

Supporting Information

Generation and Reaction of a Phenyl-Substituted Cyclopentadienyl Cation Annulated with Two Homoadamantene Frameworks

Kohei Ogawa, Toshikazu Kitagawa,* Shinya Minegishi, and Koichi Komatsu*

Table of Contents

	page
Figure S1. ^1H NMR spectrum of 4	S2
Figure S2. ^{13}C NMR spectrum of 4	S2
Figure S3. ^1H NMR spectrum of 5	S3
Figure S4. ^{13}C NMR spectrum of 5	S3
Figure S5. ^1H NMR spectrum of 6	S4
Figure S6. ^{13}C NMR spectrum of 6	S4
Figure S7. ^1H NMR spectrum of 7	S5
Figure S8. ^{13}C NMR spectrum of 7	S5
Figure S9. ^1H NMR spectrum of $\mathbf{8}^+\text{B}(\text{C}_6\text{F}_5)_4^-$	S6
Figure S10. ^{13}C NMR spectrum of $\mathbf{8}^+\text{B}(\text{C}_6\text{F}_5)_4^-$	S6
Figure S11. ^1H NMR spectrum of 14	S7
Figure S12. ^{13}C NMR spectrum of 14	S7
Table S1. Calculated molecular geometry and energy of singlet $\mathbf{2}^+$	S8
Table S2. Calculated molecular geometry and energy of triplet $\mathbf{2}^+$	S10
Table S3. Calculated molecular geometry and energy of $\mathbf{8}^+$	S12
Crystal data for 4	S14
Crystal data for 5	S22
Crystal data for 6	S30
Crystal data for $\mathbf{8}^+\text{B}(\text{C}_6\text{F}_5)_4^-$	S38
Crystal data for 14	S47

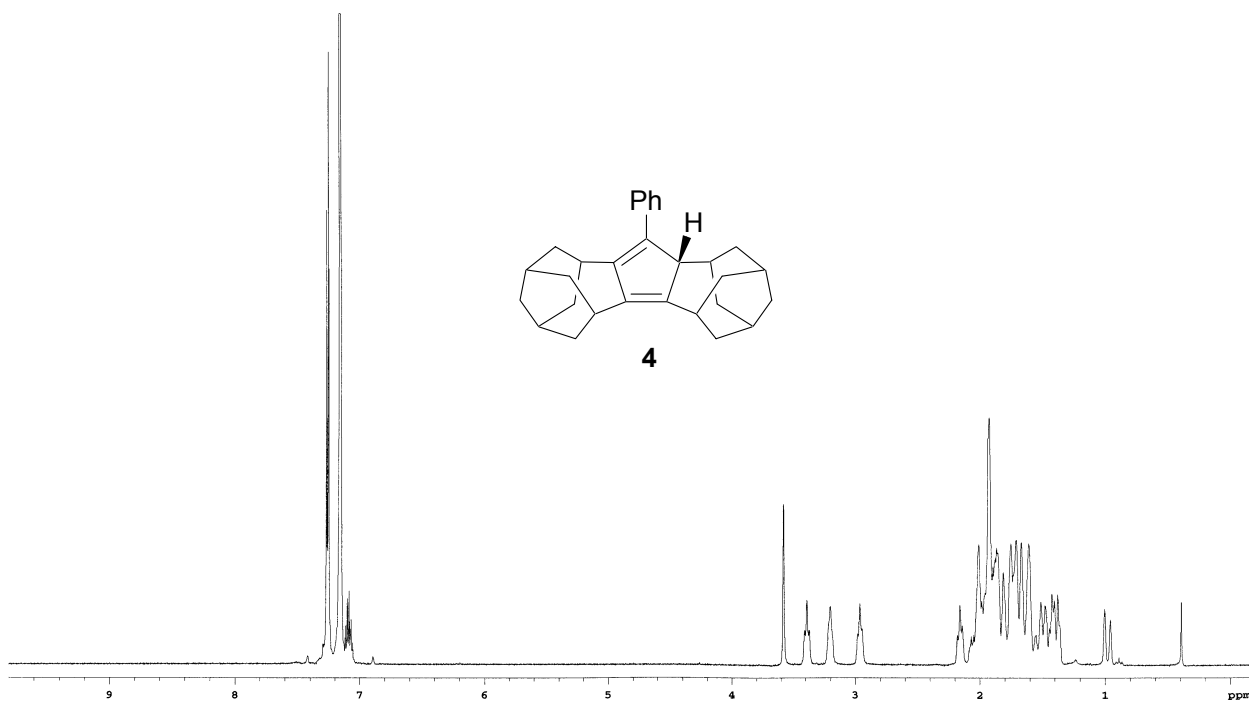


Figure S1. ^1H NMR Spectrum of **4** (300 MHz, C_6D_6)

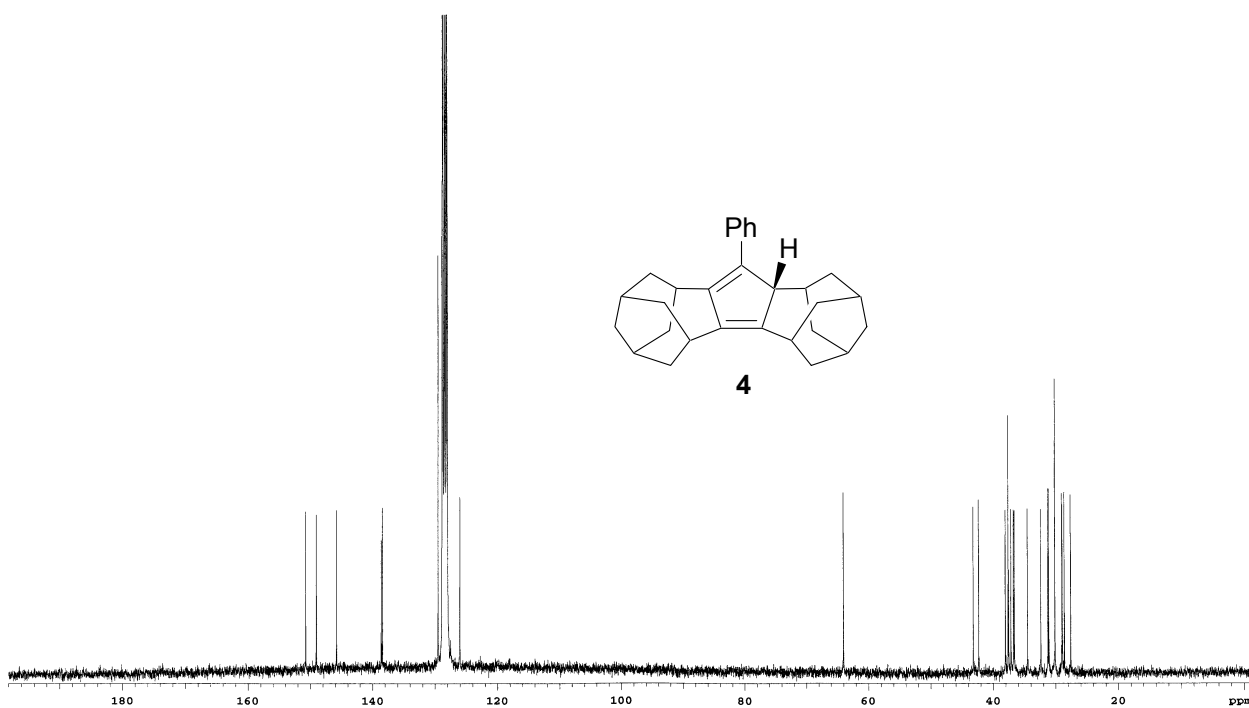


Figure S2. ^{13}C NMR Spectrum of **4** (75 MHz, C_6D_6)

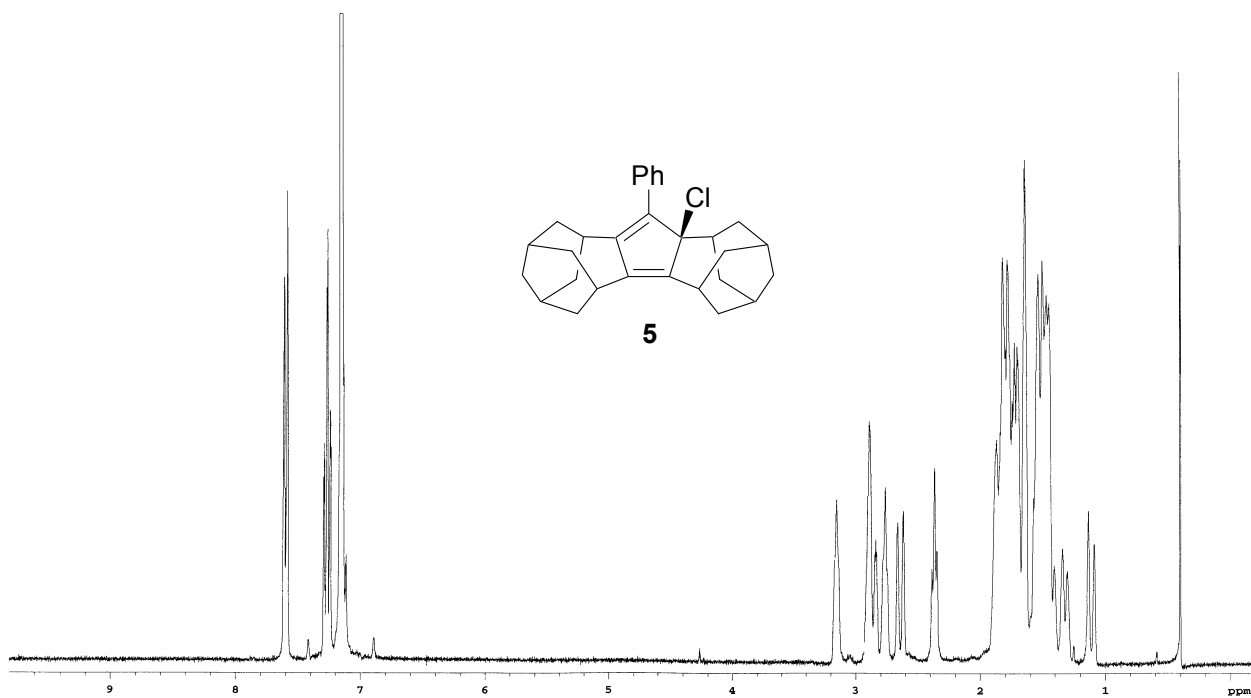


Figure S3. ¹H NMR Spectrum of **5** (300 MHz, C₆D₆)

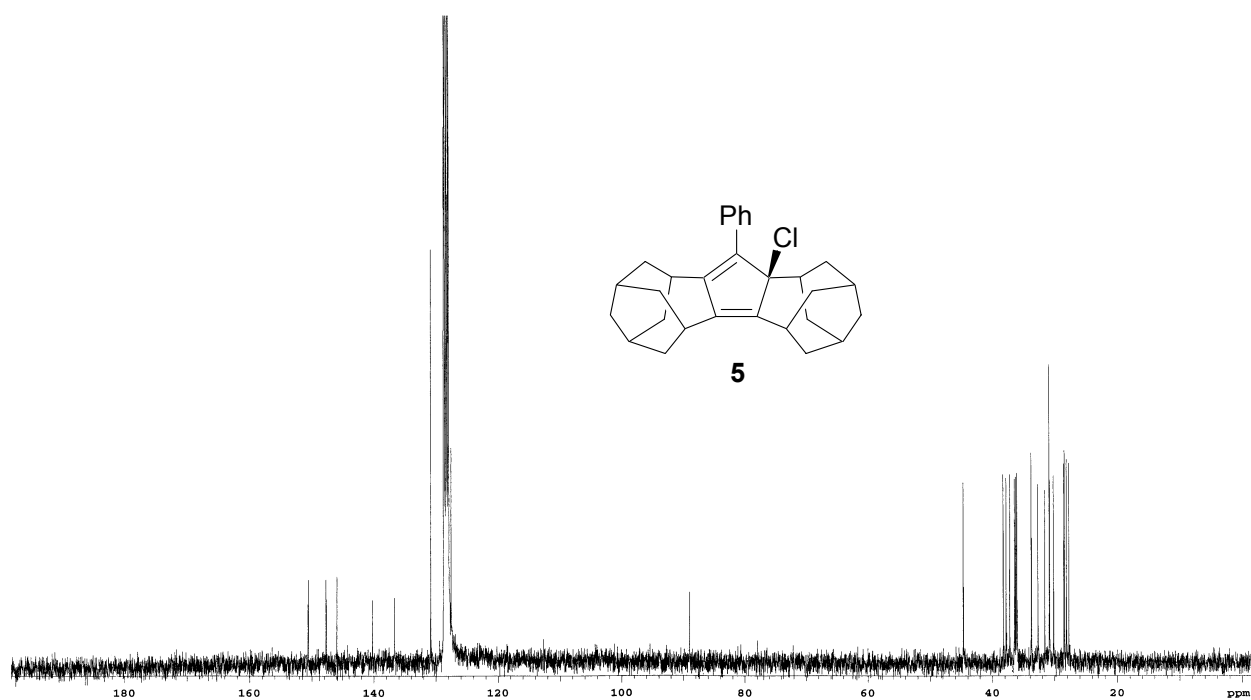


Figure S4. ¹³C NMR Spectrum of **5** (75 MHz, C₆D₆)

