Supporting Information for

C–H•••π Interactions as Modulators of Carbocation Structure—Implications for Terpene Biosynthesis

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Table S1. Gas-phase and solvation binding energies of the 2-norbornyl cation and benzene complex in Table 1 (**1**) at various levels of theory.

Method	gas-phase		DCM [e]		H_2O[e]	
	BE[a]	BE[b]	BE[a]	BE[b]	BE[a]	BE[b]
B3LYP[c]	-6.39	-8.64	+1.32	-4.24	-0.04	-6.06
CAM-B3LYP[d]	-6.78	-8.54	+0.29	-5.12	-1.28	-7.07
LC-ωPBE[d]	-6.29	-6.71	-4.07	-4.70	-6.00	-6.62
ωB97XD[d]	-12.1	-14.57	-3.18	-9.16	-4.54	-10.92
PBE1[c]	-7.58	-10.24	+1.50	-4.95	+0.23	-6.66
B971[c]	-8.25	-10.93	+0.08	-6.10	-1.47	-8.06

[a] Binding energy of complex versus separate fully optimized benzene and 2-norbornyl cation.
[b] Binding energy of complex versus separate fully optimized benzene and 2-norbornyl cation with the geometry found in the complex.
[c] Gas-phase calculations were carried out with GAUSSIAN03.
[d] Gas-phase calculations were carried out with GAUSSIAN09.
[e] Single point solvation calculations with GAUSSIAN09 on the optimized geometries in gas phase were carried out using CPCM method with UAKS radii and energies include SMD corrections.

Table S2. Fully optimized structures of benzene-complexed 2-norbornyl cation (complex **2**) at various levels of theory. Distances shown are in Å and energies are in kcal/mol. BE[a] = binding energy of complex versus separate fully optimized benzene and 2-norbornyl cation. BE[b] = binding energy of complex versus separate fully optimized benzene and 2-norbornyl cation with the geometry found in the complex. BSSE = basis set superposition error.

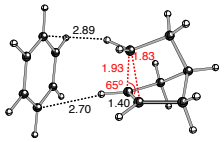
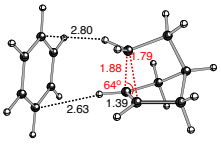
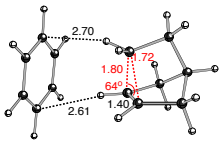
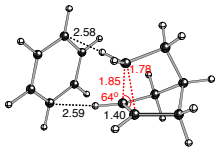
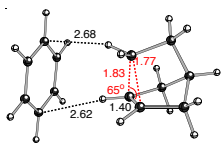
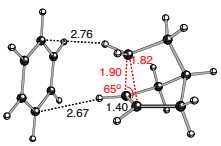
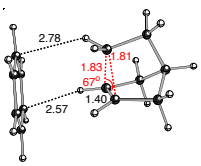
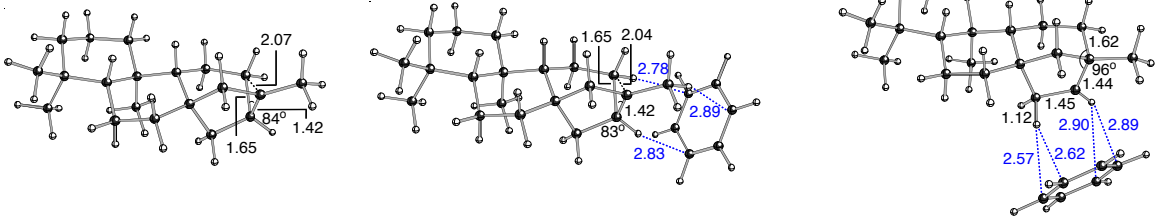
	B3LYP	**CAM-B3LYP**	**LC-ωPBE**	**ωB97XD**
norbornyl cation•benzene complex **2**				
BE[a]	-6.65	-7.84	-8.17	-12.45
BE[b]	[-6.74]	[-7.96]	[-8.37]	[-12.58]
BSSE	(+0.41)	(+0.43)	(+0.40)	(+0.44)
	PBE1	**B971**	**M06-2X**	
norbornyl cation•benzene complex **2**				
BE[a]	-8.58	-8.55	-11.63	
BE[b]	[-8.74]	[-8.62]	[-11.71]	
BSSE	(+0.45)	(+0.43)	(+0.46)	

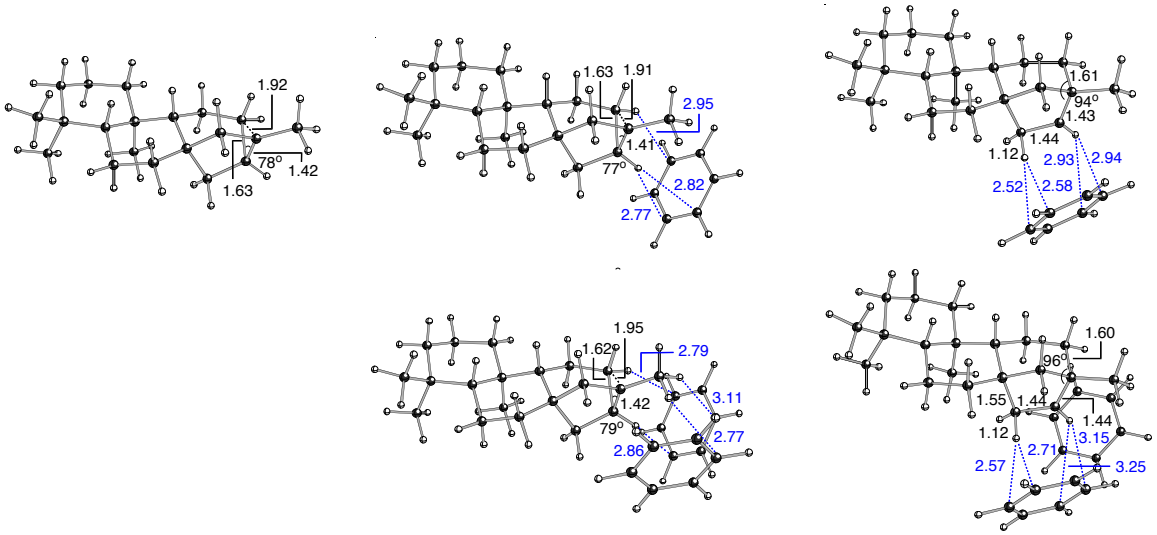
Table S3. Gas-phase binding energies of the 2-norbornyl cation and benzene complex (geometries optimized using B3LYP/6-31+G(d,p)) at various levels of theory. BE[a] = binding energy of complex versus separate fully optimized benzene and 2-norbornyl cation. BE[b] = binding energy of complex versus separate fully optimized benzene and 2-norbornyl cation with the geometry found in the complex. BSSE = basis set superposition error.

		B2PLYPD	CAM-B3LYP	LC-ωPBE	ωB97XD	PBE1	B971	M06-2X	CCSD(T)[c]
1	BE[a]	-9.60	-6.77	-4.67	-11.80	-7.46	-8.88	-9.64	-10.97
	BE[b]	[-11.77]	[-9.69]	[-9.78]	[-15.32]	[-11.29]	[-11.29]	[-14.46]	[-14.29]
	BSSE	(+1.51)	(+0.49)	(+0.44)	(+0.47)	(+0.51)	(+0.51)	(+0.44)	(+3.29)
2	BE[a]	-9.95	-8.09	-7.28	-11.56	-8.22	-8.96	-10.20	-11.03
	BE[b]	[-9.94]	[-8.36]	[-8.59]	[-11.98]	[-8.83]	[-8.70]	[-10.73]	[-10.98]
	BSSE	(+1.21)	(+0.40)	(+0.36)	(+0.37)	(+0.40)	(+0.40)	(+0.34)	(+2.13)

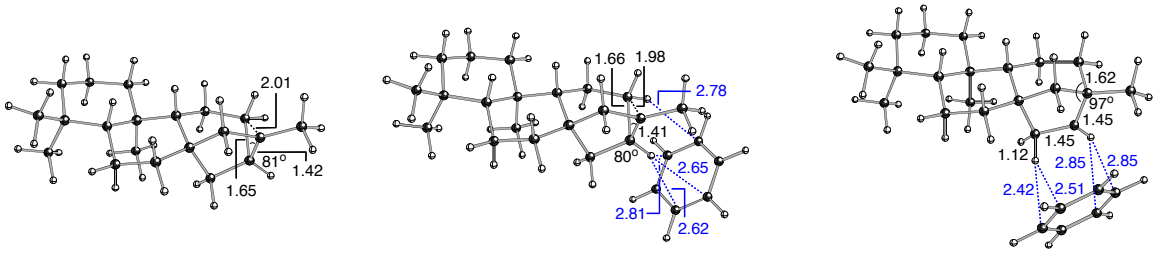
CAM-B3LYP



LC-ωPBE



ωB97X-D



PBE1

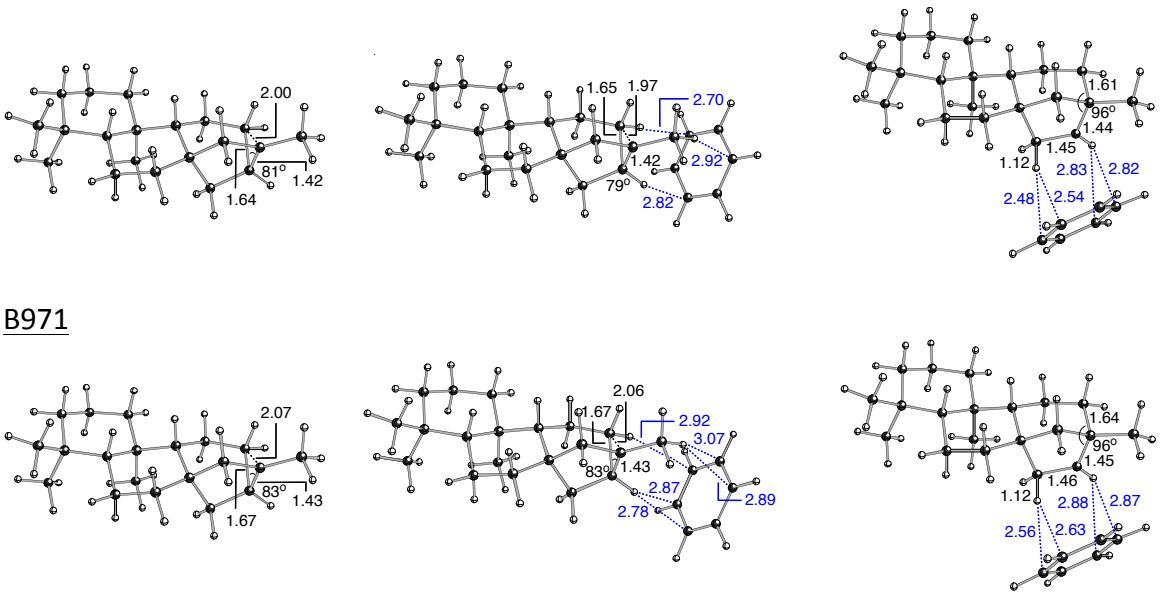


Figure S1. Fully optimized geometries of a carbocation involved in beyerene/kaurene/trachylobane/atiserene biosynthesis, complexes of this carbocation with one/two benzene molecule(s). Selected distances are shown in Å.

Binding Energy Decomposition for the 2-norbornyl cation-benzene complex (Table 1; B3LYP/TZ2P (kcal/mol), ADF program)

Pauli Repulsion

Type of energy	hartrees	eV	**kcal/mol**	kJ/mol
Kinetic (Delta T^0)	0.102570086	2.7911	**64.36**	269.3
Delta V^Pauli Coulomb	-0.060962533	-1.6589	**-38.25**	-160.06
Delta V^Pauli Hybrid-X	-0.019248126	-0.5238	**-12.08**	-50.54
Delta V^Pauli Hybrid-C	-0.006880599	-0.1872	**-4.32**	-18.07
Total Pauli Repulsion	0.015478827	0.4212	**9.71**	40.64

Steric Interaction

Type of energy	hartrees	eV	**kcal/mol**	kJ/mol
Pauli Repulsion (Delta E^Pauli)	.015478827204	0.4212	**9.71**	40.64
Electrostatic Interaction	-0.013224846	-0.3599	**-8.3**	-34.72
Total Steric Interaction	0.002253981	0.0613	**1.41**	5.92

Orbital Interactions

Type of energy	hartrees	eV	**kcal/mol**	kJ/mol
A	-0.018123107	-0.4932	**-11.37**	-47.58
(Hybrid part) HF exchange	0.002143704	0.0583	**1.35**	5.63
Total Orbital Interactions	-0.015979403	-0.4348	**-10.03**	-41.95

Alternative Decomposition Orb.Int

Type of energy	hartrees	eV	**kcal/mol**	kJ/mol
Kinetic	-0.0607176	-1.6522	**-38.1**	-159.41
Coulomb	0.035559324	0.9676	**22.31**	93.36
XC	0.009178874	0.2498	**5.76**	24.1
Total Orbital Interactions	-0.015979403	-0.4348	**-10.03**	-41.95
Residu (E=Steric+OrbInt+Res)	5.9576E-09	0	**0**	0
Total Bonding Energy:	-0.013725416	-0.3735	**-8.61**	-36.04

Summary of Bonding Energy (energy terms are taken from the energy decomposition above)

Type of energy	hartrees	eV	**kcal/mol**	kJ/mol
Electrostatic Energy	-0.013224846	-0.3599	**-8.3**	-34.72
Kinetic Energy	0.041852486	1.1389	**26.26**	109.88
Coulomb (Steric+OrbInt) Energy	-0.025403204	-0.6913	**-15.94**	-66.7
XC Energy	-0.016949852	-0.4612	**-10.64**	-44.5
Total Bonding Energy	-0.013725416	-0.3735	**-8.61**	-36.04

Coordinates and Energies

Table 1

2-Norbornyl cation and benzene complex (**1**)

B3LYP

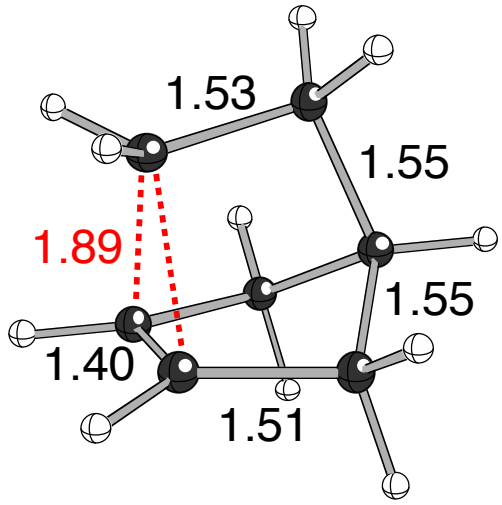
Benzene
B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -232.268418 hartrees (-145750.75497918 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.100451 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.004642	-0.972726	-0.000003
2	6	-0.340224	-1.356277	-0.000072

3	6	-1.344778	-0.383660	0.000061
4	6	-1.004560	0.972811	-0.000008
5	6	0.340111	1.356303	-0.000064
6	6	1.344810	0.383551	0.000060
7	1	1.784826	-1.728466	0.000064
8	1	-0.604294	-2.409911	-0.000080
9	1	-2.389324	-0.681549	0.000140
10	1	-1.784931	1.728349	-0.000011
11	1	0.604426	2.409869	-0.000013
12	1	2.389290	0.681697	0.000052

Free 2-norbornyl cation



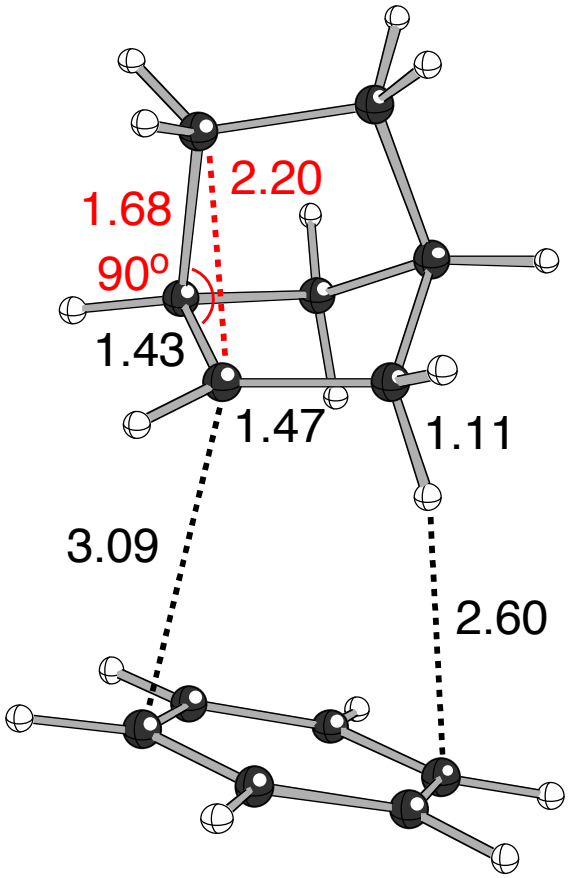
B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -273.0836446 hartrees (-171362.717822946 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.163723 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.401828	1.378716	-0.000012
2	6	1.062967	0.409126	-0.697655
3	6	-0.653168	-0.992003	0.000005
4	6	-1.491208	0.307448	-0.000012
5	1	-0.328703	2.031131	0.873959
6	1	-0.328688	2.031111	-0.873999
7	1	-2.124178	0.387654	0.886692

8	1	-2.124169	0.387642	-0.886723
9	6	0.304191	-0.797945	-1.200118
10	1	1.012120	-1.631081	-1.306797
11	1	-0.189535	-0.641288	-2.161801
12	6	1.062955	0.409141	0.697659
13	6	0.304175	-0.797923	1.200135
14	1	1.012105	-1.631056	1.306839
15	1	-0.189563	-0.641247	2.161808
16	1	1.678808	1.063301	-1.306972
17	1	1.678791	1.063326	1.306972
18	1	-1.225495	-1.918858	0.000008

2-Norbornyl cation-benzene complex



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -505.3622521 hartrees (-317119.866815271 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.265031 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000767508064

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.780094	-0.523997	1.280552
2	6	-1.963116	-1.220754	-0.083468
3	6	-0.820868	0.799065	-0.435261
4	6	-1.663685	0.903981	0.715780
5	1	-2.635449	-0.642246	1.949570
6	1	-0.868847	-0.821673	1.806988
7	1	-1.614732	1.783648	1.352172
8	6	-0.790166	-0.598220	-0.895523
9	1	-0.806128	-0.718073	-1.982889
10	6	-3.248941	-0.549510	-0.620059
11	1	-3.397876	-0.714401	-1.689797
12	1	-4.128380	-0.930041	-0.093750
13	6	-3.009233	0.934508	-0.284017
14	1	-2.915315	1.591387	-1.153751
15	1	-3.747470	1.393528	0.380420
16	1	-1.969311	-2.310486	-0.077261
17	1	-0.419378	1.647343	-0.980657
18	1	0.176819	-1.015562	-0.543690
19	6	2.002369	0.759774	1.204278
20	6	2.252611	-0.613523	1.292372
21	6	2.175225	1.427095	-0.019674
22	6	2.665087	-1.320933	0.157013
23	1	2.151159	-1.126245	2.244407
24	6	2.602805	0.719711	-1.152536
25	1	2.034519	2.503613	-0.073083
26	6	2.842671	-0.653398	-1.064782
27	1	2.878029	-2.383528	0.228015
28	1	2.769748	1.242802	-2.089624
29	1	3.188622	-1.202157	-1.935547
30	1	1.716004	1.319296	2.090446

2-Norbornyl cation in the complex
B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -273.0800614 hartrees (-171360.469329114 kcal/mol)

CAM-B3LYP

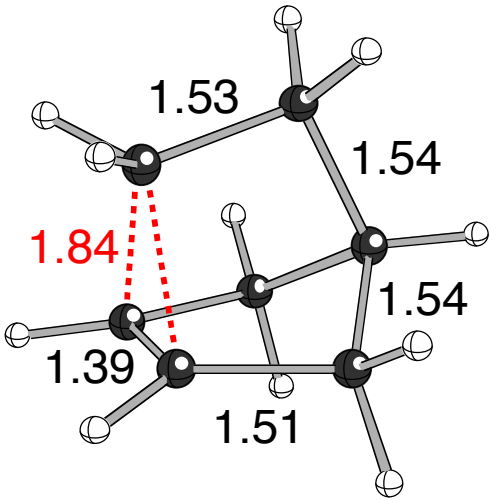
Benzene
CAM-B3LYP/6-31+G(d,p)//CAM-B3LYP/6-31+G(d,p):

HF = -232.1238481 hartrees (-145660.035921231 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.101598 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.370839	-0.245827	-0.000002
2	6	-0.898286	1.064244	-0.000038
3	6	0.472509	1.310032	0.000035
4	6	1.370845	0.245797	-0.000004
5	6	0.898309	-1.064224	-0.000037
6	6	-0.472538	-1.310022	0.000031
7	1	-2.439387	-0.437447	0.000028
8	1	-1.598518	1.893816	-0.000035
9	1	0.840861	2.331228	0.000078
10	1	2.439378	0.437496	0.000001
11	1	1.598481	-1.893847	-0.000019
12	1	-0.840815	-2.331245	0.000037

Free 2-norbornyl cation



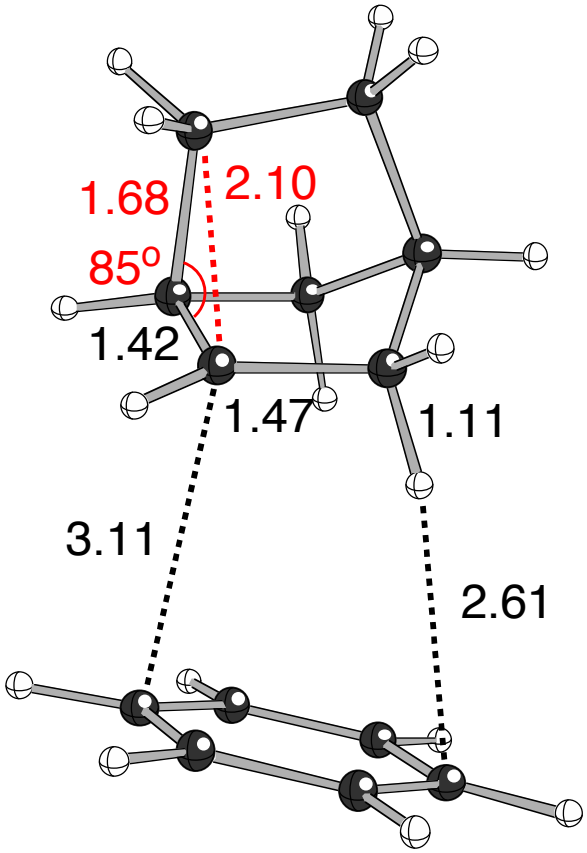
CAM-B3LYP/6-31+G(d,p)//CAM-B3LYP/6-31+G(d,p):
HF = -272.913983 hartrees (-171256.25347233 kcal/mol)
Imaginary Frequencies: none found

Zero-point correction = 0.165747 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.019399	1.410791	-0.000015
2	6	1.118152	0.136297	-0.695184
3	6	-0.882045	-0.792377	0.000005
4	6	-1.353770	0.671165	-0.000015
5	1	0.209684	2.033926	0.867673
6	1	0.209704	2.033943	-0.867683
7	1	-1.942558	0.915630	0.885627
8	1	-1.942545	0.915598	-0.885675
9	6	0.087761	-0.845805	-1.194650
10	1	0.568677	-1.825727	-1.301061
11	1	-0.353797	-0.570874	-2.154054
12	6	1.118147	0.136311	0.695187
13	6	0.087747	-0.845777	1.194668
14	1	0.568656	-1.825696	1.301122
15	1	-0.353823	-0.570811	2.154059
16	1	1.883833	0.606165	-1.303361
17	1	1.883821	0.606192	1.303363
18	1	-1.671219	-1.541977	0.000009

2-Norbornyl cation-benzene complex



CAM-B3LYP/6-31+G(d,p)//CAM-B3LYP/6-31+G(d,p):
HF = -505.0486389 hartrees (-316923.071396139 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.268185 (Hartree/Particle)
Counterpoise: BSSE energy = 0.0007237355

