62(3)	83(3)	-3(2)	31(3)	31(3)
C951	111(6)	30(3)	36(4)	-9(2)	26(4)	5(3)
C952	59(4)	77(6)	45(4)	-25(4)	27(3)	2(4)
C953	101(6)	55(4)	45(4)	-17(3)	46(4)	-37(5)
C954	127(8)	54(5)	30(3)	6(3)	16(4)	1(4)
C955	64(4)	114(7)	34(4)	-10(5)	0(3)	2(5)
C956	76(5)	72(5)	38(4)	-18(4)	19(4)	-41(4)
C942	45(3)	48(3)	62(3)	-6(3)	10(2)	2(2)
C943	53(3)	40(3)	54(3)	-2(2)	-9(2)	9(2)

C944	69(3)	38(3)	43(3)	-3(2)	7(2)	-6(2)
F941	89(5)	79(5)	75(5)	13(4)	37(4)	-10(4)

2.2.4. Bond Lengths

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Al1	O1	1.752(10)	C10C	F21C	1.353(9)
Al1	O1B	1.69(3)	C11C	F22C	1.346(8)
Al1	O2	1.739(13)	C11C	F23C	1.349(9)
Al1	O2B	1.689(17)	C11C	F24C	1.318(8)
Al1	O3	1.729(3)	C12C	F25C	1.324(7)
Al1	O4	1.720(2)	C12C	F26C	1.364(9)
Al1A	O1A	1.790(9)	C12C	F27C	1.326(9)
Al1A	O1C	1.606(15)	O4A	C13A	1.347(10)
Al1A	O2A	1.721(3)	C13A	C14A	1.547(10)
Al1A	O3A	1.72(2)	C13A	C15A	1.551(10)
Al1A	O3C	1.726(11)	C13A	C16A	1.552(11)
Al1A	O4A	1.694(13)	C14A	F28A	1.338(8)
Al1A	O4C	1.758(14)	C14A	F29A	1.326(11)
O1	C1	1.350(7)	C14A	F30A	1.326(11)
C1	C2	1.538(8)	C15A	F31A	1.326(11)
C1	C3	1.566(7)	C15A	F32A	1.346(11)
C1	C4	1.548(7)	C15A	F33A	1.338(11)
C2	F1	1.341(7)	C16A	F34A	1.328(10)
C2	F2	1.351(6)	C16A	F35A	1.346(10)
C2	F3	1.321(7)	C16A	F36A	1.347(10)
C3	F4	1.309(7)	O4C	C13C	1.354(11)
C3	F5	1.348(7)	C13C	C14C	1.540(10)
C3	F6	1.339(7)	C13C	C15C	1.539(11)
C4	F7	1.295(7)	C13C	C16C	1.544(10)
C4	F8	1.331(7)	C14C	F28C	1.330(10)
C4	F9	1.342(8)	C14C	F29C	1.321(9)
O1B	C1B	1.353(12)	C14C	F30C	1.328(9)
C1B	C2B	1.560(12)	C15C	F31C	1.331(12)
C1B	C3B	1.547(12)	C15C	F32C	1.337(11)
C1B	C4B	1.543(12)	C15C	F33C	1.335(12)
C2B	F1B	1.304(12)	C16C	F34C	1.345(9)
C2B	F2B	1.331(11)	C16C	F35C	1.324(10)
C2B	F3B	1.339(12)	C16C	F36C	1.329(11)
C3B	F4B	1.349(12)	C101	O102	1.424(6)
C3B	F5B	1.347(12)	C101	C118	1.465(7)
C3B	F6B	1.327(12)	O102	C103	1.407(5)
C4B	F7B	1.345(12)	C103	C104	1.453(7)