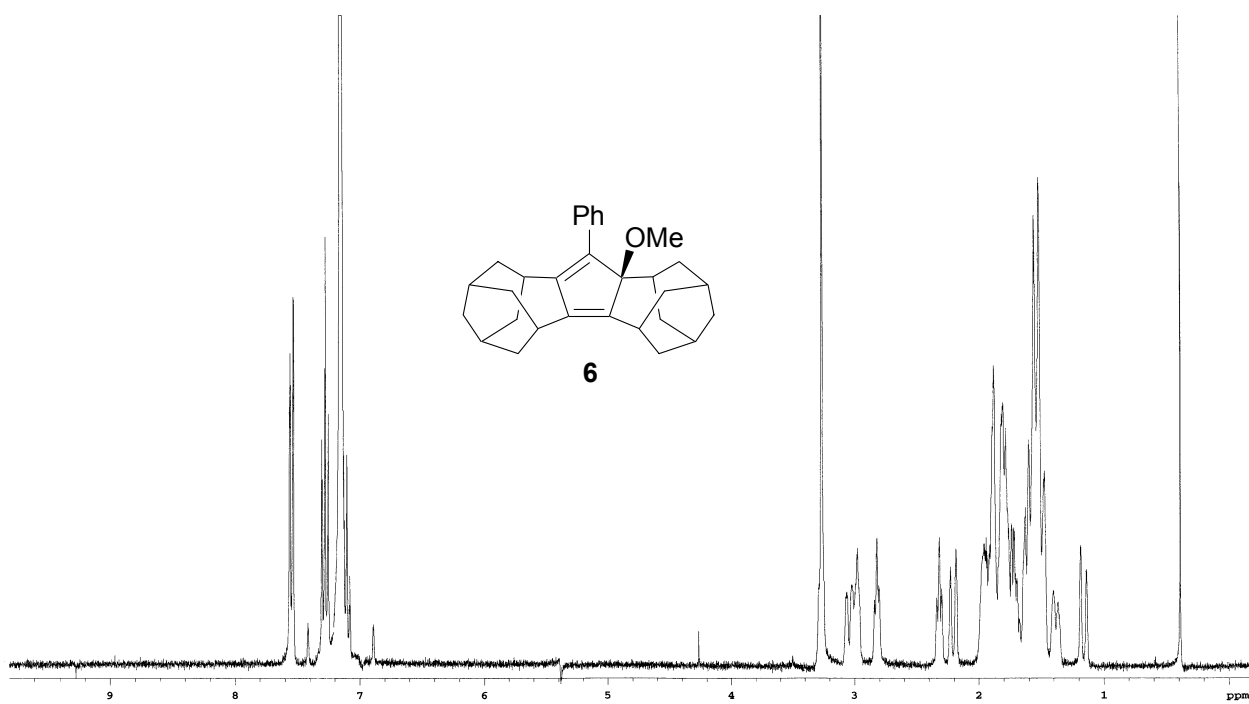


Figure S5. ^1H NMR Spectrum of **6** (300 MHz, C_6D_6)

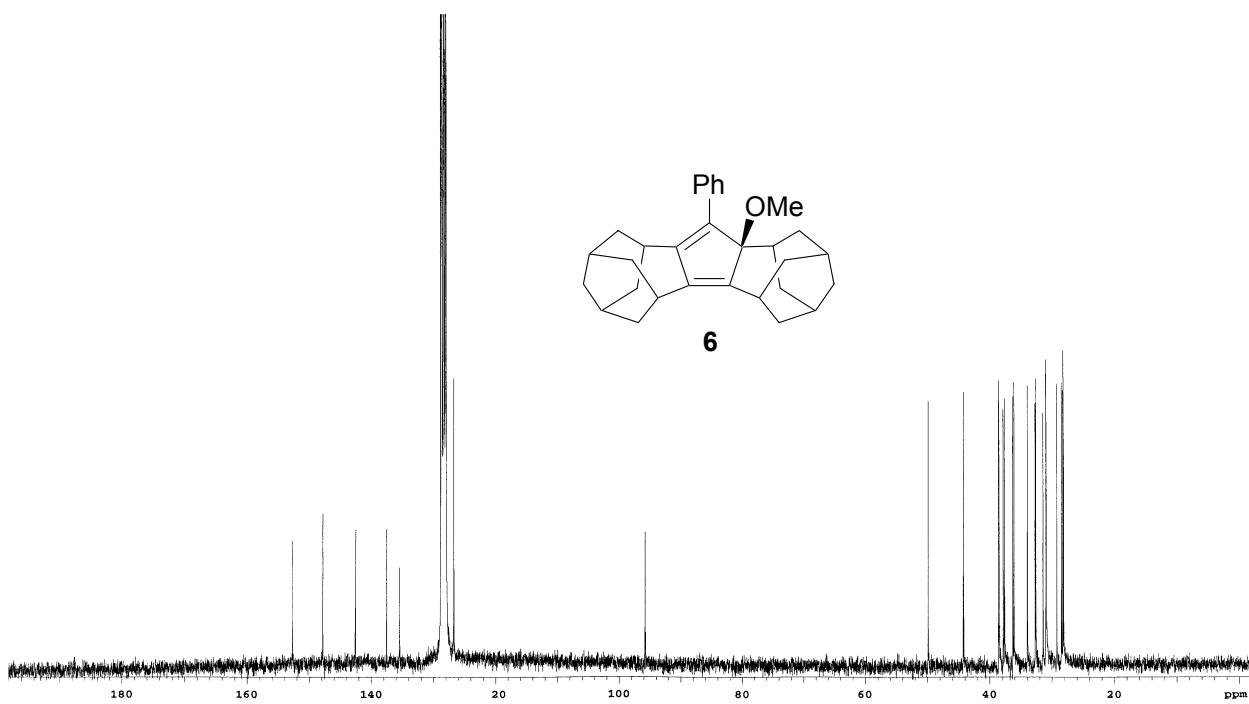


Figure S6. ^{13}C NMR Spectrum of **6** (75 MHz, C_6D_6)

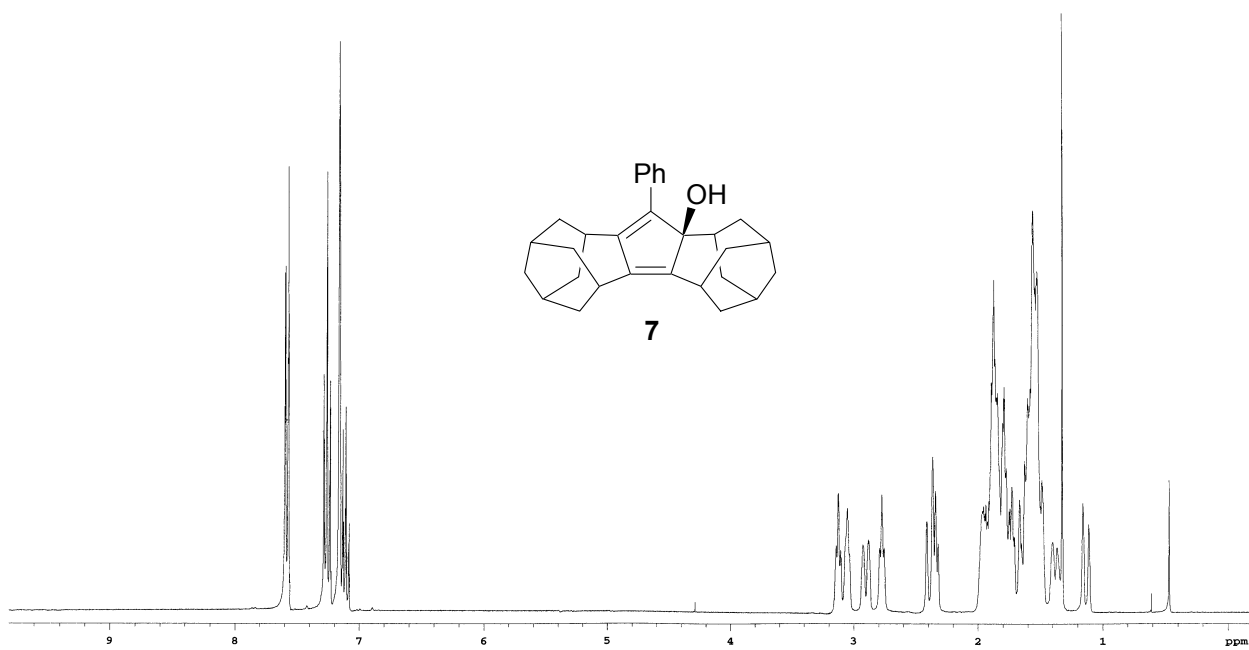


Figure S7. ^1H NMR Spectrum of **7** (300 MHz, C_6D_6)

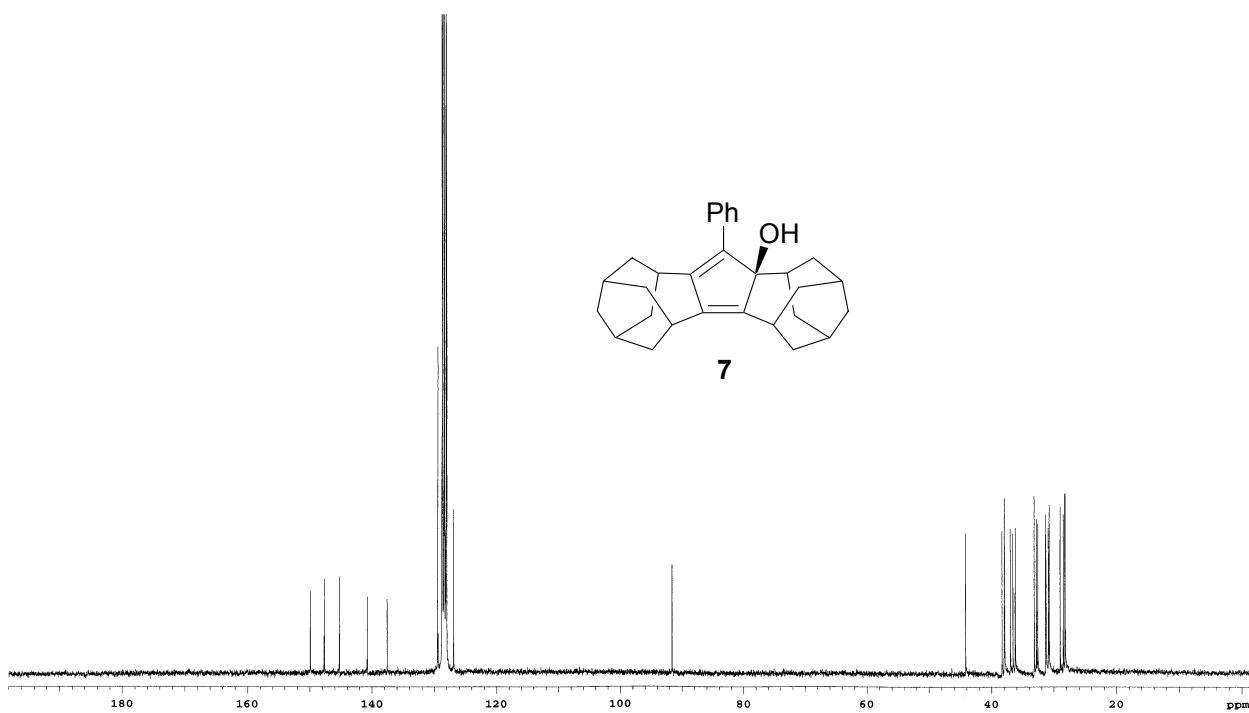


Figure S8. ^{13}C NMR Spectrum of **7** (75 MHz, C_6D_6)

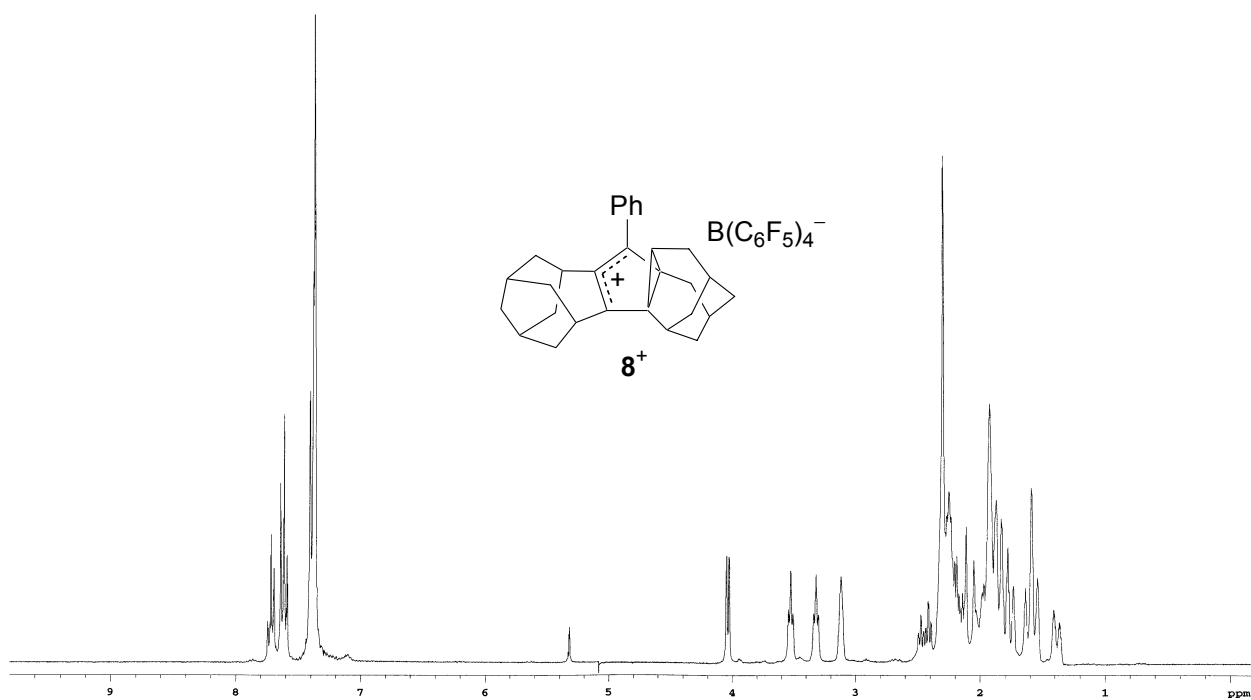


Figure S9. ^1H NMR Spectrum of $8^+\text{B}(\text{C}_6\text{F}_5)_4^-$ (300 MHz, CD_2Cl_2)

