

The Benzene + OH Potential Energy Surface: Intermediates and Transition States

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Supplementary Material

1 Comparison of Geometry Optimization Methods

Table 1: A comparison of selected geometry optimization methods with experiment for three immediately relevant covalently bonded systems.

Parameter*	6-31G*			TZVPP					Expt. [‡]
	B3LYP	M06	M062X	B3LYP	ωB97X-D	M06	M062X	RI-MP2	
•OH									
r(O–H)	0.983	0.978	0.979	0.974	0.969	0.969	0.971	0.966	0.970
H ₂ O									
r(O–H)	0.969	0.964	0.966	0.961	0.956	0.956	0.959	0.957	0.958
∠(H–O–H)	103.6	104.1	104.3	104.9	105.0	104.8	105.0	104.0	104.5
C ₆ H ₆									
r(C–C)	1.397	1.392	1.393	1.391	1.387	1.385	1.388	1.390	1.397
r(C–H)	1.087	1.089	1.086	1.082	1.082	1.083	1.082	1.079	1.084

* Bond lengths are in angstroms, angles are in degrees.

‡The experimental structures were obtained from ref. 1 for OH, ref. 2 for water, and ref. 3 for benzene

2 Additional Focal Point Tables

Table 2: Energy (in kcal/mol) of **TS₂** relative to relative to separate benzene and hydroxyl radical, giving the complexation energy. See footnote *a* in table 2 of the main paper for more details.

Basis Set	$\Delta E_e[\text{ROHF}]$	$\delta[\text{ZAPT2}]$	$\delta[\text{CCSD}]$	$\delta[\text{CCSD(T)}]$	$\Delta E_e[\text{CCSD(T)}]$
cc-pVDZ	24.57	-15.83	-2.43	-2.76	[+3.55]
cc-pVTZ	25.59	-19.00	-1.92	-3.71	[+0.97]
cc-pVQZ	25.96	-19.87	-1.95	[-3.71]	[+0.43]
cc-pV5Z	26.16	-20.20	[-1.95]	[-3.71]	[+0.30]
cc-pV6Z	26.20	-20.28	[-1.95]	[-3.71]	[+0.26]
CBS Limit	[26.21]	[-20.39]	[-1.95]	[-3.71]	[+0.16]
$\Delta E_e(\text{final}) = \Delta E_e[\text{CBS CCSD(T)}] + \Delta_{\text{core}} + \Delta_{\text{ZPVE}}$ $= 0.16 - 0.02 + 1.61 = \mathbf{1.76} \text{ kcal/mol}$					

Table 3: Energy (in kcal/mol) of **TS₃** relative to relative to separate benzene and hydroxyl radical, giving the complexation energy. See footnote *a* in table 2 of the main paper for more details.

Basis Set	ΔE_e [ROHF]	δ [ZAPT2]	δ [CCSD]	δ [CCSD(T)]	ΔE_e [CCSD(T)]
cc-pVDZ	40.06	-27.56	+4.84	-2.97	[+14.37]
cc-pVTZ	39.73	-29.60	+5.98	-3.90	[+12.20]
cc-pVQZ	39.88	-30.66	+6.08	[-3.90]	[+11.40]
cc-pV5Z	40.01	-31.01	[+6.08]	[-3.90]	[+11.17]
cc-pV6Z	40.04	-31.17	[+6.08]	[-3.90]	[+11.04]
CBS Limit	[40.05]	[-31.39]	[+6.08]	[-3.90]	[+10.83]
ΔE_e (final) = ΔE_e [CBS CCSD(T)] + Δ_{core} + Δ_{ZPVE} = 10.83 - 0.13 + 2.00 = 12.70 kcal/mol					

Table 4: Energy (in kcal/mol) of Intermediate **I2a** relative to relative to separate benzene and hydroxyl radical, giving the complexation energy. See footnote *a* in table 2 of the main paper for more details.

Basis Set	ΔE_e [ROHF]	δ [ZAPT2]	δ [CCSD]	δ [CCSD(T)]	ΔE_e [CCSD(T)]
cc-pVDZ	8.85	-13.98	+2.66	-1.03	[-3.49]
cc-pVTZ	6.85	-16.83	+3.98	-1.77	[-7.77]
cc-pVQZ	6.62	-17.88	+4.25	[-1.77]	[-8.79]
cc-pV5Z	6.73	-18.25	[+4.25]	[-1.77]	[-9.05]
cc-pV6Z	6.76	-18.32	[+4.25]	[-1.77]	[-9.09]
CBS Limit	[6.77]	[-18.43]	[+4.25]	[-1.77]	[-9.19]
ΔE_e (final) = ΔE_e [CBS CCSD(T)] + Δ_{core} + Δ_{ZPVE} = -9.19 - 0.04 + 1.22 = -8.01 kcal/mol					

Table 5: Energy (in kcal/mol) of **I3** relative to relative to separate benzene and hydroxyl radical, giving the complexation energy. See footnote *a* in table 2 of the main paper for more details.

Basis Set	ΔE_e [ROHF]	δ [ZAPT2]	δ [CCSD]	δ [CCSD(T)]	ΔE_e [CCSD(T)]
cc-pVDZ	8.65	-23.69	+0.31	-0.79	[-15.51]
cc-pVTZ	7.97	-26.33	+1.73	-1.44	[-18.08]
cc-pVQZ	8.05	-27.46	+2.04	[-1.44]	[-18.80]
cc-pV5Z	8.15	-27.86	[+2.04]	[-1.44]	[-19.11]
cc-pV6Z	8.19	-28.02	[+2.04]	[-1.44]	[-19.24]
CBS Limit	[8.19]	[-28.24]	[+2.04]	[-1.44]	[-19.45]
ΔE_e (final) = ΔE_e [CBS CCSD(T)] + Δ_{core} + Δ_{ZPVE} = -19.45 - 0.01 + 2.90 = -16.6 kcal/mol					

Table 6: Energy (in kcal/mol) of separated phenyl radical and water relative to relative to separate benzene and hydroxyl radical, giving the complexation energy. See footnote *a* in table 2 of the main paper for more details.

Basis Set	$\Delta E_e[\text{ROHF}]$	$\delta[\text{ZAPT2}]$	$\delta[\text{CCSD}]$	$\delta[\text{CCSD(T)}]$	$\Delta E_e[\text{CCSD(T)}]$
cc-pVDZ	10.05	-11.23	+1.88	-0.65	[+0.05]
cc-pVTZ	7.49	-13.15	+2.97	-1.22	[-3.90]
cc-pVQZ	6.87	-14.15	+3.24	-1.35	[-5.39]
cc-pV5Z	6.65	-14.60	[+3.24]	[-1.35]	[-6.05]
cc-pV6Z	6.61	-14.72	[+3.24]	[-1.35]	[-6.22]
CBS Limit	[6.60]	[-14.90]	[+3.24]	[-1.35]	[-6.40]
$\Delta E_e(\text{final}) = \Delta E_e[\text{CBS CCSD(T)}] + \Delta_{\text{core}} + \Delta_{\text{ZPVE}}$ $= -6.40 - 0.01 - 0.00 = \textbf{-6.41 kcal/mol}$					

Table 7: Energy (in kcal/mol) of separated phenol and H relative to relative to separate benzene and hydroxyl radical, giving the complexation energy. See footnote *a* in table 2 of the main paper for more details.

Basis Set	$\Delta E_e[\text{ROHF}]$	$\delta[\text{ZAPT2}]$	$\delta[\text{CCSD}]$	$\delta[\text{CCSD(T)}]$	$\Delta E_e[\text{CCSD(T)}]$
cc-pVDZ	-35.37	[-19.67]	[+11.15]	-2.07	[+4.75]
cc-pVTZ	15.89	-19.67	+11.15	-2.81	[+4.56]
cc-pVQZ	16.06	-20.23	+11.18	-2.90	[+4.12]
cc-pV5Z	16.20	-20.46	[+11.18]	[-2.90]	[+4.03]
cc-pV6Z	16.23	-20.59	[+11.18]	[-2.90]	[+3.93]
CBS Limit	[16.24]	[-20.76]	[+11.18]	[-2.90]	[+3.77]
$\Delta E_e(\text{final}) = \Delta E_e[\text{CBS CCSD(T)}] + \Delta_{\text{core}} + \Delta_{\text{ZPVE}}$ $= 3.77 - 0.20 - 2.64 = \textbf{0.93 kcal/mol}$					

3 Geometries

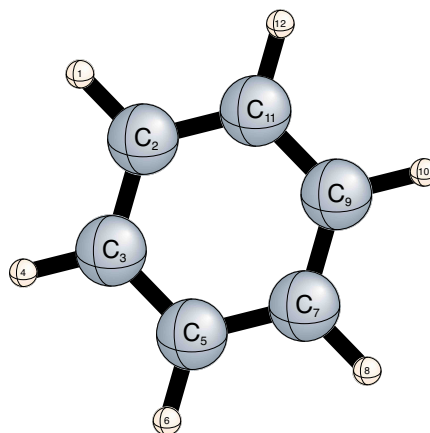
Molecule: benzene

Method: B3LYP

Basis: 6-31G*

Energy: -145738.1177878 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.727433	-1.784505	0.000000
2	C	-0.971395	-1.003484	0.000000
3	C	-1.354726	0.339500	0.000000
4	H	-2.409125	0.603759	0.000000
5	C	-0.383339	1.342975	0.000000
6	H	-0.681711	2.388234	0.000000
7	C	0.971395	1.003484	0.000000
8	H	1.727433	1.784505	0.000000
9	C	1.354726	-0.339500	0.000000
10	H	2.409125	-0.603759	0.000000
11	C	0.383339	-1.342975	0.000000
12	H	0.681711	-2.388234	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.087	2.156	2.484	3.404	4.302	3.880	4.967	3.404	4.302	2.156	2.484
2		1.397	2.156	2.419	3.404	2.793	3.880	2.419	3.404	1.397	2.156
3			1.087	1.397	2.156	2.419	3.404	2.793	3.880	2.419	3.404
4				2.156	2.484	3.404	4.302	3.880	4.967	3.404	4.302
5					1.087	1.397	2.156	2.419	3.404	2.793	3.880
6						2.156	2.484	3.404	4.302	3.880	4.967
7							1.087	1.397	2.156	2.419	3.404
8								2.156	2.484	3.404	4.302
9									1.087	1.397	2.156
10										2.156	2.484
11											1.087

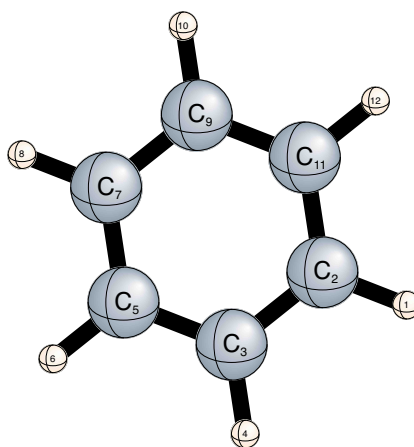
Molecule: benzene

Method: B3LYP

Basis: def2-TZVPP

Energy: -145795.443233691 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.303295	0.901091	0.000000
2	C	1.295457	0.506815	0.000000
3	C	0.208815	1.375300	0.000000
4	H	0.371268	2.445253	0.000000
5	C	-1.086639	0.868480	0.000000
6	H	-1.932010	1.544156	0.000000
7	C	-1.295457	-0.506815	0.000000
8	H	-2.303295	-0.901091	0.000000
9	C	-0.208815	-1.375300	0.000000
10	H	-0.371268	-2.445253	0.000000
11	C	1.086639	-0.868480	0.000000
12	H	1.932010	-1.544156	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.082	2.147	2.473	3.390	4.284	3.864	4.947	3.390	4.284	2.147	2.473
2		1.391	2.147	2.409	3.390	2.782	3.864	2.409	3.390	1.391	2.147
3			1.082	1.391	2.147	2.409	3.390	2.782	3.864	2.409	3.390
4				2.147	2.473	3.390	4.284	3.864	4.947	3.390	4.284
5					1.082	1.391	2.147	2.409	3.390	2.782	3.864
6						2.147	2.473	3.390	4.284	3.864	4.947
7							1.082	1.391	2.147	2.409	3.390
8								2.147	2.473	3.390	4.284
9									1.082	1.391	2.147
10										2.147	2.473
11											1.082

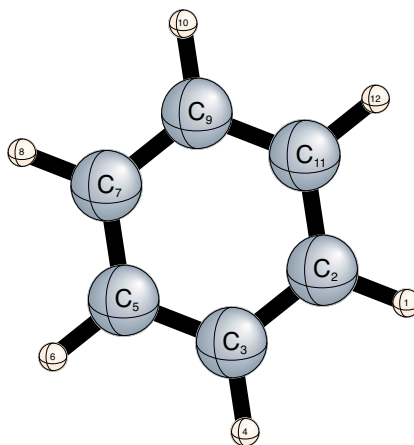
Molecule: benzene

Method: ω B97

Basis: 6-31G*

Energy: -145702.612440655 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.312944	0.904887	0.000000
2	C	1.298518	0.508068	0.000000
3	C	0.209274	1.378618	0.000000
4	H	0.372943	2.455547	0.000000
5	C	-1.089291	0.870549	0.000000
6	H	-1.940154	1.550647	0.000000
7	C	-1.298518	-0.508068	0.000000
8	H	-2.312944	-0.904887	0.000000
9	C	-0.209274	-1.378618	0.000000
10	H	-0.372943	-2.455547	0.000000
11	C	1.089291	-0.870549	0.000000
12	H	1.940154	-1.550647	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.089	2.156	2.484	3.402	4.302	3.878	4.967	3.402	4.302	2.156	2.484
2		1.394	2.156	2.415	3.402	2.789	3.878	2.415	3.402	1.394	2.156
3			1.089	1.394	2.156	2.415	3.402	2.789	3.878	2.415	3.402
4				2.156	2.484	3.402	4.302	3.878	4.967	3.402	4.302
5					1.089	1.394	2.156	2.415	3.402	2.789	3.878
6						2.156	2.484	3.402	4.302	3.878	4.967
7							1.089	1.394	2.156	2.415	3.402
8								2.156	2.484	3.402	4.302
9									1.089	1.394	2.156
10										2.156	2.484
11											1.089

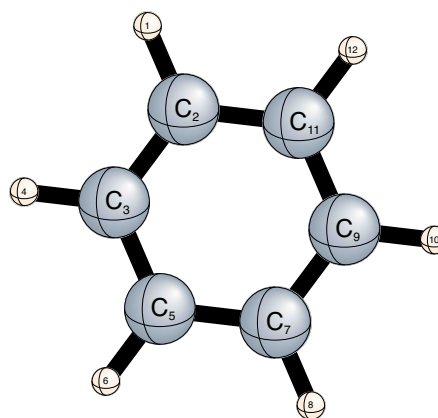
Molecule: benzene

Method: ω B97

Basis: def2-TZVPP

Energy: -145755.212464534 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-0.978656	-2.273107	0.000000
2	C	-0.549570	-1.276641	0.000000
3	C	-1.380341	-0.162344	0.000000
4	H	-2.457863	-0.289042	0.000000
5	C	-0.830803	1.114296	0.000000
6	H	-1.479296	1.984075	0.000000
7	C	0.549570	1.276641	0.000000
8	H	0.978656	2.273107	0.000000
9	C	1.380341	0.162344	0.000000
10	H	2.457863	0.289042	0.000000
11	C	0.830803	-1.114296	0.000000
12	H	1.479296	-1.984075	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.085	2.149	2.475	3.391	4.287	3.865	4.950	3.391	4.287	2.149	2.475
2		1.390	2.149	2.407	3.391	2.780	3.865	2.407	3.391	1.390	2.149
3			1.085	1.390	2.149	2.407	3.391	2.780	3.865	2.407	3.391
4				2.149	2.475	3.391	4.287	3.865	4.950	3.391	4.287
5					1.085	1.390	2.149	2.407	3.391	2.780	3.865
6						2.149	2.475	3.391	4.287	3.865	4.950
7							1.085	1.390	2.149	2.407	3.391
8								2.149	2.475	3.391	4.287
9									1.085	1.390	2.149
10										2.149	2.475
11											1.085