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.786312	-0.596841	1.255419
2	6	-1.965609	-1.211459	-0.140757
3	6	-0.855442	0.825247	-0.382841
4	6	-1.655236	0.853288	0.785574
5	1	-2.642596	-0.752133	1.913916
6	1	-0.876878	-0.925974	1.764782
7	1	-1.619831	1.697714	1.466721
8	6	-0.803321	-0.546743	-0.914191
9	1	-0.826704	-0.612309	-2.004338
10	6	-3.238864	-0.506028	-0.638244
11	1	-3.407534	-0.638305	-1.708449

12	1	-4.119349	-0.873424	-0.107390
13	6	-2.949944	0.955067	-0.273976
14	1	-2.809381	1.615519	-1.135557
15	1	-3.682895	1.450466	0.366780
16	1	-1.977981	-2.298793	-0.194597
17	1	-0.445292	1.704689	-0.868474
18	1	0.170782	-0.952094	-0.581343
19	6	2.051898	0.163696	1.410923
20	6	2.401724	-1.080769	0.891629
21	6	2.065311	1.290698	0.587322
22	6	2.765984	-1.199113	-0.450294
23	1	2.415916	-1.954483	1.535425
24	6	2.438601	1.172173	-0.753875
25	1	1.839191	2.268490	1.003096
26	6	2.787304	-0.072480	-1.272110
27	1	3.058428	-2.165389	-0.848571
28	1	2.489328	2.055279	-1.383911
29	1	3.096684	-0.162590	-2.308298
30	1	1.801552	0.262920	2.462732

2-Norbornyl cation in the complex
CAM-B3LYP/6-31+G(d,p)//CAM-B3LYP/6-31+G(d,p):
HF = -272.9111794 hartrees (-171254.494185294 kcal/mol)

LC-ωPBE

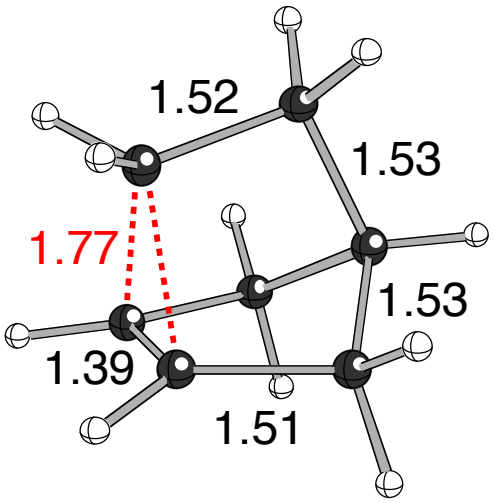
Benzene
LC-ωPBE/6-31+G(d,p)//LC-ωPBE/6-31+G(d,p):
HF = -232.0866898 hartrees (-145636.718716398 kcal/mol)
Zero-point correction = 0.102457 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.992177	-0.972470	-0.000003
2	6	0.346152	-1.345451	-0.000064
3	6	1.338338	-0.372987	0.000043
4	6	0.992157	0.972489	-0.000008
5	6	-0.346125	1.345458	-0.000048
6	6	-1.338345	0.372960	0.000054
7	1	-1.767844	-1.732727	0.000049

8	1	0.616599	-2.397359	-0.000061
9	1	2.384542	-0.664621	0.000109
10	1	1.767864	1.732707	0.000002
11	1	-0.616627	2.397353	-0.000009
12	1	-2.384534	0.664648	0.000068

Free 2-norbornyl cation



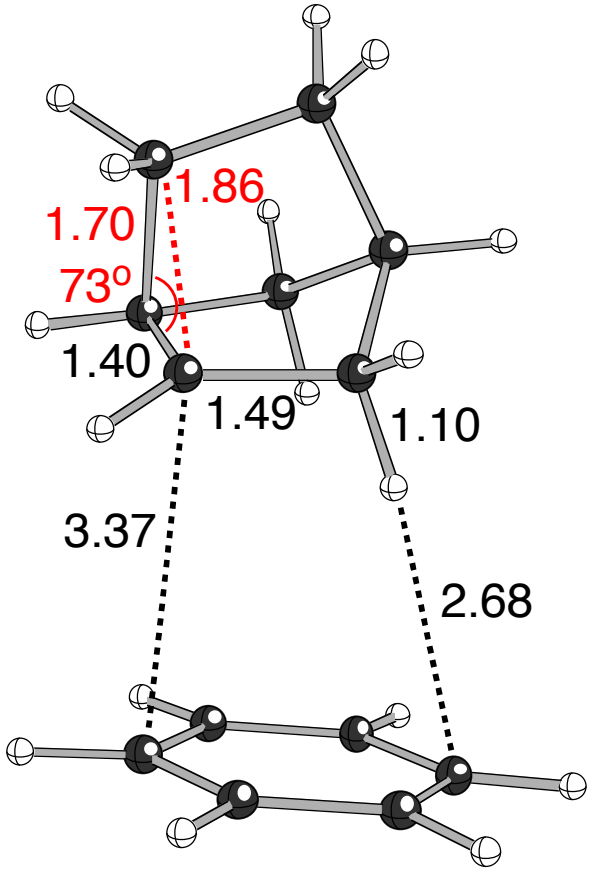
LC-ωPBE/6-31+G(d,p)//LC-ωPBE/6-31+G(d,p):
HF = -272.9127703 hartrees (-171255.492490953 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.167569 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.523167	1.266894	-0.000852
2	6	1.075687	-0.267346	-0.695536
3	6	-1.114583	-0.405270	-0.000174
4	6	-0.993336	1.120455	-0.001538
5	1	0.973033	1.782321	0.853766
6	1	0.973058	1.777692	-0.858354
7	1	-1.439678	1.576453	0.883672
8	1	-1.438618	1.575146	-0.887930
9	6	-0.238449	-0.813610	-1.189994
10	1	-0.142661	-1.900502	-1.291765
11	1	-0.553333	-0.398401	-2.148939

12	6	1.074707	-0.265161	0.697260
13	6	-0.239800	-0.811235	1.191350
14	1	-0.143748	-1.897840	1.295540
15	1	-0.555904	-0.393999	2.149012
16	1	1.966680	-0.134824	-1.301564
17	1	1.965133	-0.132028	1.303955
18	1	-2.128322	-0.802386	-0.000488

2-Norbornyl cation-benzene complex



LC-ωPBE/6-31+G(d,p)//LC-ωPBE/6-31+G(d,p):
HF = -505.009485 hartrees (-316898.50193235 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.270729 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000577112

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	-1.814982	-0.733275	1.209943
2	6	-2.002111	-1.190768	-0.238407
3	6	-1.033322	0.906702	-0.297287
4	6	-1.680160	0.749066	0.931376
5	1	-2.653456	-0.976791	1.864617
6	1	-0.887300	-1.100382	1.659275
7	1	-1.698854	1.522979	1.691685
8	6	-0.881413	-0.424628	-0.954665
9	1	-0.953713	-0.395089	-2.043380
10	6	-3.273795	-0.442335	-0.646395
11	1	-3.492173	-0.520254	-1.712765
12	1	-4.146203	-0.786466	-0.088149
13	6	-2.889146	0.978057	-0.248287
14	1	-2.726595	1.655868	-1.096655
15	1	-3.564243	1.543206	0.398384
16	1	-2.009974	-2.266809	-0.404293
17	1	-0.608266	1.839531	-0.654366
18	1	0.116697	-0.794124	-0.680300
19	6	2.112984	0.344971	1.365697
20	6	2.359285	-0.977987	1.013237
21	6	2.228773	1.351916	0.411406
22	6	2.719932	-1.294033	-0.292987
23	1	2.300127	-1.761248	1.763673
24	6	2.587277	1.034909	-0.895352
25	1	2.080579	2.390231	0.697193
26	6	2.832707	-0.288080	-1.247068
27	1	2.935457	-2.323820	-0.562356
28	1	2.707479	1.822979	-1.633480
29	1	3.134872	-0.533249	-2.260906
30	1	1.869396	0.596343	2.394557

2-Norbornyl cation in the complex
LC-ωPBE/6-31+G(d,p)//LC-ωPBE/6-31+G(d,p):
HF = -272.9121028 hartrees (-171255.073628028 kcal/mol)

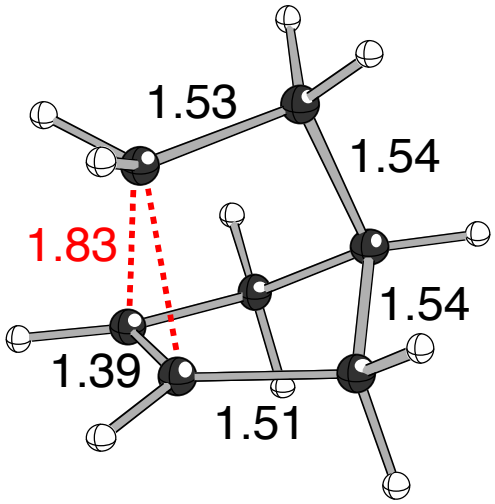
ωB97X-D

Benzene
ωB97X-D/6-31+G(d,p)//ωB97X-D/6-31+G(d,p):
HF = -232.1807124 hartrees (-145695.718838124 kcal/mol)
Zero-point correction = 0.101453 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.281162	-1.365274	0.000000
2	6	-1.041974	-0.926093	-0.000001
3	6	-1.323217	0.439334	0.000007
4	6	-0.281134	1.365280	0.000000
5	6	1.041955	0.926114	-0.000006
6	6	1.323209	-0.439361	0.000001
7	1	0.499766	-2.428854	0.000001
8	1	-1.853685	-1.647210	-0.000001
9	1	-2.353772	0.780946	0.000011
10	1	-0.499809	2.428845	-0.000001
11	1	1.853711	1.647180	-0.000008
12	1	2.353785	-0.780907	-0.000001

Free 2-norboryl cation



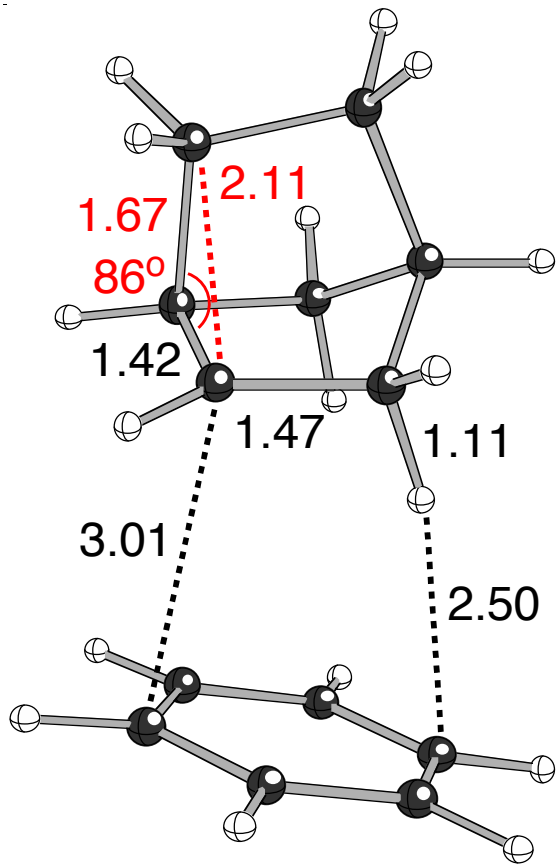
ωB97X-D/6-31+G(d,p)//ωB97X-D/6-31+G(d,p):
HF = -273.0046625 hartrees (-171313.155765375 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.165731 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	0.124170	1.397310	-0.008093
2	6	1.124920	0.025250	-0.694214
3	6	-0.955378	-0.704080	0.002147
4	6	-1.281045	0.799081	-0.008769
5	1	0.409763	2.008950	0.852667
6	1	0.414569	1.991697	-0.879479
7	1	-1.843149	1.107115	0.874412
8	1	-1.837480	1.096487	-0.899138
9	6	0.007351	-0.858611	-1.190508
10	1	0.395158	-1.879769	-1.288518
11	1	-0.404947	-0.547262	-2.151747
12	6	1.119587	0.038050	0.699159
13	6	0.000633	-0.841554	1.202130
14	1	0.388970	-1.860629	1.316864
15	1	-0.417625	-0.516441	2.156192
16	1	1.937050	0.410291	-1.301592
17	1	1.929267	0.430507	1.304973
18	1	-1.813005	-1.373618	0.004250

2-Norbornyl cation-benzene complex



ωB97X-D/6-31+G(d,p)//ωB97X-D/6-31+G(d,p):
HF = -505.2046544 hartrees (-317020.972682544 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.268294 (Hartree/Particle)
Counterpoise: BSSE energy = 0.0007639282

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.670130	-0.622698	1.226402
2	6	-1.885076	-1.209480	-0.177357
3	6	-0.802966	0.843724	-0.408096
4	6	-1.579024	0.838970	0.782324
5	1	-2.502678	-0.805680	1.908013
6	1	-0.737997	-0.947391	1.696224
7	1	-1.527703	1.667478	1.481501
8	6	-0.753791	-0.514137	-0.970936
9	1	-0.805973	-0.556035	-2.061065
10	6	-3.182470	-0.511614	-0.622091
11	1	-3.374083	-0.617473	-1.691420
12	1	-4.042687	-0.908685	-0.079404
13	6	-2.905778	0.943629	-0.222968
14	1	-2.804997	1.632244	-1.068629
15	1	-3.632365	1.400930	0.453209
16	1	-1.883164	-2.295114	-0.255440
17	1	-0.428651	1.739982	-0.891923
18	1	0.229963	-0.923324	-0.669787
19	6	1.877631	0.766721	1.189491
20	6	2.093872	-0.607381	1.294850
21	6	2.122935	1.421742	-0.021928
22	6	2.542728	-1.327424	0.187443
23	1	1.936178	-1.111788	2.243118
24	6	2.579526	0.701280	-1.128176
25	1	2.002356	2.499477	-0.089027
26	6	2.785659	-0.672794	-1.023823
27	1	2.726781	-2.393558	0.273164
28	1	2.794027	1.213720	-2.060574
29	1	3.154627	-1.232466	-1.877134
30	1	1.557672	1.334456	2.058358

2-Norbornyl cation in the complex

ωB97X-D/6-31+G(d,p)//ωB97X-D/6-31+G(d,p):
HF = -273.0007204 hartrees (-171310.682058204 kcal/mol)

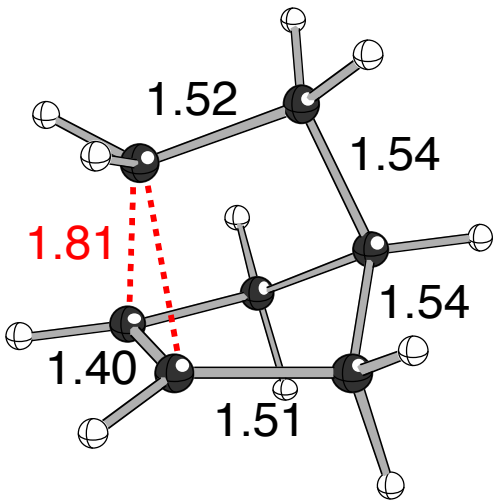
PBE1

Benzene
PBE1/6-31+G(d,p)//PBE1/6-31+G(d,p):
HF = -231.9812391 hartrees (-145570.547347641 kcal/mol)
Zero-point correction = 0.101194 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.483629	1.307339	0.000000
2	6	-1.374096	0.234830	-0.000025
3	6	-0.890479	-1.072505	0.000016
4	6	0.483676	-1.307322	-0.000004
5	6	1.374088	-0.234879	-0.000015
6	6	0.890441	1.072536	0.000020
7	1	-0.860611	2.326344	0.000004
8	1	-2.445037	0.418088	-0.000011
9	1	-1.584465	-1.908490	0.000017
10	1	0.860530	-2.326375	0.000008
11	1	2.445052	-0.418005	-0.000007
12	1	1.584529	1.908435	0.000032

Free 2-norbornyl cation

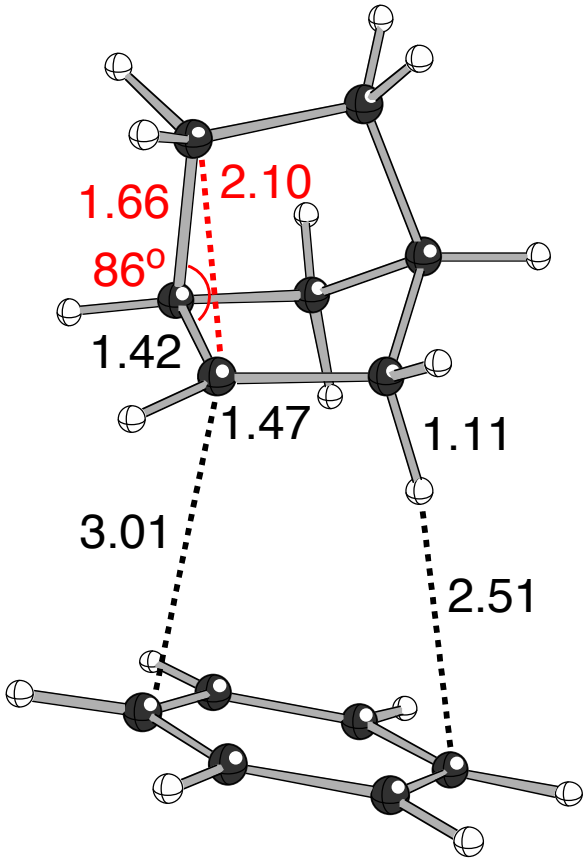


PBE1/6-31+G(d,p)//PBE1/6-31+G(d,p):
HF = -272.7589313 hartrees (-171158.956980063 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.165036 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.257425	1.367826	-0.004341
2	6	1.111340	-0.072201	-0.704979
3	6	-1.016985	-0.610582	0.008639
4	6	-1.196025	0.914297	0.000175
5	1	0.609048	1.943514	0.859754
6	1	0.604568	1.948561	-0.866672
7	1	-1.725558	1.277968	0.883870
8	1	-1.723740	1.264940	-0.889829
9	6	-0.083522	-0.850303	-1.189036
10	1	0.211522	-1.903745	-1.287126
11	1	-0.474583	-0.508136	-2.149975
12	6	1.120219	-0.066117	0.691540
13	6	-0.069538	-0.838656	1.197478
14	1	0.224894	-1.891309	1.304367
15	1	-0.449440	-0.484810	2.158734
16	1	1.950909	0.239529	-1.319447
17	1	1.970218	0.244658	1.292016
18	1	-1.935330	-1.196746	0.017447

2-Norbornyl cation-benzene complex



PBE1/6-31+G(d,p)//PBE1/6-31+G(d,p):
HF = -504.7522558 hartrees (-316737.088037058 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.267033 (Hartree/Particle)
Counterpoise: BSSE energy = 0.0008036287

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.743024	-0.616489	1.238537
2	6	-1.916862	-1.209368	-0.164977
3	6	-0.813523	0.833720	-0.375392
4	6	-1.630560	0.839604	0.791164
5	1	-2.599009	-0.792639	1.894280
6	1	-0.828264	-0.944609	1.741752
7	1	-1.595928	1.671744	1.489473
8	6	-0.760442	-0.525738	-0.927007
9	1	-0.775553	-0.578755	-2.019117
10	6	-3.191707	-0.503758	-0.649782

11	1	-3.361081	-0.617568	-1.723233
12	1	-4.070344	-0.887811	-0.124399
13	6	-2.910228	0.947933	-0.255545
14	1	-2.769782	1.625117	-1.107457
15	1	-3.657646	1.431317	0.382761
16	1	-1.921489	-2.296998	-0.236962
17	1	-0.422511	1.726579	-0.854507
18	1	0.216229	-0.938224	-0.594340
19	6	1.950326	0.429795	1.353921
20	6	2.257907	-0.904993	1.093729
21	6	2.056480	1.382433	0.334397
22	6	2.668436	-1.288468	-0.185684
23	1	2.202744	-1.642855	1.889217
24	6	2.481665	0.999163	-0.942674
25	1	1.869205	2.431266	0.552392
26	6	2.783617	-0.335699	-1.202506
27	1	2.926690	-2.324912	-0.383883
28	1	2.602213	1.745968	-1.722853
29	1	3.129152	-0.633874	-2.188067
30	1	1.662856	0.737439	2.355859

2-Norbornyl cation in the complex
PBE1/6-31+G(d,p)//PBE1/6-31+G(d,p):
HF = -272.7546953 hartrees (-171156.298847703 kcal/mol)

B971

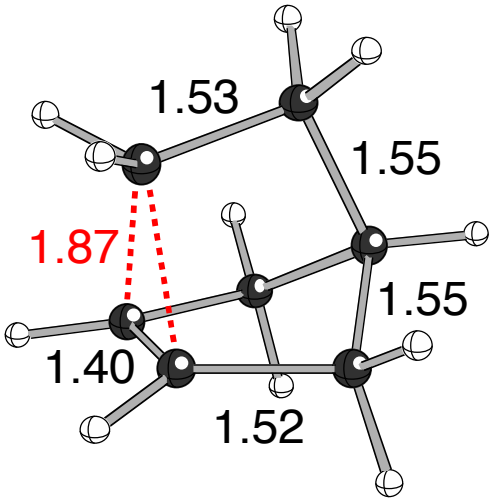
Benzene
B971/6-31+G(d,p)//B971/6-31+G(d,p):
HF = -232.1931067 hartrees (-145703.496385317 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.100143 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.814729	-1.140346	-0.000003
2	6	0.580300	-1.275717	-0.000075
3	6	1.395060	-0.135349	0.000052
4	6	0.814709	1.140360	-0.000010
5	6	-0.580278	1.275727	-0.000056

6	6	-1.395062	0.135325	0.000063
7	1	-1.447124	-2.025620	0.000056
8	1	1.030569	-2.266112	-0.000073
9	1	2.477893	-0.240425	0.000129
10	1	1.447149	2.025602	0.000002
11	1	-1.030599	2.266099	-0.000015
12	1	-2.477889	0.240456	0.000080

Free 2-norbornyl cation



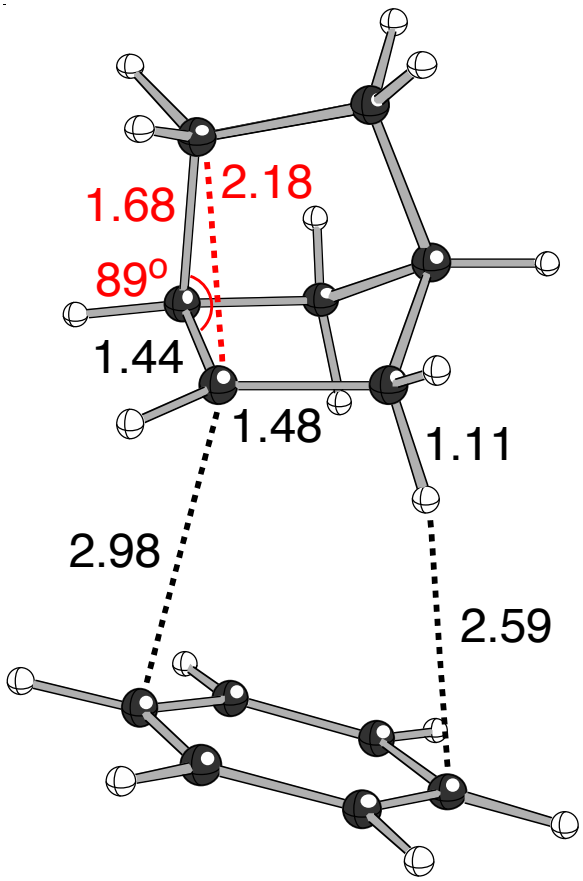
B971/6-31+G(d,p)//B971/6-31+G(d,p):
HF = -273.0025953 hartrees (-171311.858576703 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.163339 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.167750	1.414821	-0.000006
2	6	-1.108877	0.244299	0.700017
3	6	0.803384	-0.880380	0.000002
4	6	1.424311	0.537870	-0.000006
5	1	-0.005210	2.055193	-0.872685
6	1	-0.005203	2.055202	0.872668
7	1	2.035125	0.721438	-0.888909
8	1	2.035130	0.721444	0.888892

9	6	-0.173454	-0.837295	1.202815
10	1	-0.748776	-1.769028	1.307483
11	1	0.292549	-0.605894	2.165106
12	6	-1.108882	0.244290	-0.700014
13	6	-0.173460	-0.837306	-1.202806
14	1	-0.748782	-1.769040	-1.307463
15	1	0.292537	-0.605913	-2.165102
16	1	-1.823472	0.793070	1.308828
17	1	-1.823481	0.793056	-1.308827
18	1	1.514953	-1.707316	0.000003