C4B	F8B	1.367(12)	C104	O105	1.417(5)
C4B	F9B	1.333(13)	O105	C106	1.392(5)
O2	C5	1.341(9)	C106	C107	1.476(6)
C5	C6	1.554(9)	C107	O108	1.411(5)
C5	C7	1.566(9)	O108	C109	1.399(5)
C5	C8	1.552(9)	C109	C110	1.459(6)
C6	F10	1.332(7)	C110	O111	1.399(5)
C6	F11	1.338(9)	O111	C112	1.398(5)
C6	F12	1.316(11)	C112	C113	1.484(6)
C7	F13	1.348(8)	C113	O114	1.407(5)
C7	F14	1.338(9)	O114	C115	1.412(5)
C7	F15	1.316(11)	C115	C116	1.471(6)
C8	F16	1.313(8)	C116	O117	1.409(5)
C8	F17	1.338(8)	O117	C118	1.409(5)
C8	F18	1.333(10)	C201	O202	1.412(6)
O2B	C5B	1.346(11)	C201	C218	1.490(8)
C5B	C6B	1.554(10)	O202	C203	1.417(6)
C5B	C7B	1.566(11)	C203	C204	1.481(8)
C5B	C8B	1.553(10)	C204	O205	1.430(6)
C6B	F10B	1.338(9)	O205	C206	1.407(7)
C6B	F11B	1.326(11)	C206	C207	1.474(8)
C6B	F12B	1.321(12)	C207	O208	1.425(6)
C7B	F13B	1.343(10)	O208	C209	1.427(6)
C7B	F14B	1.332(12)	C209	C210	1.483(8)
C7B	F15B	1.319(10)	C210	O211	1.420(7)
C8B	F16B	1.317(10)	O211	C212	1.419(6)
C8B	F17B	1.345(12)	C212	C213	1.486(11)
C8B	F18B	1.326(10)	C213	O214	1.403(10)
O3	C9	1.348(4)	O214	C215	1.424(6)
C9	C10	1.559(5)	C215	C216	1.480(8)
C9	C11	1.563(5)	C216	O217	1.433(6)
C9	C12	1.552(5)	O217	C218	1.413(6)
C10	F19	1.342(4)	C401	O402	1.405(15)
C10	F20	1.322(5)	C401	C418	1.468(16)
C10	F21	1.322(4)	O402	C403	1.410(15)
C11	F22	1.334(4)	C403	C404	1.449(16)
C11	F23	1.342(5)	C404	O405	1.426(15)
C11	F24	1.328(5)	O405	C406	1.406(15)
C12	F25	1.333(5)	C406	C407	1.476(16)
C12	F26	1.348(5)	C407	O408	1.423(14)
C12	F27	1.320(5)	O408	C409	1.416(15)
O4	C13	1.358(4)	C409	C410	1.471(16)

C13	C14	1.543(5)	C410	O411	1.407(15)
C13	C15	1.546(5)	O411	C412	1.407(17)
C13	C16	1.572(6)	C412	C413	1.476(18)
C14	F28	1.323(5)	C413	O414	1.396(15)
C14	F29	1.332(5)	O414	C415	1.423(15)
C14	F30	1.340(4)	C415	C416	1.475(16)
C15	F31	1.332(5)	C416	O417	1.419(14)
C15	F32	1.342(4)	O417	C418	1.411(15)
C15	F33	1.317(5)	F901	C901	1.303(6)
C16	F34	1.336(4)	C901	C902	1.3900
C16	F35	1.334(5)	C901	C906	1.3900
C16	F36	1.314(5)	C902	C903	1.3900
O1A	C1A	1.363(9)	C903	C904	1.3900
C1A	C2A	1.541(9)	C904	C905	1.3900
C1A	C3A	1.554(8)	C905	C906	1.3900
C1A	C4A	1.579(9)	F971	C971	1.34(2)
C2A	F1A	1.329(8)	C971	C972	1.3900
C2A	F2A	1.336(7)	C971	C976	1.3900
C2A	F3A	1.288(7)	C972	C973	1.3900
C3A	F4A	1.339(8)	C973	C974	1.3900
C3A	F5A	1.342(8)	C974	C975	1.3900
C3A	F6A	1.321(8)	C975	C976	1.3900
C4A	F7A	1.329(7)	F911	C911	1.313(6)
C4A	F8A	1.332(9)	C911	C912	1.3900
C4A	F9A	1.319(8)	C911	C916	1.3900
O1C	C1C	1.360(11)	C912	C913	1.3900
C1C	C2C	1.553(10)	C913	C914	1.3900
C1C	C3C	1.550(11)	C914	C915	1.3900
C1C	C4C	1.565(11)	C915	C916	1.3900
C2C	F1C	1.348(10)	F961	C961	1.32(2)
C2C	F2C	1.334(10)	C961	C962	1.3900
C2C	F3C	1.330(11)	C961	C966	1.3900
C3C	F4C	1.332(10)	C962	C963	1.3900
C3C	F5C	1.358(11)	C963	C964	1.3900
C3C	F6C	1.313(12)	C964	C965	1.3900
C4C	F7C	1.330(10)	C965	C966	1.3900
C4C	F8C	1.315(10)	F921	C921	1.248(7)
C4C	F9C	1.336(11)	C921	C922	1.3900
O2A	C5A	1.343(4)	C921	C926	1.3900
C5A	C6A	1.545(6)	C922	C923	1.3900
C5A	C7A	1.567(6)	C923	C924	1.3900
C5A	C8A	1.535(5)	C924	C925	1.3900