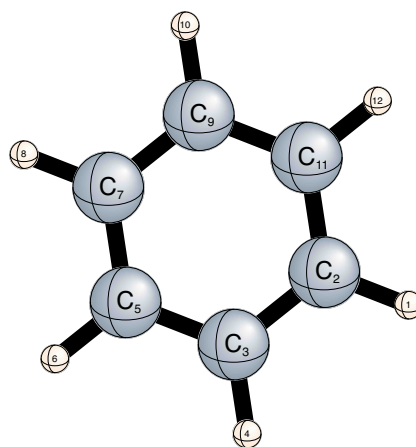
Molecule: benzene

Method: ω B97X

Basis: 6-31G*

Energy: -145694.324567219 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.309089	0.903365	0.000000
2	C	1.296614	0.507308	0.000000
3	C	0.208972	1.376607	0.000000
4	H	0.372292	2.451457	0.000000
5	C	-1.087676	0.869283	0.000000
6	H	-1.936922	1.548058	0.000000
7	C	-1.296614	-0.507308	0.000000
8	H	-2.309089	-0.903365	0.000000
9	C	-0.208972	-1.376607	0.000000
10	H	-0.372292	-2.451457	0.000000
11	C	1.087676	-0.869283	0.000000
12	H	1.936922	-1.548058	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.087	2.153	2.479	3.397	4.295	3.872	4.959	3.397	4.295	2.153	2.480
2		1.392	2.153	2.412	3.397	2.785	3.872	2.412	3.397	1.392	2.153
3			1.087	1.392	2.153	2.412	3.397	2.785	3.872	2.412	3.397
4				2.153	2.480	3.397	4.295	3.872	4.959	3.397	4.295
5					1.087	1.392	2.153	2.412	3.397	2.785	3.872
6						2.153	2.480	3.397	4.295	3.872	4.959
7							1.087	1.392	2.153	2.412	3.397
8								2.153	2.479	3.397	4.295
9									1.087	1.392	2.153
10										2.153	2.480
11											1.087

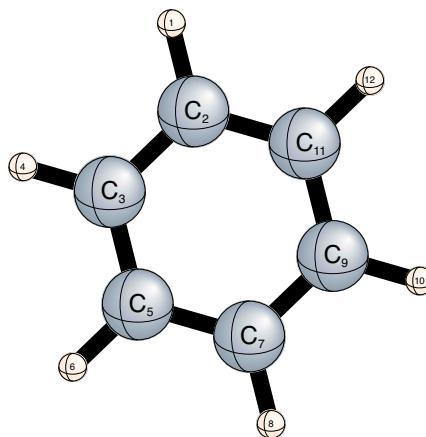
Molecule: benzene

Method: ω B97X

Basis: def2-TZVPP

Energy: -145747.060375261 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-0.596156	-2.397394	0.000000
2	C	-0.334819	-1.346398	0.000000
3	C	-1.333453	-0.383224	0.000000
4	H	-2.374310	-0.682441	0.000000
5	C	-0.998639	0.963207	0.000000
6	H	-1.778125	1.715072	0.000000
7	C	0.334819	1.346398	0.000000
8	H	0.596156	2.397394	0.000000
9	C	1.333453	0.383224	0.000000
10	H	2.374310	0.682441	0.000000
11	C	0.998639	-0.963207	0.000000
12	H	1.778125	-1.715072	0.000000

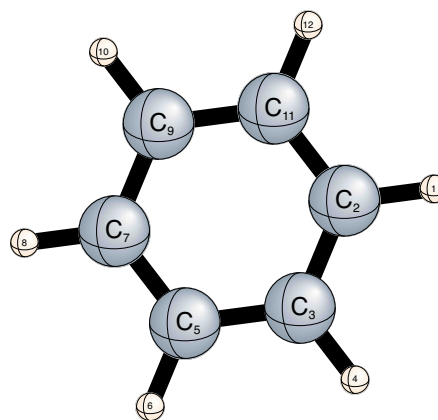


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.083	2.145	2.470	3.385	4.279	3.858	4.941	3.385	4.279	2.145	2.470
2		1.387	2.145	2.403	3.385	2.775	3.858	2.403	3.385	1.387	2.145
3			1.083	1.387	2.145	2.403	3.385	2.775	3.858	2.403	3.385
4				2.145	2.471	3.385	4.279	3.858	4.941	3.385	4.279
5					1.083	1.387	2.145	2.403	3.385	2.775	3.858
6						2.145	2.470	3.385	4.279	3.858	4.941
7							1.083	1.387	2.145	2.403	3.385
8								2.145	2.470	3.385	4.279
9									1.083	1.387	2.145
10										2.145	2.471
11											1.083

Molecule: benzene
Method: ω B97X-D
Basis: 6-31G*
Energy: -145685.266631054 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.457542	-0.324599	0.000000
2	C	1.380773	-0.182351	0.000000
3	C	0.848319	1.104657	0.000000
4	H	1.509867	1.966045	0.000000
5	C	-0.532466	1.287016	0.000000
6	H	-0.947743	2.290592	0.000000
7	C	-1.380773	0.182351	0.000000
8	H	-2.457542	0.324599	0.000000
9	C	-0.848319	-1.104657	0.000000
10	H	-1.509867	-1.966045	0.000000
11	C	0.532466	-1.287016	0.000000
12	H	0.947743	-2.290592	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.086	2.152	2.479	3.397	4.294	3.872	4.958	3.397	4.294	2.152	2.479
2		1.393	2.152	2.412	3.397	2.786	3.872	2.412	3.397	1.393	2.152
3			1.086	1.393	2.152	2.412	3.397	2.786	3.872	2.412	3.397
4				2.152	2.479	3.397	4.294	3.872	4.958	3.397	4.294
5					1.086	1.393	2.152	2.412	3.397	2.786	3.872
6						2.152	2.479	3.397	4.294	3.872	4.958
7							1.086	1.393	2.152	2.412	3.397
8								2.152	2.479	3.397	4.294
9									1.086	1.393	2.152
10										2.152	2.479
11											1.086

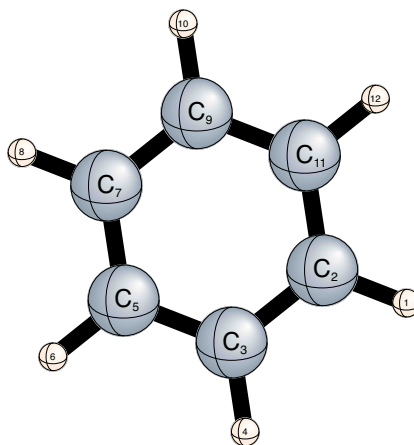
Molecule: benzene

Method: ω B97X-D

Basis: def2-TZVPP

Energy: -145738.485936663 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.299603	0.899666	0.000000
2	C	1.291974	0.505428	0.000000
3	C	0.208244	1.371611	0.000000
4	H	0.370723	2.441359	0.000000
5	C	-1.083720	0.866144	0.000000
6	H	-1.928945	1.541664	0.000000
7	C	-1.291974	-0.505428	0.000000
8	H	-2.299603	-0.899666	0.000000
9	C	-0.208244	-1.371611	0.000000
10	H	-0.370723	-2.441359	0.000000
11	C	1.083720	-0.866144	0.000000
12	H	1.928945	-1.541664	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.082	2.144	2.469	3.383	4.277	3.857	4.939	3.383	4.277	2.144	2.469
2		1.387	2.144	2.403	3.384	2.775	3.857	2.403	3.384	1.387	2.144
3			1.082	1.387	2.144	2.403	3.383	2.775	3.857	2.403	3.383
4				2.144	2.469	3.384	4.277	3.857	4.939	3.383	4.277
5					1.082	1.387	2.144	2.403	3.383	2.775	3.857
6						2.144	2.469	3.383	4.277	3.857	4.939
7							1.082	1.387	2.144	2.403	3.384
8								2.144	2.469	3.383	4.277
9									1.082	1.387	2.144
10										2.144	2.469
11											1.082

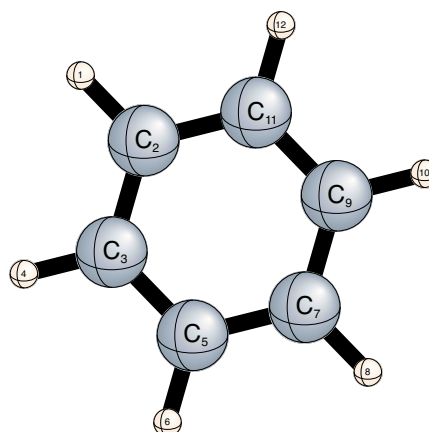
Molecule: benzene

Method: M06

Basis: 6-31G*

Energy: -145616.865318734 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.725435	-1.782346	0.000000
2	C	-0.967947	-1.000152	0.000000
3	C	-1.350037	0.338170	0.000000
4	H	-2.406197	0.603138	0.000000
5	C	-0.382085	1.338291	0.000000
6	H	-0.680854	2.385389	0.000000
7	C	0.967947	1.000152	0.000000
8	H	1.725435	1.782346	0.000000
9	C	1.350037	-0.338170	0.000000
10	H	2.406197	-0.603138	0.000000
11	C	0.382085	-1.338291	0.000000
12	H	0.680854	-2.385389	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.089	2.153	2.481	3.397	4.297	3.873	4.961	3.398	4.297	2.154	2.481
2		1.392	2.154	2.411	3.398	2.784	3.873	2.411	3.397	1.392	2.153
3			1.089	1.392	2.154	2.411	3.398	2.783	3.872	2.411	3.397
4				2.153	2.481	3.397	4.297	3.872	4.961	3.398	4.297
5					1.089	1.392	2.154	2.411	3.398	2.784	3.872
6						2.153	2.481	3.397	4.297	3.872	4.961
7							1.089	1.392	2.154	2.411	3.398
8								2.153	2.481	3.397	4.297
9									1.089	1.392	2.154
10										2.153	2.481
11											1.089

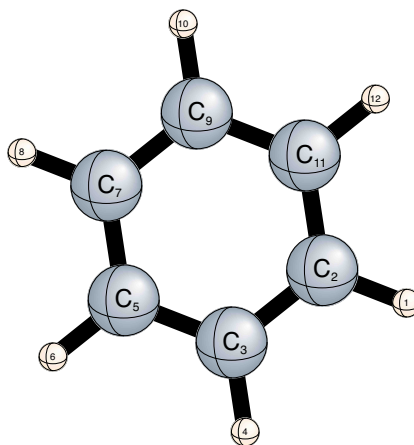
Molecule: benzene

Method: M06

Basis: def2-TZVPP

Energy: -145671.401915081 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.298471	0.899250	0.000000
2	C	1.290233	0.504722	0.000000
3	C	0.207993	1.369742	0.000000
4	H	0.370524	2.440159	0.000000
5	C	-1.082225	0.865024	0.000000
6	H	-1.928030	1.540905	0.000000
7	C	-1.290233	-0.504722	0.000000
8	H	-2.298471	-0.899250	0.000000
9	C	-0.207993	-1.369742	0.000000
10	H	-0.370524	-2.440159	0.000000
11	C	1.082225	-0.865024	0.000000
12	H	1.928030	-1.540905	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.083	2.143	2.468	3.381	4.275	3.854	4.936	3.381	4.275	2.143	2.468
2		1.385	2.143	2.400	3.381	2.771	3.854	2.400	3.381	1.385	2.143
3			1.083	1.385	2.143	2.400	3.381	2.771	3.854	2.400	3.381
4				2.143	2.468	3.381	4.275	3.854	4.936	3.381	4.275
5					1.083	1.385	2.143	2.400	3.381	2.771	3.854
6						2.143	2.468	3.381	4.275	3.854	4.936
7							1.083	1.385	2.143	2.400	3.381
8								2.143	2.468	3.381	4.275
9									1.083	1.385	2.143
10										2.143	2.468
11											1.083

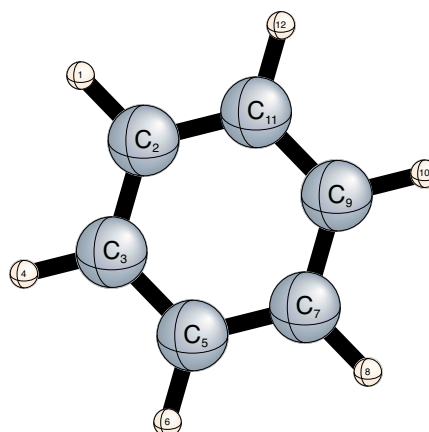
Molecule: benzene

Method: M062X

Basis: 6-31G*

Energy: -145667.741678929 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.723880	-1.781061	0.000000
2	C	-0.968780	-1.000688	0.000000
3	C	-1.351112	0.338646	0.000000
4	H	-2.404428	0.602563	0.000000
5	C	-0.382298	1.339303	0.000000
6	H	-0.680237	2.383484	0.000000
7	C	0.968780	1.000688	0.000000
8	H	1.723880	1.781061	0.000000
9	C	1.351112	-0.338646	0.000000
10	H	2.404428	-0.602563	0.000000
11	C	0.382298	-1.339303	0.000000
12	H	0.680237	-2.383484	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.086	2.152	2.479	3.397	4.293	3.872	4.957	3.396	4.293	2.152	2.478
2		1.393	2.152	2.412	3.396	2.786	3.872	2.413	3.397	1.393	2.152
3			1.086	1.393	2.152	2.413	3.396	2.786	3.872	2.413	3.397
4				2.152	2.479	3.397	4.293	3.872	4.958	3.397	4.293
5					1.086	1.393	2.152	2.413	3.397	2.786	3.871
6						2.152	2.478	3.397	4.293	3.871	4.957
7							1.086	1.393	2.152	2.412	3.396
8								2.152	2.479	3.397	4.293
9									1.086	1.393	2.152
10										2.152	2.479
11											1.086