2-Norbornyl cation-benzene complex



B971/6-31+G(d,p)//B971/6-31+G(d,p):
HF = -505.2088572 hartrees (-317023.609981572 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.264500 (Hartree/Particle)
Counterpoise: BSSE energy = 0.0008167291

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.747449	-0.619270	1.240136
2	6	-1.935948	-1.219755	-0.171397
3	6	-0.799742	0.827193	-0.389864
4	6	-1.633559	0.846986	0.777143
5	1	-2.602250	-0.786219	1.902887
6	1	-0.829738	-0.950903	1.737974
7	1	-1.586392	1.682533	1.472902
8	6	-0.767269	-0.540577	-0.947010
9	1	-0.794686	-0.585041	-2.041608
10	6	-3.225845	-0.511315	-0.655381
11	1	-3.383486	-0.607468	-1.733882
12	1	-4.103167	-0.920063	-0.143749
13	6	-2.971688	0.949465	-0.228264
14	1	-2.869064	1.657087	-1.059437
15	1	-3.710255	1.376789	0.460245
16	1	-1.941921	-2.309025	-0.239999
17	1	-0.419555	1.717144	-0.886039
18	1	0.203598	-0.979066	-0.628553
19	6	1.967895	0.256751	1.406236
20	6	2.347795	-1.023160	0.981974
21	6	2.002282	1.334288	0.502081
22	6	2.763941	-1.226713	-0.344883
23	1	2.343873	-1.855038	1.682515
24	6	2.437088	1.131568	-0.821803
25	1	1.759276	2.337674	0.846707
26	6	2.814029	-0.148201	-1.244485
27	1	3.076294	-2.216404	-0.669770
28	1	2.506479	1.974358	-1.506387
29	1	3.164823	-0.305572	-2.261607
30	1	1.676986	0.425651	2.440903

2-Norbornyl cation in the complex
B971/6-31+G(d,p)//B971/6-31+G(d,p):
HF = -272.9983361 hartrees (-171309.185886111 kcal/mol)

B3LYP-DCP

Benzene
B3LYP-DCP/6-31+G(d,p)//B971/6-31+G(d,p):
HF = -231.5611469 hartrees (-145304.6196797500 kcal/mol)

Free 2-norbornyl cation
B3LYP-DCP/6-31+G(d,p)//B971/6-31+G(d,p):
HF = -272.2833516 hartrees (-170857.8031290000 kcal/mol)
2-Norbornyl cation-benzene complex
B3LYP-DCP/6-31+G(d,p)//B971/6-31+G(d,p):
HF = -503.8610205 hartrees (-316172.7903637500 kcal/mol)
2-Norbornyl cation in the complex
B3LYP-DCP/6-31+G(d,p)//B971/6-31+G(d,p):
HF = -272.9380555 hartrees (-171268.6298262500 kcal/mol)

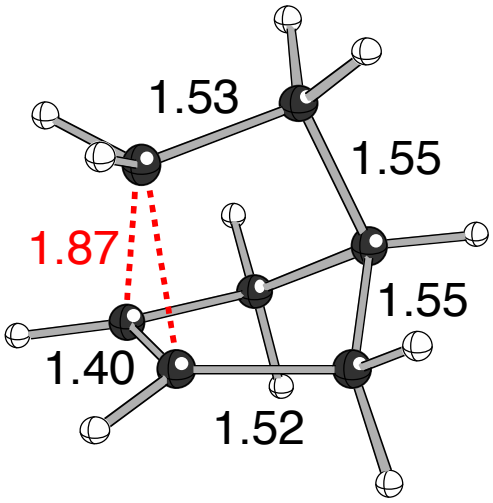
MO6-2X

Benzene
MO6-2X/6-31+G(d,p)//MO6-2X/6-31+G(d,p):
HF = -232.1520475 hartrees (-145677.731326725 kcal/mol)
Zero-point correction = 0.101285 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.173416	-1.383541	0.000055
2	6	-1.111643	-0.841940	0.000046
3	6	1.285053	-0.541667	-0.000147
4	6	-1.285062	0.541640	-0.000124
5	1	-1.977006	-1.497687	0.000148
6	6	1.111621	0.841966	0.000065
7	1	2.285611	-0.963224	-0.000092
8	6	-0.173390	1.383543	0.000038
9	1	-2.285598	0.963246	-0.000073
10	1	1.977024	1.497663	0.000178
11	1	-0.308520	2.460809	0.000104
12	1	0.308516	-2.460813	0.000140

Free 2-norbornyl cation

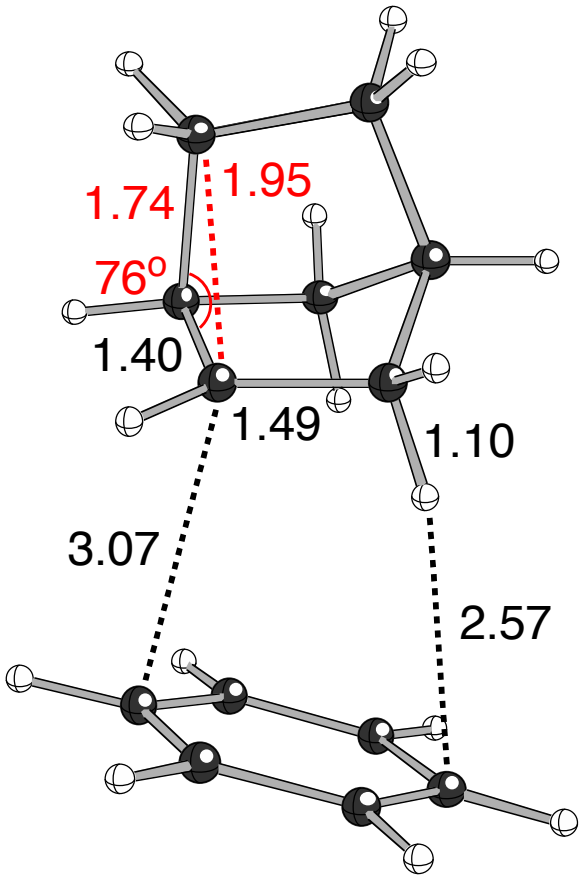


MO6-2X/6-31+G(d,p)//MO6-2X/6-31+G(d,p):
HF = -272.9457702 hartrees (-171276.200258202 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.165461 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.210465	1.385353	-0.006245
2	6	1.125021	-0.040399	-0.694775
3	6	-0.998228	-0.645247	0.001088
4	6	-1.228988	0.875359	-0.007416
5	1	0.533830	1.973880	0.857796
6	1	0.538504	1.959895	-0.878037
7	1	-1.769369	1.216493	0.877483
8	1	-1.765225	1.207923	-0.898059
9	6	-0.046339	-0.855777	-1.190966
10	1	0.280999	-1.898736	-1.286933
11	1	-0.439153	-0.518049	-2.151910
12	6	1.120647	-0.030430	0.699788
13	6	-0.052140	-0.842208	1.199899
14	1	0.275438	-1.883637	1.309587
15	1	-0.450139	-0.493623	2.154788
16	1	1.957680	0.300238	-1.302349
17	1	1.950855	0.316284	1.307243
18	1	-1.896050	-1.260575	0.002161

2-Norbornyl cation-benzene complex



MO6-2X/6-31+G(d,p)//MO6-2X/6-31+G(d,p):
HF = -505.1144004 hartrees (-316964.337395004 kcal/mol)
Zero-point correction = 0.267496 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000676759544

Coordinates (from last standard orientation):

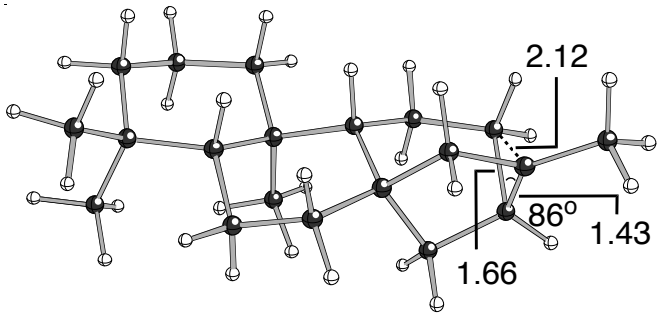
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.687392	-0.817062	1.141269
2	6	-1.900444	-1.182932	-0.336505
3	6	-0.917987	0.922707	-0.265773
4	6	-1.565931	0.688166	0.955225
5	1	-2.514277	-1.106239	1.792533
6	1	-0.747009	-1.206762	1.545159
7	1	-1.577876	1.412769	1.762704
8	6	-0.793900	-0.356985	-1.024257

9	1	-0.885659	-0.244972	-2.106798
10	6	-3.198687	-0.430349	-0.674092
11	1	-3.420872	-0.429219	-1.742705
12	1	-4.054564	-0.846065	-0.138607
13	6	-2.863385	0.972305	-0.165805
14	1	-2.739313	1.731259	-0.946410
15	1	-3.531913	1.424118	0.571397
16	1	-1.894869	-2.245786	-0.571913
17	1	-0.540825	1.888203	-0.587689
18	1	0.208763	-0.753741	-0.794856
19	6	1.917330	0.127165	1.402933
20	6	2.277616	-1.111713	0.870524
21	6	2.001509	1.277108	0.613348
22	6	2.720358	-1.201017	-0.451323
23	1	2.241347	-2.002387	1.490723
24	6	2.439944	1.186377	-0.710287
25	1	1.766121	2.247990	1.042408
26	6	2.799220	-0.052659	-1.242026
27	1	3.021805	-2.161170	-0.858306
28	1	2.531638	2.083597	-1.315672
29	1	3.160379	-0.121062	-2.263283
30	1	1.607613	0.202799	2.441930

2-Norbornyl cation in the complex
MO6-2X/6-31+G(d,p)//MO6-2X/6-31+G(d,p):
HF = -272.944381 hartrees (-171275.32852131 kcal/mol)

Figure 1

(a)



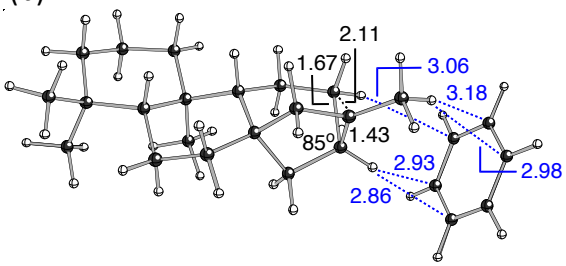
B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -781.7943597 hartrees (-490583.778655347 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.491134 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.174352	-0.550778	-0.204333
2	6	1.600782	-0.589642	-0.195476
3	6	0.838428	0.738265	0.147919
4	6	1.446785	1.903469	-0.680680
5	6	2.972350	2.003083	-0.560241
6	6	3.639294	0.696507	-0.998394
7	1	1.348507	-0.785385	-1.251611
8	1	1.197508	1.753522	-1.741697
9	1	0.991068	2.856004	-0.382968
10	1	3.328771	2.827952	-1.187781
11	1	3.261073	2.261833	0.465451
12	1	3.418655	0.535743	-2.063955
13	1	4.730206	0.781230	-0.922093
14	6	-0.661082	0.550815	-0.328737
15	6	0.993194	-1.751331	0.610283
16	1	1.558632	-2.673392	0.450021
17	1	1.039279	-1.553018	1.685953
18	6	-0.446548	-2.003130	0.157758
19	6	-1.382357	-0.771274	0.124502
20	6	3.835666	-0.568323	1.193722
21	1	3.433139	-1.363581	1.829329
22	1	4.909083	-0.756569	1.083878
23	1	3.737938	0.375128	1.735090
24	6	3.689658	-1.796732	-0.964117
25	1	3.214554	-1.895274	-1.947302
26	1	4.769263	-1.712870	-1.127894
27	1	3.522461	-2.725641	-0.409712
28	6	0.932837	1.100825	1.650907
29	1	1.969453	1.139413	1.979262
30	1	0.515904	2.091525	1.854333
31	1	0.429070	0.385030	2.304307
32	6	-2.550845	-1.115833	-0.865870
33	1	-2.806124	-2.188325	-0.772302
34	1	-0.597283	0.499515	-1.425023
35	6	-1.532640	1.784391	0.039987
36	1	-1.299158	2.119997	1.051905
37	1	-1.305389	2.623450	-0.624283
38	6	-3.038338	1.543326	-0.021062

39	1	-3.367987	1.495957	-1.070398
40	1	-3.647655	2.335736	0.421308
41	6	-3.764425	-0.416860	-0.373486
42	1	-2.340031	-0.954368	-1.929046
43	6	-5.088911	-0.453214	-1.030301
44	1	-5.531393	-1.422715	-0.748521
45	1	-5.765172	0.324179	-0.668234
46	1	-5.023460	-0.441126	-2.121211
47	6	-3.452795	0.203932	0.876158
48	6	-2.195799	-0.489739	1.421656
49	1	-4.264009	0.455277	1.557335
50	1	-2.501037	-1.420613	1.914590
51	1	-1.671406	0.114938	2.160866
52	1	-0.393079	-2.402204	-0.864566
53	1	-0.919009	-2.787894	0.763807

(b)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1014.0701728 hartrees (-636339.174133728 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.592431 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000744026756 hartrees

Coordinates (from last standard orientation):

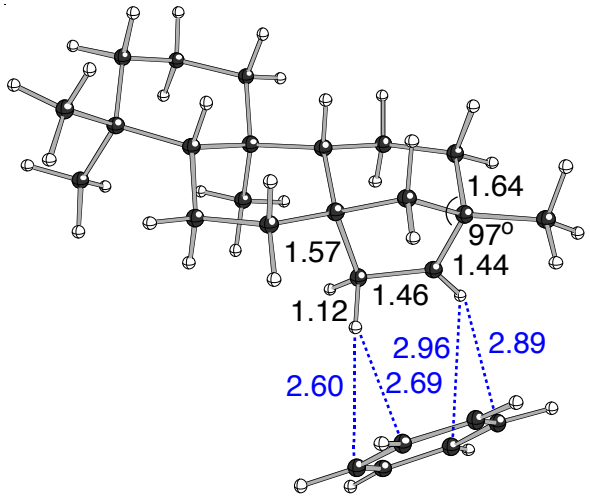
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-4.767674	0.072976	0.260550
2	6	-3.249689	0.451179	0.084119
3	6	-2.225986	-0.718215	-0.136567
4	6	-2.778571	-1.675166	-1.227772
5	6	-4.214207	-2.141201	-0.957287
6	6	-5.162486	-0.945316	-0.839720
7	1	-3.238701	1.007450	-0.868842

8	1	-2.764693	-1.154967	-2.197137
9	1	-2.121597	-2.547649	-1.331069
10	1	-4.540973	-2.791986	-1.776512
11	1	-4.253233	-2.758409	-0.051772
12	1	-5.184294	-0.423696	-1.807826
13	1	-6.187880	-1.288770	-0.655557
14	6	-0.893839	-0.072104	-0.701549
15	6	-2.703898	1.417521	1.148810
16	1	-3.438804	2.193147	1.381600
17	1	-2.507452	0.896422	2.091540
18	6	-1.443168	2.108771	0.627010
19	6	-0.336646	1.183580	0.066980
20	6	-5.144806	-0.478357	1.655880
21	1	-4.766867	0.156426	2.463870
22	1	-6.235675	-0.505885	1.751455
23	1	-4.789574	-1.495362	1.834869
24	6	-5.617555	1.346292	0.033443
25	1	-5.359311	1.840493	-0.910502
26	1	-6.679284	1.081616	-0.013215
27	1	-5.505836	2.075969	0.841772
28	6	-1.977824	-1.534406	1.156053
29	1	-2.914245	-1.903171	1.569490
30	1	-1.363686	-2.419052	0.963442
31	1	-1.494542	-0.957355	1.948100
32	6	0.542784	2.055113	-0.896964
33	1	0.628041	3.079957	-0.490562
34	1	-1.165838	0.285783	-1.704840
35	6	0.231268	-1.131688	-0.864421
36	1	0.260582	-1.785090	0.009173
37	6	1.630521	-0.551486	-1.043661
38	6	1.928896	1.522321	-0.824402
39	6	3.075186	2.036285	-1.605071
40	1	3.379806	2.967438	-1.100649
41	1	3.935786	1.364119	-1.580845
42	1	2.804357	2.305826	-2.629302
43	6	1.977816	0.518823	0.188877
44	6	0.746954	0.720313	1.083790
45	1	-1.759690	2.775264	-0.187183
46	1	-1.002039	2.758513	1.394621
47	1	0.026417	-1.774919	-1.725571
48	1	2.449370	-1.270795	-0.961816
49	1	1.733800	-0.127526	-2.053919
50	1	0.485252	-0.176308	1.645181
51	1	2.936015	0.251139	0.631235

52	1	0.158518	2.170482	-1.916600
53	1	0.976580	1.507599	1.812142
54	6	5.428839	-0.481749	1.835146
55	6	5.037427	-1.689678	1.244535
56	6	5.313916	-1.930664	-0.106573
57	6	5.982173	-0.963982	-0.867270
58	6	6.374251	0.242772	-0.276141
59	6	6.097357	0.484140	1.074630
60	1	5.238102	-0.306189	2.890107
61	1	4.544738	-2.451412	1.842447
62	1	5.040313	-2.881417	-0.556027
63	1	6.223838	-1.163370	-1.907609
64	1	6.921608	0.979510	-0.857753
65	1	6.424864	1.409724	1.539493

Kauranyl cation in the complex

(c)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1014.0681291 hartrees (-636337.891691541 kcal/mol)
Imaginary Frequencies: 1 (-10.3938 1/cm)
Zero-point correction = 0.592155 (Hartree/Particle)
Counterpoise: BSSE energy = 0.001032073148 hartrees

Coordinates (from last standard orientation):

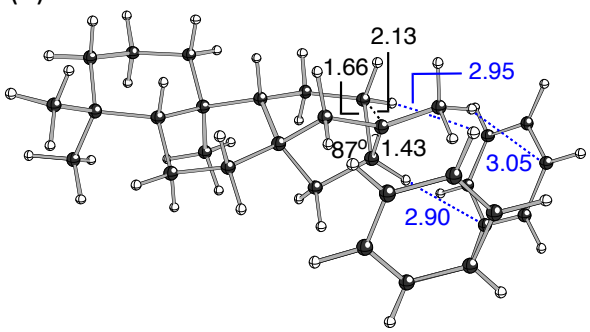
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	-3.999791	-1.253383	0.388147
2	6	-2.586185	-0.574454	0.519406
3	6	-2.209899	0.533499	-0.525463
4	6	-3.391162	1.535046	-0.650565
5	6	-4.741468	0.856731	-0.913163
6	6	-5.069696	-0.149757	0.193766
7	1	-2.655097	-0.034351	1.479024
8	1	-3.472470	2.106602	0.286102
9	1	-3.184632	2.263071	-1.444697
10	1	-5.524648	1.622091	-0.959439
11	1	-4.742664	0.368850	-1.895345
12	1	-5.179831	0.400898	1.139519
13	1	-6.040143	-0.623770	0.001939
14	6	-0.971652	1.330350	0.064571
15	6	-1.413475	-1.560066	0.668191
16	1	-1.682348	-2.385364	1.333491
17	1	-1.157354	-2.019057	-0.292226
18	6	-0.204670	-0.846239	1.273726
19	6	0.233865	0.465814	0.580965
20	6	-4.112560	-2.311456	-0.734226
21	1	-3.295762	-3.039482	-0.693856
22	1	-5.047350	-2.869320	-0.613494
23	1	-4.130462	-1.882255	-1.738285
24	6	-4.321521	-1.973284	1.720538
25	1	-4.196794	-1.305124	2.580739
26	1	-5.362169	-2.314877	1.717642
27	1	-3.695894	-2.856921	1.881185
28	6	-1.915422	-0.056221	-1.926853
29	1	-2.763617	-0.631394	-2.292626
30	1	-1.742634	0.728935	-2.668688
31	1	-1.055035	-0.728780	-1.944661
32	6	1.071202	1.274138	1.634993
33	1	1.667169	0.568808	2.243842
34	1	-1.373393	1.848465	0.947008
35	6	-0.462940	2.409896	-0.932568
36	1	-0.454946	2.008626	-1.947203
37	6	0.941819	2.936219	-0.648286
38	6	2.094991	2.042738	0.884384
39	6	3.083269	2.957684	1.494921
40	1	3.875301	2.304515	1.894999
41	1	3.553891	3.622013	0.766914
42	1	2.677258	3.522409	2.337796
43	6	2.018746	1.672866	-0.492898
44	6	1.287242	0.325020	-0.555890

45	1	-0.468982	-0.597468	2.311099
46	1	0.663377	-1.516072	1.334078
47	1	-1.141299	3.268302	-0.944482
48	1	1.377598	3.533045	-1.453654
49	1	0.918984	3.615439	0.217333
50	1	0.865450	0.122644	-1.539762
51	1	2.882564	1.842298	-1.132806
52	1	0.493909	1.871911	2.349463
53	1	2.014998	-0.462797	-0.332957
54	6	4.355009	-2.017164	-1.683427
55	6	5.131997	-0.884085	-1.417135
56	6	5.428805	-0.533405	-0.094701
57	6	4.942156	-1.313231	0.961147
58	6	4.163479	-2.444950	0.693549
59	6	3.871928	-2.799358	-0.628277
60	1	4.143192	-2.300030	-2.710492
61	1	5.532456	-0.296694	-2.238832
62	1	6.067105	0.322486	0.109155
63	1	5.199167	-1.063030	1.987209
64	1	3.804775	-3.062501	1.512205
65	1	3.285938	-3.689810	-0.836347

Beyeranyl cation in the complex

(d)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1246.3451465 hartrees (-782094.042880215 kcal/mol)
Imaginary Frequencies: 1 (-8.2328 1/cm)
Zero-point correction = 0.693656 (Hartree/Particle)
Counterpoise: BSSE energy = 0.001520014992 hartrees

Coordinates (from last standard orientation):

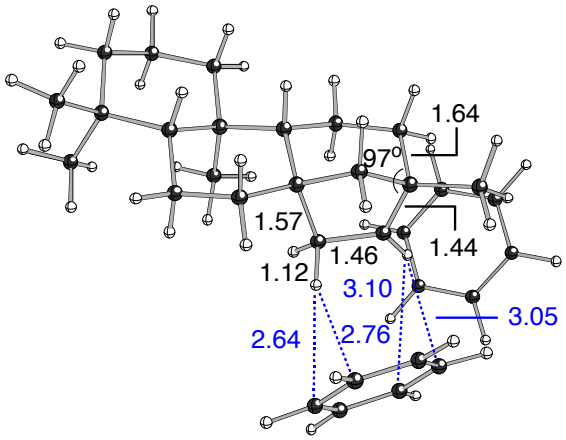
Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	6	-5.296152	0.515776	0.219105
2	6	-3.733962	0.485877	0.028860
3	6	-3.038034	-0.914585	-0.099044
4	6	-3.825856	-1.781449	-1.119499
5	6	-5.330349	-1.849125	-0.828404
6	6	-5.944876	-0.447313	-0.807118
7	1	-3.592623	0.954127	-0.960279
8	1	-3.691156	-1.356513	-2.125362
9	1	-3.410421	-2.796282	-1.150506
10	1	-5.818984	-2.454021	-1.600954
11	1	-5.515635	-2.369154	0.119224
12	1	-5.841720	-0.009396	-1.810885
13	1	-7.022288	-0.506095	-0.609432
14	6	-1.592958	-0.664863	-0.701292
15	6	-2.951676	1.355538	1.027923
16	1	-3.465179	2.305267	1.202718
17	1	-2.881704	0.866806	2.005106
18	6	-1.563333	1.668089	0.468759
19	6	-0.729663	0.458377	-0.016140
20	6	-5.784992	0.182652	1.648098
21	1	-5.250508	0.761304	2.408463
22	1	-6.846768	0.437155	1.737386
23	1	-5.693797	-0.874572	1.906236
24	6	-5.801396	1.941614	-0.109403
25	1	-5.441564	2.281457	-1.087796
26	1	-6.896178	1.950840	-0.140099
27	1	-5.496583	2.678589	0.640539
28	6	-2.986782	-1.670441	1.252170
29	1	-3.979776	-1.755306	1.688669
30	1	-2.622032	-2.694281	1.127644
31	1	-2.359629	-1.181241	2.001143
32	6	0.334107	1.015954	-1.025339
33	1	0.680988	2.011581	-0.689776
34	1	-1.779511	-0.317910	-1.727749
35	6	-0.775178	-1.984924	-0.785785
36	1	-0.915243	-2.569083	0.125485
37	6	0.727675	-1.797482	-0.975157
38	6	1.545299	0.168985	-0.900092
39	6	2.776915	0.339477	-1.690854
40	1	3.288422	1.206217	-1.235373
41	1	3.451786	-0.515887	-1.614784
42	1	2.578984	0.607188	-2.732068