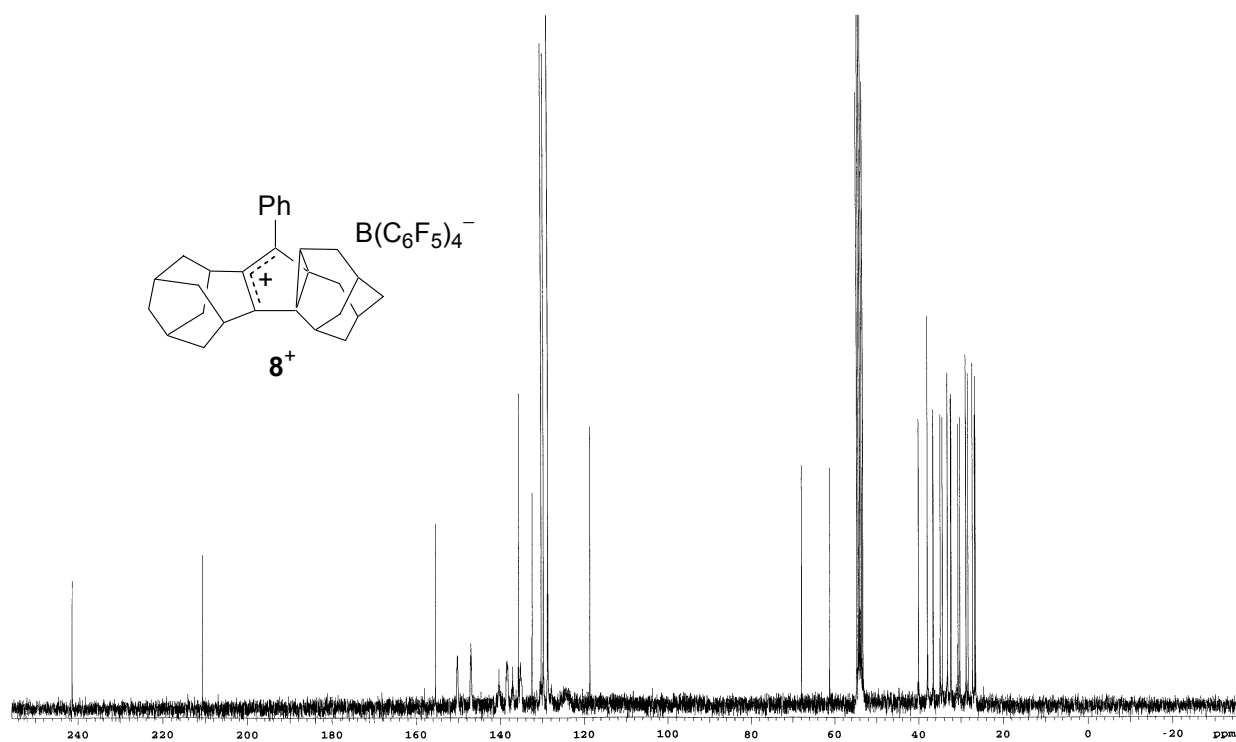


Figure S10. ^{13}C NMR Spectrum of $8^+\text{B}(\text{C}_6\text{F}_5)_4^-$ (75 MHz, CD_2Cl_2)

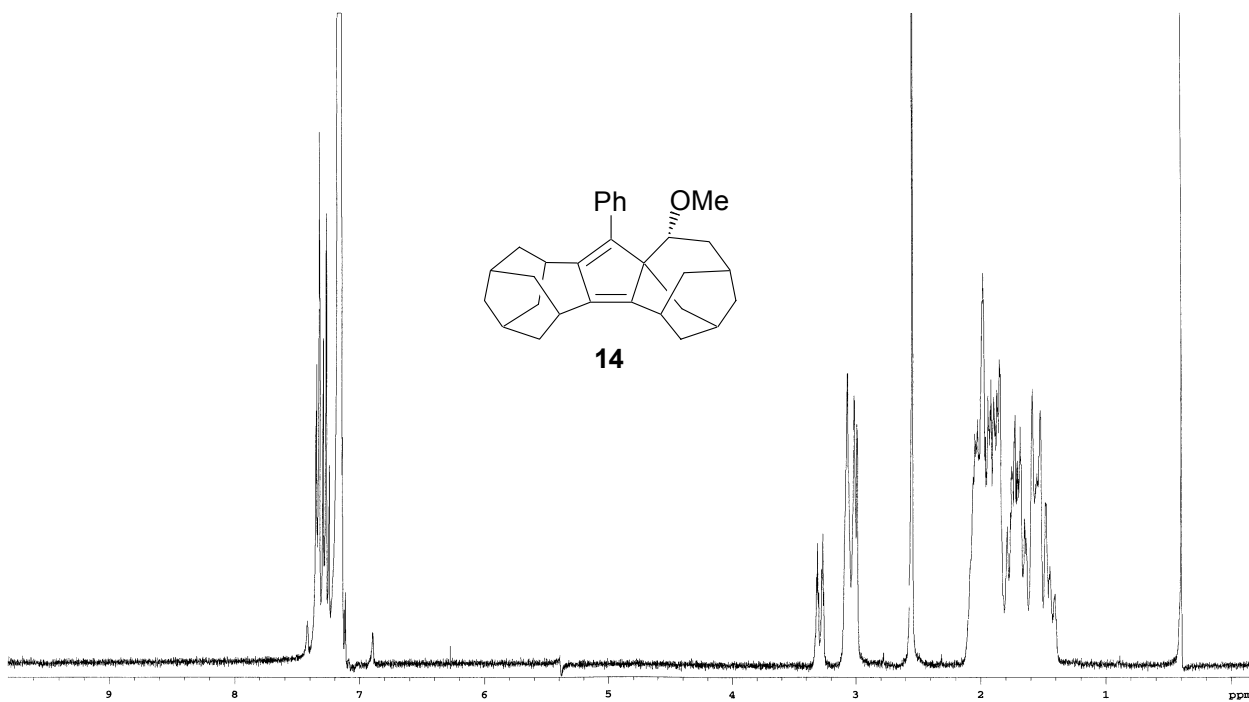


Figure S11. ^1H NMR Spectrum of **14** (300 MHz, C_6D_6)

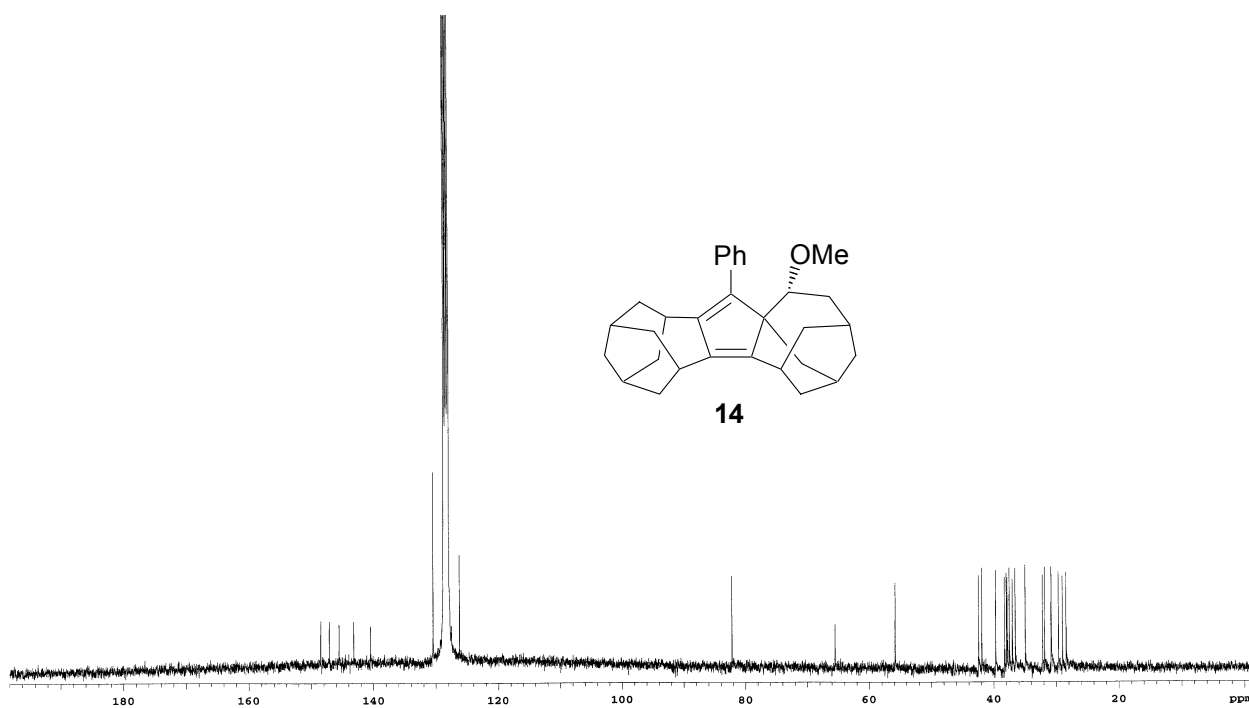


Figure S12. ^{13}C NMR Spectrum of **14** (75 MHz, C_6D_6)

Table S1. Calculated molecular geometry and energy of singlet 2^+

B3LYP/6-31+G(d,p) level

HF = -1124.7868579 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.722866	-1.347537	-1.198431
2	6	0	-4.562179	-1.596604	0.066816
3	6	0	-3.676388	-1.358589	1.302179
4	6	0	-2.514360	-2.371111	1.308540
5	6	0	-1.649998	-2.352203	0.011801
6	6	0	-2.558062	-2.356174	-1.254785
7	6	0	-3.233035	0.113754	1.345710
8	6	0	-2.528961	0.636559	0.036039
9	6	0	-3.287558	0.127217	-1.246802
10	6	0	-1.120593	0.235325	0.008326
11	6	0	-0.674606	-1.217895	0.003457
12	6	0	3.676898	-1.360207	-1.301430
13	6	0	4.562201	-1.596635	-0.065411
14	6	0	3.722387	-1.345896	1.199181
15	6	0	3.287187	0.128963	1.245512
16	6	0	2.529031	0.636552	-0.038210
17	6	0	3.233447	0.112053	-1.346969
18	6	0	2.557406	-2.354286	1.256359
19	6	0	1.649883	-2.352053	-0.010694
20	6	0	2.514896	-2.372735	-1.306992
21	6	0	0.674409	-1.217939	-0.004243
22	6	0	1.120656	0.235388	-0.010443
23	6	0	0.000125	1.082651	-0.001796
24	6	0	0.000170	2.569423	-0.001116
25	6	0	0.396882	3.282567	1.142440
26	6	0	0.398044	4.679412	1.142486
27	6	0	-0.000150	5.380897	0.001416
28	6	0	-0.398077	4.681344	-1.140951
29	6	0	-0.396692	3.284433	-1.143508
30	1	0	-4.346069	-1.517910	-2.085989
31	1	0	-4.947980	-2.622865	0.069707
32	1	0	-5.433510	-0.930319	0.085732
33	1	0	-4.267271	-1.533044	2.210826
34	1	0	-2.938958	-3.377860	1.405631
35	1	0	-1.871624	-2.219003	2.183929
36	1	0	-1.062850	-3.276126	-0.003599
37	1	0	-1.946125	-2.192393	-2.150001

38	1	0	-2.983599	-3.362703	-1.349867
39	1	0	-2.588166	0.306241	2.210614
40	1	0	-4.117457	0.749869	1.471823
41	1	0	-2.569931	1.728986	0.043554
42	1	0	-4.178983	0.760629	-1.329768
43	1	0	-2.680371	0.328597	-2.136719
44	1	0	4.268147	-1.535752	-2.209625
45	1	0	5.433545	-0.930374	-0.084840
46	1	0	4.948010	-2.622900	-0.066825
47	1	0	4.345196	-1.515246	2.087211
48	1	0	4.178595	0.762439	1.328053
49	1	0	2.679576	0.331427	2.134895
50	1	0	2.569967	1.728976	-0.047083
51	1	0	2.588783	0.303306	-2.212305
52	1	0	4.117880	0.748032	-1.473733
53	1	0	1.945103	-2.189097	2.151065
54	1	0	2.982698	-3.360765	1.353058
55	1	0	1.062878	-3.276049	0.005700
56	1	0	2.939484	-3.379653	-1.402450
57	1	0	1.872627	-2.221853	-2.182934
58	1	0	0.693218	2.743242	2.038219
59	1	0	0.704697	5.217549	2.034108
60	1	0	-0.000273	6.466393	0.002474
61	1	0	-0.704740	5.221333	-2.031444
62	1	0	-0.693085	2.746852	-2.040300

Table S2. Calculated molecular geometry and energy of triplet 2^+

UB3LYP/6-31+G(d,p) level

HF = -1124.7923136 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.769423	-1.356178	-1.158393
2	6	0	-4.565544	-1.654021	0.124686
3	6	0	-3.662472	-1.390762	1.343016
4	6	0	-2.468199	-2.364774	1.315642
5	6	0	-1.631270	-2.304619	-0.001034
6	6	0	-2.564573	-2.316648	-1.250875
7	6	0	-3.263547	0.098365	1.376120
8	6	0	-2.601150	0.625802	0.061891
9	6	0	-3.395237	0.140263	-1.190435
10	6	0	-1.161806	0.232299	-0.014566
11	6	0	-0.713969	-1.126022	-0.008121
12	6	0	3.663997	-1.389677	-1.342285
13	6	0	4.566514	-1.652002	-0.123369
14	6	0	3.769535	-1.353879	1.159103
15	6	0	3.394670	0.142422	1.190147
16	6	0	2.600907	0.626865	-0.062850
17	6	0	3.264713	0.099316	-1.376294
18	6	0	2.565040	-2.314842	1.251328
19	6	0	1.632375	-2.303800	0.001012
20	6	0	2.470081	-2.364064	-1.315182
21	6	0	0.714428	-1.125724	0.007294
22	6	0	1.161790	0.232725	0.013186
23	6	0	-0.000162	1.088225	-0.001123
24	6	0	-0.000453	2.544842	-0.000893
25	6	0	0.844909	3.270160	0.872646
26	6	0	0.830242	4.661265	0.882000
27	6	0	-0.002092	5.361838	0.000955
28	6	0	-0.833276	4.661440	-0.881327
29	6	0	-0.846700	3.270272	-0.873487
30	1	0	-4.403808	-1.549295	-2.032424
31	1	0	-4.911189	-2.694955	0.125674
32	1	0	-5.461405	-1.022754	0.170743
33	1	0	-4.225447	-1.594696	2.262511
34	1	0	-2.853570	-3.387734	1.405692
35	1	0	-1.812818	-2.201130	2.179404
36	1	0	-1.016548	-3.208696	-0.039895
37	1	0	-1.976546	-2.115717	-2.154536

38	1	0	-2.949792	-3.338597	-1.352782
39	1	0	-2.607374	0.307302	2.229550
40	1	0	-4.171572	0.693921	1.531359
41	1	0	-2.652187	1.716311	0.094213
42	1	0	-4.322304	0.725193	-1.231177
43	1	0	-2.835420	0.378907	-2.103154
44	1	0	4.227608	-1.593829	-2.261354
45	1	0	5.462187	-1.020460	-0.169288
46	1	0	4.912535	-2.692813	-0.123635
47	1	0	4.403456	-1.546347	2.033622
48	1	0	4.321425	0.727861	1.230924
49	1	0	2.834349	0.381408	2.102466
50	1	0	2.651372	1.717399	-0.095580
51	1	0	2.609451	0.307918	-2.230494
52	1	0	4.172728	0.695126	-1.530704
53	1	0	1.976501	-2.113705	2.154601
54	1	0	2.950641	-3.336570	1.354022
55	1	0	1.018197	-3.208286	0.039905
56	1	0	2.855862	-3.386930	-1.404681
57	1	0	1.815126	-2.200984	-2.179379
58	1	0	1.475171	2.738068	1.577542
59	1	0	1.465297	5.201697	1.576677
60	1	0	-0.002645	6.447280	0.001700
61	1	0	-1.468888	5.202231	-1.575210
62	1	0	-1.476366	2.738366	-1.579048