C6A	F10A	1.343(6)	C925	C926	1.3900
C6A	F11A	1.323(7)	F981	C981	1.41(3)
C6A	F12A	1.323(5)	C981	C982	1.3900
C7A	F13A	1.324(6)	C981	C986	1.3900
C7A	F14A	1.332(5)	C982	C983	1.3900
C7A	F15A	1.322(7)	C983	C984	1.3900
C8A	F16A	1.316(5)	C984	C985	1.3900
C8A	F17A	1.338(5)	C985	C986	1.3900
C8A	F18A	1.332(5)	F931	C931	1.310(6)
O3A	C9A	1.355(12)	C931	C932	1.3900
C9A	C10A	1.540(12)	C931	C936	1.3900
C9A	C11A	1.551(12)	C932	C933	1.3900
C9A	C12A	1.540(12)	C933	C934	1.3900
C10A	F19A	1.342(12)	C934	C935	1.3900
C10A	F20A	1.324(11)	C935	C936	1.3900
C10A	F21A	1.337(11)	F951	C951	1.46(4)
C11A	F22A	1.337(13)	C951	C952	1.3900
C11A	F23A	1.336(13)	C951	C956	1.3900
C11A	F24A	1.309(13)	C952	C953	1.3900
C12A	F25A	1.299(12)	C953	C954	1.3900
C12A	F26A	1.345(12)	C954	C955	1.3900
C12A	F27A	1.335(13)	C955	C956	1.3900
O3C	C9C	1.358(7)	C942	C943	1.368(8)
C9C	C10C	1.554(9)	C942	C944[1]	1.366(8)
C9C	C11C	1.552(8)	C943	C944	1.378(8)
C9C	C12C	1.534(8)	C944	C942[1]	1.366(8)
C10C	F19C	1.301(8)	C944	F941	1.273(8)
C10C	F20C	1.336(8)			

2.2.5. Bond Angles

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1B	Al1	O1	3.9(17)	C8A	C5A	C7A	109.1(3)
O1B	Al1	O2	110.2(14)	F10A	C6A	C5A	109.3(5)
O1B	Al1	O3	103.0(12)	F11A	C6A	C5A	110.4(4)
O1B	Al1	O4	115.8(14)	F11A	C6A	F10A	107.6(5)
O2	Al1	O1	108.9(8)	F11A	C6A	F12A	107.8(5)
O2B	Al1	O1	107.1(11)	F12A	C6A	C5A	114.0(4)
O2B	Al1	O1B	107.9(15)	F12A	C6A	F10A	107.4(4)
O2B	Al1	O2	7.3(15)	F13A	C7A	C5A	109.9(4)
O2B	Al1	O3	110.5(10)	F13A	C7A	F14A	108.6(4)
O2B	Al1	O4	111.5(9)	F14A	C7A	C5A	112.2(4)
O3	Al1	O1	106.8(4)	F15A	C7A	C5A	110.8(4)