43	6	1.340185	-0.763837	0.166350
44	6	0.209594	-0.195454	1.038752
45	1	-1.710117	2.332887	-0.393761
46	1	-0.965517	2.239178	1.191568
47	1	-1.140264	-2.605902	-1.609368
48	1	1.324800	-2.701451	-0.829380
49	1	0.939942	-1.489378	-2.010053
50	1	-0.267469	-0.957308	1.654896
51	1	2.206211	-1.223468	0.640281
52	1	-0.012138	1.153622	-2.055951
53	1	0.637200	0.555909	1.712889
54	6	4.250784	-2.921731	1.797680
55	6	3.546053	-3.951736	1.162854
56	6	3.771773	-4.223433	-0.191417
57	6	4.702096	-3.465138	-0.912037
58	6	5.407025	-2.436271	-0.276900
59	6	5.181820	-2.164756	1.077836
60	1	4.094403	-2.728278	2.855177
61	1	2.844378	-4.557936	1.729097
62	1	3.247309	-5.042454	-0.676023
63	1	4.897393	-3.694206	-1.955937
64	1	6.151456	-1.867868	-0.827703
65	1	5.747671	-1.382879	1.576326
66	6	4.369324	3.213545	0.885773
67	6	4.641236	3.505885	-0.455991
68	6	3.694742	4.189506	-1.228733
69	6	2.478895	4.584438	-0.658347
70	6	2.209388	4.294722	0.684114
71	6	3.153460	3.607146	1.455563
72	1	5.113119	2.704244	1.491931
73	1	5.597222	3.226690	-0.890232
74	1	3.914106	4.435594	-2.263826
75	1	1.757394	5.140364	-1.250518
76	1	1.279258	4.628727	1.135625
77	1	2.953778	3.402847	2.503710

Kauranyl cation in the complex

(e)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1246.339557 hartrees (-782090.53541307 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.693741 (Hartree/Particle)
Counterpoise: BSSE energy = 0.001971380641 hartrees

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	4.945783	0.211433	-0.471663
2	6	3.510635	0.346268	0.151072
3	6	2.529177	-0.870744	-0.018545
4	6	3.268779	-2.171588	0.401118
5	6	4.628177	-2.353338	-0.287511
6	6	5.544229	-1.151980	-0.039062
7	1	3.708034	0.379484	1.235610
8	1	3.433386	-2.149379	1.488505
9	1	2.638120	-3.045628	0.197306
10	1	5.103352	-3.263812	0.095510
11	1	4.495392	-2.519089	-1.363306
12	1	5.770157	-1.105003	1.036263
13	1	6.506012	-1.297929	-0.546223
14	6	1.347080	-0.634765	1.003869
15	6	2.791668	1.666301	-0.182628
16	1	3.484772	2.508656	-0.107992
17	1	2.429720	1.669655	-1.217164
18	6	1.638336	1.915206	0.793750
19	6	0.634791	0.755749	0.926213
20	6	4.996557	0.363841	-2.008907
21	1	4.514081	1.289531	-2.340308

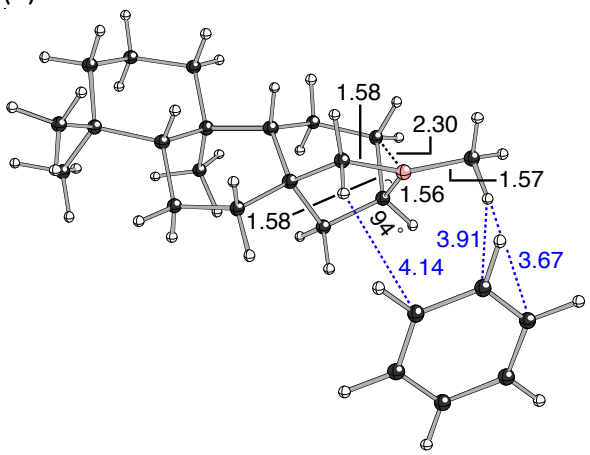
22	1	6.040910	0.411048	-2.335923
23	1	4.531915	-0.465067	-2.546078
24	6	5.855066	1.313184	0.124580
25	1	5.805793	1.327350	1.219745
26	1	6.897390	1.127219	-0.156091
27	1	5.599797	2.312885	-0.240635
28	6	2.023066	-1.047453	-1.471249
29	1	2.811848	-1.429616	-2.118053
30	1	1.210313	-1.777949	-1.526871
31	1	1.673667	-0.118056	-1.927666
32	6	-0.244709	0.945493	2.190770
33	1	-0.557759	1.992605	2.287919
34	1	1.829621	-0.642012	1.992592
35	6	0.291296	-1.768181	1.018515
36	1	-0.065243	-1.971670	0.003390
37	6	-0.918123	-1.480560	1.917895
38	6	-1.475624	0.062792	1.914231
39	6	-2.683082	0.164952	2.839889
40	1	-3.048540	1.195138	2.868880
41	1	-3.499664	-0.484924	2.511995
42	1	-2.401810	-0.123659	3.856511
43	6	-1.659596	0.165357	0.487842
44	6	-0.491999	0.733648	-0.170687
45	1	2.071630	2.083922	1.789063
46	1	1.097629	2.835715	0.538381
47	1	0.744506	-2.700441	1.366627
48	1	-1.747843	-2.158092	1.705084
49	1	-0.654144	-1.576897	2.977981
50	1	-0.276848	0.304453	-1.151597
51	1	-2.520881	-0.244455	-0.040612
52	1	0.270501	0.663513	3.113402
53	1	-0.803500	1.785414	-0.374511
54	6	-2.623972	3.054162	-2.062777
55	6	-3.607070	2.315901	-1.399790
56	6	-3.826695	2.512460	-0.028462
57	6	-3.071334	3.461909	0.674459
58	6	-2.086483	4.198970	0.011348
59	6	-1.858773	3.991139	-1.355765
60	1	-2.462400	2.914511	-3.127449
61	1	-4.215473	1.603954	-1.949183
62	1	-4.616829	1.964572	0.477406
63	1	-3.269651	3.644488	1.726668
64	1	-1.511488	4.947083	0.548926
65	1	-1.105347	4.576985	-1.874038

66	6	-4.816940	-1.687642	-1.288740
67	6	-3.728143	-2.039692	-2.095109
68	6	-2.876889	-3.080092	-1.705277
69	6	-3.115264	-3.768314	-0.510150
70	6	-4.202716	-3.414686	0.296856
71	6	-5.053281	-2.373735	-0.091846
72	1	-5.498549	-0.903446	-1.606438
73	1	-3.560828	-1.526836	-3.038215
74	1	-2.049102	-3.372737	-2.345060
75	1	-2.471123	-4.594333	-0.222025
76	1	-4.402141	-3.965729	1.211596
77	1	-5.913069	-2.117409	0.520647

Beyeranyl cation in the complex

Figure 3

(a)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1001.0881661 hartrees (-628192.835109411 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.588184 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000519842077 hartrees

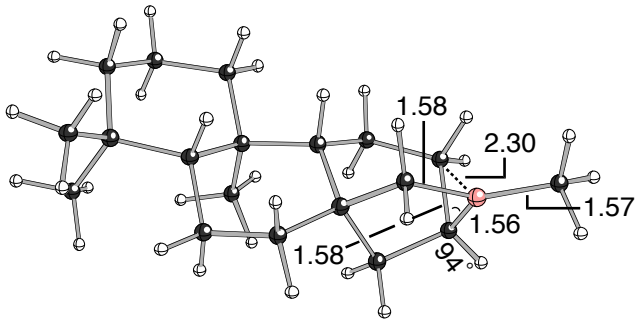
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	4.054627	-1.772258	-0.219598

2	6	2.704459	-0.962811	-0.166523
3	6	2.772121	0.572300	0.139831
4	6	3.885034	1.208662	-0.736731
5	6	5.234913	0.489719	-0.627670
6	6	5.098067	-0.977145	-1.044530
7	1	2.336624	-1.016941	-1.205005
8	1	3.566111	1.178787	-1.789303
9	1	4.005216	2.267169	-0.478150
10	1	5.969107	0.988804	-1.272758
11	1	5.629917	0.567036	0.393374
12	1	4.801310	-1.005912	-2.103500
13	1	6.068111	-1.489109	-0.983902
14	6	1.385133	1.217477	-0.290526
15	6	1.610286	-1.597672	0.707059
16	1	1.614484	-2.689041	0.611602
17	1	1.788530	-1.386407	1.767271
18	6	0.243858	-1.080379	0.255618
19	6	0.063955	0.456012	0.137705
20	6	4.647541	-2.143979	1.160045
21	1	3.897163	-2.598048	1.815318
22	1	5.452037	-2.877243	1.026420
23	1	5.080377	-1.291772	1.688728
24	6	3.795979	-3.101771	-0.969249
25	1	3.327476	-2.923739	-1.944339
26	1	4.742875	-3.626015	-1.145228
27	1	3.149644	-3.780455	-0.403087
28	6	3.102614	0.850987	1.630455
29	1	3.929246	0.235563	1.982792
30	1	3.403382	1.892070	1.779946
31	1	2.257132	0.657432	2.294110
32	6	-1.079019	0.710813	-0.913021
33	1	-1.815991	-0.108188	-0.825631
34	1	1.399913	1.188147	-1.389865
35	6	1.318254	2.712185	0.138436
36	1	1.686392	2.812700	1.162619
37	6	-0.082084	3.335347	0.110171
38	6	-3.094059	2.679546	-1.176762
39	1	-3.994275	2.148024	-0.828559
40	1	-3.237237	3.733028	-0.909598
41	1	-3.087627	2.587164	-2.269180
42	6	-1.158098	2.446922	0.859909
43	6	-0.518571	1.148492	1.405656
44	1	0.062571	-1.512333	-0.738444
45	1	-0.554421	-1.473098	0.900326

46	1	1.991987	3.309724	-0.485707
47	1	-0.058537	4.335598	0.556077
48	1	-0.371996	3.509741	-0.942444
49	1	0.226471	1.317019	2.191063
50	1	-1.692023	3.035229	1.611282
51	1	-0.726502	0.666402	-1.951906
52	1	-1.302629	0.518184	1.847043
53	5	-1.865932	2.005062	-0.462498
54	6	-6.099013	-1.103239	-1.378325
55	6	-6.761517	-0.243762	-0.496223
56	6	-6.712600	-0.481982	0.881005
57	6	-6.001900	-1.579929	1.375990
58	6	-5.339992	-2.439670	0.493723
59	6	-5.388161	-2.201051	-0.883324
60	1	-6.136637	-0.918010	-2.448144
61	1	-7.314962	0.608380	-0.880853
62	1	-7.227439	0.185616	1.566287
63	1	-5.964436	-1.765378	2.445814
64	1	-4.788785	-3.293399	0.877994
65	1	-4.873883	-2.868938	-1.568705

Boro-kauraryl cation



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -768.8192074 hartrees (-482441.740835574 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.487198 (Hartree/Particle)

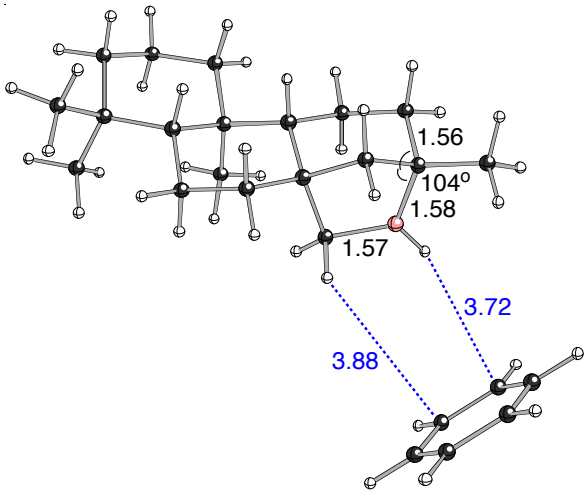
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.154831	-0.574232	-0.203789
2	6	1.580621	-0.595614	-0.156376

3	6	0.830462	0.752147	0.118742
4	6	1.442267	1.858053	-0.784120
5	6	2.968872	1.958065	-0.681051
6	6	3.623488	0.627601	-1.062500
7	1	1.301643	-0.856514	-1.191139
8	1	1.184605	1.641795	-1.831491
9	1	0.989610	2.827881	-0.546421
10	1	3.329352	2.750456	-1.349215
11	1	3.266784	2.260128	0.331149
12	1	3.384149	0.417664	-2.115745
13	1	4.717827	0.704273	-1.005781
14	6	-0.688810	0.563077	-0.307247
15	6	0.978436	-1.693916	0.735452
16	1	1.555945	-2.621853	0.663285
17	1	1.007661	-1.398806	1.789955
18	6	-0.452720	-1.980801	0.279061
19	6	-1.412630	-0.769957	0.145802
20	6	3.852020	-0.537805	1.176811
21	1	3.441033	-1.288190	1.859778
22	1	4.919188	-0.758065	1.053243
23	1	3.785745	0.434540	1.670101
24	6	3.639370	-1.861010	-0.914789
25	1	3.145794	-1.992123	-1.884922
26	1	4.719402	-1.806973	-1.095877
27	1	3.455577	-2.760359	-0.318235
28	6	0.967070	1.196294	1.599852
29	1	1.995697	1.121215	1.949864
30	1	0.669930	2.241207	1.728130
31	1	0.356461	0.596535	2.278441
32	6	-2.524520	-1.168157	-0.893214
33	1	-2.715588	-2.252640	-0.795822
34	1	-0.660046	0.524763	-1.405952
35	6	-1.530925	1.807850	0.097110
36	1	-1.263017	2.111682	1.111954
37	6	-3.049845	1.600872	0.084454
38	6	-5.279875	-0.567046	-1.140707
39	1	-5.791698	-1.449001	-0.722658
40	1	-5.931594	0.287771	-0.924867
41	1	-5.240190	-0.717903	-2.225651
42	6	-3.493793	0.294953	0.863410
43	6	-2.264487	-0.465582	1.414175
44	1	-0.374453	-2.453730	-0.709805
45	1	-0.927105	-2.727943	0.930442
46	1	-1.277016	2.655622	-0.548908

47	1	-3.553082	2.472811	0.516007
48	1	-3.395971	1.575880	-0.965567
49	1	-1.713490	0.081622	2.187276
50	1	-4.251022	0.530950	1.616055
51	1	-2.209938	-1.029287	-1.935911
52	1	-2.597677	-1.406310	1.873894
53	5	-3.872700	-0.477172	-0.442414

(b)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -1001.085153 hartrees (-628190.94435903 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.587686 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000446883545 hartrees

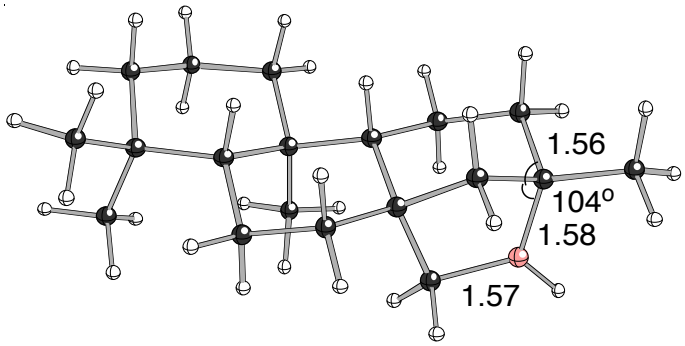
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	4.294735	-1.411743	-0.271660
2	6	2.896236	-0.731878	-0.491614
3	6	2.516916	0.465441	0.455643
4	6	3.699126	1.475049	0.462299
5	6	5.059762	0.833307	0.766661
6	6	5.376084	-0.302796	-0.209574
7	1	2.999322	-0.259216	-1.482925
8	1	3.756283	1.957679	-0.524742
9	1	3.506145	2.273916	1.188007

10	1	5.842872	1.599522	0.703988
11	1	5.087958	0.464723	1.799566
12	1	5.484190	0.126624	-1.216770
13	1	6.345273	-0.758026	0.035336
14	6	1.263802	1.175401	-0.199501
15	6	1.715628	-1.712834	-0.623000
16	1	1.997469	-2.570957	-1.241715
17	1	1.436850	-2.124610	0.354431
18	6	0.511921	-1.018994	-1.268739
19	6	0.041387	0.251714	-0.539405
20	6	4.374793	-2.322089	0.974122
21	1	3.576494	-3.071905	0.970909
22	1	5.329597	-2.861666	0.976273
23	1	4.310270	-1.773894	1.915424
24	6	4.628370	-2.294178	-1.499128
25	1	4.501419	-1.739517	-2.436490
26	1	5.671930	-2.627003	-1.448440
27	1	4.005518	-3.192626	-1.550892
28	6	2.247479	0.034358	1.918741
29	1	3.176321	-0.171809	2.452927
30	1	1.742974	0.830036	2.473906
31	1	1.630137	-0.862335	1.995843
32	6	-0.924874	1.067969	-1.439070
33	1	-1.697500	0.397818	-1.844387
34	1	1.634403	1.515331	-1.180321
35	6	0.789757	2.450063	0.539141
36	1	0.529454	2.208948	1.578530
37	6	-0.424909	3.124455	-0.133976
38	6	-1.562696	2.120330	-0.499223
39	6	-2.765207	2.857356	-1.095573
40	1	-3.561710	2.158998	-1.378703
41	1	-3.189697	3.571800	-0.379972
42	1	-2.482854	3.418571	-1.997467
43	6	-0.874500	-0.013652	0.702185
44	1	0.791407	-0.745552	-2.297499
45	1	-0.332867	-1.715698	-1.355786
46	1	1.605830	3.177251	0.600387
47	1	-0.810915	3.916036	0.521267
48	1	-0.105042	3.616362	-1.065918
49	1	-0.380578	-0.367184	1.610033
50	1	-2.455855	1.577430	1.752333
51	1	-0.409446	1.521680	-2.298143
52	1	-1.590357	-0.812814	0.428111
53	6	-5.262302	-1.306508	1.567656

54	6	-5.722697	-0.073764	1.094149
55	6	-6.324668	0.010654	-0.165380
56	6	-6.465558	-1.137420	-0.951384
57	6	-6.005292	-2.370035	-0.477796
58	6	-5.403772	-2.454663	0.781951
59	1	-4.794861	-1.371464	2.546173
60	1	-5.611140	0.817900	1.704320
61	1	-6.683539	0.968064	-0.532624
62	1	-6.933689	-1.071876	-1.929612
63	1	-6.115823	-3.262018	-1.088112
64	1	-5.047409	-3.412545	1.150585
65	5	-1.767196	1.272155	0.821404

Boro-beyerayl cation



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
HF = -768.8161647 hartrees (-482439.831510897 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.486557 (Hartree/Particle)

Coordinates (from last standard orientation):

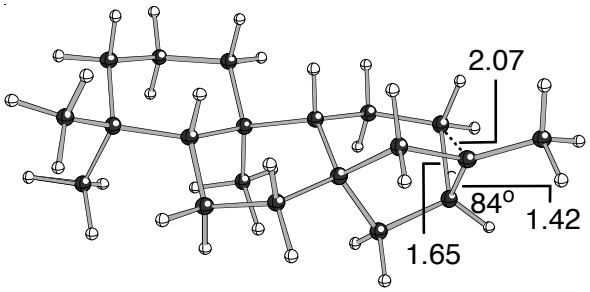
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.162492	-0.443641	-0.215198
2	6	1.597948	-0.535832	-0.311012
3	6	0.767057	0.685698	0.231777
4	6	1.347636	1.986111	-0.391710
5	6	2.866970	2.128608	-0.225959
6	6	3.611071	0.920293	-0.800090
7	1	1.410748	-0.518646	-1.398128
8	1	1.112449	1.997523	-1.466485

9	1	0.854207	2.863071	0.043561
10	1	3.201325	3.041515	-0.734936
11	1	3.126058	2.267322	0.831026
12	1	3.447017	0.897695	-1.887770
13	1	4.693918	1.034965	-0.655502
14	6	-0.708417	0.496066	-0.304309
15	6	0.997719	-1.864076	0.188783
16	1	1.605403	-2.709950	-0.148553
17	1	1.000674	-1.908334	1.284615
18	6	-0.427987	-2.041749	-0.344924
19	6	-1.385176	-0.887151	-0.002949
20	6	3.729397	-0.637098	1.209330
21	1	3.362540	-1.564289	1.662360
22	1	4.822948	-0.706728	1.164789
23	1	3.484716	0.182415	1.887296
24	6	3.792583	-1.541866	-1.105427
25	1	3.366218	-1.532418	-2.115552
26	1	4.871923	-1.373272	-1.199102
27	1	3.657911	-2.545577	-0.690408
28	6	0.819346	0.829189	1.773722
29	1	1.767416	1.257741	2.102376
30	1	0.036415	1.503687	2.131397
31	1	0.700983	-0.120627	2.298251
32	6	-2.672890	-0.975578	-0.867357
33	1	-3.071942	-2.000123	-0.820321
34	1	-0.596797	0.515133	-1.400407
35	6	-1.670143	1.654936	0.046883
36	1	-1.726872	1.779804	1.136234
37	6	-3.097372	1.447461	-0.503008
38	6	-3.665605	0.020881	-0.220067
39	6	-5.105823	-0.099037	-0.726689
40	1	-5.506682	-1.106481	-0.561412
41	1	-5.769251	0.608372	-0.215253
42	1	-5.169359	0.105162	-1.804762
43	6	-1.997912	-0.953840	1.435953
44	1	-0.369921	-2.132086	-1.440214
45	1	-0.859065	-2.985228	0.016903
46	1	-1.279499	2.601927	-0.339029
47	1	-3.763379	2.212893	-0.084327
48	1	-3.098124	1.593320	-1.594411
49	1	-1.345514	-0.659607	2.261128
50	1	-4.086409	0.115904	2.225911
51	1	-2.479278	-0.755499	-1.927396
52	1	-2.267164	-2.008641	1.640948

53	5	-3.379798	-0.217441	1.318138

Figure S1

CAM-B3LYP

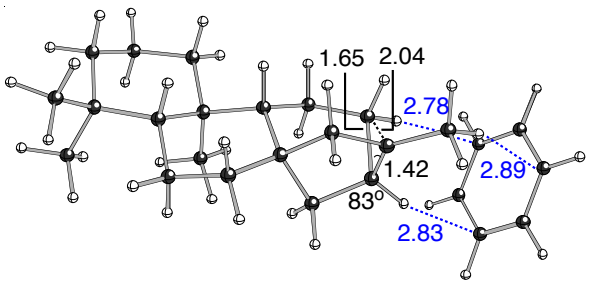


CAM-B3LYP/6-31+G(d,p)//CAM-B3LYP/6-31+G(d,p):
HF = -781.3214671 hartrees (-490287.033819921 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.497049 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.156005	-0.541910	-0.205983
2	6	1.592489	-0.584399	-0.201391
3	6	0.830761	0.731462	0.146263
4	6	1.433875	1.897352	-0.669605
5	6	2.952032	2.000400	-0.540455
6	6	3.619559	0.704064	-0.986798
7	1	1.341969	-0.776402	-1.257561
8	1	1.191036	1.751396	-1.731493
9	1	0.973162	2.845091	-0.369081
10	1	3.310359	2.831283	-1.156258
11	1	3.234081	2.247882	0.488605
12	1	3.400794	0.550842	-2.052621
13	1	4.709098	0.788239	-0.907504
14	6	-0.657256	0.544087	-0.329353
15	6	0.991888	-1.745508	0.597125
16	1	1.560934	-2.663588	0.435118
17	1	1.036862	-1.549166	1.672061
18	6	-0.440989	-1.997721	0.144184