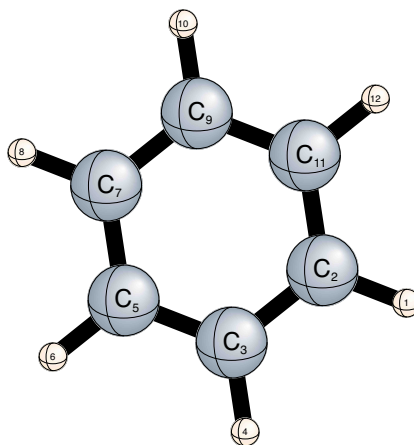
Molecule: benzene

Method: M062X

Basis: def2-TZVPP

Energy: -145724.573361205 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.300614	0.900002	0.000000
2	C	1.292951	0.505806	0.000000
3	C	0.208454	1.372542	0.000000
4	H	0.370690	2.442293	0.000000
5	C	-1.084461	0.866732	0.000000
6	H	-1.929656	1.542336	0.000000
7	C	-1.292951	-0.505806	0.000000
8	H	-2.300614	-0.900002	0.000000
9	C	-0.208454	-1.372542	0.000000
10	H	-0.370690	-2.442293	0.000000
11	C	1.084461	-0.866732	0.000000
12	H	1.929656	-1.542336	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.082	2.145	2.470	3.385	4.279	3.859	4.941	3.385	4.279	2.145	2.470
2		1.388	2.145	2.405	3.385	2.777	3.859	2.405	3.385	1.388	2.145
3			1.082	1.388	2.145	2.405	3.385	2.777	3.859	2.405	3.385
4				2.145	2.470	3.385	4.279	3.859	4.941	3.385	4.279
5					1.082	1.388	2.145	2.405	3.385	2.777	3.859
6						2.145	2.470	3.385	4.279	3.859	4.941
7							1.082	1.388	2.145	2.405	3.385
8								2.145	2.470	3.385	4.279
9									1.082	1.388	2.145
10										2.145	2.470
11											1.082

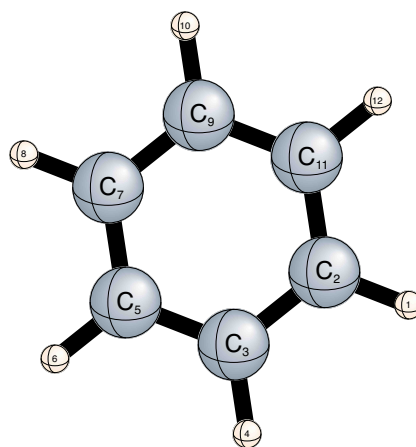
Molecule: benzene

Method: M052X

Basis: 6-31G*

Energy: -145718.255889248 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.305019	0.901752	0.000000
2	C	1.296344	0.507107	0.000000
3	C	0.209054	1.376130	0.000000
4	H	0.371350	2.447011	0.000000
5	C	-1.087227	0.869039	0.000000
6	H	-1.933335	1.545265	0.000000
7	C	-1.296344	-0.507107	0.000000
8	H	-2.305019	-0.901752	0.000000
9	C	-0.209054	-1.376130	0.000000
10	H	-0.371350	-2.447011	0.000000
11	C	1.087227	-0.869039	0.000000
12	H	1.933335	-1.545265	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.083	2.149	2.475	3.392	4.287	3.867	4.950	3.393	4.287	2.149	2.475
2		1.392	2.149	2.411	3.392	2.784	3.867	2.411	3.392	1.392	2.149
3			1.083	1.392	2.149	2.411	3.393	2.784	3.867	2.411	3.392
4				2.149	2.475	3.392	4.287	3.867	4.950	3.392	4.287
5					1.083	1.392	2.149	2.411	3.392	2.784	3.867
6						2.149	2.475	3.392	4.287	3.867	4.950
7							1.083	1.392	2.149	2.411	3.392
8								2.149	2.475	3.392	4.287
9									1.083	1.392	2.149
10										2.149	2.475
11											1.083

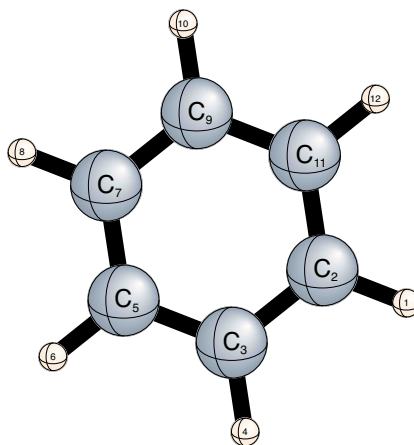
Molecule: benzene

Method: M052X

Basis: def2-TZVPP

Energy: -145776.315169263 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.296861	0.898509	0.000000
2	C	1.291458	0.505280	0.000000
3	C	0.208236	1.371010	0.000000
4	H	0.370057	2.438329	0.000000
5	C	-1.083166	0.865736	0.000000
6	H	-1.926462	1.539798	0.000000
7	C	-1.291458	-0.505280	0.000000
8	H	-2.296861	-0.898509	0.000000
9	C	-0.208236	-1.371010	0.000000
10	H	-0.370057	-2.438329	0.000000
11	C	1.083166	-0.865736	0.000000
12	H	1.926462	-1.539798	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.080	2.141	2.466	3.380	4.272	3.853	4.933	3.380	4.272	2.141	2.466
2		1.387	2.141	2.402	3.380	2.774	3.853	2.402	3.380	1.387	2.141
3			1.080	1.387	2.141	2.402	3.380	2.773	3.853	2.402	3.380
4				2.141	2.466	3.380	4.272	3.853	4.933	3.380	4.272
5					1.080	1.387	2.141	2.402	3.380	2.773	3.853
6						2.141	2.466	3.380	4.272	3.853	4.932
7							1.080	1.387	2.141	2.402	3.380
8								2.141	2.466	3.380	4.272
9									1.080	1.387	2.141
10										2.141	2.466
11											1.080

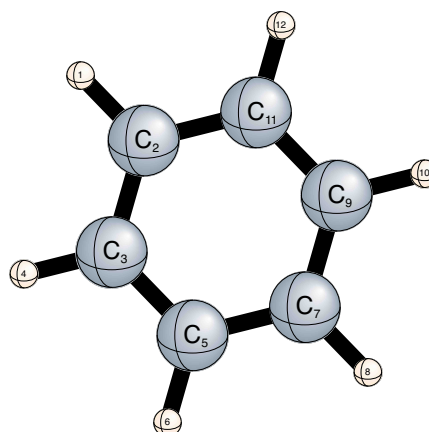
Molecule: benzene

Method: M06L

Basis: 6-31G*

Energy: -145713.084526083 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.726315	-1.783164	0.000000
2	C	-0.969074	-1.000995	0.000000
3	C	-1.351334	0.338751	0.000000
4	H	-2.407351	0.603179	0.000000
5	C	-0.382375	1.339792	0.000000
6	H	-0.681361	2.386573	0.000000
7	C	0.969074	1.000995	0.000000
8	H	1.726315	1.783164	0.000000
9	C	1.351334	-0.338751	0.000000
10	H	2.407351	-0.603179	0.000000
11	C	0.382375	-1.339792	0.000000
12	H	0.681361	-2.386573	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.089	2.155	2.482	3.400	4.299	3.875	4.964	3.400	4.299	2.155	2.482
2		1.393	2.155	2.413	3.400	2.786	3.875	2.413	3.400	1.393	2.155
3			1.089	1.393	2.155	2.413	3.400	2.786	3.875	2.413	3.400
4				2.155	2.482	3.400	4.299	3.875	4.964	3.400	4.299
5					1.089	1.393	2.155	2.413	3.400	2.787	3.875
6						2.155	2.482	3.400	4.299	3.875	4.964
7							1.089	1.393	2.155	2.413	3.400
8								2.155	2.482	3.400	4.299
9									1.089	1.393	2.155
10										2.155	2.482
11											1.089

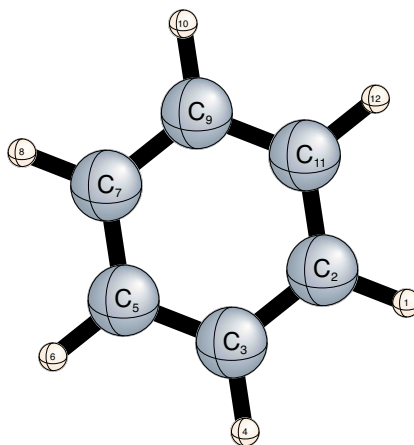
Molecule: benzene

Method: M06L

Basis: def2-TZVPP

Energy: -145768.796507028 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.299267	0.899552	0.000000
2	C	1.292318	0.505587	0.000000
3	C	0.208257	1.372023	0.000000
4	H	0.370757	2.441064	0.000000
5	C	-1.084129	0.866396	0.000000
6	H	-1.928715	1.541497	0.000000
7	C	-1.292318	-0.505587	0.000000
8	H	-2.299267	-0.899552	0.000000
9	C	-0.208257	-1.372023	0.000000
10	H	-0.370757	-2.441064	0.000000
11	C	1.084129	-0.866396	0.000000
12	H	1.928715	-1.541497	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.081	2.144	2.469	3.384	4.276	3.857	4.938	3.383	4.277	2.144	2.469
2		1.388	2.144	2.404	3.384	2.775	3.857	2.404	3.384	1.388	2.144
3			1.081	1.388	2.144	2.404	3.383	2.775	3.857	2.404	3.384
4				2.144	2.469	3.384	4.277	3.857	4.938	3.384	4.276
5					1.081	1.388	2.144	2.404	3.384	2.776	3.857
6						2.144	2.469	3.384	4.276	3.857	4.938
7							1.081	1.388	2.144	2.404	3.384
8								2.144	2.469	3.384	4.276
9									1.081	1.388	2.144
10										2.144	2.469
11											1.081

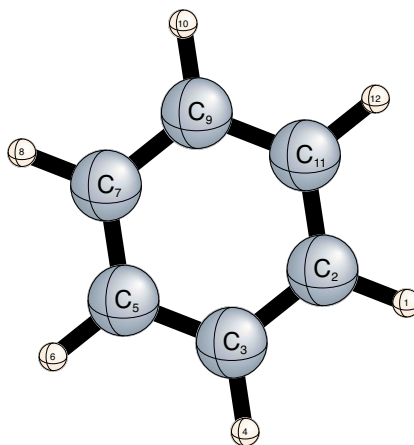
Molecule: benzene

Method: M06HF

Basis: 6-31G*

Energy: -145695.505531627 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.304544	0.901499	0.000000
2	C	1.296725	0.507263	0.000000
3	C	0.209136	1.376501	0.000000
4	H	0.371173	2.446409	0.000000
5	C	-1.087497	0.869246	0.000000
6	H	-1.932869	1.544914	0.000000
7	C	-1.296725	-0.507263	0.000000
8	H	-2.304544	-0.901499	0.000000
9	C	-0.209136	-1.376501	0.000000
10	H	-0.371173	-2.446409	0.000000
11	C	1.087497	-0.869246	0.000000
12	H	1.932869	-1.544914	0.000000

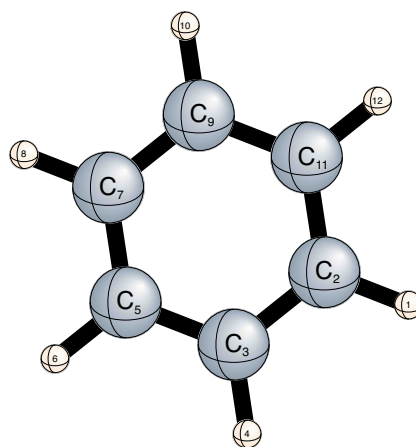


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.082	2.149	2.475	3.392	4.286	3.867	4.949	3.392	4.286	2.149	2.474
2		1.392	2.149	2.412	3.392	2.785	3.867	2.412	3.392	1.392	2.149
3			1.082	1.392	2.149	2.412	3.392	2.785	3.867	2.411	3.392
4				2.148	2.474	3.392	4.286	3.867	4.949	3.392	4.286
5					1.082	1.392	2.149	2.411	3.392	2.784	3.867
6						2.149	2.474	3.392	4.286	3.867	4.949
7							1.082	1.392	2.149	2.412	3.392
8								2.149	2.475	3.392	4.286
9									1.082	1.392	2.149
10										2.148	2.474
11											1.082

Molecule: benzene
Method: M06HF
Basis: def2-TZVPP
Energy: -145760.719209297 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.299474	0.899421	0.000000
2	C	1.292537	0.505711	0.000000
3	C	0.208438	1.372089	0.000000
4	H	0.370293	2.440952	0.000000
5	C	-1.083989	0.866378	0.000000
6	H	-1.928526	1.541509	0.000000
7	C	-1.292537	-0.505711	0.000000
8	H	-2.299474	-0.899421	0.000000
9	C	-0.208438	-1.372089	0.000000
10	H	-0.370293	-2.440952	0.000000
11	C	1.083989	-0.866378	0.000000
12	H	1.928526	-1.541509	0.000000

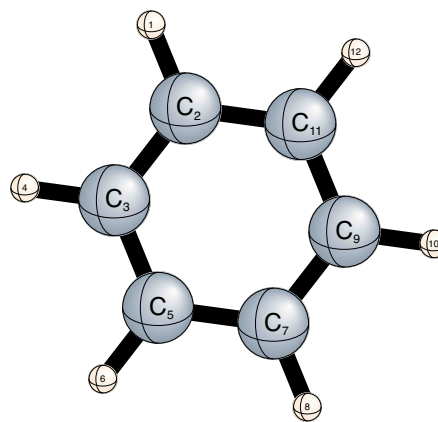


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.081	2.144	2.469	3.384	4.276	3.857	4.938	3.384	4.276	2.144	2.469
2		1.388	2.144	2.404	3.384	2.776	3.857	2.404	3.383	1.388	2.144
3			1.081	1.388	2.144	2.404	3.384	2.776	3.857	2.404	3.383
4				2.143	2.469	3.383	4.276	3.857	4.938	3.383	4.276
5					1.081	1.388	2.144	2.404	3.383	2.775	3.857
6						2.144	2.469	3.383	4.276	3.857	4.938
7							1.081	1.388	2.144	2.404	3.384
8								2.144	2.469	3.384	4.276
9									1.081	1.388	2.144
10										2.143	2.469
11											1.081

Molecule: benzene
Method: RI-MP2
Basis: def2-TZVPP
Energy: -145470.601844438 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-0.934232	-2.286024	0.000000
2	C	-0.525894	-1.286838	0.000000
3	C	-1.377382	-0.187981	0.000000
4	H	-2.446871	-0.333943	0.000000
5	C	-0.851487	1.098857	0.000000
6	H	-1.512636	1.952082	0.000000
7	C	0.525894	1.286838	0.000000
8	H	0.934232	2.286024	0.000000
9	C	1.377382	0.187981	0.000000
10	H	2.446871	0.333943	0.000000
11	C	0.851487	-1.098857	0.000000
12	H	1.512636	-1.952082	0.000000

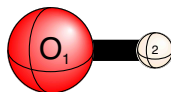


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12
1	1.079	2.144	2.470	3.386	4.277	3.860	4.939	3.386	4.277	2.144	2.470
2		1.390	2.144	2.408	3.386	2.780	3.860	2.408	3.386	1.390	2.144
3			1.079	1.390	2.144	2.408	3.386	2.780	3.860	2.408	3.386
4				2.144	2.470	3.386	4.277	3.860	4.939	3.386	4.277
5					1.079	1.390	2.144	2.408	3.386	2.780	3.860
6						2.144	2.470	3.386	4.277	3.860	4.939
7							1.079	1.390	2.144	2.408	3.386
8								2.144	2.470	3.386	4.277
9									1.079	1.390	2.144
10										2.144	2.470
11											1.079