O3	Al1	O2	115.9(7)	F15A	C7A	F13A	108.0(5)
O4	Al1	O1	113.1(5)	F15A	C7A	F14A	107.2(5)
O4	Al1	O2	104.6(6)	F16A	C8A	C5A	110.4(3)
O4	Al1	O3	107.82(13)	F16A	C8A	F17A	106.5(4)
O1C	Al1A	O1A	8.3(13)	F16A	C8A	F18A	108.8(4)
O1C	Al1A	O2A	118.3(9)	F17A	C8A	C5A	111.3(3)
O1C	Al1A	O3A	103.5(13)	F18A	C8A	C5A	113.1(4)
O1C	Al1A	O3C	101.4(9)	F18A	C8A	F17A	106.5(3)
O1C	Al1A	O4A	102.1(9)	C9A	O3A	Al1A	152(2)
O1C	Al1A	O4C	110.8(9)	O3A	C9A	C10A	110.9(15)
O2A	Al1A	O1A	110.2(5)	O3A	C9A	C11A	109.7(15)
O2A	Al1A	O3C	109.9(3)	O3A	C9A	C12A	108.8(13)
O2A	Al1A	O4C	109.2(7)	C10A	C9A	C11A	108.6(11)
O3A	Al1A	O1A	108.0(11)	C10A	C9A	C12A	110.8(10)
O3A	Al1A	O2A	101.3(9)	C12A	C9A	C11A	108.0(11)
O3A	Al1A	O3C	9.3(12)	F19A	C10A	C9A	110.8(11)
O3A	Al1A	O4C	113.4(11)	F20A	C10A	C9A	109.1(10)
O3C	Al1A	O1A	107.1(6)	F20A	C10A	F19A	105.3(11)
O3C	Al1A	O4C	106.3(7)	F20A	C10A	F21A	111.8(12)
O4A	Al1A	O1A	104.1(5)	F21A	C10A	C9A	110.1(10)
O4A	Al1A	O2A	107.4(6)	F21A	C10A	F19A	109.8(12)
O4A	Al1A	O3A	125.5(11)	F22A	C11A	C9A	110.7(16)
O4A	Al1A	O3C	117.9(6)	F23A	C11A	C9A	109.8(15)
O4A	Al1A	O4C	12.6(8)	F23A	C11A	F22A	106.8(18)
O4C	Al1A	O1A	114.0(6)	F24A	C11A	C9A	109.8(13)
C1	O1	Al1	143.9(10)	F24A	C11A	F22A	107.9(17)
O1	C1	C2	112.3(8)	F24A	C11A	F23A	111.8(16)
O1	C1	C3	111.7(7)	F25A	C12A	C9A	113.5(12)
O1	C1	C4	107.1(7)	F25A	C12A	F26A	110.5(12)
C2	C1	C3	107.5(5)	F25A	C12A	F27A	108.3(12)
C2	C1	C4	110.2(5)	F26A	C12A	C9A	109.3(11)
C4	C1	C3	108.0(5)	F27A	C12A	C9A	108.6(10)
F1	C2	C1	110.4(5)	F27A	C12A	F26A	106.3(12)
F1	C2	F2	108.3(5)	C9C	O3C	Al1A	145.2(10)
F2	C2	C1	109.7(5)	O3C	C9C	C10C	109.3(7)
F3	C2	C1	113.0(5)	O3C	C9C	C11C	106.9(7)
F3	C2	F1	108.0(6)	O3C	C9C	C12C	112.4(6)
F3	C2	F2	107.3(6)	C11C	C9C	C10C	109.4(6)
F4	C3	C1	111.8(5)	C12C	C9C	C10C	108.8(6)
F4	C3	F5	108.2(5)	C12C	C9C	C11C	110.0(6)
F4	C3	F6	106.9(6)	F19C	C10C	C9C	113.8(7)
F5	C3	C1	109.9(5)	F19C	C10C	F20C	110.2(6)

F6	C3	C1	112.7(5)	F19C	C10C	F21C	106.6(6)
F6	C3	F5	107.2(6)	F20C	C10C	C9C	111.0(6)
F7	C4	C1	112.9(5)	F20C	C10C	F21C	106.3(7)
F7	C4	F8	106.8(5)	F21C	C10C	C9C	108.6(5)
F7	C4	F9	107.7(7)	F22C	C11C	C9C	111.9(8)
F8	C4	C1	109.1(5)	F22C	C11C	F23C	107.6(9)
F8	C4	F9	107.7(8)	F23C	C11C	C9C	109.8(8)
F9	C4	C1	112.4(8)	F24C	C11C	C9C	112.6(7)
C1B	O1B	Al1	151(3)	F24C	C11C	F22C	108.8(8)
O1B	C1B	C2B	110.0(18)	F24C	C11C	F23C	105.9(8)
O1B	C1B	C3B	110.3(18)	F25C	C12C	C9C	112.5(6)
O1B	C1B	C4B	109.8(17)	F25C	C12C	F26C	106.5(6)
C3B	C1B	C2B	107.4(9)	F25C	C12C	F27C	108.2(7)
C4B	C1B	C2B	108.6(10)	F26C	C12C	C9C	110.9(6)
C4B	C1B	C3B	110.6(10)	F27C	C12C	C9C	111.8(6)
F1B	C2B	C1B	110.6(12)	F27C	C12C	F26C	106.4(6)
F1B	C2B	F2B	111.9(12)	C13A	O4A	Al1A	148.4(13)
F1B	C2B	F3B	108.1(14)	O4A	C13A	C14A	108.7(9)
F2B	C2B	C1B	108.8(10)	O4A	C13A	C15A	112.7(10)
F2B	C2B	F3B	107.5(12)	O4A	C13A	C16A	109.6(8)
F3B	C2B	C1B	109.9(12)	C14A	C13A	C15A	109.3(8)
F4B	C3B	C1B	108.3(10)	C14A	C13A	C16A	108.6(7)
F5B	C3B	C1B	111.2(10)	C15A	C13A	C16A	107.9(7)
F5B	C3B	F4B	108.3(10)	F28A	C14A	C13A	112.1(6)
F6B	C3B	C1B	114.5(13)	F29A	C14A	C13A	110.5(9)
F6B	C3B	F4B	105.0(12)	F29A	C14A	F28A	108.8(10)
F6B	C3B	F5B	109.2(13)	F30A	C14A	C13A	110.4(8)
F7B	C4B	C1B	109.9(11)	F30A	C14A	F28A	106.1(9)
F7B	C4B	F8B	113.7(12)	F30A	C14A	F29A	108.8(10)
F8B	C4B	C1B	108.8(10)	F31A	C15A	C13A	110.2(8)
F9B	C4B	C1B	112.4(18)	F31A	C15A	F32A	110.0(9)
F9B	C4B	F7B	107.0(18)	F31A	C15A	F33A	106.8(8)
F9B	C4B	F8B	105.0(18)	F32A	C15A	C13A	112.5(8)
C5	O2	Al1	149.7(15)	F33A	C15A	C13A	110.8(8)
O2	C5	C6	107.9(10)	F33A	C15A	F32A	106.3(9)
O2	C5	C7	111.8(10)	F34A	C16A	C13A	111.1(8)
O2	C5	C8	111.1(11)	F34A	C16A	F35A	107.2(9)
C6	C5	C7	108.4(6)	F34A	C16A	F36A	107.1(7)
C8	C5	C6	110.4(6)	F35A	C16A	C13A	111.1(8)
C8	C5	C7	107.2(6)	F35A	C16A	F36A	106.7(9)
F10	C6	C5	110.6(6)	F36A	C16A	C13A	113.3(8)
F10	C6	F11	107.3(7)	C13C	O4C	Al1A	149.7(15)