19	6	-1.372611	-0.771872	0.119767
20	6	3.811221	-0.566620	1.186981
21	1	3.396328	-1.354160	1.822373
22	1	4.880501	-0.771229	1.078507
23	1	3.728059	0.378367	1.725434
24	6	3.672864	-1.776738	-0.967476
25	1	3.194358	-1.875035	-1.947669
26	1	4.750059	-1.685652	-1.135319
27	1	3.514043	-2.706845	-0.415038
28	6	0.924821	1.082837	1.644715
29	1	1.960146	1.110329	1.973761
30	1	0.516256	2.074743	1.852567
31	1	0.416152	0.367710	2.292715
32	6	-2.537239	-1.109405	-0.861736
33	1	-2.802311	-2.176605	-0.762135
34	1	-0.593046	0.494665	-1.424820
35	6	-1.527935	1.767562	0.039664
36	1	-1.300027	2.100143	1.052761
37	6	-3.026155	1.510223	-0.026341
38	6	-3.740760	-0.400404	-0.368542
39	6	-5.064880	-0.428286	-1.019300
40	1	-5.507755	-1.395851	-0.740871
41	1	-5.733748	0.350310	-0.649491
42	1	-5.001874	-0.406690	-2.108857
43	6	-3.427990	0.198487	0.884083
44	6	-2.174285	-0.495897	1.416429
45	1	-0.386311	-2.388755	-0.879933
46	1	-0.911848	-2.786348	0.743897
47	1	-1.303514	2.609383	-0.619512
48	1	-3.646911	2.309546	0.382513
49	1	-3.337611	1.441937	-1.080490
50	1	-1.644955	0.104971	2.153744
51	1	-4.235172	0.450436	1.568050
52	1	-2.325371	-0.949292	-1.923304
53	1	-2.476247	-1.427941	1.906476

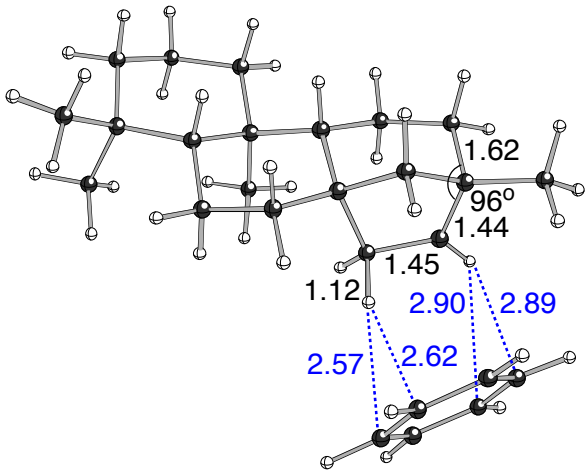


CAM-B3LYP/6-31+G(d,p)//CAM-B3LYP/6-31+G(d,p):
HF = -1013.4544597 hartrees (-635952.808006347 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.599674 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000773195875 hartrees

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-4.705934	-0.080596	0.125883
2	6	-3.220962	0.395155	0.007866
3	6	-2.113793	-0.697949	-0.093075
4	6	-2.531722	-1.744104	-1.151082
5	6	-3.938417	-2.297087	-0.930687
6	6	-4.966922	-1.170818	-0.932216
7	1	-3.195687	0.903203	-0.970075
8	1	-2.501430	-1.275599	-2.144796
9	1	-1.810289	-2.568635	-1.170432
10	1	-4.173160	-3.012014	-1.725571
11	1	-3.986116	-2.864636	0.005075
12	1	-4.965424	-0.701663	-1.925750
13	1	-5.975319	-1.573929	-0.786335
14	6	-0.810943	0.010573	-0.618916
15	6	-2.807625	1.445186	1.044118
16	1	-3.603896	2.177813	1.193909
17	1	-2.633457	0.986812	2.021944
18	6	-1.570459	2.191156	0.559705
19	6	-0.380562	1.319121	0.119874
20	6	-5.117619	-0.587431	1.520290
21	1	-4.815233	0.102635	2.313167
22	1	-6.207512	-0.671980	1.565929
23	1	-4.717675	-1.573103	1.761512
24	6	-5.625002	1.109368	-0.208456
25	1	-5.345447	1.579319	-1.157290

26	1	-6.659150	0.765166	-0.303589
27	1	-5.615194	1.877786	0.569278
28	6	-1.884151	-1.423807	1.247427
29	1	-2.815069	-1.829181	1.634313
30	1	-1.208173	-2.274657	1.132837
31	1	-1.481418	-0.778057	2.028849
32	6	0.502321	2.194795	-0.820907
33	1	0.512551	3.234728	-0.452861
34	1	-1.056178	0.311202	-1.646705
35	6	0.384075	-0.968814	-0.685557
36	1	0.410639	-1.593241	0.208047
37	6	1.740537	-0.290122	-0.802244
38	6	1.903597	1.736451	-0.646809
39	6	3.068962	2.280485	-1.373789
40	1	3.303754	3.235317	-0.882335
41	1	3.949842	1.642630	-1.280559
42	1	2.847808	2.501618	-2.419727
43	6	1.943393	0.803238	0.421329
44	6	0.651093	0.962637	1.218920
45	1	-1.878372	2.788133	-0.308437
46	1	-1.222795	2.909561	1.312340
47	1	0.275256	-1.647717	-1.534624
48	1	2.607670	-0.942882	-0.684323
49	1	1.853427	0.123503	-1.816447
50	1	0.403451	0.074216	1.797259
51	1	2.883559	0.604565	0.930232
52	1	0.172978	2.243812	-1.863175
53	1	0.782790	1.789129	1.925943
54	6	5.298029	-0.662224	1.701970
55	6	4.865141	-1.848616	1.110542
56	6	5.105920	-2.081551	-0.242886
57	6	5.777546	-1.127499	-1.005757
58	6	6.209564	0.058693	-0.414506
59	6	5.970726	0.291069	0.939420
60	1	5.137375	-0.494531	2.762577
61	1	4.366120	-2.603214	1.710766
62	1	4.795926	-3.018296	-0.695983
63	1	5.988012	-1.320398	-2.053107
64	1	6.761696	0.787038	-1.000903
65	1	6.333380	1.201691	1.406298



CAM-B3LYP/6-31+G(d,p)//CAM-B3LYP/6-31+G(d,p):
HF = -1013.4486489 hartrees (-635949.161671239 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.599260 (Hartree/Particle)
Counterpoise: BSSE energy = 0.001031837406 hartrees

Coordinates (from last standard orientation):

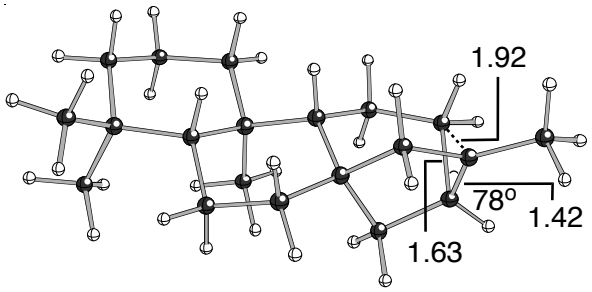
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.997250	-1.087167	-0.309531
2	6	2.572178	-0.490174	-0.536545
3	6	2.064417	0.570836	0.494168
4	6	3.159841	1.644317	0.687412
5	6	4.534656	1.059362	1.008908
6	6	4.981336	0.074895	-0.065942
7	1	2.681705	0.077906	-1.474257
8	1	3.243732	2.234613	-0.235737
9	1	2.866784	2.341201	1.480495
10	1	5.260652	1.875013	1.085367
11	1	4.528181	0.577338	1.992378
12	1	5.108112	0.624046	-1.009030
13	1	5.965718	-0.337245	0.182370
14	6	0.820216	1.267239	-0.163714
15	6	1.483694	-1.535872	-0.804900
16	1	1.853017	-2.303725	-1.487994
17	1	1.207786	-2.062137	0.114598
18	6	0.260236	-0.884157	-1.440386
19	6	-0.301874	0.317983	-0.675136
20	6	4.084615	-2.117658	0.829238

21	1	3.332204	-2.904533	0.721160
22	1	5.064126	-2.604561	0.803816
23	1	3.972252	-1.681859	1.822306
24	6	4.449693	-1.797856	-1.598581
25	1	4.325906	-1.155828	-2.477116
26	1	5.510513	-2.055840	-1.526690
27	1	3.907262	-2.730033	-1.778123
28	6	1.737936	-0.036578	1.872990
29	1	2.647796	-0.310428	2.402364
30	1	1.223247	0.680615	2.517415
31	1	1.130767	-0.941788	1.818808
32	6	-1.270798	1.117005	-1.573804
33	1	-1.923812	0.436055	-2.132279
34	1	1.215272	1.744926	-1.071109
35	6	0.205419	2.388920	0.696206
36	1	0.001875	2.022942	1.707276
37	6	-1.078234	2.979115	0.107896
38	6	-2.104465	1.928760	-0.577070
39	6	-3.332684	2.668989	-1.076399
40	1	-4.019618	1.976423	-1.567333
41	1	-3.865609	3.168764	-0.263086
42	1	-3.039167	3.427641	-1.805517
43	6	-2.211264	1.056334	0.561602
44	6	-1.272020	-0.043953	0.495143
45	1	0.549001	-0.526666	-2.436817
46	1	-0.538695	-1.617715	-1.602310
47	1	0.919068	3.206203	0.817867
48	1	-1.613903	3.586716	0.840815
49	1	-0.852818	3.618917	-0.752011
50	1	-0.863851	-0.352500	1.458212
51	1	-2.841460	1.269824	1.422263
52	1	-0.753106	1.752803	-2.296214
53	1	-1.925872	-0.886312	0.167358
54	6	-3.974213	-2.199854	1.565266
55	6	-4.652087	-0.984510	1.567674
56	6	-4.978437	-0.364502	0.358045
57	6	-4.639076	-0.971085	-0.852489
58	6	-3.960890	-2.187267	-0.854030
59	6	-3.624124	-2.798637	0.354461
60	1	-3.734146	-2.690978	2.502606
61	1	-4.952038	-0.531825	2.508016
62	1	-5.544866	0.562192	0.360302
63	1	-4.929007	-0.510858	-1.791947
64	1	-3.713051	-2.670785	-1.793453

65	1	-3.111870	-3.755430	0.352355

Beyeranyl cation in the complex
CAM-B3LYP/6-31+G(d,p)//CAM-B3LYP/6-31+G(d,p):
HF = -781.3111152 hartrees (-490280.537899152 kcal/mol)

LC-ωPBE

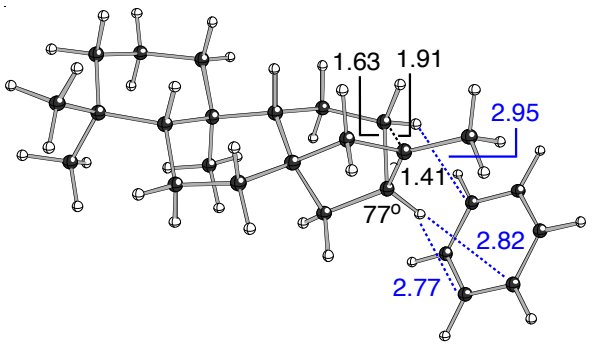


LC-ωPBE/6-31+G(d,p)//LC-ωPBE /6-31+G(d,p):
HF = -781.3247711 hartrees (-490289.107112961 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.501630 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.145259	-0.520321	-0.207098
2	6	1.590440	-0.576100	-0.216509
3	6	0.818988	0.718710	0.156069
4	6	1.411220	1.905450	-0.626422
5	6	2.923814	2.016572	-0.491318
6	6	3.598674	0.738061	-0.962555
7	1	1.349497	-0.742552	-1.280139
8	1	1.171836	1.784770	-1.692306
9	1	0.942628	2.841596	-0.301521
10	1	3.277406	2.862091	-1.088943
11	1	3.203785	2.245664	0.542340
12	1	3.380510	0.602271	-2.030751
13	1	4.687475	0.828489	-0.881755
14	6	-0.651557	0.523218	-0.339111
15	6	0.996969	-1.758976	0.545868
16	1	1.571452	-2.668273	0.355054

17	1	1.043646	-1.595842	1.626285
18	6	-0.431824	-2.005126	0.089796
19	6	-1.361512	-0.785176	0.103417
20	6	3.789626	-0.563969	1.184641
21	1	3.375229	-1.364456	1.803599
22	1	4.859987	-0.762639	1.078673
23	1	3.701173	0.371310	1.738712
24	6	3.678339	-1.732707	-0.984290
25	1	3.197146	-1.828413	-1.963063
26	1	4.752534	-1.619475	-1.156382
27	1	3.541254	-2.671876	-0.441927
28	6	0.903321	1.036902	1.655738
29	1	1.939140	1.149348	1.966182
30	1	0.416618	1.984389	1.900064
31	1	0.476298	0.262368	2.293793
32	6	-2.535324	-1.098355	-0.860054
33	1	-2.829029	-2.153801	-0.750347
34	1	-0.569215	0.467405	-1.434063
35	6	-1.537586	1.733654	0.005052
36	1	-1.320786	2.092731	1.012500
37	6	-3.024617	1.426698	-0.047699
38	6	-3.711418	-0.339651	-0.354878
39	6	-5.057345	-0.359909	-0.975731
40	1	-5.492996	-1.329985	-0.709418
41	1	-5.713860	0.413652	-0.575263
42	1	-5.018246	-0.305820	-2.064605
43	6	-3.387576	0.177195	0.925097
44	6	-2.129485	-0.519659	1.414706
45	1	-0.379861	-2.364469	-0.945988
46	1	-0.897010	-2.812894	0.667137
47	1	-1.336990	2.566111	-0.672805
48	1	-3.691648	2.226233	0.278846
49	1	-3.305276	1.296921	-1.111841
50	1	-1.580269	0.073867	2.144419
51	1	-4.176130	0.447195	1.622972
52	1	-2.320108	-0.940882	-1.920630
53	1	-2.426630	-1.454084	1.902855

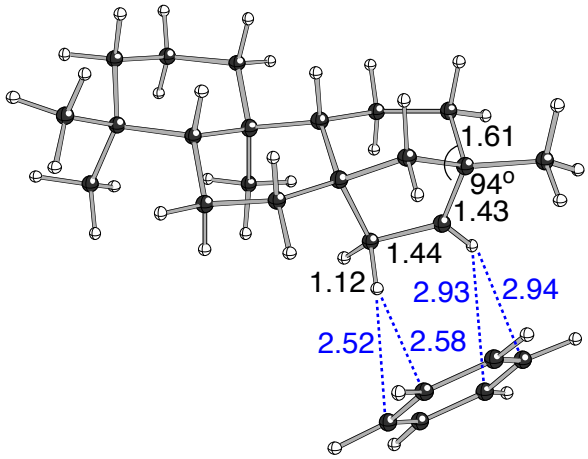


LC-ωPBE/6-31+G(d,p)//LC-ωPBE /6-31+G(d,p):
HF = -1013.4210794 hartrees (-635931.861534294 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.605102 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000665843963 hartrees

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-4.565489	-0.100427	0.381257
2	6	-3.100916	0.396377	0.211127
3	6	-2.052495	-0.615236	-0.323268
4	6	-2.623664	-1.322642	-1.566135
5	6	-4.004800	-1.920195	-1.332798
6	6	-4.986444	-0.844542	-0.894829
7	1	-3.182185	1.154298	-0.586513
8	1	-2.700491	-0.594737	-2.386015
9	1	-1.935185	-2.106057	-1.903342
10	1	-4.357131	-2.386126	-2.257959
11	1	-3.956096	-2.726598	-0.593267
12	1	-5.087684	-0.113459	-1.708605
13	1	-5.982803	-1.274481	-0.743969
14	6	-0.813419	0.218634	-0.788461
15	6	-2.534637	1.120652	1.430623
16	1	-3.286487	1.777370	1.874277
17	1	-2.253551	0.412048	2.215161
18	6	-1.349833	1.976354	1.015583
19	6	-0.252843	1.255720	0.223068
20	6	-4.817647	-0.978427	1.614321
21	1	-4.380946	-0.548536	2.519988
22	1	-5.895231	-1.057761	1.784460
23	1	-4.444733	-1.998229	1.510490

24	6	-5.479858	1.126408	0.513728
25	1	-5.294484	1.855744	-0.281467
26	1	-6.526760	0.818297	0.439596
27	1	-5.365505	1.632735	1.475793
28	6	-1.688739	-1.683034	0.718358
29	1	-2.577896	-2.207698	1.058509
30	1	-1.030719	-2.449225	0.300719
31	1	-1.212230	-1.278492	1.612032
32	6	0.553431	2.340459	-0.536493
33	1	0.678055	3.224897	0.106441
34	1	-1.178578	0.800716	-1.646817
35	6	0.331776	-0.681663	-1.283355
36	1	0.458198	-1.538047	-0.619082
37	6	1.671348	0.031129	-1.349347
38	6	1.933065	1.801846	-0.696383
39	6	3.044318	2.518928	-1.368121
40	1	3.356584	3.305988	-0.672566
41	1	3.905519	1.871164	-1.536500
42	1	2.732302	3.002440	-2.295088
43	6	2.058068	0.648717	0.112043
44	6	0.867657	0.595048	1.052432
45	1	-1.741408	2.780447	0.379391
46	1	-0.895477	2.470292	1.882630
47	1	0.108904	-1.083315	-2.274311
48	1	2.538596	-0.586232	-1.588985
49	1	1.634496	0.748629	-2.191063
50	1	0.644758	-0.417153	1.387088
51	1	3.036242	0.289897	0.424667
52	1	0.095691	2.688198	-1.466833
53	1	1.113063	1.189602	1.939132
54	6	4.977477	-1.057072	1.867653
55	6	4.513050	-2.079541	1.046581
56	6	4.768171	-2.044452	-0.320381
57	6	5.485504	-0.984903	-0.867341
58	6	5.947626	0.038835	-0.045965
59	6	5.694191	0.002307	1.321537
60	1	4.798790	-1.096965	2.938149
61	1	3.973755	-2.918385	1.476905
62	1	4.434155	-2.860418	-0.955496
63	1	5.714699	-0.974772	-1.929622
64	1	6.535491	0.850024	-0.466670
65	1	6.076899	0.788214	1.966117



LC-ωPBE/6-31+G(d,p)//LC-ωPBE /6-31+G(d,p):
HF = -1013.412429 hartrees (-635926.43332179 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.604203 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000846927285 hartrees

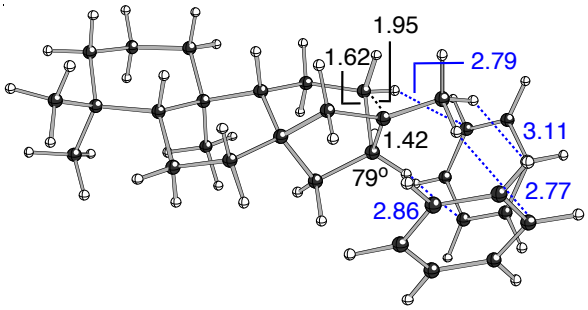
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.963420	-1.080397	-0.313086
2	6	2.544050	-0.487144	-0.532023
3	6	2.046648	0.574244	0.490913
4	6	3.138359	1.646157	0.669653
5	6	4.511874	1.064586	0.980557
6	6	4.945575	0.080350	-0.093533
7	1	2.645934	0.075262	-1.475250
8	1	3.214753	2.233272	-0.256151
9	1	2.851576	2.344641	1.463801
10	1	5.238157	1.880281	1.046997
11	1	4.517309	0.585875	1.965548
12	1	5.056119	0.624194	-1.041638
13	1	5.934515	-0.327978	0.142046
14	6	0.807369	1.265577	-0.163580
15	6	1.458406	-1.533228	-0.781560
16	1	1.824921	-2.307148	-1.459555
17	1	1.187623	-2.051438	0.143921
18	6	0.236689	-0.887890	-1.415259
19	6	-0.313648	0.319923	-0.659695
20	6	4.062128	-2.095705	0.831224

21	1	3.307667	-2.882342	0.739506
22	1	5.040027	-2.584657	0.797877
23	1	3.964300	-1.650404	1.821422
24	6	4.402400	-1.802589	-1.594928
25	1	4.257064	-1.176228	-2.481046
26	1	5.467146	-2.046156	-1.536058
27	1	3.870456	-2.744758	-1.750593
28	6	1.732698	-0.022509	1.871063
29	1	2.649460	-0.264982	2.404573
30	1	1.201725	0.688262	2.509173
31	1	1.150766	-0.944812	1.828833
32	6	-1.280317	1.106717	-1.561693
33	1	-1.937507	0.418104	-2.106427
34	1	1.199850	1.740222	-1.074810
35	6	0.195869	2.382003	0.694052
36	1	-0.000986	2.018463	1.707645
37	6	-1.088555	2.963623	0.106854
38	6	-2.107123	1.928915	-0.578785
39	6	-3.331591	2.665859	-1.077955
40	1	-4.021092	1.970776	-1.560273
41	1	-3.859619	3.173771	-0.267238
42	1	-3.038826	3.416719	-1.814754
43	6	-2.196469	1.085688	0.577311
44	6	-1.266606	-0.016214	0.516874
45	1	0.520804	-0.540143	-2.416298
46	1	-0.566140	-1.619463	-1.564875
47	1	0.905480	3.203710	0.809848
48	1	-1.620003	3.579619	0.836842
49	1	-0.857414	3.603363	-0.751737
50	1	-0.857830	-0.333754	1.476298
51	1	-2.826919	1.310384	1.436987
52	1	-0.763860	1.731238	-2.295377
53	1	-1.955744	-0.833649	0.194846
54	6	-3.909192	-2.198467	1.561856
55	6	-4.616471	-1.002566	1.552907
56	6	-4.950309	-0.399484	0.341114
57	6	-4.584508	-1.000385	-0.860630
58	6	-3.876409	-2.196878	-0.851056
59	6	-3.536108	-2.793728	0.359997
60	1	-3.664505	-2.678914	2.504374
61	1	-4.935722	-0.553891	2.489693
62	1	-5.540415	0.513380	0.334541
63	1	-4.879322	-0.553260	-1.805819
64	1	-3.608877	-2.678177	-1.787126

65	1	-2.999935	-3.738120	0.366710

Beyeranyl cation in the complex
LC-ωPBE/6-31+G(d,p)//LC-ωPBE /6-31+G(d,p):
HF = -781.3120969 hartrees (-490281.153925719 kcal/mol)



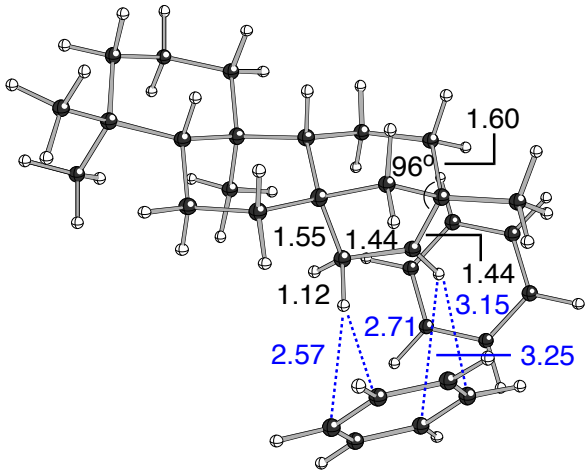
LC-ωPBE/6-31+G(d,p)//LC-ωPBE /6-31+G(d,p):
HF = -1245.5152771 hartrees (-781573.291533021 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.707774 (Hartree/Particle)
Counterpoise: BSSE energy = 0.001448561207 hartrees

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-5.263001	0.640280	0.286877
2	6	-3.727807	0.646544	0.034025
3	6	-3.015772	-0.722827	-0.128633
4	6	-3.813632	-1.591811	-1.118040
5	6	-5.292059	-1.694255	-0.768137
6	6	-5.926487	-0.313340	-0.718058
7	1	-3.636213	1.122004	-0.957217
8	1	-3.730186	-1.154871	-2.122995
9	1	-3.376738	-2.595421	-1.173307
10	1	-5.799325	-2.305697	-1.520537
11	1	-5.428334	-2.219714	0.183152
12	1	-5.863288	0.134938	-1.719119
13	1	-6.994063	-0.390636	-0.484053
14	6	-1.622589	-0.433647	-0.779153
15	6	-2.933139	1.520665	1.001749
16	1	-3.459482	2.457722	1.198239