Molecule: hydroxyl radical
Method: B3LYP
Basis: 6-31G*
Energy: -47517.148825805 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.106374
2	H	0.000000	0.000000	0.876540



Distance Matrix

		2
1		0.983

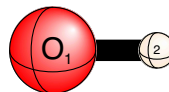
Molecule: hydroxyl radical

Method: B3LYP

Basis: def2-TZVPP

Energy: -47546.2599836245 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.111568
2	H	0.000000	0.000000	0.862675



Distance Matrix

		2
1		0.974

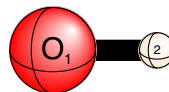
Molecule: hydroxyl radical

Method: ω B97

Basis: 6-31G*

Energy: -47507.4793959244 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.114319
2	H	0.000000	0.000000	0.865426



Distance Matrix

		2
1		0.980

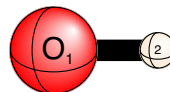
Molecule: hydroxyl radical

Method: ω B97

Basis: def2-TZVPP

Energy: -47535.7488809424 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.104695
2	H	0.000000	0.000000	0.866719



Distance Matrix

		2
1		0.971

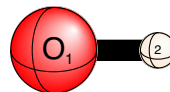
Molecule: hydroxyl radical

Method: ω B97X

Basis: 6-31G*

Energy: -47503.8316974026 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.113393
2	H	0.000000	0.000000	0.864500



Distance Matrix

		2
1		0.978

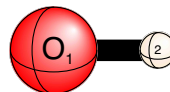
Molecule: hydroxyl radical

Method: ω B97X

Basis: def2-TZVPP

Energy: -47531.7352016015 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.104581
2	H	0.000000	0.000000	0.865164



Distance Matrix

		2
1		0.970

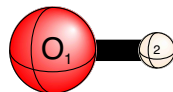
Molecule: hydroxyl radical

Method: ω B97X-D

Basis: 6-31G*

Energy: -47501.5118317701 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.106227
2	H	0.000000	0.000000	0.870716



Distance Matrix

		2
1		0.977

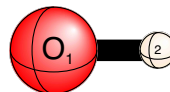
Molecule: hydroxyl radical

Method: ω B97X-D

Basis: def2-TZVPP

Energy: -47529.2833526285 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.108938
2	H	0.000000	0.000000	0.860045

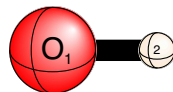


Distance Matrix

		2
1		0.969

Molecule: hydroxyl radical
Method: M06
Basis: 6-31G*
Energy: -47494.484560537 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.103704
2	H	0.000000	0.000000	0.873869

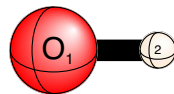


Distance Matrix

		2
1		0.978

Molecule: hydroxyl radical
Method: M06
Basis: def2-TZVPP
Energy: -47521.033870821 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.108705
2	H	0.000000	0.000000	0.859812



Distance Matrix

		2
1		0.969

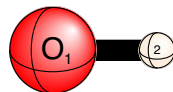
Molecule: hydroxyl radical

Method: M062X

Basis: 6-31G*

Energy: -47495.3180412086 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.104371
2	H	0.000000	0.000000	0.874537



Distance Matrix

		2
1		0.979

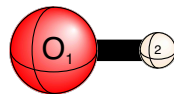
Molecule: hydroxyl radical

Method: M062X

Basis: def2-TZVPP

Energy: -47523.4477875024 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.110066
2	H	0.000000	0.000000	0.861173



Distance Matrix

		2
1		0.971

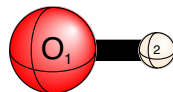
Molecule: hydroxyl radical

Method: M052X

Basis: 6-31G*

Energy: -47508.0311275651 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.112718
2	H	0.000000	0.000000	0.863825



Distance Matrix

		2
1		0.977

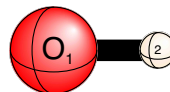
Molecule: hydroxyl radical

Method: M052X

Basis: def2-TZVPP

Energy: -47535.6545839099 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.109082
2	H	0.000000	0.000000	0.860189



Distance Matrix

		2
1		0.969

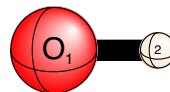
Molecule: hydroxyl radical

Method: M06L

Basis: 6-31G*

Energy: -47511.6957230218 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.103698
2	H	0.000000	0.000000	0.873864



Distance Matrix

		2
1		0.978

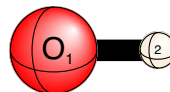
Molecule: hydroxyl radical

Method: M06L

Basis: def2-TZVPP

Energy: -47536.8111011947 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.108788
2	H	0.000000	0.000000	0.859895



Distance Matrix

		2
1		0.969

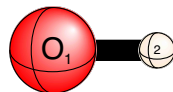
Molecule: hydroxyl radical

Method: M06HF

Basis: 6-31G*

Energy: -47493.3020166889 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.114610
2	H	0.000000	0.000000	0.865717



Distance Matrix

		2
1		0.980

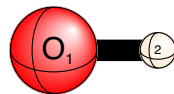
Molecule: hydroxyl radical

Method: M06HF

Basis: def2-TZVPP

Energy: -47525.6218790291 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.110287
2	H	0.000000	0.000000	0.861394



Distance Matrix

		2
1		0.972

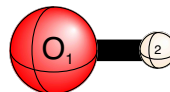
Molecule: hydroxyl radical

Method: RI-MP2

Basis: def2-TZVPP

Energy: -47462.9466064138 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	O	0.000000	0.000000	-0.103820
2	H	0.000000	0.000000	0.861889



Distance Matrix

		2
1		0.966

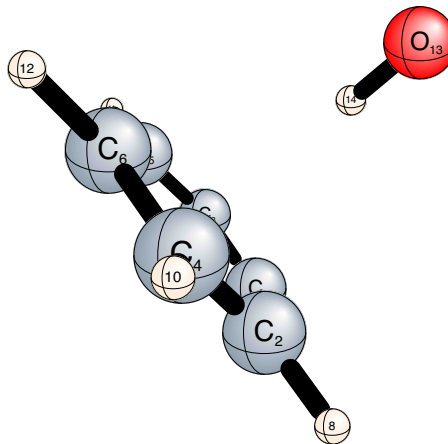
Molecule: $[\text{C}_6\text{H}_6 \cdots \text{OH}]$ (Intermediate 1, C_{6v} input geometry)

Method: B3LYP

Basis: 6-31G*

Energy: -193258.535728417 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.397856	0.000000	-0.564727
2	C	0.698928	1.210579	-0.564727
3	C	0.698928	-1.210579	-0.564727
4	C	-0.698928	1.210579	-0.564727
5	C	-0.698928	-1.210579	-0.564727
6	C	-1.397856	0.000000	-0.564727
7	H	2.484386	0.000000	-0.559210
8	H	1.242193	2.151542	-0.559210
9	H	1.242193	-2.151542	-0.559210
10	H	-1.242193	2.151542	-0.559210
11	H	-1.242193	-2.151542	-0.559210
12	H	-2.484386	0.000000	-0.559210
13	O	0.000000	0.000000	2.752347
14	H	0.000000	0.000000	1.769710



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.398	1.398	2.421	2.421	2.796	1.087	2.157	2.157	3.406	3.406	3.882	3.600	2.721
2		2.421	1.398	2.796	2.421	2.157	1.087	3.406	2.157	3.882	3.406	3.600	2.721
3			2.796	1.398	2.421	2.157	3.406	1.087	3.882	2.157	3.406	3.600	2.721
4				2.421	1.398	3.406	2.157	3.882	1.087	3.406	2.157	3.600	2.721
5					1.398	3.406	3.882	2.157	3.406	1.087	2.157	3.600	2.721
6						3.882	3.406	3.406	2.157	2.157	1.087	3.600	2.721
7							2.484	2.484	4.303	4.303	4.969	4.140	3.405
8								4.303	2.484	4.969	4.303	4.140	3.405
9									4.969	2.484	4.303	4.140	3.405
10										4.303	2.484	4.140	3.405
11											2.484	4.140	3.405
12												4.140	3.405
13													0.983

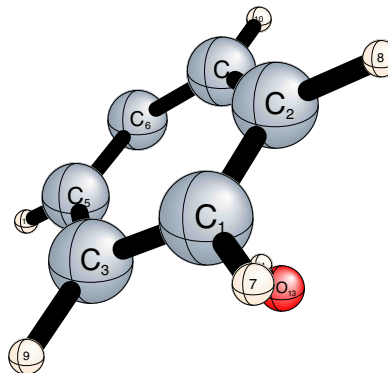
Molecule: $[\text{C}_6\text{H}_6 \cdots \text{OH}]$ (Intermediate 1, C_{6v} input geometry)

Method: B3LYP

Basis: def2-TZVPP

Energy: -193344.172071783 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	-0.581002	1.392280	0.011653
2	C	-0.580606	0.686454	1.210944
3	C	-0.579912	0.705962	-1.199372
4	C	-0.580201	-0.705905	1.199321
5	C	-0.580491	-0.686395	-1.210994
6	C	-0.581176	-1.392222	-0.011704
7	H	-0.576535	2.474054	0.020451
8	H	-0.576886	1.219464	2.152401
9	H	-0.576651	1.254529	-2.131914
10	H	-0.577163	-1.254468	2.131866
11	H	-0.576682	-1.219410	-2.152449
12	H	-0.576842	-2.473996	-0.020498
13	O	2.849018	-0.000148	0.000104
14	H	1.873560	-0.000079	0.000057



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.392	1.392	2.411	2.412	2.785	1.082	2.148	2.148	3.391	3.392	3.866	3.702	2.822
2		2.410	1.392	2.784	2.412	2.148	1.082	3.391	2.148	3.866	3.392	3.701	2.821
3			2.783	1.392	2.411	2.148	3.391	1.082	3.865	2.148	3.391	3.701	2.821
4				2.410	1.392	3.391	2.148	3.865	1.082	3.391	2.148	3.701	2.821
5					1.392	3.392	3.866	2.148	3.391	1.082	2.148	3.701	2.821
6						3.866	3.392	3.391	2.148	2.148	1.082	3.702	2.822
7							2.474	2.474	4.285	4.285	4.948	4.226	3.482
8								4.284	2.474	4.948	4.285	4.226	3.482
9									4.947	2.474	4.285	4.226	3.482
10										4.284	2.474	4.226	3.482
11											2.474	4.226	3.482
12												4.226	3.482
13													0.975

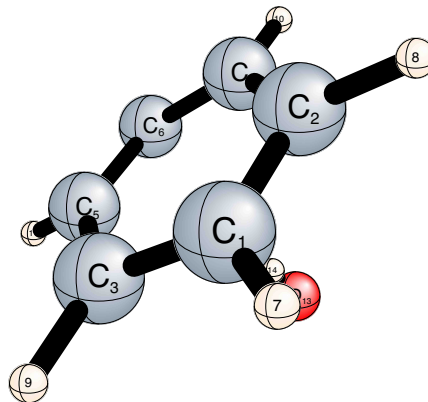
Molecule: $[\text{C}_6\text{H}_6 \cdots \text{OH}]$ (Intermediate 1, C_{6v} input geometry)

Method: ωB97

Basis: 6-31G*

Energy: -193215.019349747 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	-0.544960	1.395393	0.011445
2	C	-0.545669	0.687765	1.214545
3	C	-0.545491	0.707655	-1.203166
4	C	-0.545738	-0.707600	1.203095
5	C	-0.545590	-0.687705	-1.214615
6	C	-0.545128	-1.395335	-0.011511
7	H	-0.538255	2.484223	0.020470
8	H	-0.538145	1.224440	2.161891
9	H	-0.537861	1.259868	-2.141539
10	H	-0.538298	-1.259808	2.141473
11	H	-0.538008	-1.224386	-2.161957
12	H	-0.538555	-2.484166	-0.020542
13	O	2.630709	-0.000147	0.000171
14	H	1.649420	-0.000078	0.000105



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.396	1.396	2.417	2.417	2.791	1.089	2.157	2.157	3.404	3.404	3.880	3.469	2.601
2		2.418	1.395	2.792	2.417	2.157	1.089	3.405	2.157	3.880	3.404	3.469	2.601
3			2.792	1.395	2.417	2.157	3.405	1.089	3.880	2.157	3.404	3.469	2.601
4				2.418	1.396	3.404	2.157	3.880	1.089	3.405	2.157	3.469	2.601
5					1.396	3.404	3.880	2.157	3.405	1.089	2.157	3.469	2.601
6						3.880	3.404	3.404	2.157	2.157	1.089	3.469	2.601
7							2.484	2.485	4.303	4.303	4.969	4.027	3.310
8								4.304	2.484	4.969	4.303	4.027	3.310
9									4.969	2.484	4.303	4.027	3.310
10										4.304	2.485	4.027	3.310
11											2.484	4.027	3.310
12												4.027	3.310
13													0.981

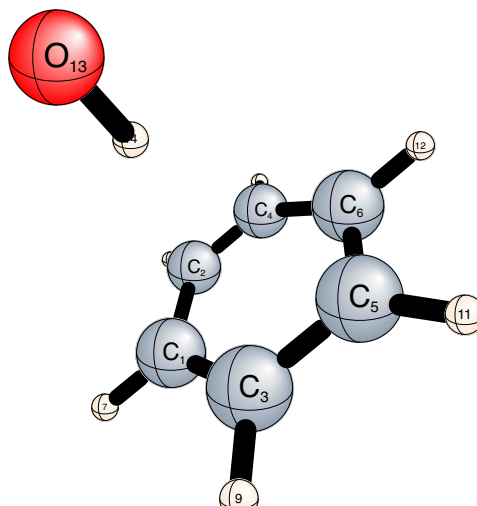
Molecule: $[\text{C}_6\text{H}_6 \cdots \text{OH}]$ (Intermediate 1, C_{6v} input geometry)

Method: ωB97

Basis: def2-TZVPP

Energy: -193295.608118648 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.550646	0.004602	-1.391209
2	C	0.550180	-1.202057	-0.700040
3	C	0.549425	1.206671	-0.691258
4	C	0.549470	-1.206661	0.691234
5	C	0.550194	1.202066	0.700016
6	C	0.550705	-0.004592	1.391185
7	H	0.544140	0.008492	-2.475705
8	H	0.544271	-2.139492	-1.245529
9	H	0.544417	2.147903	-1.230339
10	H	0.544497	-2.147893	1.230315
11	H	0.544296	2.139501	1.245506
12	H	0.544245	-0.008483	2.475682
13	O	-2.683061	-0.000029	0.000066
14	H	-1.708382	-0.000013	0.000025



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.391	1.391	2.409	2.410	2.782	1.085	2.149	2.149	3.392	3.393	3.867	3.520	2.653
2		2.409	1.391	2.782	2.410	2.149	1.085	3.392	2.150	3.867	3.393	3.520	2.653
3			2.781	1.391	2.409	2.149	3.392	1.085	3.866	2.150	3.392	3.519	2.652
4				2.409	1.391	3.392	2.150	3.866	1.085	3.392	2.149	3.519	2.652
5					1.391	3.393	3.867	2.150	3.392	1.085	2.149	3.520	2.653
6						3.867	3.393	3.392	2.149	2.149	1.085	3.520	2.653
7							2.475	2.475	4.288	4.288	4.951	4.067	3.347
8								4.287	2.476	4.951	4.288	4.067	3.347
9									4.951	2.476	4.288	4.067	3.347
10										4.287	2.475	4.067	3.347
11											2.475	4.067	3.347
12												4.067	3.347
13													0.975