F11	C6	C5	111.5(8)	O4C	C13C	C14C	106.4(9)
F12	C6	C5	111.2(10)	O4C	C13C	C15C	109.6(12)
F12	C6	F10	108.0(8)	O4C	C13C	C16C	111.3(10)
F12	C6	F11	108.1(10)	C14C	C13C	C16C	108.9(8)
F13	C7	C5	110.0(6)	C15C	C13C	C14C	110.3(8)
F14	C7	C5	110.2(6)	C15C	C13C	C16C	110.2(8)
F14	C7	F13	108.0(6)	F28C	C14C	C13C	112.4(8)
F15	C7	C5	113.9(10)	F29C	C14C	C13C	110.0(10)
F15	C7	F13	108.3(10)	F29C	C14C	F28C	108.4(11)
F15	C7	F14	106.3(10)	F29C	C14C	F30C	108.6(11)
F16	C8	C5	112.1(6)	F30C	C14C	C13C	109.2(7)
F16	C8	F17	106.6(6)	F30C	C14C	F28C	108.1(8)
F16	C8	F18	107.2(8)	F31C	C15C	C13C	111.5(9)
F17	C8	C5	109.3(6)	F31C	C15C	F32C	106.9(10)
F18	C8	C5	113.4(9)	F31C	C15C	F33C	105.8(11)
F18	C8	F17	108.0(8)	F32C	C15C	C13C	112.5(10)
C5B	O2B	Al1	155(2)	F33C	C15C	C13C	111.4(9)
O2B	C5B	C6B	109.9(14)	F33C	C15C	F32C	108.4(10)
O2B	C5B	C7B	109.1(13)	F34C	C16C	C13C	110.5(8)
O2B	C5B	C8B	111.1(14)	F35C	C16C	C13C	111.5(8)
C6B	C5B	C7B	108.3(8)	F35C	C16C	F34C	108.4(9)
C8B	C5B	C6B	110.0(8)	F35C	C16C	F36C	107.2(11)
C8B	C5B	C7B	108.3(8)	F36C	C16C	C13C	111.3(9)
F10B	C6B	C5B	110.2(7)	F36C	C16C	F34C	107.7(11)
F11B	C6B	C5B	112.7(11)	O102	C101	C118	111.3(4)
F11B	C6B	F10B	107.5(8)	C103	O102	C101	114.8(4)
F12B	C6B	C5B	110.5(11)	O102	C103	C104	110.5(4)
F12B	C6B	F10B	106.8(11)	O105	C104	C103	111.2(4)
F12B	C6B	F11B	108.8(12)	C106	O105	C104	115.0(3)
F13B	C7B	C5B	107.7(8)	O105	C106	C107	110.8(4)
F14B	C7B	C5B	110.2(13)	O108	C107	C106	111.5(4)
F14B	C7B	F13B	110.1(13)	C109	O108	C107	115.2(3)
F15B	C7B	C5B	109.6(7)	O108	C109	C110	111.8(3)
F15B	C7B	F13B	106.8(9)	O111	C110	C109	112.4(4)
F15B	C7B	F14B	112.3(13)	C112	O111	C110	115.0(3)
F16B	C8B	C5B	111.2(8)	O111	C112	C113	111.3(3)
F16B	C8B	F17B	109.3(12)	O114	C113	C112	110.5(3)
F16B	C8B	F18B	108.2(9)	C113	O114	C115	113.6(3)
F17B	C8B	C5B	111.5(11)	O114	C115	C116	110.8(4)
F18B	C8B	C5B	111.8(8)	O117	C116	C115	111.7(3)
F18B	C8B	F17B	104.6(11)	C116	O117	C118	115.0(3)
C9	O3	Al1	146.6(2)	O117	C118	C101	110.5(4)