17	1	-2.819305	1.030017	1.972732
18	6	-1.580831	1.857996	0.396846
19	6	-0.756235	0.666703	-0.106037
20	6	-5.686335	0.280669	1.717068
21	1	-5.110717	0.831916	2.465667
22	1	-6.737281	0.548770	1.858917
23	1	-5.604453	-0.783082	1.943900
24	6	-5.806180	2.048297	0.002210
25	1	-5.470630	2.421691	-0.970754
26	1	-6.899738	2.027672	-0.013195
27	1	-5.513022	2.773006	0.766370
28	6	-2.901976	-1.482406	1.201181
29	1	-3.882072	-1.624265	1.649915
30	1	-2.489271	-2.484521	1.060863
31	1	-2.294987	-0.968687	1.947551
32	6	0.272450	1.221797	-1.124051
33	1	0.656370	2.192034	-0.773842
34	1	-1.860858	-0.056905	-1.784321
35	6	-0.787716	-1.715959	-0.942183
36	1	-0.873418	-2.341112	-0.051856
37	6	0.692036	-1.453464	-1.159698
38	6	1.459803	0.331730	-1.056842
39	6	2.685076	0.503682	-1.861857
40	1	3.217641	1.343235	-1.394462
41	1	3.337967	-0.368403	-1.808992
42	1	2.474635	0.779888	-2.896031
43	6	1.298218	-0.546875	0.043883
44	6	0.186440	0.006058	0.920723
45	1	-1.768735	2.514195	-0.462738
46	1	-0.969509	2.441736	1.095476
47	1	-1.156608	-2.313329	-1.779038
48	1	1.336526	-2.334082	-1.163932
49	1	0.824915	-1.039023	-2.176657
50	1	-0.283636	-0.761740	1.533933
51	1	2.164323	-1.034622	0.485714
52	1	-0.112814	1.380407	-2.135274
53	1	0.625538	0.749741	1.594009
54	6	3.721279	-3.023537	1.829311
55	6	2.974629	-3.967411	1.131711
56	6	3.207532	-4.174957	-0.223673
57	6	4.182458	-3.433862	-0.883952
58	6	4.926726	-2.487967	-0.186683
59	6	4.697623	-2.284853	1.170167
60	1	3.556894	-2.879981	2.893308

61	1	2.228394	-4.561179	1.651662
62	1	2.646861	-4.935369	-0.760521
63	1	4.383129	-3.615774	-1.936202
64	1	5.708320	-1.929645	-0.694484
65	1	5.297640	-1.566030	1.720456
66	6	4.702252	2.318555	0.958189
67	6	5.209272	2.861556	-0.217253
68	6	4.469282	3.803066	-0.924721
69	6	3.223729	4.205176	-0.454443
70	6	2.718969	3.665431	0.724084
71	6	3.456810	2.719930	1.429089
72	1	5.289865	1.599507	1.521257
73	1	6.191060	2.564413	-0.574011
74	1	4.872942	4.239588	-1.833489
75	1	2.658194	4.959560	-0.993869
76	1	1.762328	4.006983	1.110921
77	1	3.076202	2.319280	2.364648



LC-ωPBE/6-31+G(d,p)//LC-ωPBE /6-31+G(d,p):
HF = -1245.5086936 hartrees (-781569.160320936 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.707445 (Hartree/Particle)
Counterpoise: BSSE energy = 0.00179749779 hartrees

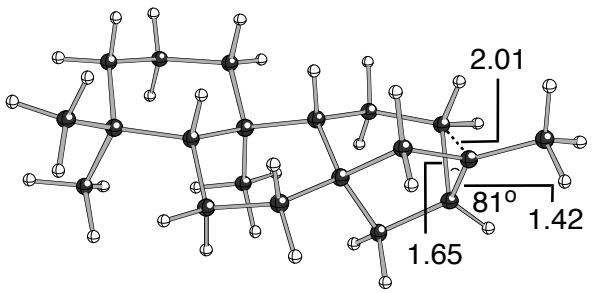
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	4.786064	0.377393	-0.520770

2	6	3.375022	0.459718	0.123085
3	6	2.478833	-0.808772	0.042883
4	6	3.295272	-2.027185	0.512919
5	6	4.642727	-2.160234	-0.185735
6	6	5.475286	-0.899570	-0.016396
7	1	3.591770	0.567980	1.199019
8	1	3.474525	-1.938582	1.593454
9	1	2.717074	-2.945980	0.363640
10	1	5.180385	-3.015655	0.234347
11	1	4.508365	-2.390498	-1.248056
12	1	5.703288	-0.771234	1.050560
13	1	6.439778	-1.009956	-0.524315
14	6	1.320640	-0.592417	1.069062
15	6	2.575631	1.701197	-0.270809
16	1	3.216578	2.585669	-0.258038
17	1	2.198616	1.621185	-1.295515
18	6	1.432841	1.930063	0.706108
19	6	0.521159	0.723561	0.919360
20	6	4.792449	0.425061	-2.052911
21	1	4.233194	1.285132	-2.432411
22	1	5.821839	0.530890	-2.407503
23	1	4.386217	-0.472123	-2.520117
24	6	5.626494	1.564898	-0.029968
25	1	5.579607	1.669549	1.058880
26	1	6.675376	1.413307	-0.300932
27	1	5.317312	2.512456	-0.478630
28	6	1.966360	-1.095216	-1.377050
29	1	2.753650	-1.522953	-1.995130
30	1	1.160250	-1.833078	-1.374310
31	1	1.611612	-0.206607	-1.902109
32	6	-0.347653	0.935539	2.170946
33	1	-0.736726	1.960473	2.193500
34	1	1.822923	-0.506896	2.043912
35	6	0.350644	-1.777099	1.168462
36	1	-0.008738	-2.060852	0.174294
37	6	-0.850812	-1.507475	2.070969
38	6	-1.500365	-0.047184	1.981157
39	6	-2.703922	0.036896	2.896652
40	1	-3.138868	1.037169	2.862305
41	1	-3.472490	-0.686839	2.614758
42	1	-2.403420	-0.166542	3.926708
43	6	-1.697533	-0.068557	0.558842
44	6	-0.594294	0.542347	-0.142010
45	1	1.868572	2.181271	1.681285

46	1	0.827174	2.795077	0.411810
47	1	0.865821	-2.656904	1.559748
48	1	-1.628015	-2.261610	1.930274
49	1	-0.550705	-1.529167	3.124195
50	1	-0.364948	0.103880	-1.113484
51	1	-2.545430	-0.552918	0.068210
52	1	0.198445	0.760108	3.101706
53	1	-1.038850	1.543142	-0.358585
54	6	-2.664275	2.874646	-2.006610
55	6	-3.660712	2.123350	-1.395726
56	6	-3.917762	2.280131	-0.036307
57	6	-3.183384	3.199335	0.708453
58	6	-2.185357	3.950276	0.097766
59	6	-1.922941	3.785030	-1.258839
60	1	-2.474521	2.764854	-3.070149
61	1	-4.252828	1.429512	-1.983924
62	1	-4.718801	1.715157	0.433224
63	1	-3.409902	3.354703	1.759558
64	1	-1.625186	4.681057	0.673798
65	1	-1.155311	4.384152	-1.739742
66	6	-4.533941	-1.697861	-1.493140
67	6	-3.384731	-1.948031	-2.236100
68	6	-2.446064	-2.865488	-1.775822
69	6	-2.658261	-3.533267	-0.573844
70	6	-3.805809	-3.279744	0.170766
71	6	-4.743423	-2.360522	-0.288084
72	1	-5.284046	-1.006881	-1.866679
73	1	-3.232653	-1.447508	-3.188057
74	1	-1.562697	-3.082364	-2.369919
75	1	-1.940426	-4.273003	-0.230224
76	1	-3.984441	-3.821067	1.095698
77	1	-5.652454	-2.182439	0.279075

ωB97XD

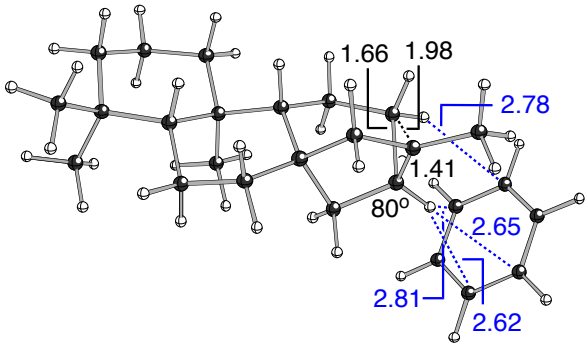


ωB97XD/6-31+G(d,p)//ωB97XD /6-31+G(d,p):
HF = -781.6042526 hartrees (-490464.484549026 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.497431 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.158459	-0.528862	-0.202774
2	6	1.597375	-0.584123	-0.222200
3	6	0.823739	0.718455	0.149495
4	6	1.425012	1.911541	-0.628780
5	6	2.942948	2.018928	-0.493030
6	6	3.619766	0.733657	-0.959485
7	1	1.361905	-0.749894	-1.287580
8	1	1.185879	1.795231	-1.696010
9	1	0.958550	2.847908	-0.299424
10	1	3.298409	2.862404	-1.093226
11	1	3.221396	2.248851	0.541635
12	1	3.407994	0.596394	-2.029664
13	1	4.708432	0.824709	-0.869693
14	6	-0.652663	0.528748	-0.356411
15	6	0.997461	-1.771328	0.538580
16	1	1.562970	-2.684743	0.337781
17	1	1.052927	-1.615305	1.620169
18	6	-0.440082	-2.007572	0.091261
19	6	-1.368180	-0.779504	0.100363
20	6	3.787606	-0.567821	1.201825
21	1	3.367658	-1.370542	1.815718
22	1	4.861811	-0.757293	1.110505
23	1	3.680222	0.369040	1.751442
24	6	3.698647	-1.748375	-0.974937
25	1	3.220890	-1.847845	-1.956248
26	1	4.774498	-1.634548	-1.141671
27	1	3.556969	-2.686116	-0.429251
28	6	0.899477	1.030756	1.657371
29	1	1.931293	1.178420	1.968543
30	1	0.377831	1.958030	1.909363
31	1	0.499835	0.236203	2.289744
32	6	-2.554930	-1.108306	-0.856477
33	1	-2.829360	-2.171702	-0.750242

34	1	-0.566416	0.461064	-1.450458
35	6	-1.530192	1.759607	-0.026251
36	1	-1.295759	2.141696	0.968535
37	6	-3.026875	1.481270	-0.057006
38	6	-3.739382	-0.375728	-0.337510
39	6	-5.083345	-0.399812	-0.957356
40	1	-5.514158	-1.374217	-0.688807
41	1	-5.744107	0.371849	-0.558740
42	1	-5.041255	-0.352294	-2.047228
43	6	-3.398348	0.196836	0.917586
44	6	-2.132094	-0.494125	1.417450
45	1	-0.394901	-2.371210	-0.944337
46	1	-0.908210	-2.810140	0.674998
47	1	-1.326856	2.572224	-0.727905
48	1	-3.663899	2.280497	0.325879
49	1	-3.345245	1.373131	-1.108304
50	1	-1.579337	0.113151	2.132775
51	1	-4.181483	0.474297	1.618269
52	1	-2.359114	-0.944191	-1.920614
53	1	-2.425752	-1.420510	1.923763



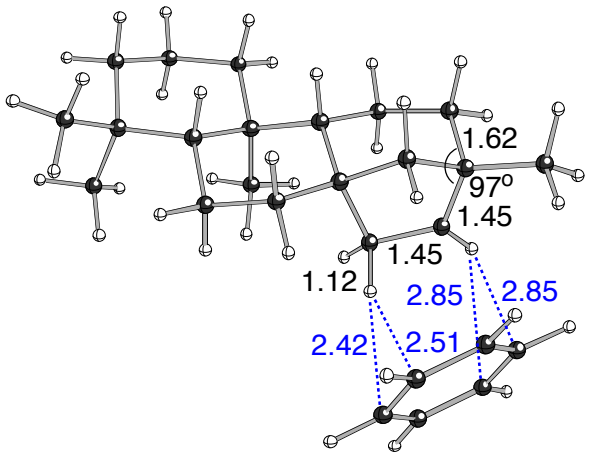
ωB97XD/6-31+G(d,p)//ωB97XD /6-31+G(d,p):
HF = -1013.8024822 hartrees (-636171.195605322 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.600855 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000795635142 hartrees

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	-4.500413	-0.111164	0.400368
2	6	-3.037219	0.409040	0.229269
3	6	-1.986143	-0.576097	-0.368410
4	6	-2.572779	-1.240567	-1.634997
5	6	-3.952499	-1.856735	-1.409632
6	6	-4.937739	-0.806785	-0.905151
7	1	-3.135848	1.201185	-0.532909
8	1	-2.661557	-0.480314	-2.424884
9	1	-1.883852	-2.007268	-2.009878
10	1	-4.316203	-2.282144	-2.350347
11	1	-3.888574	-2.694684	-0.705967
12	1	-5.058736	-0.040865	-1.684873
13	1	-5.927220	-1.254539	-0.756418
14	6	-0.755147	0.290805	-0.821245
15	6	-2.456636	1.084566	1.476157
16	1	-3.202085	1.727703	1.950677
17	1	-2.172889	0.344173	2.230385
18	6	-1.266394	1.953811	1.089869
19	6	-0.176591	1.272851	0.244029
20	6	-4.715224	-1.049953	1.601692
21	1	-4.281657	-0.641524	2.519887
22	1	-5.788612	-1.174218	1.776879
23	1	-4.304703	-2.049964	1.451130
24	6	-5.427811	1.102748	0.605001
25	1	-5.262590	1.868891	-0.161079
26	1	-6.473974	0.787618	0.536146
27	1	-5.297702	1.567411	1.587091
28	6	-1.593278	-1.684405	0.628566
29	1	-2.464947	-2.261431	0.928740
30	1	-0.896474	-2.401731	0.186351
31	1	-1.145502	-1.303150	1.547707
32	6	0.628911	2.410684	-0.456909
33	1	0.740302	3.262911	0.233799
34	1	-1.141196	0.921369	-1.635230
35	6	0.379038	-0.585247	-1.402908
36	1	0.505635	-1.492868	-0.810663
37	6	1.732548	0.107964	-1.449667
38	6	2.014747	1.896357	-0.637420
39	6	3.124260	2.641664	-1.277725
40	1	3.445397	3.388495	-0.539624
41	1	3.980292	1.997187	-1.486683
42	1	2.807522	3.179703	-2.173350
43	6	2.136237	0.672872	0.062381
44	6	0.956281	0.553259	1.017416

45	1	-1.660810	2.791681	0.499147
46	1	-0.799207	2.399857	1.976853
47	1	0.131756	-0.906616	-2.417777
48	1	2.588913	-0.526776	-1.683805
49	1	1.721288	0.858449	-2.257459
50	1	0.738883	-0.480998	1.280443
51	1	3.113538	0.291479	0.340464
52	1	0.174994	2.806602	-1.370603
53	1	1.215874	1.082508	1.941432
54	6	4.843726	-0.916054	1.898541
55	6	4.198381	-1.995315	1.293013
56	6	4.331765	-2.207926	-0.079553
57	6	5.107929	-1.338988	-0.848430
58	6	5.747120	-0.255181	-0.244055
59	6	5.616759	-0.045160	1.129905
60	1	4.754856	-0.762377	2.969258
61	1	3.609451	-2.681021	1.894067
62	1	3.852530	-3.064253	-0.544585
63	1	5.238558	-1.521822	-1.911124
64	1	6.373080	0.404770	-0.837467
65	1	6.132487	0.784303	1.603639



ωB97XD/6-31+G(d,p)//ωB97XD /6-31+G(d,p):
HF = -1013.8011896 hartrees (-636170.3844858960 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.600855 (Hartree/Particle)
Counterpoise: BSSE energy = 0.001071668783 hartrees

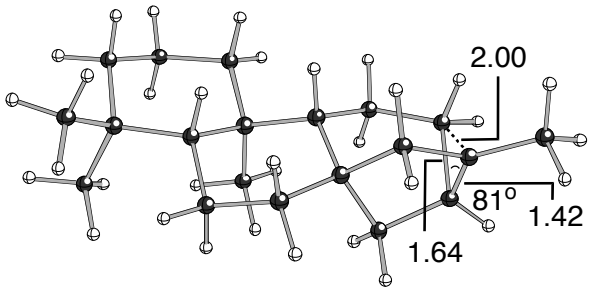
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.947868	-1.064673	-0.295492
2	6	2.517431	-0.488190	-0.528346
3	6	2.024791	0.618659	0.459677
4	6	3.113704	1.711096	0.573751
5	6	4.504024	1.155743	0.884328
6	6	4.929837	0.115547	-0.147165
7	1	2.605445	0.033100	-1.496637
8	1	3.166615	2.258230	-0.378687
9	1	2.833300	2.439996	1.343159
10	1	5.223879	1.980337	0.893202
11	1	4.533091	0.726963	1.892640
12	1	5.024983	0.610772	-1.124200
13	1	5.924358	-0.275058	0.097862
14	6	0.761124	1.271060	-0.203857
15	6	1.433640	-1.555521	-0.723728
16	1	1.796397	-2.349970	-1.380313
17	1	1.181561	-2.041812	0.225299
18	6	0.190306	-0.944169	-1.359055
19	6	-0.361017	0.284705	-0.631175
20	6	4.057950	-2.018884	0.906331
21	1	3.300710	-2.808277	0.862134
22	1	5.037018	-2.508375	0.894317
23	1	3.962982	-1.517425	1.870326
24	6	4.376488	-1.858095	-1.545356
25	1	4.204404	-1.287435	-2.465008
26	1	5.446642	-2.082482	-1.491051
27	1	3.854345	-2.815485	-1.633809
28	6	1.738765	0.075330	1.874799
29	1	2.666432	-0.106542	2.415038
30	1	1.178842	0.793873	2.480040
31	1	1.192913	-0.870935	1.876394
32	6	-1.377327	1.021226	-1.529975
33	1	-2.041184	0.301801	-2.024868
34	1	1.128844	1.703938	-1.146218
35	6	0.159006	2.432266	0.612038
36	1	-0.005670	2.124229	1.650114
37	6	-1.153361	2.971537	0.037198
38	6	-2.182275	1.870401	-0.541263
39	6	-3.443295	2.561391	-1.031554
40	1	-4.120342	1.834735	-1.486044

41	1	-3.969810	3.068934	-0.217994
42	1	-3.187102	3.306256	-1.788733
43	6	-2.242635	1.035153	0.637628
44	6	-1.273097	-0.039737	0.593451
45	1	0.450861	-0.627463	-2.377633
46	1	-0.607370	-1.690275	-1.465478
47	1	0.865897	3.263581	0.660222
48	1	-1.671683	3.611202	0.756180
49	1	-0.963173	3.566391	-0.863184
50	1	-0.817459	-0.271185	1.557574
51	1	-2.834667	1.285941	1.515588
52	1	-0.897752	1.627052	-2.303585
53	1	-1.890917	-0.931849	0.339947
54	6	-3.841475	-2.213920	1.561324
55	6	-4.534590	-1.007133	1.528190
56	6	-4.800519	-0.387273	0.301340
57	6	-4.392543	-0.990857	-0.891834
58	6	-3.697147	-2.196705	-0.858043
59	6	-3.415592	-2.804429	0.368815
60	1	-3.643305	-2.702299	2.509650
61	1	-4.888414	-0.556859	2.450713
62	1	-5.375625	0.533863	0.274778
63	1	-4.634076	-0.531187	-1.845217
64	1	-3.386545	-2.672719	-1.782470
65	1	-2.884781	-3.750724	0.393799

Beyeranyl cation in the complex
ωB97XD/6-31+G(d,p)//ωB97XD /6-31+G(d,p):
HF = -781.5934851 hartrees (-490457.727835101 kcal/mol)

PBE1



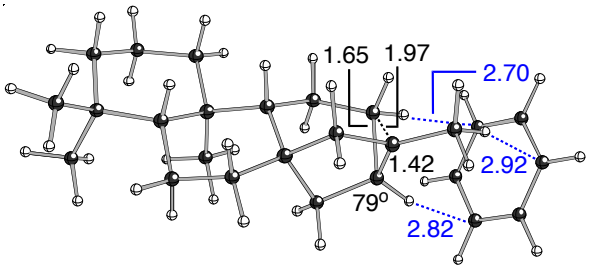
PBE1/6-31+G(d,p)//PBE1/6-31+G(d,p):
HF = -780.8644222 hartrees (-490000.233574722 kcal/mol)
Imaginary Frequencies: none found

Zero-point correction = 0.494235 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.154191	-0.529609	-0.206262
2	6	1.594496	-0.582705	-0.213571
3	6	0.824407	0.720897	0.153750
4	6	1.422436	1.906455	-0.633444
5	6	2.937964	2.012039	-0.503525
6	6	3.609119	0.727671	-0.969775
7	1	1.351338	-0.754082	-1.277955
8	1	1.178030	1.784220	-1.699845
9	1	0.956845	2.846422	-0.309779
10	1	3.293197	2.855883	-1.105654
11	1	3.221485	2.245019	0.530108
12	1	3.387205	0.586699	-2.038400
13	1	4.700062	0.815285	-0.893425
14	6	-0.652147	0.528925	-0.343576
15	6	0.996631	-1.761820	0.555773
16	1	1.565616	-2.676469	0.364680
17	1	1.051490	-1.595342	1.636933
18	6	-0.437765	-2.003048	0.108624
19	6	-1.367283	-0.778846	0.109430
20	6	3.796579	-0.565295	1.189023
21	1	3.398059	-1.379102	1.803604
22	1	4.873320	-0.738305	1.086060
23	1	3.682011	0.365517	1.748985
24	6	3.686021	-1.748545	-0.977833
25	1	3.218232	-1.836429	-1.965590
26	1	4.765530	-1.647619	-1.133261
27	1	3.528789	-2.688799	-0.439675
28	6	0.904649	1.043961	1.655380
29	1	1.939605	1.178850	1.966570
30	1	0.398276	1.982996	1.899429
31	1	0.491338	0.261319	2.295711
32	6	-2.544341	-1.106387	-0.854930
33	1	-2.823168	-2.170083	-0.742691
34	1	-0.568644	0.466248	-1.439707
35	6	-1.530575	1.751639	-0.004784
36	1	-1.304925	2.114577	1.001096
37	6	-3.022672	1.471207	-0.053983

38	6	-3.731923	-0.371608	-0.352393
39	6	-5.070017	-0.396809	-0.978499
40	1	-5.507491	-1.366805	-0.698301
41	1	-5.733996	0.378937	-0.591208
42	1	-5.029648	-0.366662	-2.069808
43	6	-3.401148	0.196329	0.910672
44	6	-2.142854	-0.495953	1.417354
45	1	-0.391407	-2.374585	-0.924971
46	1	-0.907641	-2.803676	0.695806
47	1	-1.320503	2.579283	-0.688615
48	1	-3.672961	2.270627	0.311509
49	1	-3.328320	1.360937	-1.112391
50	1	-1.594791	0.105930	2.142857
51	1	-4.192446	0.470313	1.605912
52	1	-2.335957	-0.956886	-1.919945
53	1	-2.443140	-1.425208	1.917369



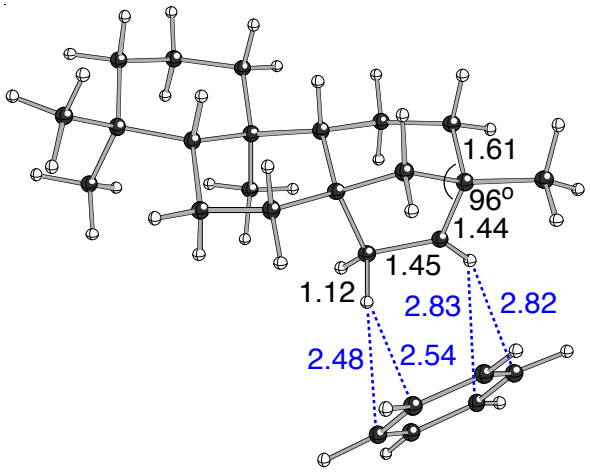
PBE1/6-31+G(d,p)//PBE1/6-31+G(d,p):
HF = -1012.8559451 hartrees (-635577.234109701 kcal/mol)
Imaginary Frequencies: 1 (-1.0949 1/cm)
Zero-point correction = 0.596301 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000835467066 hartrees

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-4.651814	-0.149435	0.122503
2	6	-3.187762	0.376438	0.002210
3	6	-2.046989	-0.677919	-0.104932
4	6	-2.428886	-1.729683	-1.168561
5	6	-3.817276	-2.325204	-0.957606
6	6	-4.877779	-1.232382	-0.947514