Table S3. Calculated molecular geometry and energy of 8^+

B3LYP/6-31+G(d,p) level

HF = -1124.8051413 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.412155	-1.749026	-1.868443
2	6	0	-1.005001	0.348199	-0.082926
3	6	0	0.785334	-1.199041	-0.043664
4	6	0	1.528447	-2.347811	-0.752236
5	6	0	1.386425	-0.648397	1.299927
6	6	0	0.192421	1.098942	-0.044267
7	6	0	1.364607	0.182150	-0.008312
8	6	0	-2.484686	-2.111405	1.314650
9	6	0	-0.307051	4.776128	-0.738242
10	6	0	-3.743087	-1.056786	-1.164083
11	6	0	1.505287	4.511864	0.849425
12	6	0	-1.660630	-2.131417	-0.010208
13	6	0	2.658168	0.505572	-0.753725
14	6	0	3.410725	-0.752101	-1.252037
15	6	0	2.648744	-1.252862	1.866459
16	6	0	2.409827	-3.143467	0.229654
17	6	0	-2.432498	0.845295	0.016913
18	6	0	-2.605204	-2.095304	-1.254870
19	6	0	-0.671242	-1.017242	-0.065650
20	6	0	-3.615196	-1.063952	1.338289
21	6	0	-0.490619	3.396247	-0.765304
22	6	0	0.336248	2.547247	0.005447
23	6	0	-4.543339	-1.287727	0.130519
24	6	0	3.414265	-2.192899	0.906676
25	6	0	4.249462	-1.448893	-0.157946
26	6	0	1.351961	3.130610	0.797656
27	6	0	-3.269868	0.412377	-1.216704
28	6	0	-3.117580	0.396571	1.338582
29	6	0	0.679800	5.338207	0.077931
30	1	0	2.948609	-2.559208	-2.375413
31	1	0	1.793075	-1.251995	-2.625986
32	1	0	0.782501	-3.016169	-1.194305
33	1	0	0.652172	-0.340088	2.039593
34	1	0	-2.930010	-3.107769	1.423287
35	1	0	-1.810147	-1.978907	2.169068
36	1	0	-0.932108	5.413824	-1.355074
37	1	0	-4.396426	-1.223144	-2.029361

38	1	0	2.270354	4.946829	1.484440
39	1	0	-1.103608	-3.073136	-0.037937
40	1	0	2.388109	1.114096	-1.624042
41	1	0	3.319664	1.125275	-0.138099
42	1	0	4.101821	-0.410076	-2.030874
43	1	0	2.361382	-1.818418	2.761562
44	1	0	3.305072	-0.444965	2.220701
45	1	0	2.941140	-3.925991	-0.323760
46	1	0	1.792432	-3.647287	0.984139
47	1	0	-2.402475	1.936149	0.037564
48	1	0	-2.015369	-1.945162	-2.167128
49	1	0	-3.052713	-3.093348	-1.336091
50	1	0	-4.180866	-1.221273	2.264832
51	1	0	-1.236733	2.971151	-1.427193
52	1	0	-4.953970	-2.304871	0.149341
53	1	0	-5.397137	-0.600883	0.175923
54	1	0	4.104481	-2.777619	1.524913
55	1	0	4.911368	-0.720550	0.327347
56	1	0	4.903964	-2.181121	-0.647540
57	1	0	1.992706	2.496252	1.401308
58	1	0	-4.160277	1.051497	-1.261992
59	1	0	-2.704054	0.600211	-2.138021
60	1	0	-3.986424	1.047893	1.493884
61	1	0	-2.443830	0.576876	2.185805
62	1	0	0.810061	6.415444	0.108036

Crystal data for 4

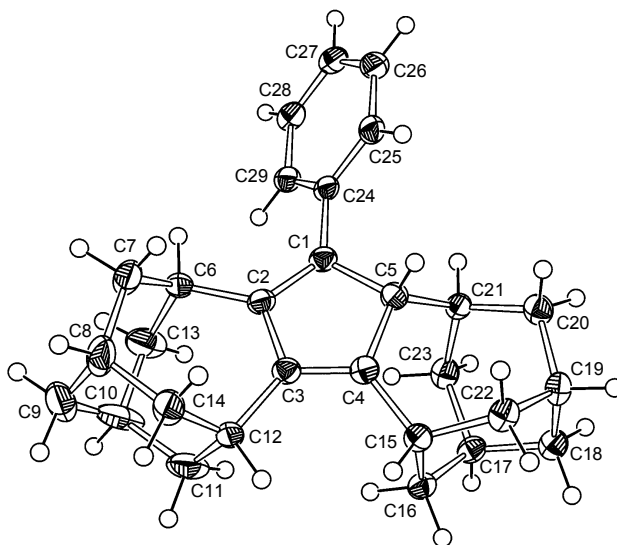


Table 1. Crystal data and structure refinement for 4.

Identification code	4	
Empirical formula	C ₂₉ H ₃₄	
Formula weight	382.56	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 6.3533(12) Å	α = 90°.
	b = 17.527(3) Å	β = 96.512(4)°.
	c = 18.820(4) Å	γ = 90°.
Volume	2082.2(7) Å ³	
Z	4	
Density (calculated)	1.220 Mg/m ³	
Absorption coefficient	0.068 mm ⁻¹	
F(000)	832	
Crystal size	0.10 x 0.10 x 0.10 mm ³	
Theta range for data collection	1.59 to 25.00°.	
Index ranges	-7 ≤ h ≤ 7, -16 ≤ k ≤ 20, -16 ≤ l ≤ 22	
Reflections collected	10646	

Independent reflections	3672 [R(int) = 0.0440]
Completeness to theta = 25.00°	99.9 %
Absorption correction	Empirical (SADABS)
Max. and min. transmission	0.9932 and 0.9932
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3672 / 0 / 262
Goodness-of-fit on F ²	1.013
Final R indices [I>2sigma(I)]	R ₁ = 0.0528, wR ₂ = 0.1067
R indices (all data)	R ₁ = 0.0906, wR ₂ = 0.1161
Largest diff. peak and hole	0.285 and -0.247 e.Å ⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(1)	4885(3)	2408(1)	2828(1)	23(1)
C(24)	5383(3)	3133(1)	3199(1)	23(1)
C(3)	3900(3)	1182(1)	2506(1)	23(1)
C(16)	1990(3)	1338(1)	857(1)	26(1)
C(4)	4607(3)	1474(1)	1915(1)	23(1)
C(19)	5408(4)	2254(1)	348(1)	27(1)
C(29)	3953(4)	3487(1)	3609(1)	26(1)
C(5)	5407(4)	2271(1)	2070(1)	25(1)
C(21)	4560(3)	2873(1)	1514(1)	23(1)
C(22)	5856(4)	1452(1)	661(1)	28(1)
C(6)	3472(3)	1597(1)	3808(1)	26(1)
C(25)	7294(4)	3505(1)	3141(1)	27(1)
C(12)	2955(4)	406(1)	2598(1)	28(1)
C(15)	4282(3)	1159(1)	1166(1)	24(1)
C(17)	1697(3)	2172(1)	632(1)	25(1)
C(2)	4071(3)	1758(1)	3076(1)	24(1)
C(7)	4797(4)	942(1)	4173(1)	39(1)
C(28)	4459(4)	4171(1)	3960(1)	28(1)

C(26)	7792(4)	4186(1)	3490(1)	32(1)
C(18)	3096(4)	2328(1)	43(1)	28(1)
C(20)	5904(4)	2903(1)	891(1)	28(1)
C(14)	4349(4)	-69(1)	3159(1)	39(1)
C(23)	2192(3)	2753(1)	1247(1)	28(1)
C(27)	6378(4)	4518(1)	3903(1)	31(1)
C(13)	1100(4)	1430(2)	3801(1)	48(1)
C(11)	678(4)	441(2)	2779(1)	48(1)
C(8)	4087(5)	139(2)	3933(1)	52(1)
C(9)	1807(6)	44(2)	4050(2)	70(1)
C(10)	470(5)	606(2)	3576(2)	61(1)

Table 3. Bond lengths [Å] and angles [°] for **4**.

C(1)-C(2)	1.356(3)
C(1)-C(24)	1.469(3)
C(1)-C(5)	1.518(3)
C(24)-C(25)	1.393(3)
C(24)-C(29)	1.401(3)
C(3)-C(4)	1.347(3)
C(3)-C(2)	1.468(3)
C(3)-C(12)	1.505(3)
C(16)-C(17)	1.527(3)
C(16)-C(15)	1.537(3)
C(4)-C(5)	1.504(3)
C(4)-C(15)	1.506(3)
C(19)-C(18)	1.521(3)
C(19)-C(20)	1.539(3)
C(19)-C(22)	1.539(3)
C(29)-C(28)	1.389(3)
C(5)-C(21)	1.539(3)
C(21)-C(20)	1.527(3)
C(21)-C(23)	1.546(3)

C(22)-C(15)	1.543(3)
C(6)-C(2)	1.498(3)
C(6)-C(13)	1.533(3)
C(6)-C(7)	1.538(3)
C(25)-C(26)	1.382(3)
C(12)-C(11)	1.525(3)
C(12)-C(14)	1.542(3)
C(17)-C(18)	1.523(3)
C(17)-C(23)	1.547(3)
C(7)-C(8)	1.530(3)
C(28)-C(27)	1.378(3)
C(26)-C(27)	1.380(3)
C(14)-C(8)	1.528(3)
C(13)-C(10)	1.545(4)
C(11)-C(10)	1.548(3)
C(8)-C(9)	1.499(4)
C(9)-C(10)	1.522(4)

C(2)-C(1)-C(24)	129.28(19)
C(2)-C(1)-C(5)	108.89(18)
C(24)-C(1)-C(5)	121.70(19)
C(25)-C(24)-C(29)	117.5(2)
C(25)-C(24)-C(1)	120.7(2)
C(29)-C(24)-C(1)	121.8(2)
C(4)-C(3)-C(2)	109.85(19)
C(4)-C(3)-C(12)	127.81(19)
C(2)-C(3)-C(12)	122.28(19)
C(17)-C(16)-C(15)	112.37(18)
C(3)-C(4)-C(5)	109.16(18)
C(3)-C(4)-C(15)	127.7(2)
C(5)-C(4)-C(15)	122.00(18)
C(18)-C(19)-C(20)	107.70(18)
C(18)-C(19)-C(22)	110.57(18)
C(20)-C(19)-C(22)	113.90(17)
C(28)-C(29)-C(24)	121.0(2)

C(4)-C(5)-C(1)	102.97(17)
C(4)-C(5)-C(21)	114.80(17)
C(1)-C(5)-C(21)	115.69(18)
C(20)-C(21)-C(5)	111.31(18)
C(20)-C(21)-C(23)	111.29(17)
C(5)-C(21)-C(23)	112.39(18)
C(19)-C(22)-C(15)	115.83(18)
C(2)-C(6)-C(13)	112.34(18)
C(2)-C(6)-C(7)	111.55(18)
C(13)-C(6)-C(7)	110.4(2)
C(26)-C(25)-C(24)	121.5(2)
C(3)-C(12)-C(11)	113.0(2)
C(3)-C(12)-C(14)	111.18(19)
C(11)-C(12)-C(14)	110.8(2)
C(4)-C(15)-C(16)	107.60(17)
C(4)-C(15)-C(22)	115.10(18)
C(16)-C(15)-C(22)	110.61(17)
C(18)-C(17)-C(16)	108.16(18)
C(18)-C(17)-C(23)	109.86(18)
C(16)-C(17)-C(23)	114.51(17)
C(1)-C(2)-C(3)	108.93(18)
C(1)-C(2)-C(6)	128.5(2)
C(3)-C(2)-C(6)	122.55(19)
C(8)-C(7)-C(6)	115.3(2)
C(27)-C(28)-C(29)	120.1(2)
C(27)-C(26)-C(25)	120.1(2)
C(19)-C(18)-C(17)	109.19(17)
C(21)-C(20)-C(19)	113.22(18)
C(8)-C(14)-C(12)	114.0(2)
C(21)-C(23)-C(17)	116.14(18)
C(28)-C(27)-C(26)	119.8(2)
C(6)-C(13)-C(10)	113.9(2)
C(12)-C(11)-C(10)	114.3(2)
C(9)-C(8)-C(14)	109.0(2)
C(9)-C(8)-C(7)	108.4(2)

C(14)-C(8)-C(7)	116.1(2)
C(8)-C(9)-C(10)	109.0(2)
C(9)-C(10)-C(13)	109.5(2)
C(9)-C(10)-C(11)	110.1(2)
C(13)-C(10)-C(11)	113.1(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
C(1)	28(1)	19(1)	22(1)	-2(1)	-1(1)	0(1)
C(24)	32(1)	17(1)	19(1)	3(1)	-4(1)	-1(1)
C(3)	27(1)	19(1)	24(1)	-1(1)	1(1)	0(1)
C(16)	32(1)	24(1)	22(1)	-3(1)	3(1)	-2(1)
C(4)	25(1)	19(1)	24(1)	2(1)	-1(1)	4(1)
C(19)	32(1)	26(1)	24(1)	3(1)	8(1)	4(1)
C(29)	30(1)	23(1)	24(1)	3(1)	-3(1)	-1(1)
C(5)	31(1)	20(1)	24(1)	1(1)	2(1)	-1(1)
C(21)	33(1)	15(1)	20(1)	0(1)	3(1)	0(1)
C(22)	32(1)	25(1)	26(1)	0(1)	5(1)	7(1)
C(6)	35(1)	20(1)	23(1)	-5(1)	4(1)	-6(1)
C(25)	36(1)	23(1)	23(1)	2(1)	3(1)	-3(1)
C(12)	41(2)	23(1)	22(1)	-7(1)	9(1)	-10(1)
C(15)	32(1)	15(1)	24(1)	1(1)	2(1)	2(1)
C(17)	25(1)	28(1)	22(1)	1(1)	-3(1)	3(1)
C(2)	28(1)	22(1)	21(1)	-2(1)	-1(1)	-2(1)
C(7)	72(2)	22(1)	21(1)	0(1)	3(1)	-3(1)
C(28)	39(2)	20(1)	24(1)	-1(1)	0(1)	5(1)
C(26)	40(2)	25(1)	29(1)	4(1)	-3(1)	-8(1)
C(18)	37(1)	22(1)	26(1)	2(1)	3(1)	4(1)
C(20)	34(1)	21(1)	30(1)	3(1)	5(1)	1(1)