O3	C9	C10	110.3(3)	O202	C201	C218	109.3(4)
O3	C9	C11	110.3(3)	C201	O202	C203	113.4(4)
O3	C9	C12	108.3(3)	O202	C203	C204	109.9(4)
C10	C9	C11	109.5(3)	O205	C204	C203	109.0(4)
C12	C9	C10	109.2(3)	C206	O205	C204	113.1(4)
C12	C9	C11	109.2(3)	O205	C206	C207	109.7(5)
F19	C10	C9	112.4(3)	O208	C207	C206	109.1(4)
F20	C10	C9	111.0(3)	C207	O208	C209	112.7(4)
F20	C10	F19	108.3(3)	O208	C209	C210	109.0(4)
F21	C10	C9	110.3(3)	O211	C210	C209	109.3(5)
F21	C10	F19	107.0(3)	C212	O211	C210	112.8(4)
F21	C10	F20	107.6(3)	O211	C212	C213	109.6(5)
F22	C11	C9	112.6(3)	O214	C213	C212	109.5(8)
F22	C11	F23	106.9(3)	C213	O214	C215	113.8(6)
F23	C11	C9	111.4(3)	O214	C215	C216	108.7(5)
F24	C11	C9	110.8(3)	O217	C216	C215	109.0(4)
F24	C11	F22	107.4(3)	C218	O217	C216	113.5(4)
F24	C11	F23	107.5(3)	O217	C218	C201	109.6(4)
F25	C12	C9	110.7(3)	O402	C401	C418	110.0(16)
F25	C12	F26	107.4(3)	C401	O402	C403	115.3(13)
F26	C12	C9	111.8(3)	O402	C403	C404	112.6(16)
F27	C12	C9	111.2(3)	O405	C404	C403	111.8(17)
F27	C12	F25	107.8(4)	C406	O405	C404	113.3(13)
F27	C12	F26	107.7(3)	O405	C406	C407	108.8(16)
C13	O4	Al1	147.4(3)	O408	C407	C406	109.2(15)
O4	C13	C14	111.5(3)	C409	O408	C407	113.0(13)
O4	C13	C15	108.3(3)	O408	C409	C410	109.8(15)
O4	C13	C16	109.0(3)	O411	C410	C409	110.7(17)
C14	C13	C15	110.6(3)	C410	O411	C412	113.2(15)
C14	C13	C16	108.5(3)	O411	C412	C413	108.9(19)
C15	C13	C16	108.9(3)	O414	C413	C412	114(2)
F28	C14	C13	112.2(4)	C413	O414	C415	113.8(14)
F28	C14	F29	108.3(4)	O414	C415	C416	110.9(16)
F28	C14	F30	107.2(4)	O417	C416	C415	109.4(16)
F29	C14	C13	110.2(3)	C418	O417	C416	113.9(13)
F29	C14	F30	107.1(4)	O417	C418	C401	109.9(16)
F30	C14	C13	111.7(3)	F901	C901	C902	117.0(4)
F31	C15	C13	109.6(3)	F901	C901	C906	123.0(4)
F31	C15	F32	107.5(3)	C902	C901	C906	120.0
F32	C15	C13	112.1(3)	C903	C902	C901	120.0
F33	C15	C13	111.7(3)	C902	C903	C904	120.0
F33	C15	F31	108.0(4)	C905	C904	C903	120.0