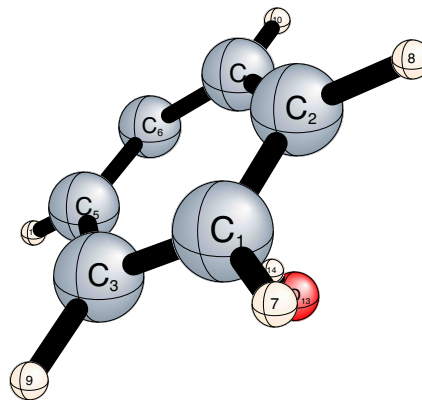
Molecule: $[\text{C}_6\text{H}_6 \cdots \text{OH}]$ (Intermediate 1, C_{6v} input geometry)

Method: ωB97X

Basis: 6-31G*

Energy: -193202.824056834 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	-0.549261	1.393333	0.011458
2	C	-0.549952	0.686752	1.212770
3	C	-0.549728	0.706605	-1.201377
4	C	-0.549975	-0.706550	1.201307
5	C	-0.549873	-0.686691	-1.212840
6	C	-0.549429	-1.393275	-0.011519
7	H	-0.543005	2.480069	0.020437
8	H	-0.542891	1.222396	2.158271
9	H	-0.542644	1.257730	-2.137947
10	H	-0.543080	-1.257671	2.137881
11	H	-0.542754	-1.222341	-2.158337
12	H	-0.543305	-2.480012	-0.020518
13	O	2.656865	-0.000148	0.000172
14	H	1.677464	-0.000078	0.000107



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.394	1.394	2.414	2.414	2.787	1.087	2.154	2.154	3.398	3.399	3.873	3.496	2.627
2		2.414	1.393	2.787	2.414	2.154	1.087	3.399	2.153	3.874	3.398	3.497	2.627
3			2.787	1.393	2.414	2.154	3.399	1.087	3.874	2.153	3.398	3.496	2.627
4				2.414	1.394	3.398	2.153	3.874	1.087	3.399	2.154	3.497	2.627
5					1.394	3.398	3.874	2.153	3.399	1.087	2.154	3.497	2.627
6						3.873	3.398	3.398	2.154	2.154	1.087	3.496	2.627
7							2.480	2.480	4.296	4.296	4.960	4.049	3.329
8								4.296	2.480	4.961	4.296	4.049	3.329
9									4.961	2.480	4.296	4.049	3.329
10										4.296	2.480	4.049	3.329
11											2.480	4.049	3.329
12												4.049	3.329
13													0.979

Molecule: $[\text{C}_6\text{H}_6 \cdots \text{OH}]$ (Intermediate 1, C_{6v} input geometry)

Method: ωB97X

Basis: def2-TZVPP

Energy: not available kcal/mol

(This calculation failed to converge to a suitable accuracy after multiple attempts)

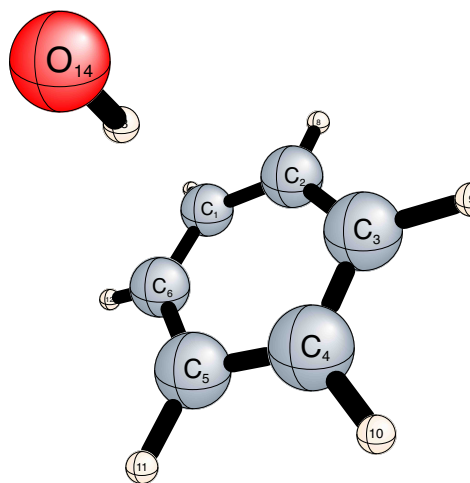
Molecule: $[\text{C}_6\text{H}_6 \cdots \text{OH}]$ (Intermediate 1, C_{6v} input geometry)

Method: $\omega\text{B97X-D}$

Basis: 6-31G*

Energy: -193191.528855929 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.316822	-1.457608	0.000000
2	C	0.433280	-0.769692	1.207537
3	C	0.667049	0.604628	1.206672
4	C	0.784406	1.290892	0.000000
5	C	0.667049	0.604628	-1.206672
6	C	0.433280	-0.769692	-1.207537
7	H	0.130148	-2.527169	0.000000
8	H	0.337102	-1.304024	2.147755
9	H	0.750555	1.141128	2.146716
10	H	0.957113	2.362524	0.000000
11	H	0.750555	1.141128	-2.146716
12	H	0.337102	-1.304024	-2.147755
13	H	-1.745948	0.054218	0.000000
14	O	-2.637770	0.456695	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.395	2.415	2.788	2.415	1.395	1.086	2.153	3.399	3.873	3.399	2.153	2.557	3.521
2		1.394	2.414	2.788	2.415	2.154	1.086	2.153	3.398	3.873	3.399	2.624	3.520
3			1.393	2.413	2.788	3.399	2.153	1.086	2.152	3.397	3.873	2.753	3.521
4				1.393	2.414	3.874	3.398	2.152	1.085	2.152	3.398	2.816	3.522
5					1.394	3.399	3.873	3.397	2.152	1.086	2.153	2.753	3.521
6						2.154	3.399	3.873	3.398	2.153	1.086	2.624	3.520
7							2.480	4.295	4.959	4.295	2.480	3.191	4.070
8								2.480	4.294	4.959	4.296	3.286	4.070
9									2.478	4.293	4.959	3.467	4.069
10										2.478	4.294	3.555	4.069
11											2.480	3.467	4.069
12												3.286	4.070
13													0.978

Molecule: $[\text{C}_6\text{H}_6 \cdots \text{OH}]$ (Intermediate 1, C_{6v} input geometry)

Method: $\omega\text{B97X-D}$

Basis: def2-TZVPP

Energy: not available kcal/mol

(This calculation failed to converge to a suitable accuracy after multiple attempts)

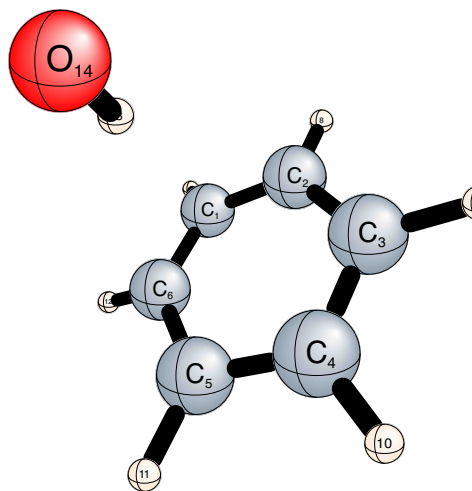
Molecule: $[\text{C}_6\text{H}_6 \cdots \text{OH}]$ (Intermediate 1, C_{6v} input geometry)

Method: M06

Basis: 6-31G*

Energy: -193115.795463643 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.280314	-1.429613	0.000000
2	C	0.413282	-0.744665	1.207046
3	C	0.682543	0.621929	1.205700
4	C	0.818766	1.303780	0.000000
5	C	0.682543	0.621929	-1.205700
6	C	0.413282	-0.744665	-1.207046
7	H	0.070914	-2.497987	0.000000
8	H	0.305467	-1.278162	2.149795
9	H	0.781335	1.157190	2.148166
10	H	1.021839	2.372885	0.000000
11	H	0.781335	1.157190	-2.148166
12	H	0.305467	-1.278162	-2.149795
13	H	-1.773962	-0.131544	0.000000
14	O	-2.602382	0.393525	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.394	2.413	2.786	2.413	1.394	1.089	2.155	3.400	3.874	3.400	2.155	2.430	3.411
2		1.393	2.412	2.786	2.414	2.156	1.089	2.154	3.398	3.874	3.401	2.572	3.442
3			1.392	2.411	2.786	3.400	2.155	1.088	2.153	3.398	3.875	2.838	3.507
4				1.392	2.412	3.875	3.399	2.153	1.088	2.153	3.399	2.964	3.540
5					1.393	3.400	3.875	3.398	2.153	1.088	2.155	2.838	3.507
6						2.156	3.401	3.874	3.398	2.154	1.089	2.572	3.442
7							2.483	4.299	4.963	4.299	2.483	3.001	3.938
8								2.481	4.297	4.963	4.300	3.203	3.984
9									2.480	4.296	4.963	3.578	4.080
10										2.480	4.297	3.753	4.130
11											2.481	3.578	4.080
12												3.203	3.984
13													0.981

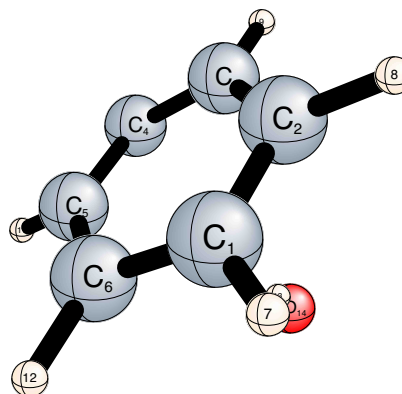
Molecule: $[\text{C}_6\text{H}_6 \cdots \text{OH}]$ (Intermediate 1, C_{6v} input geometry)

Method: M06

Basis: def2-TZVPP

Energy: -193196.139690404 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	-0.467002	1.346594	0.000000
2	C	-0.516391	0.654168	1.201121
3	C	-0.617501	-0.728735	1.200096
4	C	-0.669445	-1.419208	0.000000
5	C	-0.617501	-0.728735	-1.200096
6	C	-0.516391	0.654168	-1.201121
7	H	-0.388861	2.426281	0.000000
8	H	-0.475674	1.193909	2.138526
9	H	-0.652490	-1.268690	2.137455
10	H	-0.743101	-2.498945	0.000000
11	H	-0.652490	-1.268690	-2.137455
12	H	-0.475674	1.193909	-2.138526
13	H	1.790652	0.360656	0.000000
14	O	2.735856	0.129656	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.387	2.402	2.773	2.402	1.387	1.083	2.144	3.383	3.855	3.383	2.144	2.464	3.426
2		1.387	2.401	2.773	2.402	2.145	1.082	2.143	3.382	3.855	3.383	2.617	3.506
3			1.386	2.400	2.773	3.383	2.144	1.082	2.142	3.381	3.855	2.903	3.664
4				1.386	2.401	3.856	3.382	2.143	1.082	2.143	3.382	3.036	3.741
5					1.387	3.383	3.855	3.381	2.142	1.082	2.144	2.903	3.664
6						2.145	3.383	3.855	3.382	2.143	1.082	2.617	3.506
7							2.470	4.277	4.938	4.277	2.470	3.003	3.878
8								2.469	4.276	4.938	4.277	3.225	4.002
9									2.468	4.275	4.938	3.632	4.243
10										2.468	4.276	3.821	4.360
11											2.469	3.632	4.243
12												3.225	4.002
13													0.973

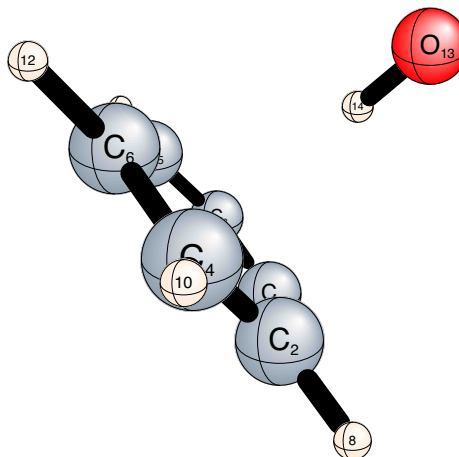
Molecule: $[\text{C}_6\text{H}_6 \cdots \text{OH}]$ (Intermediate 1, C_{6v} input geometry)

Method: M062X

Basis: 6-31G*

Energy: -193168.3632185 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.394322	0.000000	-0.540615
2	C	0.697161	1.207519	-0.540615
3	C	0.697161	-1.207519	-0.540615
4	C	-0.697161	1.207519	-0.540615
5	C	-0.697161	-1.207519	-0.540615
6	C	-1.394322	0.000000	-0.540615
7	H	2.479691	0.000000	-0.531642
8	H	1.239845	2.147475	-0.531642
9	H	1.239845	-2.147475	-0.531642
10	H	-1.239845	2.147475	-0.531642
11	H	-1.239845	-2.147475	-0.531642
12	H	-2.479691	0.000000	-0.531642
13	O	0.000000	0.000000	2.595882
14	H	0.000000	0.000000	1.616089



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.394	1.394	2.415	2.415	2.789	1.085	2.153	2.153	3.399	3.399	3.874	3.432	2.568
2		2.415	1.394	2.789	2.415	2.153	1.085	3.399	2.153	3.874	3.399	3.432	2.568
3			2.789	1.394	2.415	2.153	3.399	1.085	3.874	2.153	3.399	3.432	2.568
4				2.415	1.394	3.399	2.153	3.874	1.085	3.399	2.153	3.432	2.568
5					1.394	3.399	3.874	2.153	3.399	1.085	2.153	3.432	2.568
6						3.874	3.399	3.399	2.153	2.153	1.085	3.432	2.568
7							2.480	2.480	4.295	4.295	4.959	3.991	3.280
8								4.295	2.480	4.959	4.295	3.991	3.280
9									4.959	2.480	4.295	3.991	3.280
10										4.295	2.480	3.991	3.280
11											2.480	3.991	3.280
12												3.991	3.280
13													0.980

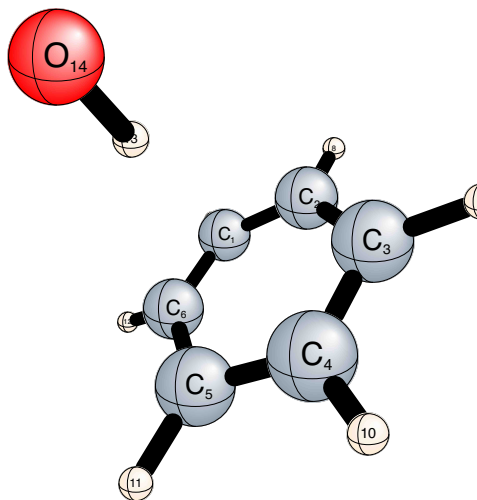
Molecule: $[\text{C}_6\text{H}_6 \cdots \text{OH}]$ (Intermediate 1, C_{6v} input geometry)

Method: M062X

Basis: def2-TZVPP

Energy: -193252.813935065 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.561556	-1.384781	0.000000
2	C	0.555195	-0.690142	1.203744
3	C	0.539067	0.698810	1.203702
4	C	0.529454	1.393348	0.000000
5	C	0.539067	0.698810	-1.203702
6	C	0.555195	-0.690142	-1.203744
7	H	0.567774	-2.466487	0.000000
8	H	0.554254	-1.230996	2.140309
9	H	0.525332	1.239511	2.140251
10	H	0.510628	2.474884	0.000000
11	H	0.525332	1.239511	-2.140251
12	H	0.554254	-1.230996	-2.140309
13	H	-1.677857	-0.036335	0.000000
14	O	-2.651640	-0.017096	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.390	2.406	2.778	2.406	1.390	1.082	2.146	3.387	3.860	3.387	2.146	2.614	3.492
2		1.389	2.406	2.779	2.407	2.146	1.082	2.145	3.386	3.861	3.388	2.620	3.491
3			1.390	2.407	2.779	3.387	2.145	1.082	2.146	3.387	3.861	2.628	3.485
4				1.390	2.406	3.860	3.387	2.146	1.082	2.146	3.387	2.630	3.480
5					1.389	3.387	3.861	3.387	2.146	1.082	2.145	2.628	3.485
6						2.146	3.388	3.861	3.386	2.145	1.082	2.620	3.491
7							2.471	4.280	4.942	4.280	2.471	3.309	4.045
8								2.471	4.280	4.942	4.281	3.315	4.041
9									2.471	4.281	4.942	3.326	4.031
10										2.471	4.280	3.331	4.026
11											2.471	3.326	4.031
12												3.315	4.041
13													0.974