C(14)	72(2)	17(1)	30(1)	-1(1)	8(1)	-4(1)
C(23)	33(1)	24(1)	28(1)	3(1)	4(1)	5(1)
C(27)	48(2)	17(1)	25(1)	1(1)	-7(1)	-1(1)
C(13)	46(2)	53(2)	49(2)	-27(1)	25(1)	-19(2)
C(11)	49(2)	48(2)	50(2)	-28(1)	18(1)	-24(1)
C(8)	104(3)	24(2)	27(1)	4(1)	10(2)	-9(2)
C(9)	141(3)	40(2)	36(2)	-15(1)	41(2)	-43(2)
C(10)	56(2)	67(2)	68(2)	-48(2)	42(2)	-44(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **4**.

	x	y	z	U(eq)
H(16A)	1591	1007	438	31
H(16B)	1030	1219	1221	31
H(19)	6302	2329	-52	32
H(29)	2619	3256	3647	31
H(5)	6985	2260	2085	30
H(21)	4689	3381	1757	27
H(22A)	7294	1452	927	33
H(22B)	5866	1088	260	33
H(6)	3792	2066	4104	31
H(25)	8276	3285	2856	32
H(12)	2931	134	2130	34
H(15)	4431	592	1198	29
H(17)	188	2244	427	30
H(7A)	6288	1011	4080	46
H(7B)	4754	980	4696	46
H(28)	3479	4400	4241	34
H(26)	9111	4427	3446	38
H(18A)	2768	1959	-353	34
H(18B)	2821	2849	-150	34

H(20A)	7420	2877	1083	34
H(20B)	5664	3399	642	34
H(14A)	3999	-615	3083	47
H(14B)	5852	1	3082	47
H(23A)	1582	3252	1085	34
H(23B)	1459	2585	1657	34
H(27)	6728	4983	4146	37
H(13A)	293	1789	3469	57
H(13B)	688	1524	4286	57
H(11A)	-23	-52	2647	57
H(11B)	-86	843	2484	57
H(8)	4935	-233	4250	62
H(9A)	1632	140	4559	84
H(9B)	1341	-485	3931	84
H(10)	-1045	529	3655	73

Crystal data for 5

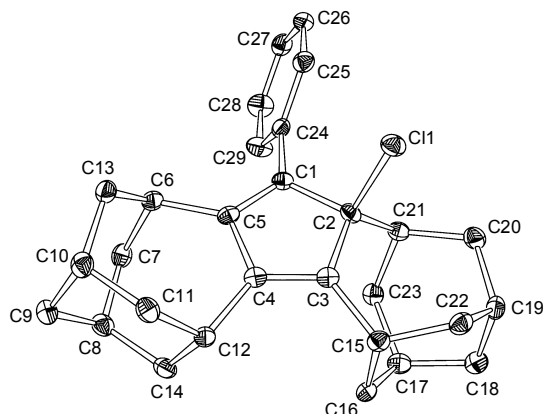


Table 1. Crystal data and structure refinement for **5**.

Identification code	5	
Empirical formula	C ₂₉ H ₃₃ Cl	
Formula weight	417.00	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 6.5347(13) Å	α = 74.790(4)°.
	b = 10.784(2) Å	β = 82.116(4)°.
	c = 15.777(3) Å	γ = 81.619(4)°.
Volume	1055.7(4) Å ³	
Z	2	
Density (calculated)	1.312 Mg/m ³	
Absorption coefficient	0.196 mm ⁻¹	
F(000)	448	
Crystal size	0.20 x 0.20 x 0.20 mm ³	
Theta range for data collection	1.34 to 25.00°.	
Index ranges	-7 ≤ h ≤ 7, -11 ≤ k ≤ 12, -15 ≤ l ≤ 18	
Reflections collected	5472	
Independent reflections	3630 [R(int) = 0.0200]	
Completeness to theta = 25.00°	97.8 %	
Absorption correction	None	

Max. and min. transmission	0.9619 and 0.9619
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3630 / 0 / 271
Goodness-of-fit on F ²	1.082
Final R indices [I>2sigma(I)]	R ₁ = 0.0406, wR ₂ = 0.0869
R indices (all data)	R ₁ = 0.0576, wR ₂ = 0.0929
Largest diff. peak and hole	0.303 and -0.210 e.Å ⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cl(1)	5050(1)	1169(1)	8186(1)	20(1)
C(1)	7025(3)	3084(2)	8359(1)	15(1)
C(4)	5619(3)	4450(2)	7146(1)	14(1)
C(24)	8102(3)	2541(2)	9171(1)	16(1)
C(5)	6151(3)	4298(2)	8055(1)	14(1)
C(3)	6093(3)	3321(2)	6913(1)	14(1)
C(12)	4925(3)	5756(2)	6577(1)	16(1)
C(10)	2906(3)	6964(2)	7708(1)	20(1)
C(2)	6975(3)	2319(2)	7679(1)	15(1)
C(15)	6320(3)	3120(2)	5990(1)	16(1)
C(21)	9081(3)	1595(2)	7424(1)	16(1)
C(19)	8489(3)	865(2)	6067(1)	19(1)
C(27)	10441(3)	1514(2)	10604(1)	21(1)
C(17)	10273(3)	2829(2)	5800(1)	19(1)
C(22)	6400(3)	1719(2)	5913(1)	19(1)
C(13)	3553(3)	6006(2)	8561(1)	18(1)
C(26)	8602(3)	1046(2)	10578(1)	20(1)
C(25)	7429(3)	1554(2)	9873(1)	19(1)
C(6)	5831(3)	5384(2)	8505(1)	17(1)
C(23)	10497(3)	2560(2)	6795(1)	18(1)
C(29)	9965(3)	3003(2)	9208(1)	24(1)

C(14)	6586(3)	6694(2)	6440(1)	19(1)
C(8)	6589(3)	7331(2)	7198(1)	19(1)
C(16)	8305(3)	3703(2)	5503(1)	17(1)
C(18)	10289(3)	1567(2)	5528(1)	20(1)
C(11)	2805(3)	6340(2)	6948(1)	19(1)
C(20)	8950(3)	459(2)	7032(1)	20(1)
C(9)	4412(3)	7994(2)	7401(1)	21(1)
C(7)	7289(3)	6420(2)	8060(1)	19(1)
C(28)	11122(3)	2496(2)	9917(1)	25(1)

Table 3. Bond lengths [Å] and angles [°] for **5**.

Cl(1)-C(2)	1.8485(19)
C(1)-C(5)	1.341(3)
C(1)-C(24)	1.488(3)
C(1)-C(2)	1.522(3)
C(4)-C(3)	1.344(3)
C(4)-C(5)	1.483(3)
C(4)-C(12)	1.503(3)
C(24)-C(29)	1.395(3)
C(24)-C(25)	1.393(3)
C(5)-C(6)	1.498(3)
C(3)-C(2)	1.512(3)
C(3)-C(15)	1.512(3)
C(12)-C(11)	1.541(3)
C(12)-C(14)	1.545(3)
C(10)-C(9)	1.531(3)
C(10)-C(11)	1.534(3)
C(10)-C(13)	1.535(3)
C(2)-C(21)	1.538(3)
C(15)-C(22)	1.540(3)
C(15)-C(16)	1.542(3)
C(21)-C(20)	1.527(3)

C(21)-C(23)	1.553(3)
C(19)-C(18)	1.525(3)
C(19)-C(20)	1.530(3)
C(19)-C(22)	1.542(3)
C(27)-C(26)	1.379(3)
C(27)-C(28)	1.378(3)
C(17)-C(18)	1.529(3)
C(17)-C(16)	1.531(3)
C(17)-C(23)	1.542(3)
C(13)-C(6)	1.542(3)
C(26)-C(25)	1.384(3)
C(6)-C(7)	1.537(3)
C(29)-C(28)	1.383(3)
C(14)-C(8)	1.529(3)
C(8)-C(9)	1.528(3)
C(8)-C(7)	1.537(3)

C(5)-C(1)-C(24)	128.15(19)
C(5)-C(1)-C(2)	109.03(17)
C(24)-C(1)-C(2)	122.52(17)
C(3)-C(4)-C(5)	110.22(17)
C(3)-C(4)-C(12)	128.02(18)
C(5)-C(4)-C(12)	121.28(18)
C(29)-C(24)-C(25)	118.01(18)
C(29)-C(24)-C(1)	117.71(17)
C(25)-C(24)-C(1)	124.18(18)
C(1)-C(5)-C(4)	108.80(18)
C(1)-C(5)-C(6)	127.80(18)
C(4)-C(5)-C(6)	123.32(17)
C(4)-C(3)-C(2)	108.35(17)
C(4)-C(3)-C(15)	127.12(18)
C(2)-C(3)-C(15)	122.47(18)
C(4)-C(12)-C(11)	111.95(16)
C(4)-C(12)-C(14)	111.32(15)
C(11)-C(12)-C(14)	110.91(17)

C(9)-C(10)-C(11)	108.93(17)
C(9)-C(10)-C(13)	109.54(16)
C(11)-C(10)-C(13)	114.36(17)
C(3)-C(2)-C(1)	103.41(16)
C(3)-C(2)-C(21)	113.63(16)
C(1)-C(2)-C(21)	114.64(16)
C(3)-C(2)-Cl(1)	109.03(13)
C(1)-C(2)-Cl(1)	104.85(13)
C(21)-C(2)-Cl(1)	110.67(13)
C(3)-C(15)-C(22)	116.77(16)
C(3)-C(15)-C(16)	106.87(16)
C(22)-C(15)-C(16)	109.99(16)
C(20)-C(21)-C(2)	115.08(16)
C(20)-C(21)-C(23)	110.64(17)
C(2)-C(21)-C(23)	110.04(16)
C(18)-C(19)-C(20)	107.51(16)
C(18)-C(19)-C(22)	110.67(16)
C(20)-C(19)-C(22)	113.89(17)
C(26)-C(27)-C(28)	119.43(19)
C(18)-C(17)-C(16)	107.47(16)
C(18)-C(17)-C(23)	110.91(16)
C(16)-C(17)-C(23)	114.67(17)
C(19)-C(22)-C(15)	115.93(16)
C(10)-C(13)-C(6)	114.86(16)
C(27)-C(26)-C(25)	120.90(19)
C(26)-C(25)-C(24)	120.36(19)
C(5)-C(6)-C(7)	111.53(16)
C(5)-C(6)-C(13)	112.63(16)
C(7)-C(6)-C(13)	110.34(16)
C(17)-C(23)-C(21)	116.18(16)
C(28)-C(29)-C(24)	121.27(19)
C(8)-C(14)-C(12)	115.16(16)
C(9)-C(8)-C(14)	109.47(17)
C(9)-C(8)-C(7)	108.33(17)
C(14)-C(8)-C(7)	115.45(17)

C(17)-C(16)-C(15)	111.61(16)
C(19)-C(18)-C(17)	108.42(16)
C(10)-C(11)-C(12)	114.57(16)
C(21)-C(20)-C(19)	113.73(16)
C(8)-C(9)-C(10)	108.65(17)
C(8)-C(7)-C(6)	114.10(16)
C(27)-C(28)-C(29)	120.02(19)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl(1)	21(1)	20(1)	19(1)	-2(1)	-2(1)	-8(1)
C(1)	14(1)	17(1)	13(1)	-2(1)	-1(1)	-4(1)
C(4)	10(1)	18(1)	15(1)	-4(1)	-2(1)	-2(1)
C(24)	19(1)	16(1)	13(1)	-5(1)	-2(1)	1(1)
C(5)	10(1)	20(1)	13(1)	-4(1)	2(1)	-4(1)
C(3)	10(1)	18(1)	15(1)	-3(1)	-2(1)	-3(1)
C(12)	18(1)	16(1)	13(1)	-3(1)	-4(1)	-1(1)
C(10)	15(1)	19(1)	23(1)	-6(1)	1(1)	1(1)
C(2)	16(1)	13(1)	17(1)	-2(1)	-2(1)	-5(1)
C(15)	16(1)	18(1)	14(1)	-3(1)	-5(1)	0(1)
C(21)	15(1)	16(1)	14(1)	0(1)	-6(1)	0(1)
C(19)	24(1)	16(1)	19(1)	-7(1)	-4(1)	-1(1)
C(27)	24(1)	22(1)	17(1)	-6(1)	-8(1)	3(1)
C(17)	16(1)	22(1)	18(1)	-2(1)	-1(1)	-4(1)
C(22)	20(1)	23(1)	15(1)	-6(1)	-3(1)	-5(1)
C(13)	22(1)	17(1)	18(1)	-7(1)	0(1)	-4(1)
C(26)	26(1)	17(1)	16(1)	-2(1)	0(1)	-1(1)
C(25)	17(1)	20(1)	18(1)	-5(1)	-1(1)	0(1)
C(6)	20(1)	18(1)	12(1)	-4(1)	-4(1)	-1(1)

C(23)	15(1)	18(1)	20(1)	-5(1)	-4(1)	0(1)
C(29)	27(1)	25(1)	19(1)	1(1)	-5(1)	-10(1)
C(14)	19(1)	15(1)	18(1)	0(1)	0(1)	-1(1)
C(8)	19(1)	16(1)	21(1)	-2(1)	0(1)	-6(1)
C(16)	21(1)	18(1)	13(1)	-5(1)	-3(1)	-2(1)
C(18)	17(1)	22(1)	19(1)	-5(1)	-3(1)	4(1)
C(11)	17(1)	17(1)	21(1)	-3(1)	-4(1)	1(1)
C(20)	21(1)	16(1)	21(1)	-2(1)	-3(1)	2(1)
C(9)	26(1)	16(1)	21(1)	-5(1)	-3(1)	-1(1)
C(7)	18(1)	20(1)	22(1)	-9(1)	-3(1)	-3(1)
C(28)	22(1)	32(1)	24(1)	-5(1)	-9(1)	-7(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5**.

	x	y	z	U(eq)
H(12)	4753	5636	5984	19
H(10)	1492	7407	7845	23
H(15)	5110	3637	5687	19
H(21)	9772	1233	7979	19
H(19)	8456	65	5864	23
H(27)	11232	1162	11092	25
H(17)	11500	3259	5467	23
H(22A)	5304	1300	6345	23
H(22B)	6056	1745	5317	23
H(13A)	2634	5308	8724	22
H(13B)	3324	6462	9040	22
H(26)	8134	366	11050	25
H(25)	6158	1227	9869	22
H(6)	6194	5013	9123	20
H(23A)	10205	3393	6967	21
H(23B)	11963	2224	6889	21

H(29)	10449	3680	8737	29
H(14A)	7974	6212	6347	22
H(14B)	6369	7382	5894	22
H(8)	7554	8015	6995	23
H(16A)	8291	3829	4859	20
H(16B)	8319	4561	5618	20
H(18A)	10134	1754	4890	24
H(18B)	11624	1017	5640	24
H(11A)	2172	7001	6462	23
H(11B)	1877	5649	7157	23
H(20A)	7847	-51	7388	24
H(20B)	10285	-110	7077	24
H(9A)	3968	8638	6866	25
H(9B)	4419	8451	7869	25
H(7A)	7390	6944	8480	23
H(7B)	8696	5984	7932	23
H(28)	12386	2824	9930	30

Crystal data for **6**

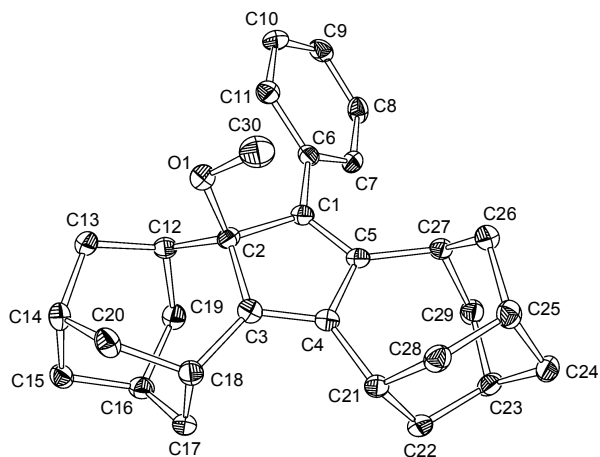


Table 1. Crystal data and structure refinement for **6**.