7	1	-3.181468	0.887209	-0.977927
8	1	-2.408471	-1.253369	-2.160839
9	1	-1.680571	-2.532524	-1.189635
10	1	-4.028897	-3.039082	-1.761688
11	1	-3.850935	-2.907299	-0.028295
12	1	-4.889392	-0.749045	-1.936035
13	1	-5.875400	-1.667567	-0.809011
14	6	-0.774814	0.079411	-0.630217
15	6	-2.810256	1.438789	1.036593
16	1	-3.629807	2.149890	1.177485
17	1	-2.632695	0.988560	2.019568
18	6	-1.592523	2.216730	0.561832
19	6	-0.379175	1.378277	0.132122
20	6	-5.035623	-0.684068	1.511098
21	1	-4.764636	0.016281	2.308098
22	1	-6.121497	-0.820450	1.558621
23	1	-4.588206	-1.652044	1.747678
24	6	-5.612402	1.009363	-0.192658
25	1	-5.356136	1.500074	-1.139071
26	1	-6.635406	0.628987	-0.285343
27	1	-5.625776	1.769657	0.594706
28	6	-1.795309	-1.403546	1.227267
29	1	-2.692280	-1.924578	1.558645
30	1	-1.022773	-2.172857	1.132883
31	1	-1.508575	-0.735544	2.042656
32	6	0.498594	2.282060	-0.781316
33	1	0.496341	3.313930	-0.387641
34	1	-1.044150	0.395882	-1.649960
35	6	0.448059	-0.856842	-0.732670
36	1	0.497405	-1.514031	0.139154
37	6	1.777964	-0.127279	-0.812184
38	6	1.903762	1.827415	-0.609054
39	6	3.074539	2.409181	-1.301465
40	1	3.282005	3.359690	-0.788952
41	1	3.965790	1.784508	-1.201673
42	1	2.873340	2.643737	-2.349455
43	6	1.944196	0.900631	0.466379
44	6	0.638522	1.016108	1.238097
45	1	-1.908402	2.804645	-0.311806
46	1	-1.268977	2.946959	1.316027
47	1	0.365202	-1.506243	-1.609226
48	1	2.681662	-0.740812	-0.739585
49	1	1.868060	0.337278	-1.812946
50	1	0.394740	0.108876	1.792099

51	1	2.881347	0.692698	0.979531
52	1	0.169637	2.349907	-1.823948
53	1	0.746137	1.829300	1.966883
54	6	5.084744	-0.920356	1.697659
55	6	4.681201	-2.025567	0.945901
56	6	4.995215	-2.098675	-0.412547
57	6	5.709293	-1.064569	-1.020280
58	6	6.111587	0.040703	-0.268762
59	6	5.801282	0.112152	1.090601
60	1	4.867985	-0.879289	2.761829
61	1	4.149113	-2.842899	1.425212
62	1	4.708413	-2.973426	-0.990141
63	1	5.976900	-1.133955	-2.071142
64	1	6.698364	0.828710	-0.733828
65	1	6.141913	0.957836	1.682096



PBE1/6-31+G(d,p)//PBE1/6-31+G(d,p):
HF = -1012.8501988 hartrees (-635573.628248988 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.596171 (Hartree/Particle)
Counterpoise: BSSE energy = 0.001034187456 hartrees

Coordinates (from last standard orientation):

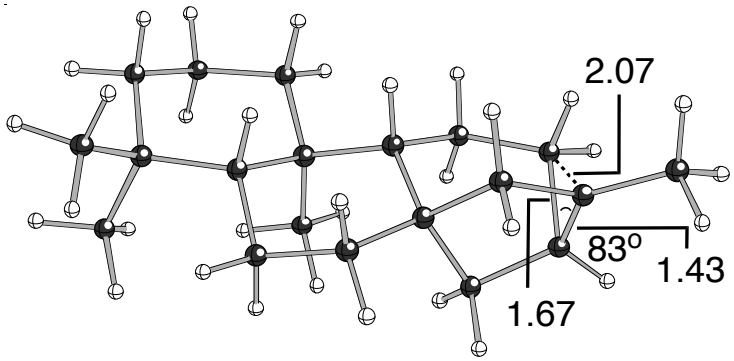
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.984028	-1.054611	-0.312974
2	6	2.554230	-0.474404	-0.536486

3	6	2.035583	0.576302	0.495155
4	6	3.117339	1.660031	0.690158
5	6	4.495157	1.088671	1.010977
6	6	4.952402	0.117574	-0.067507
7	1	2.656371	0.099663	-1.474798
8	1	3.195295	2.252296	-0.234392
9	1	2.815178	2.354349	1.484365
10	1	5.213387	1.912156	1.095262
11	1	4.492613	0.600171	1.993247
12	1	5.068609	0.673057	-1.010200
13	1	5.944477	-0.283419	0.174911
14	6	0.787258	1.259507	-0.161307
15	6	1.479969	-1.530731	-0.803990
16	1	1.859417	-2.296099	-1.487349
17	1	1.210801	-2.060751	0.117589
18	6	0.252019	-0.893398	-1.438157
19	6	-0.322691	0.301061	-0.674129
20	6	4.083469	-2.085698	0.820590
21	1	3.340663	-2.882815	0.708437
22	1	5.070344	-2.560467	0.794876
23	1	3.963943	-1.654399	1.816622
24	6	4.442587	-1.754000	-1.603125
25	1	4.315294	-1.107575	-2.479472
26	1	5.506505	-2.004642	-1.530916
27	1	3.908052	-2.691128	-1.789461
28	6	1.716209	-0.036659	1.869280
29	1	2.631417	-0.297837	2.400170
30	1	1.189647	0.672701	2.515669
31	1	1.122687	-0.952835	1.812812
32	6	-1.298720	1.086351	-1.573081
33	1	-1.948659	0.394106	-2.124773
34	1	1.178423	1.744059	-1.070396
35	6	0.159291	2.369079	0.697899
36	1	-0.051995	1.993204	1.706344
37	6	-1.118883	2.950111	0.097987
38	6	-2.135438	1.896658	-0.582103
39	6	-3.361802	2.631544	-1.085501
40	1	-4.042258	1.935865	-1.583523
41	1	-3.903064	3.126861	-0.273663
42	1	-3.068414	3.394509	-1.811733
43	6	-2.235743	1.024763	0.563724
44	6	-1.286053	-0.065750	0.498165
45	1	0.538726	-0.529776	-2.434814
46	1	-0.541338	-1.634525	-1.604317

47	1	0.867492	3.191441	0.832949
48	1	-1.662812	3.562689	0.823108
49	1	-0.886568	3.584739	-0.767478
50	1	-0.871035	-0.368363	1.462254
51	1	-2.841743	1.257268	1.437978
52	1	-0.786716	1.721118	-2.302829
53	1	-1.923507	-0.925826	0.169656
54	6	-3.892328	-2.193933	1.577990
55	6	-4.567262	-0.976291	1.571631
56	6	-4.887880	-0.359952	0.354645
57	6	-4.552361	-0.977919	-0.854332
58	6	-3.875633	-2.195710	-0.847110
59	6	-3.539208	-2.799621	0.368739
60	1	-3.654473	-2.681140	2.518996
61	1	-4.868391	-0.515994	2.509073
62	1	-5.454871	0.567623	0.350801
63	1	-4.842792	-0.523378	-1.797495
64	1	-3.627547	-2.687469	-1.783314
65	1	-3.026393	-3.757308	0.372969

Beyeranyl cation in the complex
PBE1/6-31+G(d,p)//PBE1/6-31+G(d,p):
HF = -780.8526838 hartrees (-489992.867611338 kcal/mol)

B971

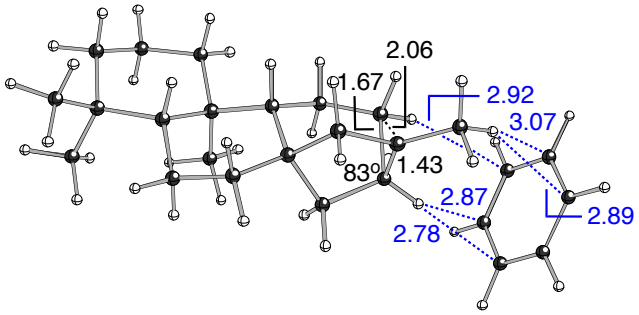


B971/6-31+G(d,p)//B971/6-31+G(d,p):
HF = -781.5565375 hartrees (-490434.542846625 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.489630 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.180195	-0.542780	-0.207051
2	6	1.605456	-0.589056	-0.206912
3	6	0.836199	0.733462	0.153979
4	6	1.442559	1.917265	-0.655260
5	6	2.971148	2.018882	-0.530622
6	6	3.642599	0.717172	-0.987969
7	1	1.356884	-0.771092	-1.269165
8	1	1.194014	1.784480	-1.720855
9	1	0.982880	2.864405	-0.338943
10	1	3.326461	2.854407	-1.147469
11	1	3.258588	2.263382	0.500836
12	1	3.419973	0.568260	-2.056882
13	1	4.735194	0.803622	-0.910242
14	6	-0.659238	0.542987	-0.338573
15	6	0.999858	-1.766939	0.583466
16	1	1.567084	-2.686921	0.404017
17	1	1.049982	-1.585853	1.663975
18	6	-0.444706	-2.013758	0.131156
19	6	-1.381106	-0.778457	0.116418
20	6	3.835120	-0.572396	1.196758
21	1	3.433115	-1.380170	1.820094
22	1	4.911992	-0.752695	1.088902
23	1	3.727362	0.365547	1.749537
24	6	3.705807	-1.780463	-0.979343
25	1	3.232990	-1.870373	-1.966471
26	1	4.787302	-1.687693	-1.138172
27	1	3.541161	-2.716877	-0.433171
28	6	0.921489	1.074446	1.665047
29	1	1.959984	1.168587	1.984241
30	1	0.449959	2.037663	1.891118
31	1	0.466856	0.316227	2.309766
32	6	-2.561014	-1.115376	-0.866339
33	1	-2.825900	-2.186388	-0.768673
34	1	-0.584673	0.486328	-1.436520
35	6	-1.539812	1.777876	0.015199
36	1	-1.312248	2.130411	1.025277
37	6	-3.045743	1.515403	-0.044117
38	6	-3.767527	-0.398097	-0.360895
39	6	-5.104966	-0.424924	-1.006478
40	1	-5.543695	-1.399939	-0.735173
41	1	-5.776093	0.349589	-0.624318

42	1	-5.048900	-0.392186	-2.098960
43	6	-3.443904	0.196420	0.899629
44	6	-2.178066	-0.496340	1.427002
45	1	-0.395484	-2.398317	-0.899094
46	1	-0.916691	-2.806836	0.729966
47	1	-1.322117	2.610187	-0.663675
48	1	-3.678200	2.308791	0.367448
49	1	-3.364423	1.435454	-1.099285
50	1	-1.641960	0.110386	2.159155
51	1	-4.244459	0.464760	1.589045
52	1	-2.352869	-0.950804	-1.931141
53	1	-2.480163	-1.428302	1.924249



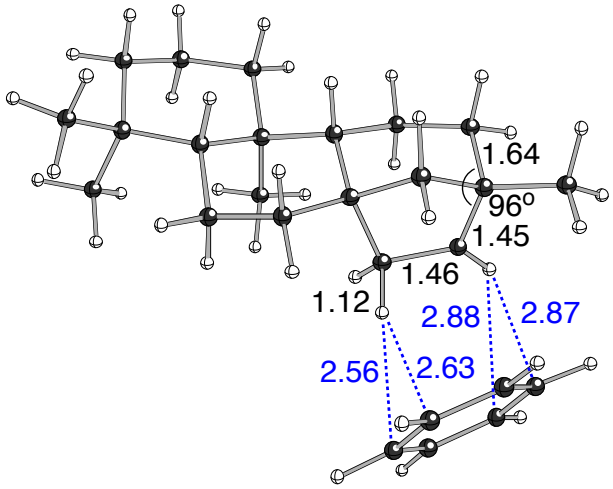
B971/6-31+G(d,p)//B971/6-31+G(d,p):
HF = -1013.7600496 hartrees (-636144.568724496 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.590699 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000753754177 hartrees

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-4.750019	0.062852	0.245690
2	6	-3.232990	0.453144	0.071577
3	6	-2.199049	-0.712626	-0.134431
4	6	-2.738331	-1.681884	-1.225683
5	6	-4.174730	-2.158191	-0.957598
6	6	-5.133557	-0.964980	-0.853766
7	1	-3.221605	1.003040	-0.888148
8	1	-2.724205	-1.165243	-2.199232
9	1	-2.072269	-2.551243	-1.319508
10	1	-4.493240	-2.817483	-1.775462

11	1	-4.213349	-2.769614	-0.045822
12	1	-5.151593	-0.447387	-1.826305
13	1	-6.159522	-1.314257	-0.672337
14	6	-0.868120	-0.058811	-0.697244
15	6	-2.699115	1.433287	1.134682
16	1	-3.442944	2.206195	1.357978
17	1	-2.501238	0.918794	2.083227
18	6	-1.438954	2.131619	0.610686
19	6	-0.321400	1.203655	0.070749
20	6	-5.128948	-0.485910	1.644856
21	1	-4.746686	0.150309	2.452286
22	1	-6.221834	-0.507969	1.739960
23	1	-4.777745	-1.506417	1.824272
24	6	-5.610116	1.331471	0.009520
25	1	-5.346908	1.826813	-0.934543
26	1	-6.670661	1.056108	-0.045215
27	1	-5.510326	2.063188	0.820138
28	6	-1.952418	-1.520768	1.166646
29	1	-2.890948	-1.897601	1.573750
30	1	-1.326431	-2.401416	0.981826
31	1	-1.481554	-0.933046	1.960956
32	6	0.569343	2.068397	-0.892086
33	1	0.658256	3.095708	-0.488911
34	1	-1.137472	0.294160	-1.705856
35	6	0.268608	-1.110770	-0.850137
36	1	0.304695	-1.760397	0.029122
37	6	1.661610	-0.506468	-1.026096
38	6	1.956812	1.522413	-0.806136
39	6	3.117483	2.027592	-1.583123
40	1	3.429407	2.955744	-1.075710
41	1	3.969352	1.341442	-1.551963
42	1	2.854033	2.295202	-2.611228
43	6	1.996936	0.543907	0.233561
44	6	0.750118	0.746753	1.107744
45	1	-1.755354	2.784101	-0.217512
46	1	-1.006390	2.795620	1.373608
47	1	0.076104	-1.759494	-1.712472
48	1	2.500500	-1.208008	-0.963311
49	1	1.748209	-0.065240	-2.035016
50	1	0.481454	-0.149645	1.670396
51	1	2.950270	0.266246	0.685474
52	1	0.190657	2.175085	-1.916455
53	1	0.969918	1.540547	1.835122
54	6	5.354831	-0.533860	1.835532

55	6	4.940998	-1.723790	1.216867
56	6	5.207968	-1.936739	-0.144121
57	6	5.888992	-0.960055	-0.886438
58	6	6.303214	0.228751	-0.267129
59	6	6.035471	0.442350	1.093326
60	1	5.171402	-0.380603	2.896822
61	1	4.438584	-2.493097	1.799600
62	1	4.917861	-2.873823	-0.615402
63	1	6.124488	-1.138993	-1.933550
64	1	6.859991	0.971835	-0.834484
65	1	6.379287	1.352812	1.579227



B971/6-31+G(d,p)//B971/6-31+G(d,p):
HF = -1013.7554369 hartrees (-636141.674209119 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.590665 (Hartree/Particle)
Counterpoise: BSSE energy = 0.00104597225 hartrees

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	4.022782	-1.084592	-0.311954
2	6	2.582330	-0.492047	-0.536445
3	6	2.070944	0.580108	0.498884
4	6	3.169738	1.668191	0.678932
5	6	4.557755	1.088256	0.999703
6	6	5.007950	0.093114	-0.077291

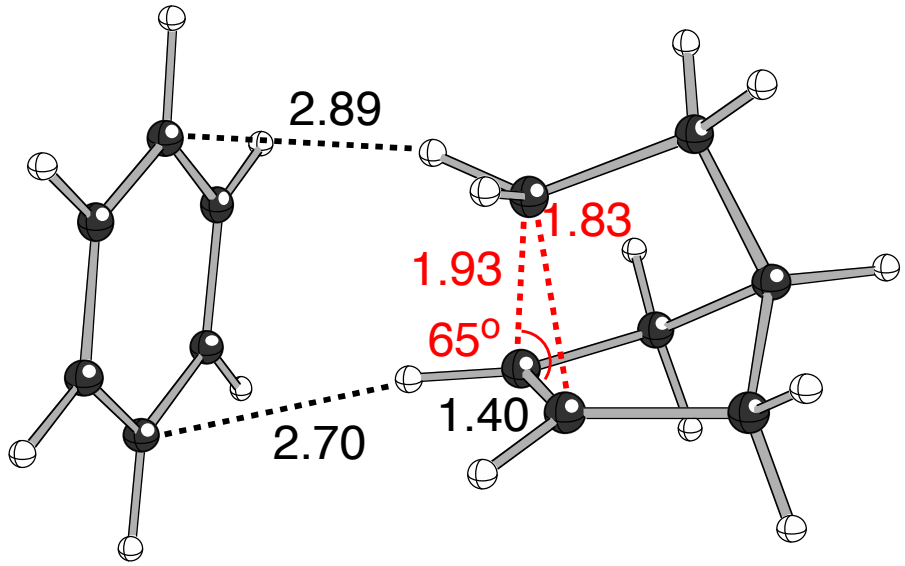
7	1	2.684286	0.073896	-1.480667
8	1	3.246063	2.252622	-0.252371
9	1	2.876495	2.371367	1.470926
10	1	5.280985	1.911518	1.065491
11	1	4.558691	0.612519	1.989780
12	1	5.128080	0.639163	-1.026689
13	1	5.998143	-0.313185	0.171371
14	6	0.810924	1.271357	-0.163827
15	6	1.490244	-1.551181	-0.794145
16	1	1.861482	-2.324968	-1.474995
17	1	1.217395	-2.071434	0.133546
18	6	0.255721	-0.905287	-1.436379
19	6	-0.315054	0.307531	-0.673160
20	6	4.122321	-2.116817	0.837858
21	1	3.371905	-2.910504	0.734841
22	1	5.107857	-2.598281	0.810115
23	1	4.010384	-1.675153	1.832093
24	6	4.475502	-1.801962	-1.610065
25	1	4.350380	-1.158235	-2.490865
26	1	5.539047	-2.061735	-1.538506
27	1	3.929329	-2.736020	-1.788013
28	6	1.751015	-0.022712	1.892000
29	1	2.667485	-0.296227	2.417511
30	1	1.239931	0.701995	2.536572
31	1	1.139480	-0.929488	1.845305
32	6	-1.295368	1.101704	-1.582757
33	1	-1.948000	0.411935	-2.137118
34	1	1.201586	1.749283	-1.077659
35	6	0.186903	2.401649	0.696790
36	1	-0.021567	2.037271	1.711123
37	6	-1.101842	2.989714	0.097824
38	6	-2.137814	1.920076	-0.583450
39	6	-3.371677	2.664900	-1.090683
40	1	-4.056548	1.966539	-1.583186
41	1	-3.908981	3.165432	-0.276951
42	1	-3.075838	3.424148	-1.822296
43	6	-2.245295	1.045161	0.566711
44	6	-1.292294	-0.058030	0.508422
45	1	0.543143	-0.551141	-2.437902
46	1	-0.543084	-1.645259	-1.592751
47	1	0.900649	3.223921	0.816074
48	1	-1.645124	3.600677	0.826509
49	1	-0.876870	3.619856	-0.774092
50	1	-0.876393	-0.345283	1.478824

51	1	-2.859007	1.276335	1.437574
52	1	-0.779724	1.737677	-2.310817
53	1	-1.919992	-0.926987	0.187263
54	6	-3.978238	-2.216106	1.575605
55	6	-4.643289	-0.984982	1.581119
56	6	-4.960341	-0.351661	0.363987
57	6	-4.629563	-0.965253	-0.856952
58	6	-3.963704	-2.196902	-0.861324
59	6	-3.631966	-2.818683	0.354654
60	1	-3.744417	-2.714687	2.513109
61	1	-4.938405	-0.529035	2.523951
62	1	-5.518085	0.582969	0.368617
63	1	-4.915315	-0.497971	-1.796819
64	1	-3.721235	-2.683171	-1.803305
65	1	-3.130320	-3.783637	0.350052

Beyeranyl cation in the complex
B971/6-31+G(d,p)//B971/6-31+G(d,p):
HF = -781.5460492 hartrees (-490427.961333492 kcal/mol)

Table S2
2-Norbornyl cation and benzene complex (**2**)

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):
2-Norbornyl cation-bezene complex



HF = -505.3626532 hartrees (-317120.118509532 kcal/mol)
Imaginary Frequencies: none found

Zero-point correction = 0.264982 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000656336 hartrees

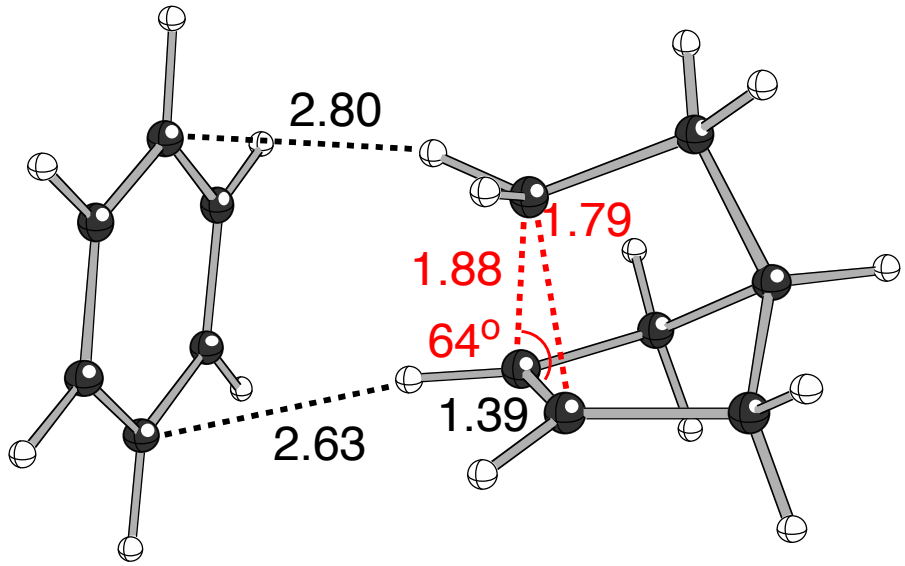
2-Norbornyl cation in the complex
HF = -273.0834936 hartrees (-171362.623068936 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.786691	-0.869793	1.155436
2	6	-3.058140	-0.140428	0.654958
3	6	-1.700522	-0.504236	-1.184081
4	6	-0.903928	-0.687657	-0.051081
5	1	-1.357576	-0.479243	2.080918
6	1	-1.958586	-1.948159	1.284920
7	1	0.177663	-0.797242	-0.066207
8	6	-3.161226	-0.656490	-0.798573
9	1	-3.844273	-0.087164	-1.432910
10	6	-2.588891	1.320677	0.467588
11	1	-3.354000	1.933446	-0.015020
12	1	-2.312439	1.792623	1.413249
13	6	-1.372458	1.137799	-0.440173
14	1	-1.389051	1.601874	-1.429187
15	1	-0.389517	1.368888	-0.017226
16	1	-3.946729	-0.273627	1.270996
17	1	-1.316114	-0.537061	-2.198250
18	1	-3.437937	-1.716846	-0.852596
19	6	2.450825	1.343506	0.496686
20	6	2.540479	0.279874	1.403336
21	6	2.537362	1.099669	-0.879941
22	6	2.719512	-1.027076	0.933593
23	1	2.503056	0.472390	2.471765
24	6	2.712963	-0.207737	-1.349694
25	1	2.502708	1.928362	-1.581883
26	6	2.805887	-1.270894	-0.442727
27	1	2.818304	-1.848377	1.637573
28	1	2.809768	-0.393762	-2.415575
29	1	2.971703	-2.281155	-0.805743
30	1	2.351990	2.361766	0.863213

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

2-Norbornyl cation-bezene complex



HF = -505.0503319 hartrees (-316924.133770569 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.268339 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000682181 hartrees

2-Norbornyl cation in the complex
HF = -272.9138056 hartrees (-171256.142152056 kcal/mol)