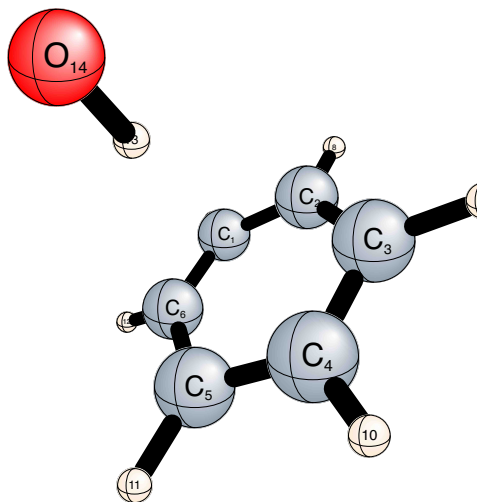
Molecule: [C₆H₆⋯OH] (Intermediate 1, C_{6v} input geometry)

Method: M052X

Basis: 6-31G*

Energy: -193231.394919992 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.558171	-1.389960	0.000000
2	C	0.551646	-0.693245	1.206946
3	C	0.536706	0.699790	1.206887
4	C	0.528444	1.396392	0.000000
5	C	0.536706	0.699790	-1.206887
6	C	0.551646	-0.693245	-1.206946
7	H	0.562624	-2.472665	0.000000
8	H	0.549161	-1.234429	2.144552
9	H	0.522281	1.240812	2.144466
10	H	0.509548	2.478912	0.000000
11	H	0.522281	1.240812	-2.144466
12	H	0.549161	-1.234429	-2.144552
13	H	-1.656092	-0.032798	0.000000
14	O	-2.633332	-0.010130	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.394	2.413	2.787	2.413	1.394	1.083	2.150	3.394	3.869	3.394	2.150	2.597	3.477
2		1.393	2.413	2.787	2.414	2.150	1.083	2.150	3.394	3.870	3.395	2.601	3.474
3			1.394	2.414	2.787	3.394	2.150	1.083	2.150	3.395	3.870	2.608	3.466
4				1.394	2.413	3.869	3.394	2.150	1.083	2.150	3.394	2.611	3.461
5					1.393	3.394	3.870	3.395	2.150	1.083	2.150	2.608	3.466
6						2.150	3.395	3.870	3.394	2.150	1.083	2.601	3.474
7							2.476	4.288	4.952	4.288	2.476	3.298	4.035
8								2.475	4.288	4.952	4.289	3.302	4.028
9									2.476	4.289	4.952	3.312	4.015
10										2.476	4.288	3.316	4.009
11											2.475	3.312	4.015
12												3.302	4.028
13													0.978

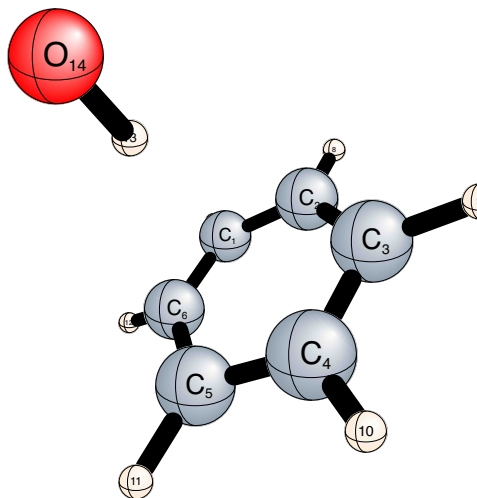
Molecule: [C₆H₆...OH] (Intermediate 1, C_{6v} input geometry)

Method: M052X

Basis: def2-TZVPP

Energy: -193316.617923179 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.579763	-1.376990	0.000000
2	C	0.564766	-0.683228	1.202354
3	C	0.531668	0.703820	1.202314
4	C	0.513816	1.397453	0.000000
5	C	0.531668	0.703820	-1.202314
6	C	0.564766	-0.683228	-1.202354
7	H	0.599674	-2.456045	0.000000
8	H	0.570681	-1.222741	2.136815
9	H	0.511466	1.243001	2.136771
10	H	0.482112	2.476199	0.000000
11	H	0.511466	1.243001	-2.136771
12	H	0.570681	-1.222741	-2.136815
13	H	-1.695643	-0.056631	0.000000
14	O	-2.667813	-0.047367	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.388	2.404	2.775	2.404	1.388	1.079	2.142	3.382	3.854	3.382	2.142	2.631	3.509
2		1.387	2.404	2.776	2.405	2.142	1.079	2.142	3.381	3.855	3.382	2.636	3.507
3			1.388	2.405	2.776	3.382	2.142	1.079	2.142	3.382	3.855	2.643	3.500
4				1.388	2.404	3.854	3.382	2.142	1.079	2.142	3.382	2.645	3.494
5					1.387	3.382	3.855	3.382	2.142	1.079	2.142	2.643	3.500
6						2.142	3.382	3.855	3.381	2.142	1.079	2.636	3.507
7							2.467	4.273	4.934	4.273	2.467	3.320	4.059
8								2.466	4.273	4.934	4.274	3.326	4.054
9									2.467	4.274	4.934	3.336	4.042
10										2.467	4.273	3.340	4.036
11											2.466	3.336	4.042
12												3.326	4.054
13													0.972

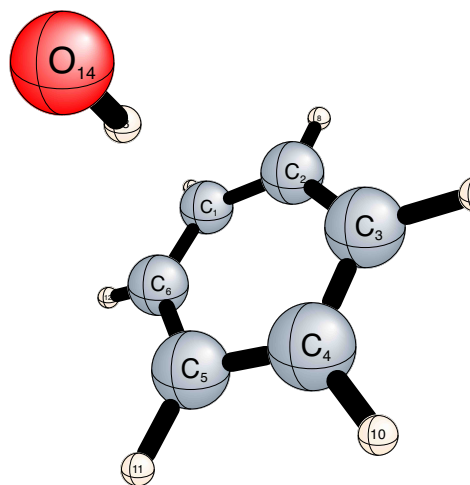
Molecule: $[\text{C}_6\text{H}_6 \cdots \text{OH}]$ (Intermediate 1, C_{6v} input geometry)

Method: M06L

Basis: 6-31G*

Energy: -193228.923685384 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.319319	-1.466107	0.000000
2	C	0.428473	-0.776362	1.207878
3	C	0.650066	0.600881	1.206988
4	C	0.762613	1.288489	0.000000
5	C	0.650066	0.600881	-1.206988
6	C	0.428473	-0.776362	-1.207878
7	H	0.141885	-2.539709	0.000000
8	H	0.336072	-1.312328	2.150313
9	H	0.727755	1.139283	2.149206
10	H	0.925166	2.364120	0.000000
11	H	0.727755	1.139283	-2.149206
12	H	0.336072	-1.312328	-2.150313
13	H	-1.689444	0.065364	0.000000
14	O	-2.563529	0.508527	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.395	2.416	2.790	2.416	1.395	1.088	2.156	3.402	3.878	3.402	2.156	2.526	3.494
2		1.395	2.415	2.789	2.416	2.157	1.088	2.155	3.401	3.877	3.402	2.579	3.473
3			1.394	2.414	2.789	3.403	2.156	1.088	2.154	3.400	3.877	2.686	3.434
4				1.394	2.415	3.878	3.401	2.155	1.088	2.155	3.401	2.740	3.416
5					1.395	3.403	3.877	3.400	2.154	1.088	2.156	2.686	3.434
6						2.157	3.402	3.877	3.401	2.155	1.088	2.579	3.473
7							2.484	4.301	4.966	4.301	2.484	3.184	4.076
8								2.483	4.300	4.965	4.301	3.260	4.043
9									2.482	4.298	4.965	3.408	3.981
10										2.482	4.300	3.481	3.951
11											2.483	3.408	3.981
12												3.260	4.043
13													0.980

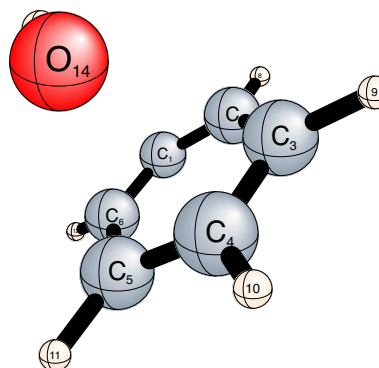
Molecule: [C₆H₆⋯OH] (Intermediate 1, C_{6v} input geometry)

Method: M06L

Basis: def2-TZVPP

Energy: -193310.812858756 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.807169	-1.478078	0.000000
2	C	0.674126	-0.798455	1.205353
3	C	0.408341	0.560669	1.207157
4	C	0.270374	1.245800	0.000000
5	C	0.408341	0.560669	-1.207157
6	C	0.674126	-0.798455	-1.205353
7	H	1.014880	-2.539312	0.000000
8	H	0.776593	-1.331502	2.140092
9	H	0.294151	1.093856	2.139893
10	H	0.090411	2.309807	0.000000
11	H	0.294151	1.093856	-2.139893
12	H	0.776593	-1.331502	-2.140092
13	H	-2.133771	0.221817	0.000000
14	O	-2.163330	1.188517	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.390	2.403	2.776	2.403	1.390	1.081	2.145	3.385	3.855	3.385	2.145	3.397	3.992
2		1.385	2.407	2.782	2.411	2.145	1.081	2.144	3.385	3.862	3.389	3.222	3.668
3			1.395	2.414	2.782	3.382	2.142	1.080	2.149	3.391	3.863	2.834	2.909
4				1.395	2.407	3.858	3.388	2.145	1.079	2.145	3.388	2.613	2.434
5					1.385	3.382	3.863	3.391	2.149	1.080	2.142	2.834	2.909
6						2.145	3.389	3.862	3.385	2.144	1.081	3.222	3.668
7							2.469	4.278	4.936	4.278	2.469	4.188	4.899
8								2.473	4.279	4.943	4.280	3.932	4.424
9									2.470	4.280	4.943	3.352	3.260
10										2.470	4.279	3.051	2.517
11											2.473	3.352	3.260
12												3.932	4.424
13													0.967

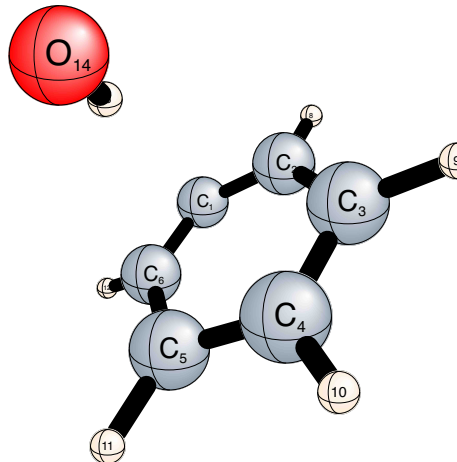
Molecule: $[\text{C}_6\text{H}_6 \cdots \text{OH}]$ (Intermediate 1, C_{6v} input geometry)

Method: M06HF

Basis: 6-31G*

Energy: -193195.155189024 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.578096	-1.403644	0.000000
2	C	0.552818	-0.706321	1.208057
3	C	0.497233	0.685968	1.207066
4	C	0.467812	1.381771	0.000000
5	C	0.497233	0.685968	-1.207066
6	C	0.552818	-0.706321	-1.208057
7	H	0.618093	-2.484930	0.000000
8	H	0.569377	-1.246754	2.144953
9	H	0.463169	1.225989	2.143447
10	H	0.410789	2.461770	0.000000
11	H	0.463169	1.225989	-2.143447
12	H	0.569377	-1.246754	-2.144953
13	H	-1.651229	-0.255712	0.000000
14	O	-2.399804	0.378589	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.395	2.415	2.788	2.415	1.395	1.082	2.151	3.394	3.869	3.394	2.151	2.508	3.470
2		1.393	2.414	2.788	2.416	2.151	1.082	2.149	3.394	3.870	3.396	2.553	3.370
3			1.394	2.414	2.788	3.395	2.149	1.081	2.149	3.394	3.870	2.638	3.153
4				1.394	2.414	3.870	3.394	2.149	1.082	2.149	3.394	2.678	3.038
5					1.393	3.395	3.870	3.394	2.149	1.081	2.149	2.638	3.153
6						2.151	3.396	3.870	3.394	2.149	1.082	2.553	3.370
7							2.477	4.288	4.951	4.288	2.477	3.181	4.160
8								2.475	4.287	4.951	4.290	3.243	4.007
9									2.475	4.287	4.951	3.356	3.675
10										2.475	4.287	3.411	3.498
11											2.475	3.356	3.675
12												3.243	4.007
13													0.981

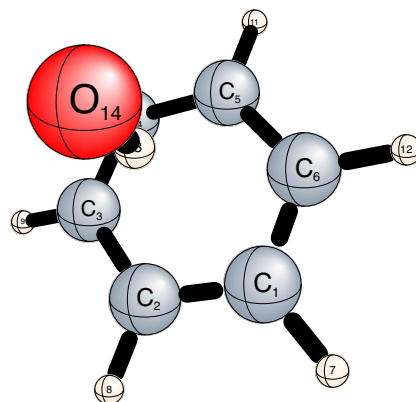
Molecule: $[\text{C}_6\text{H}_6 \cdots \text{OH}]$ (Intermediate 1, C_{6v} input geometry)

Method: M06HF

Basis: def2-TZVPP

Energy: -193291.284360127 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.249944	0.847975	0.000000
2	C	0.842520	0.284717	-1.203045
3	C	0.031062	-0.843355	-1.202600
4	C	-0.373352	-1.407826	0.000000
5	C	0.031062	-0.843355	1.202600
6	C	0.842520	0.284717	1.203045
7	H	1.875660	1.729197	0.000000
8	H	1.152858	0.727165	-2.138919
9	H	-0.290273	-1.277643	-2.138537
10	H	-1.011421	-2.280097	0.000000
11	H	-0.290273	-1.277643	2.138537
12	H	1.152858	0.727165	2.138919
13	H	-1.237359	1.121820	0.000000
14	O	-2.075400	1.620773	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.389	2.407	2.779	2.407	1.389	1.081	2.145	3.386	3.860	3.386	2.145	2.502	3.414
2		1.390	2.406	2.778	2.406	2.145	1.081	2.145	3.386	3.859	3.385	2.544	3.427
3			1.389	2.405	2.778	3.386	2.145	1.081	2.144	3.385	3.859	2.630	3.458
4				1.389	2.406	3.860	3.386	2.144	1.081	2.144	3.386	2.673	3.474
5					1.390	3.386	3.859	3.385	2.144	1.081	2.145	2.630	3.458
6						2.145	3.385	3.859	3.386	2.145	1.081	2.544	3.427
7							2.470	4.279	4.941	4.279	2.470	3.172	3.953
8								2.470	4.278	4.939	4.278	3.232	3.974
9									2.469	4.277	4.939	3.351	4.020
10										2.469	4.278	3.409	4.043
11											2.470	3.351	4.020
12												3.232	3.974
13													0.975