Identification code	6	
Empirical formula	C ₃₀ H ₃₆ O	
Formula weight	412.59	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 11.0557(16) Å	α = 90°.
	b = 17.650(3) Å	β = 97.847(3)°.
	c = 22.609(3) Å	γ = 90°.
Volume	4370.6(11) Å ³	
Z	8	
Density (calculated)	1.254 Mg/m ³	
Absorption coefficient	0.073 mm ⁻¹	
F(000)	1792	
Crystal size	0.20 x 0.20 x 0.20 mm ³	
Theta range for data collection	1.82 to 25.00°.	
Index ranges	-13 ≤ h ≤ 10, -20 ≤ k ≤ 20, -26 ≤ l ≤ 26	
Reflections collected	11232	
Independent reflections	3847 [R(int) = 0.0432]	
Completeness to theta = 25.00°	99.7 %	

Absorption correction	Empirical (SADABS)
Max. and min. transmission	0.9855 and 0.9855
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3847 / 0 / 281
Goodness-of-fit on F ²	1.012
Final R indices [I>2sigma(I)]	R ₁ = 0.0429, wR ₂ = 0.0857
R indices (all data)	R ₁ = 0.0648, wR ₂ = 0.0908
Largest diff. peak and hole	0.193 and -0.206 e.Å ⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for **6**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
O(1)	3728(1)	3559(1)	570(1)	23(1)
C(1)	4137(2)	4673(1)	1212(1)	17(1)
C(2)	3429(2)	3924(1)	1116(1)	18(1)
C(23)	1752(2)	6730(1)	1398(1)	21(1)
C(5)	3337(2)	5250(1)	1098(1)	17(1)
C(17)	874(2)	3717(1)	1788(1)	22(1)
C(10)	7508(2)	4265(1)	1268(1)	24(1)
C(27)	3596(2)	6079(1)	1024(1)	18(1)
C(26)	3078(2)	6353(1)	393(1)	21(1)
C(14)	2021(2)	2350(1)	1383(1)	21(1)
C(13)	3383(2)	2522(1)	1411(1)	22(1)
C(18)	1061(2)	3674(1)	1127(1)	20(1)
C(9)	8023(2)	4834(1)	1644(1)	23(1)
C(4)	2074(2)	4949(1)	1005(1)	17(1)
C(25)	1712(2)	6546(1)	304(1)	21(1)
C(28)	863(2)	5864(1)	311(1)	21(1)
C(16)	1840(2)	3271(1)	2194(1)	21(1)
C(11)	6250(2)	4206(1)	1130(1)	21(1)
C(12)	3729(2)	3332(1)	1611(1)	19(1)
C(8)	7264(2)	5339(1)	1883(1)	22(1)

C(3)	2109(2)	4187(1)	1040(1)	17(1)
C(6)	5474(2)	4721(1)	1358(1)	18(1)
C(15)	1692(2)	2437(1)	2013(1)	21(1)
C(29)	3126(2)	6570(1)	1510(1)	21(1)
C(19)	3167(2)	3535(1)	2182(1)	22(1)
C(24)	1452(2)	7107(1)	786(1)	23(1)
C(22)	942(2)	6029(1)	1430(1)	21(1)
C(20)	1189(2)	2841(1)	938(1)	23(1)
C(21)	975(2)	5451(1)	918(1)	19(1)
C(7)	6010(2)	5279(1)	1749(1)	20(1)
C(30)	3571(2)	4000(1)	44(1)	32(1)

Table 3. Bond lengths [Å] and angles [°] for **6**.

O(1)-C(30)	1.412(2)
O(1)-C(2)	1.4696(18)
C(1)-C(5)	1.351(2)
C(1)-C(6)	1.473(2)
C(1)-C(2)	1.536(2)
C(2)-C(3)	1.518(2)
C(2)-C(12)	1.534(2)
C(23)-C(24)	1.531(2)
C(23)-C(29)	1.531(2)
C(23)-C(22)	1.535(2)
C(5)-C(4)	1.482(2)
C(5)-C(27)	1.505(2)
C(17)-C(16)	1.529(2)
C(17)-C(18)	1.538(2)
C(10)-C(11)	1.387(2)
C(10)-C(9)	1.388(2)
C(27)-C(26)	1.541(2)
C(27)-C(29)	1.543(2)
C(26)-C(25)	1.535(2)

C(14)-C(15)	1.526(2)
C(14)-C(13)	1.529(2)
C(14)-C(20)	1.535(2)
C(13)-C(12)	1.532(2)
C(18)-C(3)	1.505(2)
C(18)-C(20)	1.543(2)
C(9)-C(8)	1.383(2)
C(4)-C(3)	1.346(2)
C(4)-C(21)	1.496(2)
C(25)-C(28)	1.528(2)
C(25)-C(24)	1.528(2)
C(28)-C(21)	1.543(2)
C(16)-C(15)	1.530(2)
C(16)-C(19)	1.542(2)
C(11)-C(6)	1.396(2)
C(12)-C(19)	1.548(2)
C(8)-C(7)	1.382(2)
C(6)-C(7)	1.400(2)
C(22)-C(21)	1.547(2)

C(30)-O(1)-C(2)	116.71(12)
C(5)-C(1)-C(6)	127.59(15)
C(5)-C(1)-C(2)	108.33(14)
C(6)-C(1)-C(2)	123.92(15)
O(1)-C(2)-C(3)	111.24(13)
O(1)-C(2)-C(12)	105.31(12)
C(3)-C(2)-C(12)	113.54(13)
O(1)-C(2)-C(1)	109.07(12)
C(3)-C(2)-C(1)	102.48(13)
C(12)-C(2)-C(1)	115.29(13)
C(24)-C(23)-C(29)	108.52(14)
C(24)-C(23)-C(22)	109.79(14)
C(29)-C(23)-C(22)	114.52(14)
C(1)-C(5)-C(4)	109.60(14)
C(1)-C(5)-C(27)	128.74(16)

C(4)-C(5)-C(27)	121.54(15)
C(16)-C(17)-C(18)	112.51(14)
C(11)-C(10)-C(9)	120.42(17)
C(5)-C(27)-C(26)	110.80(14)
C(5)-C(27)-C(29)	112.29(13)
C(26)-C(27)-C(29)	111.39(14)
C(25)-C(26)-C(27)	115.22(14)
C(15)-C(14)-C(13)	107.47(14)
C(15)-C(14)-C(20)	110.95(14)
C(13)-C(14)-C(20)	114.39(14)
C(14)-C(13)-C(12)	113.73(14)
C(3)-C(18)-C(17)	107.78(13)
C(3)-C(18)-C(20)	115.87(14)
C(17)-C(18)-C(20)	110.22(13)
C(8)-C(9)-C(10)	119.09(17)
C(3)-C(4)-C(5)	109.34(15)
C(3)-C(4)-C(21)	128.02(16)
C(5)-C(4)-C(21)	122.58(14)
C(28)-C(25)-C(24)	109.14(14)
C(28)-C(25)-C(26)	114.73(14)
C(24)-C(25)-C(26)	109.06(14)
C(25)-C(28)-C(21)	114.04(14)
C(17)-C(16)-C(15)	107.11(14)
C(17)-C(16)-C(19)	114.89(14)
C(15)-C(16)-C(19)	110.67(14)
C(10)-C(11)-C(6)	121.09(17)
C(13)-C(12)-C(2)	113.46(14)
C(13)-C(12)-C(19)	110.50(13)
C(2)-C(12)-C(19)	112.30(13)
C(7)-C(8)-C(9)	120.57(17)
C(4)-C(3)-C(18)	126.29(16)
C(4)-C(3)-C(2)	109.36(15)
C(18)-C(3)-C(2)	123.11(14)
C(11)-C(6)-C(7)	117.57(16)
C(11)-C(6)-C(1)	121.85(15)

C(7)-C(6)-C(1)	120.55(15)
C(14)-C(15)-C(16)	108.46(13)
C(23)-C(29)-C(27)	114.09(14)
C(16)-C(19)-C(12)	115.87(14)
C(25)-C(24)-C(23)	108.90(14)
C(23)-C(22)-C(21)	114.95(14)
C(14)-C(20)-C(18)	115.19(14)
C(4)-C(21)-C(28)	111.23(13)
C(4)-C(21)-C(22)	113.20(14)
C(28)-C(21)-C(22)	110.31(13)
C(8)-C(7)-C(6)	121.20(16)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **6**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(1)	25(1)	19(1)	26(1)	-1(1)	8(1)	0(1)
C(1)	15(1)	19(1)	17(1)	-1(1)	4(1)	0(1)
C(2)	16(1)	16(1)	21(1)	-3(1)	5(1)	1(1)
C(23)	20(1)	19(1)	25(1)	-3(1)	5(1)	5(1)
C(5)	15(1)	19(1)	17(1)	-1(1)	4(1)	0(1)
C(17)	15(1)	19(1)	33(1)	1(1)	7(1)	0(1)
C(10)	17(1)	25(1)	31(1)	-1(1)	8(1)	4(1)
C(27)	12(1)	18(1)	24(1)	0(1)	3(1)	-1(1)
C(26)	21(1)	18(1)	24(1)	0(1)	6(1)	-1(1)
C(14)	23(1)	15(1)	23(1)	-1(1)	2(1)	-2(1)
C(13)	23(1)	17(1)	26(1)	2(1)	7(1)	3(1)
C(18)	13(1)	19(1)	26(1)	2(1)	0(1)	0(1)
C(9)	13(1)	27(1)	31(1)	7(1)	3(1)	-1(1)
C(4)	15(1)	19(1)	17(1)	0(1)	3(1)	0(1)
C(25)	22(1)	21(1)	20(1)	4(1)	1(1)	2(1)

C(28)	17(1)	21(1)	25(1)	0(1)	0(1)	2(1)
C(16)	20(1)	24(1)	20(1)	0(1)	7(1)	0(1)
C(11)	18(1)	20(1)	24(1)	-1(1)	4(1)	-2(1)
C(12)	12(1)	20(1)	26(1)	1(1)	2(1)	1(1)
C(8)	20(1)	18(1)	28(1)	2(1)	-1(1)	-3(1)
C(3)	16(1)	20(1)	15(1)	1(1)	0(1)	-1(1)
C(6)	16(1)	17(1)	20(1)	4(1)	4(1)	0(1)
C(15)	16(1)	20(1)	26(1)	4(1)	2(1)	-1(1)
C(29)	21(1)	18(1)	24(1)	0(1)	2(1)	0(1)
C(19)	21(1)	20(1)	23(1)	0(1)	0(1)	0(1)
C(24)	18(1)	17(1)	33(1)	3(1)	3(1)	2(1)
C(22)	16(1)	22(1)	27(1)	3(1)	5(1)	4(1)
C(20)	21(1)	22(1)	26(1)	2(1)	0(1)	-5(1)
C(21)	12(1)	18(1)	26(1)	1(1)	3(1)	0(1)
C(7)	18(1)	17(1)	25(1)	1(1)	4(1)	2(1)
C(30)	38(1)	36(1)	24(1)	-3(1)	8(1)	0(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **6**.

	x	y	z	U(eq)
H(23)	1557	7098	1707	25
H(17A)	902	4254	1915	26
H(17B)	56	3516	1833	26
H(10)	8020	3913	1103	29
H(27)	4503	6141	1068	22
H(26A)	3538	6809	299	25
H(26B)	3224	5955	103	25
H(14)	1888	1808	1262	25
H(13A)	3627	2438	1010	26
H(13B)	3849	2162	1690	26
H(18)	311	3884	885	24

H(9)	8884	4877	1736	28
H(25)	1515	6802	-93	25
H(28A)	1043	5499	2	26
H(28B)	9	6036	204	26
H(16)	1656	3320	2613	25
H(11)	5910	3809	876	25
H(12)	4635	3339	1724	23
H(8)	7608	5730	2142	27
H(15A)	2237	2118	2295	25
H(15B)	839	2273	2024	25
H(29A)	3318	6310	1900	25
H(29B)	3569	7058	1538	25
H(19A)	3686	3312	2529	26
H(19B)	3195	4093	2231	26
H(24A)	583	7259	719	27
H(24B)	1958	7567	768	27
H(22A)	89	6199	1429	26
H(22B)	1198	5768	1815	26
H(20A)	366	2609	875	28
H(20B)	1509	2833	550	28
H(21)	241	5118	911	23
H(7)	5503	5623	1925	24
H(30A)	2727	4184	-31	48
H(30B)	3744	3690	-294	48
H(30C)	4131	4433	92	48

Crystal data for 8^+SbF_6^-

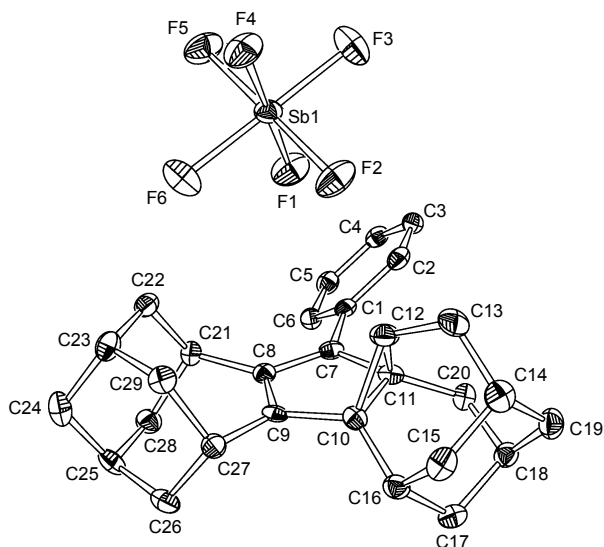


Table 1. Crystal data and structure refinement for 8^+SbF_6^- .