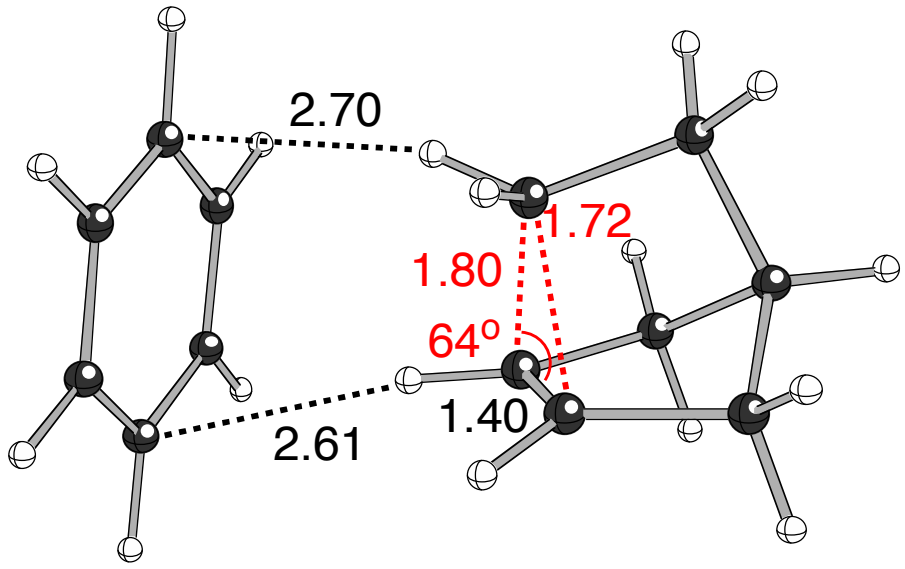
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.666008	-0.990539	-1.018614
2	6	2.978952	-0.266296	-0.662660
3	6	1.693811	-0.327451	1.248217
4	6	0.844754	-0.616857	0.183004
5	1	1.215373	-0.695962	-1.967903
6	1	1.783591	-2.082049	-1.015409
7	1	-0.236981	-0.687206	0.255060
8	6	3.124446	-0.601438	0.831334
9	1	3.857849	0.010740	1.358865
10	6	2.573136	1.216660	-0.633942
11	1	3.374912	1.850910	-0.251719
12	1	2.275903	1.588269	-1.616065
13	6	1.390457	1.176481	0.329733
14	1	1.440728	1.781116	1.237160
15	1	0.404284	1.387932	-0.096337

16	1	3.833705	-0.510170	-1.291018
17	1	1.353088	-0.226209	2.272666
18	1	3.355308	-1.657251	1.010850
19	6	-2.354689	1.305365	-0.580341
20	6	-2.448448	0.193631	-1.417407
21	6	-2.478515	1.151310	0.800725
22	6	-2.669839	-1.071521	-0.874029
23	1	-2.380761	0.317416	-2.493749
24	6	-2.696984	-0.114456	1.344093
25	1	-2.438998	2.020651	1.450109
26	6	-2.794939	-1.225477	0.506262
27	1	-2.770093	-1.932680	-1.527065
28	1	-2.821602	-0.231124	2.416084
29	1	-2.992302	-2.206322	0.927099
30	1	-2.222900	2.295470	-1.006877

LC-ωPBE

2-Norbornyl cation-bezene complex



LC-ωPBE/6-31+G(d,p)//LC-ωPBE/6-31+G(d,p):
HF = -505.0124865 hartrees (-316900.385403615 kcal/mol)
Zero-point correction = 0.270906 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000631162 hartrees

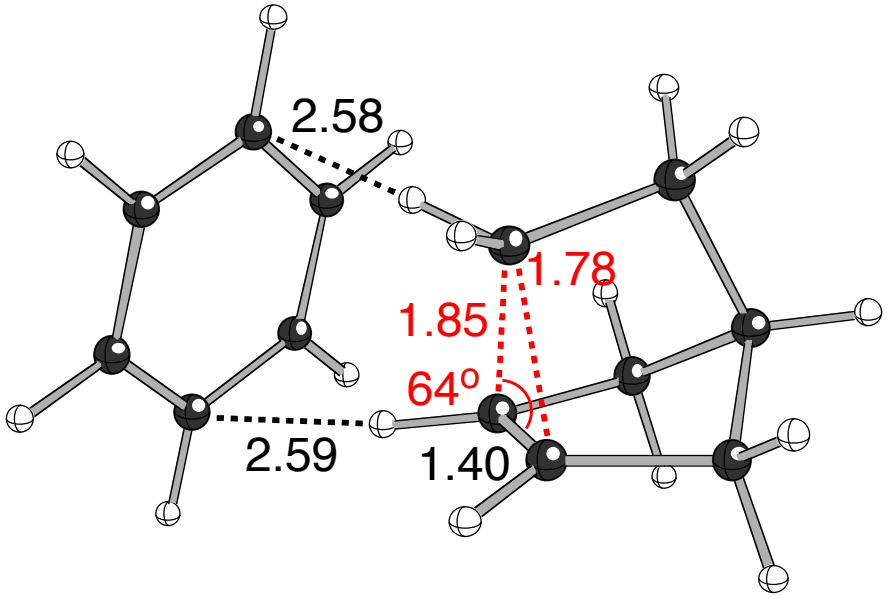
2-Norbornyl cation in the complex
LC-ωPBE/6-31+G(d,p)//LC-ωPBE/6-31+G(d,p):
HF = -272.9124511 hartrees (-171255.292189761 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.597978	-1.252493	-0.623545
2	6	2.917731	-0.470840	-0.580276
3	6	1.737401	0.112831	1.296814
4	6	0.833412	-0.490642	0.421057
5	1	1.104795	-1.272560	-1.596932
6	1	1.712641	-2.283254	-0.267700
7	1	-0.241805	-0.544563	0.578591
8	6	3.139960	-0.313647	0.926568
9	1	3.902262	0.421538	1.190076
10	6	2.498290	0.942869	-0.991189
11	1	3.301705	1.668093	-0.850975
12	1	2.154867	1.000187	-2.025462
13	6	1.359527	1.174455	-0.005962
14	1	1.377562	2.065572	0.625754
15	1	0.354209	1.216777	-0.450557
16	1	3.741781	-0.906608	-1.142860
17	1	1.448966	0.528750	2.256574
18	1	3.372279	-1.258941	1.427657
19	6	-2.275305	0.979961	-1.036663
20	6	-2.380681	-0.363939	-1.383393
21	6	-2.428650	1.370390	0.291004
22	6	-2.645832	-1.316272	-0.403973
23	1	-2.289561	-0.665560	-2.422943
24	6	-2.689391	0.417081	1.270890
25	1	-2.380142	2.422746	0.557420
26	6	-2.801436	-0.925917	0.922498
27	1	-2.756433	-2.361243	-0.678454
28	1	-2.836978	0.724287	2.302192
29	1	-3.032818	-1.666202	1.682740
30	1	-2.111351	1.727963	-1.808091

ωB97X-D

2-Norbornyl cation-bezene complex



ωB97X-D/6-31+G(d,p)//ωB97X-D/6-31+G(d,p):
HF = -505.2052168 hartrees (-317021.325594168 kcal/mol)
Zero-point correction = 0.268431 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000702605 hartrees

2-Norbornyl cation in the complex
ωB97X-D/6-31+G(d,p)//ωB97X-D/6-31+G(d,p):
HF = -273.0044637 hartrees (-171313.031016387 kcal/mol)

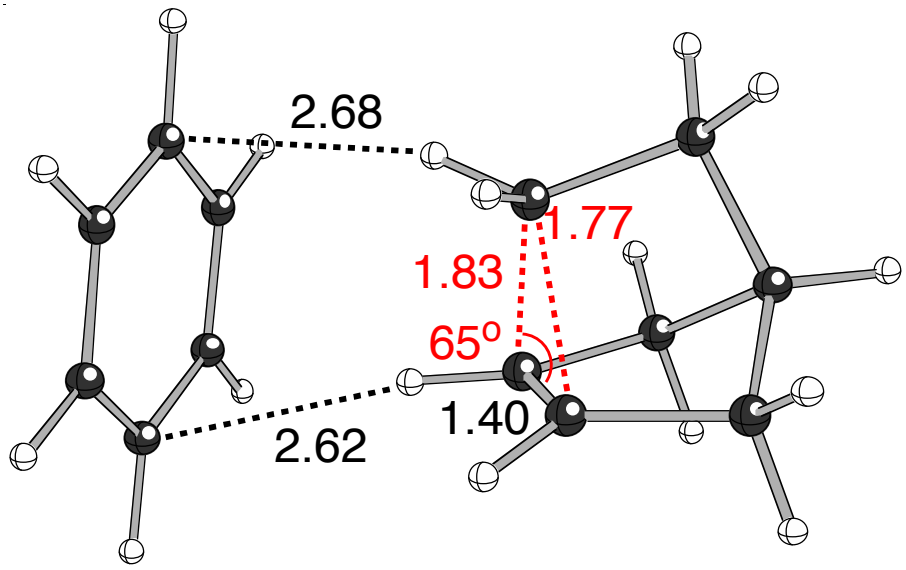
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.344875	-1.223455	0.521708
2	6	-2.696792	-0.505967	0.704127
3	6	-1.881053	0.100274	-1.363773
4	6	-0.813034	-0.440165	-0.646855
5	1	-0.684099	-1.200483	1.389592
6	1	-1.467794	-2.265485	0.200303
7	1	0.225140	-0.425202	-0.968106
8	6	-3.182203	-0.374245	-0.750585
9	1	-4.008305	0.325822	-0.886612
10	6	-2.287062	0.935591	1.050794
11	1	-3.141721	1.614349	1.062603
12	1	-1.772048	1.004559	2.010595
13	6	-1.344021	1.248095	-0.108401
14	1	-1.568744	2.104833	-0.747809

15	1	-0.283570	1.362681	0.152109
16	1	-3.390864	-0.979842	1.395272
17	1	-1.780135	0.533983	-2.352347
18	1	-3.456175	-1.336502	-1.196982
19	6	2.124563	1.014446	1.009362
20	6	2.146806	-0.324785	1.403249
21	6	2.414060	1.358199	-0.313086
22	6	2.464361	-1.319433	0.477595
23	1	1.951172	-0.587819	2.438550
24	6	2.728407	0.362603	-1.240016
25	1	2.427050	2.401973	-0.612676
26	6	2.757019	-0.976034	-0.843333
27	1	2.509640	-2.358126	0.789992
28	1	2.977941	0.630488	-2.261889
29	1	3.028183	-1.747110	-1.557416
30	1	1.917268	1.791128	1.740105

PBE1

2-Norbornyl cation-bezene complex



PBE1/6-31+G(d,p)//PBE1/6-31+G(d,p):
HF = -504.7538434 hartrees (-316738.084271934 kcal/mol)
Zero-point correction = 0.267165 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000717505 hartrees

2-Norbornyl cation in the complex

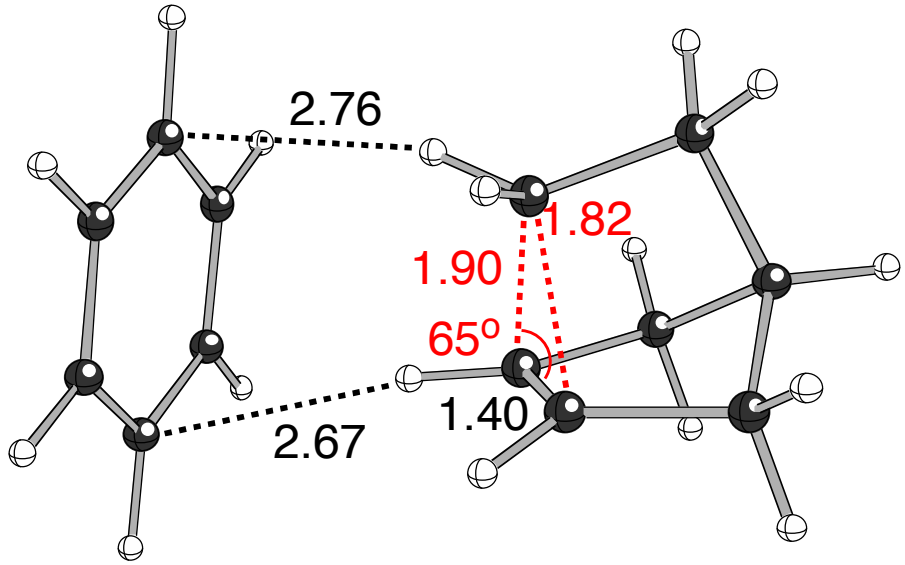
PBE1/6-31+G(d,p)//PBE1/6-31+G(d,p):
HF = -272.7586776 hartrees (-171158.797780776 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.714401	-0.909218	1.104427
2	6	-2.980808	-0.149781	0.671305
3	6	-1.695740	-0.450035	-1.213342
4	6	-0.864319	-0.678091	-0.112099
5	1	-1.258495	-0.558079	2.033129
6	1	-1.889451	-1.990773	1.190036
7	1	0.213022	-0.823617	-0.169627
8	6	-3.136703	-0.606915	-0.786698
9	1	-3.836180	-0.007057	-1.373517
10	6	-2.484576	1.293741	0.510609
11	1	-3.237178	1.937551	0.048917
12	1	-2.177872	1.742366	1.458461
13	6	-1.295303	1.076602	-0.415827
14	1	-1.268048	1.605832	-1.373527
15	1	-0.297628	1.263760	0.009856
16	1	-3.853026	-0.285615	1.310060
17	1	-1.344113	-0.461389	-2.240337
18	1	-3.420494	-1.663195	-0.873942
19	6	2.330006	1.325147	0.537669
20	6	2.430967	0.239884	1.411030
21	6	2.449657	1.126598	-0.840121
22	6	2.656875	-1.042786	0.907365
23	1	2.367892	0.398600	2.484106
24	6	2.670315	-0.157004	-1.343830
25	1	2.406654	1.975421	-1.517685
26	6	2.777286	-1.241156	-0.469626
27	1	2.765223	-1.882315	1.588397
28	1	2.792517	-0.307843	-2.412912
29	1	2.979056	-2.234971	-0.859518
30	1	2.198584	2.329412	0.932927

B971

2-Norbornyl cation-bezene complex



B971/6-31+G(d,p)//B971/6-31+G(d,p):
HF = -505.209325 hartrees (-317023.90353075 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.264591 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000682149 hartrees

2-Norbornyl cation in the complex
B971/6-31+G(d,p)//B971/6-31+G(d,p):
HF = -273.0024873 hartrees (-171311.790805623 kcal/mol)

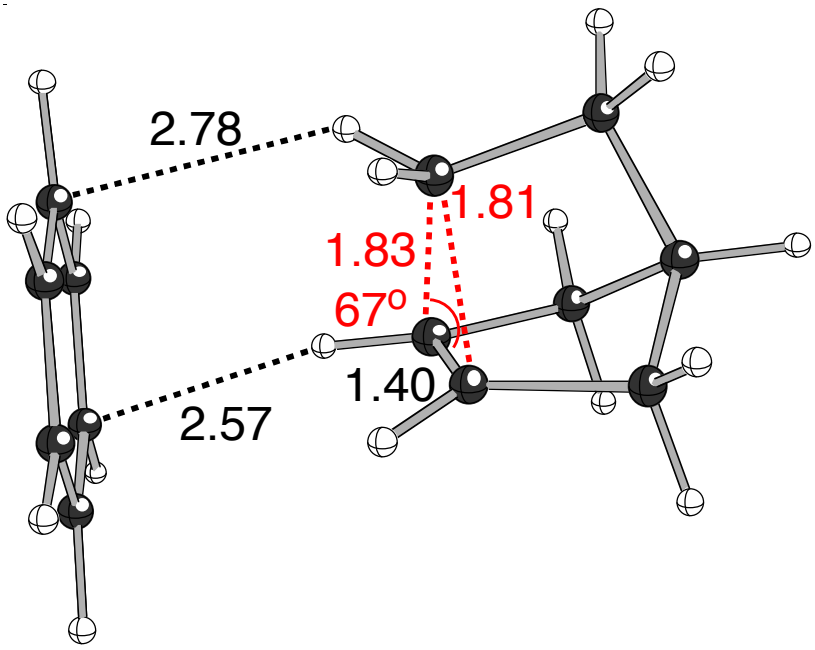
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.730349	-0.881900	1.140261
2	6	-3.005085	-0.120337	0.689868
3	6	-1.730200	-0.511191	-1.206692
4	6	-0.889509	-0.711793	-0.103140
5	1	-1.255258	-0.499758	2.048685
6	1	-1.919973	-1.958271	1.272830
7	1	0.189165	-0.852080	-0.163470
8	6	-3.180100	-0.631809	-0.761712
9	1	-3.875355	-0.042936	-1.367091
10	6	-2.503255	1.328821	0.479434
11	1	-3.265903	1.960869	0.014366
12	1	-2.180434	1.799303	1.413000
13	6	-1.319665	1.098076	-0.467205

14	1	-1.338757	1.573931	-1.453538
15	1	-0.314611	1.297720	-0.069568
16	1	-3.872870	-0.231432	1.341714
17	1	-1.386991	-0.552820	-2.237212
18	1	-3.481322	-1.687659	-0.806372
19	6	2.371878	1.322101	0.565736
20	6	2.475966	0.214050	1.421296
21	6	2.481709	1.149268	-0.823246
22	6	2.694238	-1.065755	0.888439
23	1	2.421069	0.352179	2.498934
24	6	2.694555	-0.131532	-1.356381
25	1	2.436095	2.012315	-1.484504
26	6	2.803984	-1.238569	-0.500158
27	1	2.806094	-1.919607	1.552921
28	1	2.808741	-0.261735	-2.430341
29	1	2.999986	-2.226381	-0.911239
30	1	2.245317	2.319789	0.981888

MO6-2X

2-Norbornyl cation-bezene complex



MO6-2X/6-31+G(d,p)//MO6-2X /6-31+G(d,p):
HF = -505.1163485 hartrees (-316965.559847235 kcal/mol)
Zero-point correction = 0.268169 (Hartree/Particle)
Counterpoise: BSSE energy = 0.000733063 hartrees

2-Norbornyl cation in the complex
MO6-2X/6-31+G(d,p)//MO6-2X /6-31+G(d,p):
HF = -272.945638 hartrees (-171276.11730138 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.925222	-0.417168	1.451099
2	6	-3.069784	-0.110555	0.466383
3	6	-1.240429	-0.754788	-0.789876
4	6	-0.769557	-0.412774	0.477576
5	1	-1.816112	0.306353	2.261464
6	1	-2.004224	-1.423103	1.881748
7	1	0.284414	-0.351333	0.737810
8	6	-2.725659	-1.034649	-0.715582
9	1	-3.261935	-0.805237	-1.638368
10	6	-2.697450	1.279539	-0.075355
11	1	-3.329784	1.577985	-0.913536
12	1	-2.744518	2.052323	0.694172
13	6	-1.259440	1.031910	-0.525124
14	1	-1.014519	1.177273	-1.581286
15	1	-0.466636	1.565857	0.010244
16	1	-4.076606	-0.209983	0.868087
17	1	-0.586592	-1.008799	-1.617789
18	1	-2.867510	-2.095226	-0.475569
19	6	2.312403	1.425260	0.050640
20	6	2.644249	0.679838	1.184341
21	6	2.139979	0.785564	-1.179829
22	6	2.805793	-0.704668	1.087156
23	1	2.802272	1.178899	2.135369
24	6	2.298754	-0.598709	-1.275544
25	1	1.921475	1.370178	-2.069667
26	6	2.631351	-1.344153	-0.141772
27	1	3.086119	-1.280708	1.963381
28	1	2.201482	-1.091622	-2.238997
29	1	2.779229	-2.416727	-0.220978
30	1	2.223512	2.505992	0.119225

NBO analysis (B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)) using NBO method implemented in Gaussian09.

1) Natural atomic charge

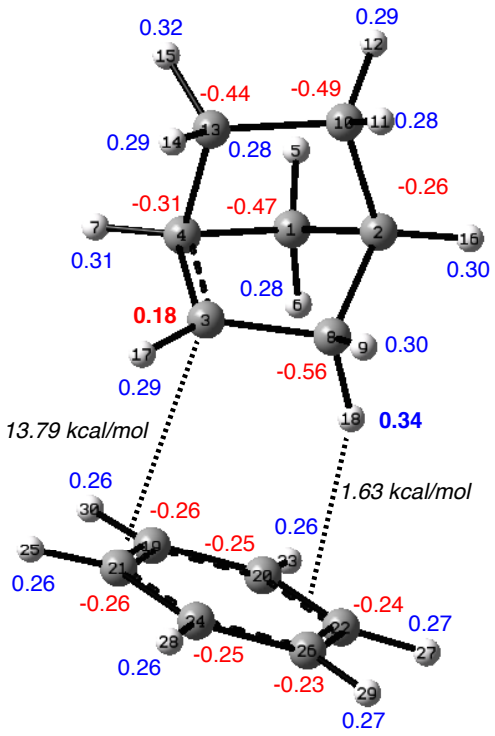


Figure S2. Computed natural charge (carbon in red and hydrogen in blue) and selected intermolecular interaction energies (See Table S4 for details).

2) Second Order Perturbation Theory Analysis of fock Matrix in NBO Basis

The strongest interaction between benzene and 2-norbornyl cation involves the interaction of C19-C21 bond with a vacant p orbital of C3, which is predicted to be 13.79 kcal/mol (Table S4; box). The second largest interaction energy is the interaction between C20-C22 bond and C8-H18 antibond, which is predicted to be 1.63 kcal/mol (Table S4; box).

Table S4. Second Order Perturbation Theory Analysis of fock Matrix in NBO Basis. E(2): Estimated strength of the donor-acceptor interactions. E(j)-E(i): The energy splitting (in atomic units) of the donor and acceptor orbitals. F(I,j): The element of the Fock (or Kohn-Sham) matrix describing the donor-acceptor interaction. Atom number is shown in Figure S2.

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
21. BD (1) C 19 - C 21	/ 48. LP*(1) C 3	0.18	0.52	0.010
21. BD (1) C 19 - C 21	/ 78. RY*(2) C 3	0.23	1.41	0.016
21. BD (1) C 19 - C 21	/ 80. RY*(4) C 3	0.09	2.07	0.012
22. BD (2) C 19 - C 21	/ 48. LP*(1) C 3	13.79	0.08	0.030
22. BD (2) C 19 - C 21	/ 85. RY*(9) C 3	0.06	1.35	0.009
22. BD (2) C 19 - C 21	/310. BD*(1) C 4 - C 13	0.06	0.43	0.005
24. BD (1) C 20 - C 22	/187. RY*(1) H 18	0.15	1.61	0.014
25. BD (2) C 20 - C 22	/187. RY*(1) H 18	0.05	1.16	0.008
25. BD (2) C 20 - C 22	/302. BD*(1) C 1 - H 6	0.10	0.69	0.008
25. BD (2) C 20 - C 22	/312. BD*(1) C 8 - H 18	1.63	0.64	0.032
27. BD (1) C 21 - C 24	/ 48. LP*(1) C 3	0.06	0.52	0.006
27. BD (1) C 21 - C 24	/ 79. RY*(3) C 3	0.14	1.57	0.013
28. BD (1) C 21 - H 25	/ 48. LP*(1) C 3	0.11	0.35	0.006
28. BD (1) C 21 - H 25	/308. BD*(1) C 3 - H 17	0.07	0.97	0.008
29. BD (1) C 22 - C 26	/187. RY*(1) H 18	0.16	1.61	0.014
32. BD (2) C 24 - C 26	/303. BD*(1) C 2 - C 8	0.10	0.56	0.007
32. BD (2) C 24 - C 26	/312. BD*(1) C 8 - H 18	0.23	0.64	0.012
320. BD*(2) C 19 - C 21	/308. BD*(1) C 3 - H 17	0.08	0.43	0.012
320. BD*(2) C 19 - C 21	/310. BD*(1) C 4 - C 13	0.06	0.16	0.006
323. BD*(2) C 20 - C 22	/302. BD*(1) C 1 - H 6	0.09	0.41	0.013
323. BD*(2) C 20 - C 22	/312. BD*(1) C 8 - H 18	0.11	0.36	0.013
330. BD*(2) C 24 - C 26	/312. BD*(1) C 8 - H 18	0.05	0.36	0.010