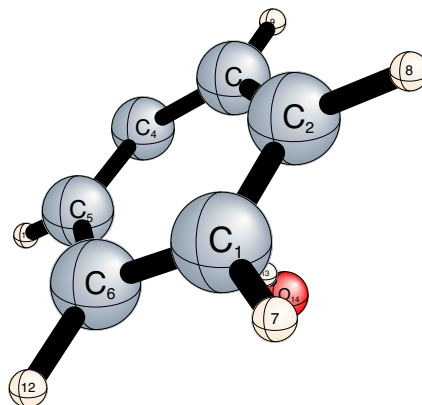
Molecule: $[\text{C}_6\text{H}_6 \cdots \text{OH}]$ (Intermediate 1, C_{6v} input geometry)

Method: RI-MP2

Basis: def2-TZVPP

Energy: -192938.393127184 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	-0.490557	1.411534	0.000000
2	C	-0.519101	0.716725	1.205047
3	C	-0.574219	-0.672915	1.205002
4	C	-0.600794	-1.367723	0.000000
5	C	-0.574219	-0.672915	-1.205002
6	C	-0.519101	0.716725	-1.205047
7	H	-0.443427	2.489776	0.000000
8	H	-0.491876	1.255752	2.139535
9	H	-0.589676	-1.212387	2.139491
10	H	-0.639057	-2.446297	0.000000
11	H	-0.589676	-1.212387	-2.139491
12	H	-0.491876	1.255752	-2.139535
13	H	1.692071	-0.048328	0.000000
14	O	2.658747	-0.115230	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.391	2.409	2.781	2.409	1.391	1.079	2.145	3.387	3.861	3.387	2.145	2.626	3.500
2		1.391	2.409	2.783	2.410	2.145	1.079	2.145	3.387	3.862	3.388	2.632	3.499
3			1.391	2.410	2.783	3.387	2.145	1.079	2.145	3.388	3.862	2.642	3.495
4				1.391	2.409	3.861	3.387	2.145	1.079	2.145	3.387	2.645	3.492
5					1.391	3.387	3.862	3.388	2.145	1.079	2.145	2.642	3.495
6						2.145	3.388	3.862	3.387	2.145	1.079	2.632	3.499
7							2.470	4.278	4.940	4.278	2.470	3.317	4.051
8								2.470	4.278	4.941	4.279	3.324	4.048
9									2.470	4.279	4.941	3.337	4.041
10										2.470	4.278	3.344	4.038
11											2.470	3.337	4.041
12												3.324	4.048
13													0.969

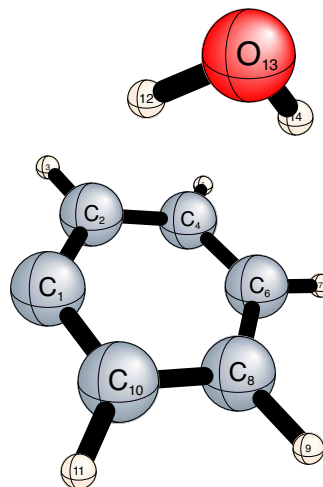
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: B3LYP

Basis: 6-31G*

Energy: -193256.922614249 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.766846	0.166335	-1.251769
2	C	0.817039	-1.111771	-0.736731
3	H	0.980283	-1.985481	-1.361731
4	C	0.642164	-1.238277	0.651465
5	H	0.670887	-2.223792	1.109890
6	C	0.431644	-0.101873	1.439729
7	H	0.302123	-0.208461	2.513263
8	C	0.392546	1.170936	0.860484
9	H	0.228146	2.048867	1.480518
10	C	0.564948	1.321062	-0.525707
11	H	0.535726	2.303119	-0.989762
12	H	-2.014414	-0.125469	-1.168816
13	O	-2.678052	-0.247295	-0.473370
14	H	-2.136835	-0.256523	0.330579



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.379	2.165	2.369	3.361	2.726	3.812	2.369	3.361	1.379	2.165	2.798	3.556	3.334
2		1.087	1.405	2.161	2.430	3.412	2.818	3.905	2.455	3.436	3.029	3.610	3.255
3			2.174	2.502	3.420	4.317	3.905	4.992	3.436	4.328	3.531	4.147	3.946
4				1.087	1.399	2.155	2.431	3.415	2.818	3.905	3.407	3.643	2.965
5					2.161	2.483	3.415	4.311	3.905	4.992	4.100	4.199	3.516
6						1.087	1.399	2.161	2.430	3.420	3.576	3.654	2.802
7							2.155	2.483	3.412	4.317	4.351	4.219	3.273
8								1.087	1.405	2.174	3.405	3.636	2.952
9									2.161	2.502	4.096	4.188	3.497
10										1.087	3.026	3.603	3.244
11											3.526	4.135	3.929
12												0.969	1.510
13													0.969

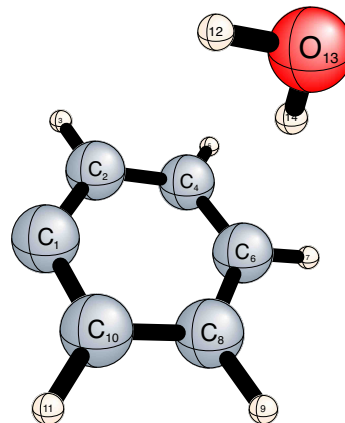
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: B3LYP

Basis: def2-TZVPP

Energy: -193348.357717455 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.896332	-0.000251	-1.382380
2	C	0.808167	-1.222335	-0.767211
3	H	0.882390	-2.154448	-1.311669
4	C	0.614266	-1.211000	0.618859
5	H	0.535345	-2.147140	1.156815
6	C	0.520687	-0.000557	1.301985
7	H	0.373433	-0.000684	2.373731
8	C	0.617640	1.210041	0.619604
9	H	0.541319	2.146067	1.158133
10	C	0.811557	1.221691	-0.766457
11	H	0.888316	2.153929	-1.310348
12	H	-2.792032	0.000332	-0.864588
13	O	-2.889750	0.003748	0.091044
14	H	-1.986643	0.002725	0.424084



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.371	2.155	2.356	3.345	2.711	3.792	2.356	3.345	1.371	2.155	3.725	4.063	3.402
2		1.082	1.400	2.152	2.420	3.398	2.806	3.889	2.444	3.421	3.803	3.989	3.276
3			2.165	2.493	3.406	4.299	3.888	4.971	3.421	4.308	4.283	4.567	3.987
4				1.083	1.393	2.145	2.421	3.401	2.806	3.888	3.908	3.746	2.877
5					2.152	2.473	3.401	4.293	3.889	4.971	4.446	4.183	3.394
6						1.082	1.393	2.152	2.420	3.406	3.958	3.619	2.657
7							2.145	2.473	3.398	4.299	4.528	3.982	3.061
8								1.083	1.400	2.165	3.911	3.747	2.877
9									2.152	2.493	4.450	4.183	3.395
10										1.082	3.806	3.990	3.276
11											4.287	4.567	3.988
12												0.961	1.520
13													0.963

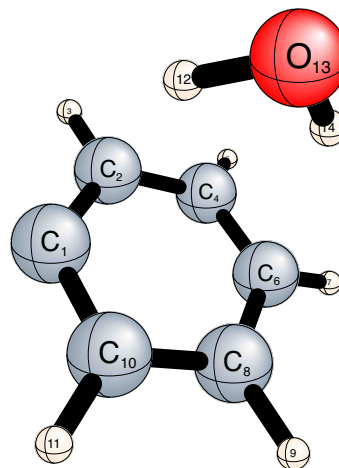
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: ωB97

Basis: 6-31G*

Energy: -193213.100375769 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.604124	-0.000578	-1.376267
2	C	0.590382	-1.227897	-0.748845
3	H	0.596055	-2.165148	-1.302520
4	C	0.565307	-1.214610	0.651946
5	H	0.551704	-2.156049	1.199943
6	C	0.555542	-0.000866	1.344084
7	H	0.539497	-0.000979	2.432778
8	C	0.567202	1.213023	0.652242
9	H	0.554999	2.154351	1.200465
10	C	0.592364	1.226612	-0.748561
11	H	0.599588	2.163995	-1.302001
12	H	-2.022360	0.004359	-0.987629
13	O	-2.567773	0.003301	-0.189706
14	H	-1.905605	0.002602	0.515673



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.378	2.166	2.364	3.359	2.721	3.810	2.364	3.359	1.378	2.166	2.655	3.387	3.143
2		1.089	1.401	2.159	2.426	3.410	2.815	3.904	2.455	3.437	2.899	3.435	3.057
3			2.174	2.503	3.419	4.317	3.903	4.992	3.437	4.329	3.415	3.994	3.777
4				1.089	1.397	2.155	2.428	3.413	2.815	3.903	3.297	3.465	2.758
5					2.160	2.483	3.413	4.310	3.904	4.992	4.010	4.040	3.342
6						1.089	1.397	2.160	2.426	3.419	3.476	3.480	2.597
7							2.155	2.483	3.410	4.317	4.273	4.066	3.107
8								1.089	1.401	2.174	3.295	3.464	2.757
9									2.159	2.503	4.007	4.039	3.340
10										1.089	2.896	3.434	3.056
11											3.411	3.992	3.775
12												0.967	1.508
13													0.967

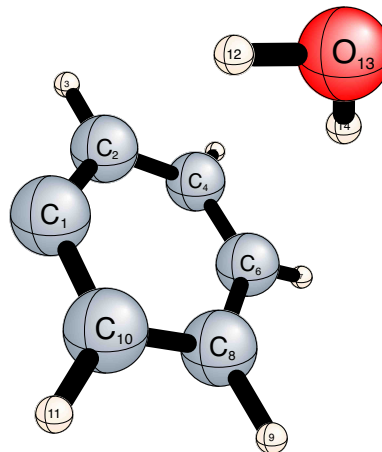
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: ωB97

Basis: def2-TZVPP

Energy: -193298.833671785 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.412711	0.000425	-1.430643
2	C	0.503449	-1.222858	-0.815446
3	H	0.423299	-2.156592	-1.360889
4	C	0.703503	-1.208365	0.566830
5	H	0.780450	-2.145559	1.108357
6	C	0.800803	0.001890	1.248228
7	H	0.958798	0.002481	2.321204
8	C	0.699902	1.211402	0.566027
9	H	0.774077	2.149182	1.106930
10	C	0.499806	1.224381	-0.816255
11	H	0.416881	2.157507	-1.362321
12	H	-2.275324	-0.004268	-0.616082
13	O	-2.596743	-0.004499	0.287826
14	H	-1.793382	-0.002661	0.814737



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.372	2.158	2.353	3.345	2.707	3.791	2.353	3.345	1.372	2.158	2.809	3.466	3.148
2		1.084	1.397	2.152	2.418	3.398	2.806	3.891	2.447	3.425	3.041	3.509	3.069
3			2.167	2.495	3.407	4.302	3.890	4.975	3.425	4.314	3.531	4.058	3.780
4				1.085	1.392	2.147	2.420	3.401	2.806	3.890	3.424	3.524	2.784
5					2.152	2.473	3.401	4.295	3.891	4.975	4.111	4.082	3.362
6						1.085	1.392	2.152	2.418	3.407	3.597	3.531	2.630
7							2.147	2.473	3.398	4.302	4.369	4.096	3.138
8								1.085	1.397	2.167	3.425	3.525	2.784
9									2.152	2.495	4.112	4.083	3.363
10										1.084	3.042	3.510	3.070
11											3.532	4.059	3.780
12												0.959	1.510
13													0.961

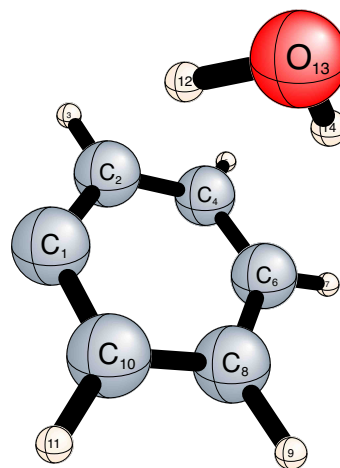
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: ωB97X

Basis: 6-31G*

Energy: -193201.3842914 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.618673	-0.000732	-1.376249
2	C	0.603151	-1.225646	-0.748679
3	H	0.611924	-2.161168	-1.301261
4	C	0.572240	-1.212907	0.650075
5	H	0.557165	-2.152510	1.196946
6	C	0.559105	-0.000914	1.340952
7	H	0.539199	-0.000983	2.427519
8	C	0.573888	1.211172	0.650282
9	H	0.560024	2.150707	1.197305
10	C	0.604886	1.224103	-0.748489
11	H	0.615041	2.159712	-1.300907
12	H	-2.048693	0.005032	-0.980610
13	O	-2.599490	0.003478	-0.188247
14	H	-1.946085	0.002774	0.522965



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.376	2.162	2.362	3.355	2.718	3.805	2.362	3.355	1.376	2.162	2.697	3.430	3.191
2		1.087	1.399	2.156	2.422	3.405	2.810	3.897	2.450	3.430	2.933	3.476	3.102
3			2.170	2.499	3.413	4.310	3.896	4.984	3.430	4.321	3.446	4.030	3.815
4				1.087	1.395	2.152	2.424	3.408	2.810	3.897	3.318	3.499	2.799
5					2.156	2.479	3.408	4.303	3.897	4.984	4.023	4.066	3.371
6						1.087	1.395	2.156	2.423	3.413	3.491	3.509	2.635
7							2.152	2.479	3.405	4.310	4.279	4.086	3.131
8								1.087	1.399	2.170	3.315	3.497	2.798
9									2.156	2.499	4.019	4.064	3.369
10										1.087	2.929	3.474	3.101
11											3.441	4.027	3.813
12												0.965	1.507
13													0.966

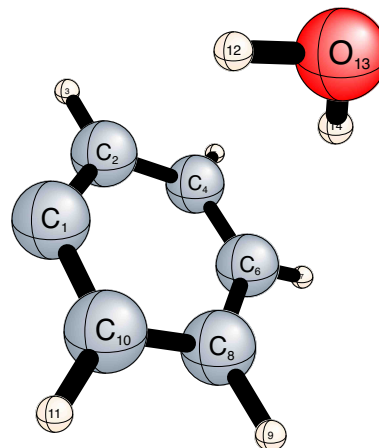
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: ωB97X

Basis: def2-TZVPP

Energy: -193286.87819336 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.464014	0.000685	-1.423409
2	C	0.539088	-1.219573	-0.805782
3	H	0.474375	-2.151850	-1.352196
4	C	0.702467	-1.205745	0.579007
5	H	0.765410	-2.141251	1.121333
6	C	0.780978	0.002400	1.261442
7	H	0.910414	0.003094	2.336267
8	C	0.697974	1.209672	0.578001
9	H	0.757473	2.145861	1.119538
10	C	0.534551	1.221727	-0.806791
11	H	0.466430	2.153298	-1.353996
12	H	-2.373238	-0.003622	-0.647252
13	O	-2.643337	-0.006386	0.271554
14	H	-1.814752	-0.005337	0.755142