Identification code	8^+SbF_6^-	
Empirical formula	$\text{C}_{29} \text{H}_{33} \text{F}_6 \text{Sb}$	
Formula weight	617.30	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	$a = 10.0120(13)$ Å	$\alpha = 90^\circ$.
	$b = 21.486(3)$ Å	$\beta = 100.848(2)^\circ$.
	$c = 11.6831(16)$ Å	$\gamma = 90^\circ$.
Volume	$2468.3(6)$ Å ³	
Z	4	
Density (calculated)	1.661 Mg/m ³	
Absorption coefficient	1.180 mm ⁻¹	
F(000)	1248	
Crystal size	0.10 x 0.10 x 0.10 mm ³	
Theta range for data collection	2.01 to 25.00°.	
Index ranges	$-11 \leq h \leq 11, -25 \leq k \leq 17, -13 \leq l \leq 12$	
Reflections collected	12263	

Independent reflections	4333 [R(int) = 0.0423]
Completeness to theta = 25.00°	100.0 %
Absorption correction	None
Max. and min. transmission	0.8911 and 0.8911
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4333 / 0 / 325
Goodness-of-fit on F ²	1.061
Final R indices [I>2sigma(I)]	R ₁ = 0.0378, wR ₂ = 0.0726
R indices (all data)	R ₁ = 0.0558, wR ₂ = 0.0759
Largest diff. peak and hole	1.335 and -0.810 e.Å ⁻³

Table 2. Atomic coordinates (x 10⁴) and equivalent isotropic displacement parameters (Å² x 10³) for **8**⁺SbF₆⁻. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Sb(1)	2310(1)	1668(1)	104(1)	21(1)
F(1)	3931(2)	2094(1)	47(2)	37(1)
F(5)	1400(2)	2144(1)	-1149(2)	39(1)
F(3)	1865(3)	2251(1)	1145(2)	45(1)
F(4)	712(2)	1226(1)	161(2)	36(1)
F(2)	3227(2)	1189(1)	1345(2)	38(1)
F(6)	2729(3)	1076(1)	-946(2)	42(1)
C(17)	10016(4)	916(2)	2825(3)	24(1)
C(8)	7558(3)	1581(2)	-466(3)	16(1)
C(10)	7925(4)	1052(2)	1322(3)	18(1)
C(16)	8753(4)	588(2)	2164(3)	21(1)
C(12)	6705(4)	1403(2)	1724(4)	25(1)
C(7)	7797(4)	2036(2)	410(3)	17(1)
C(11)	8023(4)	1733(2)	1566(3)	18(1)
C(29)	5821(4)	372(2)	-1190(3)	21(1)
C(5)	8363(4)	3655(2)	-590(3)	21(1)
C(25)	7936(4)	664(2)	-2566(3)	25(1)
C(3)	7235(4)	3707(2)	1046(3)	20(1)

C(27)	7327(4)	399(2)	-556(3)	20(1)
C(20)	9011(4)	1984(2)	2609(3)	22(1)
C(18)	9610(4)	1481(2)	3476(3)	21(1)
C(13)	6376(4)	1259(2)	2901(4)	28(1)
C(15)	7927(4)	341(2)	3036(4)	26(1)
C(21)	7115(4)	1681(2)	-1767(3)	19(1)
C(26)	8307(4)	292(2)	-1424(4)	25(1)
C(9)	7616(3)	995(2)	63(3)	16(1)
C(23)	5529(4)	739(2)	-2326(3)	23(1)
C(6)	8350(4)	3014(2)	-544(3)	21(1)
C(1)	7771(4)	2707(2)	300(3)	17(1)
C(24)	6463(4)	514(2)	-3133(4)	29(1)
C(14)	7443(4)	889(2)	3711(4)	27(1)
C(19)	8666(4)	1272(2)	4304(3)	27(1)
C(2)	7223(4)	3067(2)	1102(3)	20(1)
C(28)	8120(4)	1360(2)	-2445(3)	23(1)
C(22)	5654(4)	1445(2)	-2197(3)	21(1)
C(4)	7813(4)	4000(2)	204(3)	20(1)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for $\mathbf{8}^+\text{SbF}_6^-$.

Sb(1)-F(3)	1.858(2)
Sb(1)-F(6)	1.868(2)
Sb(1)-F(2)	1.871(2)
Sb(1)-F(4)	1.873(2)
Sb(1)-F(5)	1.874(2)
Sb(1)-F(1)	1.875(2)
C(17)-C(16)	1.524(5)
C(17)-C(18)	1.528(5)
C(8)-C(9)	1.398(5)
C(8)-C(7)	1.404(5)
C(8)-C(21)	1.517(5)
C(10)-C(9)	1.450(5)

C(10)-C(11)	1.490(5)
C(10)-C(16)	1.530(5)
C(10)-C(12)	1.580(5)
C(16)-C(15)	1.523(5)
C(12)-C(13)	1.506(5)
C(12)-C(11)	1.539(5)
C(7)-C(1)	1.447(5)
C(7)-C(11)	1.478(5)
C(11)-C(20)	1.516(5)
C(29)-C(23)	1.524(5)
C(29)-C(27)	1.551(5)
C(5)-C(6)	1.377(5)
C(5)-C(4)	1.381(5)
C(25)-C(28)	1.509(5)
C(25)-C(24)	1.533(6)
C(25)-C(26)	1.539(5)
C(3)-C(2)	1.376(5)
C(3)-C(4)	1.384(5)
C(27)-C(9)	1.472(5)
C(27)-C(26)	1.555(5)
C(20)-C(18)	1.525(5)
C(18)-C(19)	1.541(5)
C(13)-C(14)	1.513(6)
C(15)-C(14)	1.545(5)
C(21)-C(22)	1.540(5)
C(21)-C(28)	1.554(5)
C(23)-C(22)	1.527(5)
C(23)-C(24)	1.527(5)
C(6)-C(1)	1.400(5)
C(1)-C(2)	1.404(5)
C(14)-C(19)	1.528(6)
F(3)-Sb(1)-F(6)	179.05(12)
F(3)-Sb(1)-F(2)	90.36(12)
F(6)-Sb(1)-F(2)	89.81(12)

F(3)-Sb(1)-F(4)	90.41(11)
F(6)-Sb(1)-F(4)	88.65(11)
F(2)-Sb(1)-F(4)	89.51(10)
F(3)-Sb(1)-F(5)	90.13(12)
F(6)-Sb(1)-F(5)	89.69(11)
F(2)-Sb(1)-F(5)	179.48(12)
F(4)-Sb(1)-F(5)	90.62(11)
F(3)-Sb(1)-F(1)	90.57(11)
F(6)-Sb(1)-F(1)	90.37(11)
F(2)-Sb(1)-F(1)	89.69(10)
F(4)-Sb(1)-F(1)	178.74(11)
F(5)-Sb(1)-F(1)	90.17(10)
C(16)-C(17)-C(18)	110.3(3)
C(9)-C(8)-C(7)	108.5(3)
C(9)-C(8)-C(21)	123.4(3)
C(7)-C(8)-C(21)	127.5(3)
C(9)-C(10)-C(11)	105.7(3)
C(9)-C(10)-C(16)	125.7(3)
C(11)-C(10)-C(16)	120.6(3)
C(9)-C(10)-C(12)	108.2(3)
C(11)-C(10)-C(12)	60.1(2)
C(16)-C(10)-C(12)	118.4(3)
C(15)-C(16)-C(17)	108.9(3)
C(15)-C(16)-C(10)	111.1(3)
C(17)-C(16)-C(10)	108.8(3)
C(13)-C(12)-C(11)	122.9(4)
C(13)-C(12)-C(10)	119.2(3)
C(11)-C(12)-C(10)	57.0(2)
C(8)-C(7)-C(1)	129.2(4)
C(8)-C(7)-C(11)	109.6(3)
C(1)-C(7)-C(11)	121.2(3)
C(7)-C(11)-C(10)	105.3(3)
C(7)-C(11)-C(20)	122.8(3)
C(10)-C(11)-C(20)	120.8(3)
C(7)-C(11)-C(12)	108.9(3)

C(10)-C(11)-C(12)	62.9(2)
C(20)-C(11)-C(12)	120.8(3)
C(23)-C(29)-C(27)	114.0(3)
C(6)-C(5)-C(4)	120.2(4)
C(28)-C(25)-C(24)	109.8(3)
C(28)-C(25)-C(26)	115.3(3)
C(24)-C(25)-C(26)	108.8(3)
C(2)-C(3)-C(4)	119.8(4)
C(9)-C(27)-C(29)	110.5(3)
C(9)-C(27)-C(26)	111.0(3)
C(29)-C(27)-C(26)	111.0(3)
C(11)-C(20)-C(18)	113.4(3)
C(20)-C(18)-C(17)	109.9(3)
C(20)-C(18)-C(19)	114.4(3)
C(17)-C(18)-C(19)	109.4(3)
C(12)-C(13)-C(14)	115.4(3)
C(16)-C(15)-C(14)	109.8(3)
C(8)-C(21)-C(22)	111.2(3)
C(8)-C(21)-C(28)	110.6(3)
C(22)-C(21)-C(28)	110.7(3)
C(25)-C(26)-C(27)	114.1(3)
C(8)-C(9)-C(10)	110.8(3)
C(8)-C(9)-C(27)	125.3(3)
C(10)-C(9)-C(27)	123.8(3)
C(29)-C(23)-C(22)	115.4(3)
C(29)-C(23)-C(24)	109.6(3)
C(22)-C(23)-C(24)	109.1(3)
C(5)-C(6)-C(1)	120.4(4)
C(6)-C(1)-C(2)	118.4(4)
C(6)-C(1)-C(7)	122.0(3)
C(2)-C(1)-C(7)	119.5(3)
C(23)-C(24)-C(25)	108.5(3)
C(13)-C(14)-C(19)	114.4(3)
C(13)-C(14)-C(15)	109.5(3)
C(19)-C(14)-C(15)	109.9(3)

C(14)-C(19)-C(18)	113.9(3)
C(3)-C(2)-C(1)	120.7(4)
C(25)-C(28)-C(21)	114.1(3)
C(23)-C(22)-C(21)	114.5(3)
C(5)-C(4)-C(3)	120.4(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\mathbf{8}^+\text{SbF}_6^-$. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Sb(1)	17(1)	26(1)	22(1)	3(1)	7(1)	2(1)
F(1)	24(1)	42(2)	44(2)	11(1)	7(1)	-8(1)
F(5)	33(1)	45(2)	36(2)	19(1)	2(1)	9(1)
F(3)	56(2)	42(2)	43(2)	-14(1)	21(2)	3(1)
F(4)	19(1)	53(2)	37(2)	8(1)	5(1)	-9(1)
F(2)	32(1)	42(2)	37(2)	18(1)	-3(1)	-1(1)
F(6)	48(2)	39(2)	44(2)	-7(1)	21(1)	6(1)
C(17)	21(2)	24(2)	25(2)	4(2)	2(2)	4(2)
C(8)	11(2)	18(2)	19(2)	-1(2)	4(2)	-1(2)
C(10)	16(2)	18(2)	20(2)	-1(2)	7(2)	-2(2)
C(16)	23(2)	18(2)	24(2)	0(2)	5(2)	3(2)
C(12)	18(2)	28(2)	28(2)	1(2)	6(2)	5(2)
C(7)	9(2)	19(2)	23(2)	2(2)	4(2)	0(2)
C(11)	16(2)	16(2)	23(2)	1(2)	5(2)	2(2)
C(29)	21(2)	18(2)	25(2)	1(2)	5(2)	-3(2)
C(5)	18(2)	25(3)	20(2)	2(2)	2(2)	-3(2)
C(25)	30(2)	24(3)	25(2)	-5(2)	15(2)	5(2)
C(3)	17(2)	22(3)	20(2)	-5(2)	2(2)	0(2)
C(27)	22(2)	19(2)	19(2)	1(2)	4(2)	2(2)
C(20)	23(2)	23(2)	18(2)	0(2)	2(2)	-2(2)
C(18)	19(2)	22(2)	21(2)	-1(2)	0(2)	-1(2)

C(13)	20(2)	38(3)	29(3)	-2(2)	13(2)	0(2)
C(15)	28(2)	24(3)	26(2)	4(2)	1(2)	-6(2)
C(21)	21(2)	19(2)	16(2)	-1(2)	2(2)	-2(2)
C(26)	23(2)	22(2)	31(3)	-5(2)	10(2)	4(2)
C(9)	8(2)	19(2)	23(2)	-1(2)	8(2)	2(2)
C(23)	22(2)	25(2)	21(2)	1(2)	1(2)	-6(2)
C(6)	17(2)	26(3)	19(2)	-3(2)	3(2)	1(2)
C(1)	11(2)	20(2)	19(2)	-1(2)	-1(2)	1(2)
C(24)	40(3)	28(3)	20(2)	-5(2)	6(2)	-4(2)
C(14)	27(2)	30(3)	25(2)	7(2)	11(2)	-3(2)
C(19)	28(2)	32(3)	19(2)	0(2)	5(2)	-1(2)
C(2)	15(2)	25(2)	19(2)	2(2)	-1(2)	-2(2)
C(28)	21(2)	26(2)	23(2)	0(2)	7(2)	1(2)
C(22)	17(2)	25(2)	20(2)	1(2)	1(2)	0(2)
C(4)	18(2)	15(2)	26(2)	-1(2)	-3(2)	-1(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\mathbf{8}^+\text{SbF}_6^-$.

	x	y	z	U(eq)
H(17A)	10594	1051	2271	28
H(17B)	10549	623	3387	28
H(16)	9035	232	1711	26
H(12)	5899	1483	1092	29
H(29A)	5567	-68	-1358	26
H(29B)	5240	535	-661	26
H(5)	8751	3859	-1170	25
H(25)	8535	514	-3103	30
H(3)	6848	3946	1585	24
H(27)	7478	57	35	24
H(20A)	8535	2294	3014	26
H(20B)	9762	2200	2330	26

H(18)	10456	1653	3966	25
H(13A)	5510	1025	2786	33
H(13B)	6230	1657	3288	33
H(15A)	8493	54	3588	32
H(15B)	7130	107	2620	32
H(21)	7130	2138	-1923	22
H(26A)	9240	407	-1035	30
H(26B)	8311	-157	-1615	30
H(23)	4573	644	-2715	28
H(6)	8737	2779	-1089	25
H(24A)	6227	725	-3898	35
H(24B)	6355	60	-3261	35
H(14)	7002	710	4337	32
H(19A)	9201	1021	4941	32
H(19B)	8333	1645	4660	32
H(2)	6838	2867	1689	24
H(28A)	8004	1545	-3233	28
H(28B)	9061	1447	-2039	28
H(22A)	5080	1585	-1643	25
H(22B)	5292	1639	-2961	25
H(4)	7832	4442	172	24

Crystal data for 14

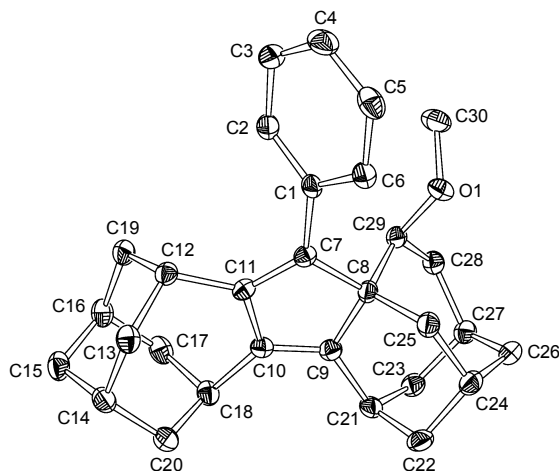


Table 1. Crystal data and structure refinement for **14**.