F33	C15	F32	107.8(3)	C906	C905	C904	120.0
F34	C16	C13	111.9(4)	C905	C906	C901	120.0
F35	C16	C13	110.4(3)	F971	C971	C972	131.8(14)
F35	C16	F34	107.2(4)	F971	C971	C976	108.0(14)
F36	C16	C13	110.7(3)	C972	C971	C976	120.0
F36	C16	F34	108.2(4)	C971	C972	C973	120.0
F36	C16	F35	108.3(4)	C972	C973	C974	120.0
C1A	O1A	Al1A	142.7(7)	C975	C974	C973	120.0
O1A	C1A	C2A	114.9(6)	C974	C975	C976	120.0
O1A	C1A	C3A	106.7(8)	C975	C976	C971	120.0
O1A	C1A	C4A	107.6(7)	F911	C911	C912	121.1(4)
C2A	C1A	C3A	109.6(6)	F911	C911	C916	118.9(4)
C2A	C1A	C4A	108.4(6)	C912	C911	C916	120.0
C3A	C1A	C4A	109.5(6)	C911	C912	C913	120.0
F1A	C2A	C1A	111.5(6)	C912	C913	C914	120.0
F1A	C2A	F2A	106.2(5)	C915	C914	C913	120.0
F2A	C2A	C1A	113.3(5)	C914	C915	C916	120.0
F3A	C2A	C1A	111.8(5)	C915	C916	C911	120.0
F3A	C2A	F1A	105.0(5)	F961	C961	C962	120.0(8)
F3A	C2A	F2A	108.5(6)	F961	C961	C966	120.0(8)
F4A	C3A	C1A	110.6(6)	C962	C961	C966	120.0
F4A	C3A	F5A	108.9(7)	C961	C962	C963	120.0
F5A	C3A	C1A	111.4(6)	C964	C963	C962	120.0
F6A	C3A	C1A	111.6(6)	C965	C964	C963	120.0
F6A	C3A	F4A	107.9(7)	C964	C965	C966	120.0
F6A	C3A	F5A	106.3(7)	C965	C966	C961	120.0
F7A	C4A	C1A	111.5(6)	F921	C921	C922	122.2(5)
F7A	C4A	F8A	110.8(7)	F921	C921	C926	117.8(5)
F8A	C4A	C1A	109.5(6)	C922	C921	C926	120.0
F9A	C4A	C1A	109.5(6)	C923	C922	C921	120.0
F9A	C4A	F7A	108.7(6)	C922	C923	C924	120.0
F9A	C4A	F8A	106.8(7)	C925	C924	C923	120.0
C1C	O1C	Al1A	157.4(17)	C924	C925	C926	120.0
O1C	C1C	C2C	108.6(12)	C925	C926	C921	120.0
O1C	C1C	C3C	108.1(12)	C982	C981	F981	119.7(8)
O1C	C1C	C4C	114.0(12)	C982	C981	C986	120.0
C2C	C1C	C4C	109.0(8)	C986	C981	F981	120.2(8)
C3C	C1C	C2C	108.7(9)	C981	C982	C983	120.0
C3C	C1C	C4C	108.4(8)	C982	C983	C984	120.0
F1C	C2C	C1C	112.0(8)	C985	C984	C983	120.0
F2C	C2C	C1C	113.2(9)	C984	C985	C986	120.0
F2C	C2C	F1C	107.8(9)	C985	C986	C981	120.0

F3C	C2C	C1C	115.2(9)	F931	C931	C932	118.2(6)
F3C	C2C	F1C	102.4(9)	F931	C931	C936	121.8(6)
F3C	C2C	F2C	105.3(9)	C932	C931	C936	120.0
F4C	C3C	C1C	110.5(9)	C933	C932	C931	120.0
F4C	C3C	F5C	108.9(10)	C932	C933	C934	120.0
F5C	C3C	C1C	113.7(9)	C933	C934	C935	120.0
F6C	C3C	C1C	111.1(9)	C936	C935	C934	120.0
F6C	C3C	F4C	106.6(11)	C935	C936	C931	120.0
F6C	C3C	F5C	105.8(11)	C952	C951	F951	118.6(8)
F7C	C4C	C1C	113.1(8)	C952	C951	C956	120.0
F7C	C4C	F9C	109.1(9)	C956	C951	F951	121.4(8)
F8C	C4C	C1C	111.3(8)	C953	C952	C951	120.0
F8C	C4C	F7C	108.3(9)	C952	C953	C954	120.0
F8C	C4C	F9C	104.0(9)	C953	C954	C955	120.0
F9C	C4C	C1C	110.6(8)	C954	C955	C956	120.0
C5A	O2A	Al1A	150.5(3)	C955	C956	C951	120.0
O2A	C5A	C6A	110.3(3)	C944[1]	C942	C943	119.1(5)
O2A	C5A	C7A	108.3(3)	C942	C943	C944	119.4(5)
O2A	C5A	C8A	111.3(3)	C942[1]	C944	C943	121.5(5)
C6A	C5A	C7A	109.7(4)	F941	C944	C942[1]	118.4(6)
C8A	C5A	C6A	108.2(3)	F941	C944	C943	120.1(6)

2.2.6. Hydrogen Atom Coordinates and Isotropic Displacement Parameters

Atom	***x***	***y***	***z***	**U(eq)**
H10A	7380	1096	1236	61
H10B	8136	1408	1373	61
H10C	8123	793	1978	59
H10D	7375	424	1863	59
H10E	7599	576	2512	58
H10F	7712	1564	2458	58
H10G	6775	1822	2832	55
H10H	6661	831	2872	55
H10I	5560	966	2567	52
H10J	5653	1523	2943	52
H10K	4768	2454	2705	48
H10L	4641	1910	2327	48
H11A	4260	3273	2228	45
H11B	5007	3622	2358	45
H11C	5022	4283	1755	37
H11D	4279	3918	1625	37
H11E	4714	3188	1132	45
H11F	4844	4177	1098	45

H11G	5787	3945	750	45
H11H	5660	2952	768	45
H11I	6787	3245	675	47
H11J	6875	3768	1060	47
H11K	7786	2799	1289	54
H11L	7663	2281	903	54
H20A	1735	9320	132	45
H20B	1437	10028	389	45
H20C	2609	10258	629	45
H20D	2887	9458	419	45
H20E	3581	9805	983	48
H20F	2950	9593	1217	48
H20G	3593	8437	1530	49
H20H	4217	8704	1301	49
H20I	4155	7359	1009	54
H20J	4359	7312	1455	54
H20K	3900	5915	1482	50
H20L	3725	5943	1032	50
H21A	3015	4987	1324	49
H21B	2718	5762	1544	49
H21C	1595	5520	1231	49
H21D	1895	4724	1027	49
H21E	1579	5359	434	53
H21F	929	5186	659	53
H21G	359	6240	288	47
H21H	1003	6577	93	47
H21I	169	7641	168	44
H21J	345	7553	616	44
H21K	784	8977	662	46
H21L	572	9076	218	46
H40A	2534	9501	340	45
H40B	2438	10239	637	45
H40C	3529	9813	963	45
H40D	3585	9041	681	45
H40E	4212	8819	1258	48
H40F	3528	8879	1462	48
H40G	3605	7440	1687	49
H40H	4344	7465	1537	49
H40I	3981	6351	1113	54
H40J	4032	6080	1548	54
H40K	3155	4995	1394	50
H40L	3191	5273	965	50

H41A	2144	4633	1057	49
H41B	1996	5379	1339	49
H41C	995	5499	890	49
H41D	1267	4937	563	49
H41E	1283	6103	176	53
H41F	535	5970	300	53
H41G	216	7413	208	47
H41H	921	7495	25	47
H41I	518	8798	240	44
H41J	625	8439	663	44
H41K	1443	9566	797	46
H41L	1380	9859	365	46
H902	4330	1332	1266	41
H903	4579	439	1783	45
H904	5585	-348	1839	48
H905	6342	-242	1378	43
H906	6093	651	861	37
H972	4808	1530	881	41
H973	4262	1275	1422	45
H974	4727	316	1874	48
H975	5738	-389	1786	43
H976	6284	-135	1246	37
H912	8260	3794	2048	47
H913	7169	4048	1747	47
H914	6228	4051	2095	49
H915	6378	3802	2745	49
H916	7468	3548	3046	42
H962	7529	3454	3012	47
H963	8412	3232	2633	47
H964	8235	3493	1985	49
H965	7175	3975	1716	49
H966	6292	4196	2094	42
H922	459	8402	1357	63
H923	1363	9326	1520	67
H924	2363	8836	1859	54
H925	2459	7421	2035	43
H926	1555	6497	1872	40
H982	1390	9386	1526	63
H983	2371	8985	1908	67
H984	2505	7592	2112	54
H985	1658	6601	1934	43
H986	676	7002	1552	40

H932	2169	7687	-59	71
H933	2492	6399	220	77
H934	3644	6036	321	84
H935	4474	6960	142	85
H936	4152	8248	-138	73
H952	2813	6100	238	71
H953	2081	7166	-7	77
H954	2529	8440	-198	84
H955	3708	8646	-143	85
H956	4440	7580	102	73
H942	6064	-284	-201	62
H943	5729	-951	331	60
H944	4658	-683	518	60

[1] I. Krossing, *Chemistry – A European Journal* **2001**, *7*, 490.
[2] A. J. Lehner, N. Trapp, H. Scherer, I. Krossing, *Dalton Transactions* **2011**, *40*, 1448.