Identification code	14	
Empirical formula	$C_{30} H_{36} O$	
Formula weight	412.59	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	$a = 16.001(2)$ Å	$\alpha = 90^\circ$.
	$b = 9.9744(14)$ Å	$\beta = 95.655(3)^\circ$.
	$c = 14.124(2)$ Å	$\gamma = 90^\circ$.
Volume	$2243.3(6)$ Å ³	
Z	4	
Density (calculated)	1.222 Mg/m ³	
Absorption coefficient	0.071 mm ⁻¹	
F(000)	896	
Crystal size	0.10 x 0.10 x 0.10 mm ³	
Theta range for data collection	2.41 to 25.00°.	
Index ranges	-19 ≤ h ≤ 14, -11 ≤ k ≤ 11, -11 ≤ l ≤ 16	
Reflections collected	11342	
Independent reflections	3941 [R(int) = 0.0447]	
Completeness to theta = 25.00°	99.9 %	

Absorption correction	None
Max. and min. transmission	0.9929 and 0.9929
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3941 / 0 / 281
Goodness-of-fit on F ²	1.012
Final R indices [I>2sigma(I)]	R ₁ = 0.0441, wR ₂ = 0.0798
R indices (all data)	R ₁ = 0.0712, wR ₂ = 0.0851
Largest diff. peak and hole	0.171 and -0.196 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **14**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
C(21)	839(1)	994(2)	2518(1)	23(1)
C(26)	1077(1)	3715(2)	3280(1)	24(1)
C(8)	2328(1)	1941(2)	2222(1)	18(1)
C(7)	2981(1)	1394(2)	1598(1)	17(1)
C(1)	3778(1)	2097(2)	1451(1)	18(1)
C(9)	1703(1)	786(2)	2204(1)	19(1)
C(10)	1977(1)	-238(2)	1698(1)	18(1)
C(25)	1866(1)	3218(2)	1825(1)	21(1)
C(20)	1293(1)	-1825(2)	452(1)	25(1)
C(2)	4546(1)	1446(2)	1663(1)	22(1)
C(24)	1014(1)	3432(2)	2206(1)	23(1)
C(6)	3792(1)	3411(2)	1111(1)	21(1)
C(19)	3518(1)	-2086(2)	1247(1)	24(1)
C(17)	2135(1)	-2721(2)	1939(1)	26(1)
C(13)	2677(1)	-1173(2)	-221(1)	22(1)
C(23)	811(1)	1258(2)	3580(1)	25(1)
C(11)	2770(1)	129(2)	1325(1)	18(1)
C(18)	1562(1)	-1580(2)	1511(1)	22(1)
C(14)	2010(1)	-2258(2)	-123(1)	23(1)
C(29)	2785(1)	2167(2)	3229(1)	19(1)

C(22)	453(1)	2212(2)	1966(1)	26(1)
C(28)	2261(1)	2191(2)	4078(1)	21(1)
C(27)	1317(1)	2501(2)	3922(1)	22(1)
C(5)	4543(1)	4040(2)	988(1)	26(1)
C(4)	5300(1)	3380(2)	1190(1)	28(1)
C(12)	3217(1)	-806(2)	706(1)	19(1)
C(16)	2831(1)	-3142(2)	1329(1)	25(1)
C(15)	2434(1)	-3504(2)	337(1)	26(1)
C(3)	5297(1)	2080(2)	1526(1)	26(1)
O(1)	3250(1)	3393(1)	3188(1)	23(1)
C(30)	4032(1)	3360(2)	3768(1)	30(1)

Table 3. Bond lengths [Å] and angles [°] for **14**.

C(21)-C(9)	1.508(2)
C(21)-C(23)	1.528(2)
C(21)-C(22)	1.540(2)
C(26)-C(24)	1.537(2)
C(26)-C(27)	1.539(2)
C(8)-C(9)	1.524(2)
C(8)-C(7)	1.533(2)
C(8)-C(25)	1.550(2)
C(8)-C(29)	1.550(2)
C(7)-C(11)	1.352(2)
C(7)-C(1)	1.488(2)
C(1)-C(2)	1.396(2)
C(1)-C(6)	1.398(2)
C(9)-C(10)	1.344(2)
C(10)-C(11)	1.469(2)
C(10)-C(18)	1.506(2)
C(25)-C(24)	1.530(2)
C(20)-C(14)	1.532(2)
C(20)-C(18)	1.534(2)

C(2)-C(3)	1.389(2)
C(24)-C(22)	1.530(2)
C(6)-C(5)	1.382(2)
C(19)-C(16)	1.535(2)
C(19)-C(12)	1.541(2)
C(17)-C(16)	1.533(2)
C(17)-C(18)	1.547(2)
C(13)-C(14)	1.536(2)
C(13)-C(12)	1.540(2)
C(23)-C(27)	1.533(2)
C(11)-C(12)	1.506(2)
C(14)-C(15)	1.530(2)
C(29)-O(1)	1.4349(18)
C(29)-C(28)	1.530(2)
C(28)-C(27)	1.537(2)
C(5)-C(4)	1.383(2)
C(4)-C(3)	1.381(2)
C(16)-C(15)	1.523(2)
O(1)-C(30)	1.4261(19)

C(9)-C(21)-C(23)	115.41(14)
C(9)-C(21)-C(22)	107.06(14)
C(23)-C(21)-C(22)	108.22(14)
C(24)-C(26)-C(27)	115.14(14)
C(9)-C(8)-C(7)	101.78(13)
C(9)-C(8)-C(25)	109.11(13)
C(7)-C(8)-C(25)	114.32(14)
C(9)-C(8)-C(29)	112.02(14)
C(7)-C(8)-C(29)	106.98(13)
C(25)-C(8)-C(29)	112.21(14)
C(11)-C(7)-C(1)	126.38(15)
C(11)-C(7)-C(8)	109.36(14)
C(1)-C(7)-C(8)	123.69(15)
C(2)-C(1)-C(6)	117.81(16)
C(2)-C(1)-C(7)	119.96(15)

C(6)-C(1)-C(7)	122.23(15)
C(10)-C(9)-C(21)	128.08(15)
C(10)-C(9)-C(8)	109.66(15)
C(21)-C(9)-C(8)	120.66(14)
C(9)-C(10)-C(11)	109.86(14)
C(9)-C(10)-C(18)	127.47(16)
C(11)-C(10)-C(18)	122.67(15)
C(24)-C(25)-C(8)	113.36(14)
C(14)-C(20)-C(18)	114.12(14)
C(3)-C(2)-C(1)	120.93(17)
C(22)-C(24)-C(25)	109.56(14)
C(22)-C(24)-C(26)	110.23(15)
C(25)-C(24)-C(26)	113.48(14)
C(5)-C(6)-C(1)	120.86(16)
C(16)-C(19)-C(12)	114.49(14)
C(16)-C(17)-C(18)	114.65(15)
C(14)-C(13)-C(12)	115.33(15)
C(21)-C(23)-C(27)	112.49(15)
C(7)-C(11)-C(10)	109.27(15)
C(7)-C(11)-C(12)	128.62(15)
C(10)-C(11)-C(12)	122.07(14)
C(10)-C(18)-C(20)	112.94(15)
C(10)-C(18)-C(17)	110.58(14)
C(20)-C(18)-C(17)	111.26(14)
C(15)-C(14)-C(20)	109.17(15)
C(15)-C(14)-C(13)	109.08(14)
C(20)-C(14)-C(13)	114.39(14)
O(1)-C(29)-C(28)	110.11(14)
O(1)-C(29)-C(8)	106.70(13)
C(28)-C(29)-C(8)	118.39(13)
C(24)-C(22)-C(21)	108.54(13)
C(29)-C(28)-C(27)	119.84(15)
C(23)-C(27)-C(28)	111.35(14)
C(23)-C(27)-C(26)	110.98(14)
C(28)-C(27)-C(26)	115.30(14)

C(6)-C(5)-C(4)	120.82(17)
C(3)-C(4)-C(5)	119.08(17)
C(11)-C(12)-C(13)	112.41(14)
C(11)-C(12)-C(19)	111.61(15)
C(13)-C(12)-C(19)	110.30(14)
C(15)-C(16)-C(17)	108.75(14)
C(15)-C(16)-C(19)	109.30(15)
C(17)-C(16)-C(19)	114.84(14)
C(16)-C(15)-C(14)	108.99(14)
C(4)-C(3)-C(2)	120.50(17)
C(30)-O(1)-C(29)	112.73(13)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **14**. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(21)	17(1)	23(1)	30(1)	-6(1)	5(1)	-5(1)
C(26)	19(1)	24(1)	30(1)	-3(1)	2(1)	5(1)
C(8)	17(1)	14(1)	22(1)	-1(1)	4(1)	1(1)
C(7)	17(1)	16(1)	18(1)	3(1)	1(1)	1(1)
C(1)	19(1)	18(1)	17(1)	-5(1)	3(1)	-1(1)
C(9)	17(1)	20(1)	20(1)	0(1)	2(1)	0(1)
C(10)	17(1)	19(1)	19(1)	1(1)	1(1)	-1(1)
C(25)	23(1)	19(1)	21(1)	-1(1)	1(1)	2(1)
C(20)	23(1)	21(1)	32(1)	-4(1)	2(1)	-4(1)
C(2)	22(1)	19(1)	24(1)	-3(1)	5(1)	0(1)
C(24)	21(1)	23(1)	24(1)	0(1)	-1(1)	6(1)
C(6)	22(1)	19(1)	23(1)	-3(1)	3(1)	0(1)
C(19)	25(1)	18(1)	27(1)	-2(1)	0(1)	4(1)
C(17)	34(1)	18(1)	27(1)	1(1)	6(1)	-6(1)
C(13)	26(1)	21(1)	21(1)	-1(1)	5(1)	0(1)

C(23)	19(1)	27(1)	29(1)	-2(1)	8(1)	0(1)
C(11)	15(1)	18(1)	19(1)	3(1)	2(1)	2(1)
C(18)	23(1)	19(1)	24(1)	-2(1)	8(1)	-5(1)
C(14)	24(1)	24(1)	22(1)	-5(1)	3(1)	-3(1)
C(29)	18(1)	14(1)	23(1)	2(1)	2(1)	1(1)
C(22)	16(1)	37(1)	25(1)	-8(1)	1(1)	5(1)
C(28)	24(1)	19(1)	20(1)	0(1)	1(1)	1(1)
C(27)	21(1)	26(1)	20(1)	-3(1)	6(1)	1(1)
C(5)	34(1)	19(1)	25(1)	-1(1)	7(1)	-7(1)
C(4)	23(1)	31(1)	32(1)	-6(1)	9(1)	-11(1)
C(12)	18(1)	18(1)	23(1)	0(1)	5(1)	-1(1)
C(16)	32(1)	15(1)	29(1)	1(1)	4(1)	2(1)
C(15)	29(1)	18(1)	33(1)	-5(1)	11(1)	-3(1)
C(3)	19(1)	31(1)	30(1)	-7(1)	4(1)	-1(1)
O(1)	21(1)	22(1)	25(1)	0(1)	0(1)	-6(1)
C(30)	24(1)	35(1)	31(1)	-6(1)	1(1)	-9(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **14**.

	x	y	z	U(eq)
H(21)	489	186	2337	28
H(26A)	529	4065	3441	29
H(26B)	1500	4429	3427	29
H(25A)	2226	4008	1990	25
H(25B)	1782	3155	1122	25
H(20A)	853	-2527	395	30
H(20B)	1041	-991	171	30
H(2)	4555	556	1904	26
H(24)	741	4225	1870	27
H(6)	3279	3879	962	26
H(19A)	3975	-2495	921	28

H(19B)	3756	-1832	1896	28
H(17A)	2397	-2431	2570	31
H(17B)	1781	-3514	2039	31
H(13A)	2391	-351	-479	27
H(13B)	3054	-1482	-692	27
H(23A)	1036	466	3943	30
H(23B)	219	1379	3712	30
H(18)	1041	-1588	1848	26
H(14)	1761	-2507	-777	28
H(29)	3205	1428	3345	22
H(22A)	413	2033	1273	31
H(22B)	-119	2385	2146	31
H(28A)	2519	2858	4537	25
H(28B)	2324	1304	4392	25
H(27)	1139	2727	4562	26
H(5)	4540	4938	762	31
H(4)	5814	3815	1099	34
H(12)	3727	-328	524	23
H(16)	3104	-3967	1619	30
H(15A)	2014	-4225	379	31
H(15B)	2871	-3833	-56	31
H(3)	5813	1616	1664	32
H(30A)	3930	3189	4430	45
H(30B)	4317	4224	3725	45
H(30C)	4384	2645	3546	45