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.370	2.154	2.350	3.340	2.703	3.786	2.350	3.340	1.370	2.154	2.942	3.540	3.153
2		1.083	1.394	2.148	2.414	3.392	2.800	3.883	2.441	3.418	3.160	3.572	3.074
3			2.163	2.491	3.401	4.294	3.883	4.966	3.418	4.305	3.636	4.118	3.780
4				1.083	1.390	2.143	2.415	3.395	2.800	3.883	3.523	3.568	2.794
5					2.148	2.469	3.395	4.287	3.883	4.966	4.189	4.111	3.369
6						1.083	1.390	2.148	2.414	3.401	3.687	3.565	2.645
7							2.143	2.469	3.392	4.294	4.437	4.110	3.151
8								1.083	1.394	2.163	3.522	3.569	2.797
9									2.148	2.491	4.188	4.113	3.373
10										1.083	3.159	3.574	3.076
11											3.635	4.120	3.783
12												0.958	1.510
13													0.959

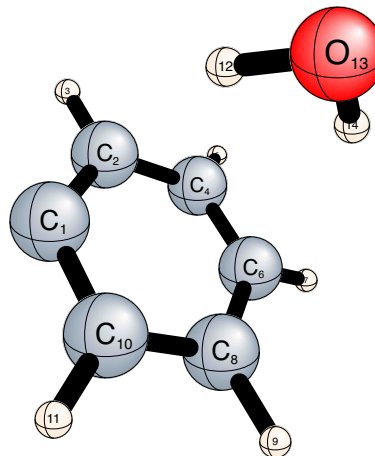
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: $\omega\text{B97X-D}$

Basis: 6-31G*

Energy: -193190.908108966 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.448346	-0.001876	-1.434562
2	C	0.528651	-1.223634	-0.805949
3	H	0.468958	-2.161321	-1.349664
4	C	0.688786	-1.204637	0.584823
5	H	0.754808	-2.140968	1.131369
6	C	0.760326	0.010800	1.266327
7	H	0.887987	0.015910	2.344425
8	C	0.670608	1.219778	0.575503
9	H	0.722650	2.161184	1.114825
10	C	0.510189	1.225722	-0.815353
11	H	0.436206	2.158175	-1.366236
12	H	-2.150703	-0.025986	-0.634489
13	O	-2.608513	-0.019289	0.213906
14	H	-1.881100	-0.004695	0.847112



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.376	2.161	2.363	3.355	2.719	3.805	2.363	3.355	1.376	2.161	2.720	3.473	3.261
2		1.086	1.400	2.155	2.423	3.404	2.810	3.897	2.449	3.429	2.940	3.512	3.166
3			2.169	2.498	3.413	4.308	3.896	4.982	3.429	4.320	3.455	4.062	3.873
4				1.086	1.395	2.151	2.425	3.407	2.811	3.896	3.307	3.523	2.848
5					2.156	2.478	3.407	4.302	3.897	4.982	4.004	4.081	3.405
6						1.086	1.395	2.156	2.423	3.413	3.477	3.530	2.675
7							2.151	2.478	3.404	4.308	4.256	4.095	3.148
8								1.086	1.400	2.169	3.313	3.524	2.843
9									2.155	2.498	4.012	4.082	3.397
10										1.086	2.946	3.512	3.162
11											3.464	4.063	3.866
12												0.964	1.506
13													0.965

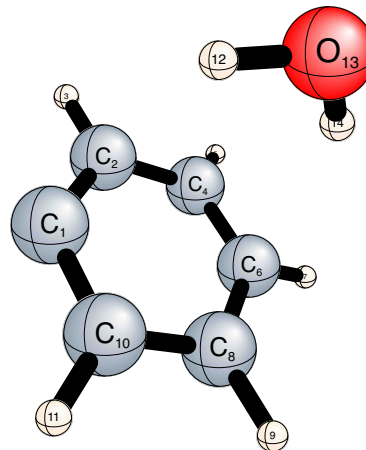
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: $\omega\text{B97X-D}$

Basis: def2-TZVPP

Energy: -193276.459360228 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.507927	-0.000097	-1.412547
2	C	0.558717	-1.219842	-0.792878
3	H	0.510471	-2.151505	-1.340418
4	C	0.673283	-1.207305	0.597099
5	H	0.714718	-2.142717	1.139798
6	C	0.730433	0.000095	1.282047
7	H	0.821661	0.000172	2.359818
8	C	0.673299	1.207400	0.596926
9	H	0.714750	2.142890	1.139489
10	C	0.558728	1.219737	-0.793052
11	H	0.510488	2.151321	-1.340728
12	H	-2.274757	-0.000273	-0.727745
13	O	-2.665033	-0.000058	0.146118
14	H	-1.906653	0.000167	0.731671



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.369	2.153	2.350	3.339	2.704	3.785	2.350	3.339	1.369	2.153	2.866	3.535	3.229
2		1.082	1.395	2.147	2.413	3.391	2.799	3.882	2.440	3.416	3.085	3.572	3.145
3			2.161	2.489	3.399	4.292	3.881	4.963	3.416	4.303	3.572	4.114	3.843
4				1.082	1.389	2.142	2.415	3.394	2.799	3.881	3.450	3.578	2.852
5					2.148	2.468	3.394	4.286	3.882	4.963	4.125	4.123	3.410
6						1.082	1.389	2.148	2.413	3.399	3.615	3.580	2.694
7							2.142	2.468	3.391	4.292	4.373	4.130	3.177
8								1.082	1.395	2.161	3.450	3.578	2.852
9									2.147	2.489	4.125	4.123	3.410
10										1.082	3.086	3.572	3.145
11											3.572	4.114	3.843
12												0.957	1.505
13													0.958

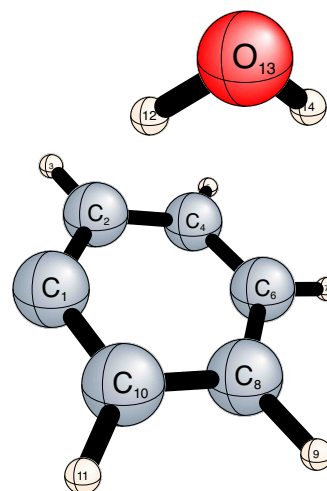
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: M06

Basis: 6-31G*

Energy: -193118.739430275 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.729427	0.159779	-1.250740
2	C	0.789890	-1.112932	-0.733116
3	H	0.945675	-1.989252	-1.360048
4	C	0.636744	-1.236311	0.651756
5	H	0.675590	-2.221449	1.114716
6	C	0.435438	-0.101971	1.437051
7	H	0.322335	-0.206505	2.514659
8	C	0.382164	1.165084	0.857758
9	H	0.222704	2.044162	1.480703
10	C	0.533496	1.311330	-0.525128
11	H	0.492547	2.293947	-0.992093
12	H	-1.832148	-0.084525	-1.106668
13	O	-2.607833	-0.216359	-0.546091
14	H	-2.222978	-0.293618	0.335283



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.375	2.163	2.362	3.357	2.716	3.805	2.362	3.357	1.375	2.163	2.577	3.432	3.382
2		1.089	1.399	2.158	2.420	3.404	2.808	3.897	2.447	3.430	2.841	3.519	3.300
3			2.170	2.500	3.413	4.310	3.897	4.986	3.429	4.323	3.378	4.054	3.974
4				1.089	1.394	2.152	2.424	3.409	2.808	3.897	3.243	3.606	3.028
5					2.157	2.479	3.409	4.305	3.897	4.986	3.974	4.190	3.567
6						1.089	1.394	2.157	2.420	3.412	3.408	3.634	2.884
7							2.152	2.479	3.404	4.310	4.216	4.237	3.352
8								1.089	1.399	2.170	3.213	3.580	3.031
9									2.158	2.500	3.930	4.151	3.572
10										1.089	2.808	3.493	3.304
11											3.328	4.014	3.979
12												0.966	1.509
13													0.965

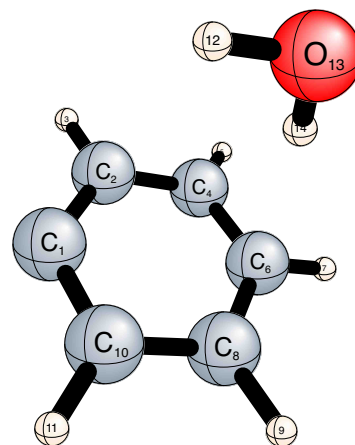
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: M06

Basis: def2-TZVPP

Energy: -193203.100679744 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.793240	-0.000355	-1.372235
2	C	0.726066	-1.217627	-0.755118
3	H	0.781603	-2.150703	-1.301840
4	C	0.579783	-1.206900	0.629973
5	H	0.517649	-2.142102	1.172749
6	C	0.509269	-0.000514	1.312851
7	H	0.396238	-0.000579	2.389259
8	C	0.582603	1.205957	0.630413
9	H	0.522669	2.141104	1.173531
10	C	0.728905	1.216847	-0.754673
11	H	0.786616	2.149988	-1.301058
12	H	-2.571329	0.002236	-0.915660
13	O	-2.715427	0.002677	0.029689
14	H	-1.830234	0.001959	0.401402



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.366	2.152	2.347	3.338	2.700	3.782	2.347	3.338	1.366	2.152	3.395	3.778	3.167
2		1.083	1.393	2.148	2.409	3.388	2.795	3.878	2.434	3.412	3.519	3.735	3.059
3			2.159	2.489	3.396	4.289	3.878	4.961	3.412	4.301	4.003	4.317	3.789
4				1.083	1.388	2.141	2.413	3.392	2.795	3.878	3.712	3.561	2.706
5					2.146	2.466	3.392	4.283	3.878	4.961	4.301	4.045	3.272
6						1.082	1.388	2.146	2.409	3.396	3.802	3.471	2.511
7							2.141	2.466	3.388	4.289	4.442	3.905	2.985
8								1.083	1.393	2.159	3.713	3.562	2.706
9									2.148	2.489	4.303	4.046	3.272
10										1.083	3.520	3.735	3.060
11											4.005	4.318	3.789
12												0.956	1.511
13													0.960

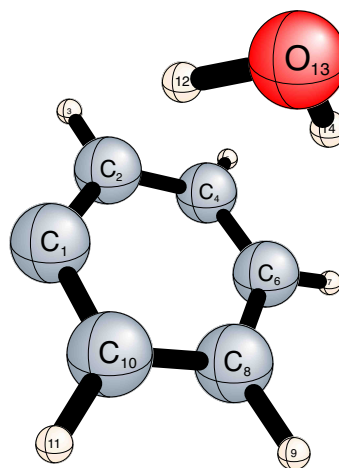
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: M062X

Basis: 6-31G*

Energy: -193167.955151907 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.597019	-0.000952	-1.379672
2	C	0.583485	-1.224427	-0.747924
3	H	0.587386	-2.158887	-1.300344
4	C	0.560101	-1.213754	0.651279
5	H	0.546046	-2.152517	1.197078
6	C	0.551990	-0.001681	1.343186
7	H	0.536999	-0.001950	2.428578
8	C	0.560859	1.210744	0.651916
9	H	0.547157	2.149220	1.198219
10	C	0.584373	1.222186	-0.747288
11	H	0.588794	2.156954	-1.299179
12	H	-1.991569	0.004306	-0.985231
13	O	-2.542327	0.007667	-0.191300
14	H	-1.889286	0.005209	0.522283



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.377	2.159	2.366	3.357	2.723	3.809	2.366	3.357	1.377	2.159	2.618	3.357	3.130
2		1.086	1.399	2.155	2.423	3.404	2.809	3.895	2.447	3.426	2.863	3.406	3.040
3			2.169	2.498	3.412	4.308	3.894	4.980	3.426	4.316	3.381	3.965	3.760
4				1.086	1.396	2.151	2.424	3.407	2.809	3.894	3.267	3.439	2.739
5					2.156	2.478	3.407	4.302	3.895	4.980	3.982	4.016	3.323
6						1.085	1.396	2.156	2.423	3.412	3.448	3.454	2.576
7							2.151	2.478	3.404	4.308	4.248	4.043	3.086
8								1.086	1.399	2.169	3.264	3.433	2.734
9									2.155	2.498	3.977	4.008	3.315
10										1.086	2.859	3.400	3.035
11											3.375	3.956	3.753
12												0.966	1.511
13													0.967

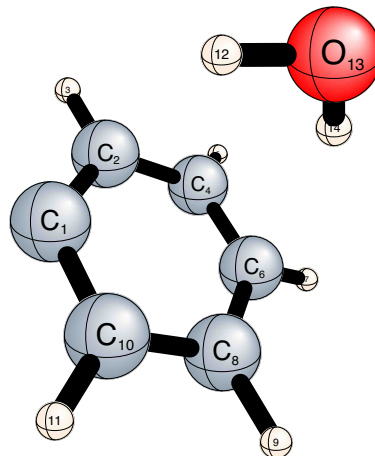
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: M062X

Basis: def2-TZVPP

Energy: -193258.161107427 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.434016	-0.000162	-1.427281
2	C	0.505560	-1.219449	-0.805044
3	H	0.435939	-2.150621	-1.351383
4	C	0.669866	-1.208630	0.580401
5	H	0.729509	-2.144125	1.121106
6	C	0.752409	-0.000652	1.264272
7	H	0.880728	-0.000840	2.338279
8	C	0.671826	1.207569	0.580602
9	H	0.732986	2.142873	1.121475
10	C	0.507520	1.218902	-0.804843
11	H	0.439348	2.150278	-1.351008
12	H	-2.281487	0.000729	-0.749054
13	O	-2.598991	0.002025	0.156459
14	H	-1.792381	0.001509	0.679631



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.371	2.152	2.355	3.343	2.710	3.792	2.355	3.343	1.371	2.152	2.799	3.422	3.065
2		1.082	1.395	2.148	2.414	3.392	2.800	3.882	2.438	3.414	3.043	3.472	2.996
3			2.162	2.490	3.401	4.293	3.881	4.964	3.414	4.301	3.518	4.015	3.704
4				1.082	1.391	2.143	2.416	3.395	2.800	3.881	3.456	3.512	2.745
5					2.148	2.469	3.395	4.287	3.882	4.964	4.143	4.076	3.340
6						1.082	1.391	2.148	2.414	3.401	3.641	3.530	2.611
7							2.143	2.469	3.392	4.293	4.419	4.107	3.146
8								1.082	1.395	2.162	3.456	3.512	2.745
9									2.148	2.490	4.144	4.076	3.340
10										1.082	3.044	3.472	2.996
11											3.519	4.015	3.704
12												0.960	1.510
13													0.961

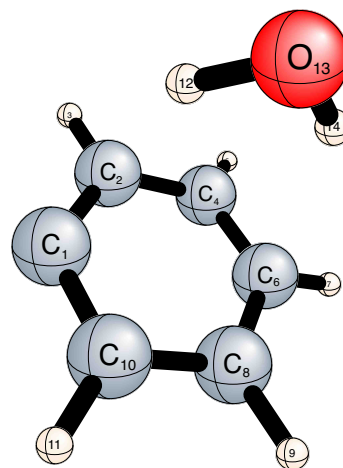
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: M052X

Basis: 6-31G*

Energy: -193229.453633677 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.619340	-0.000086	-1.375260
2	C	0.601648	-1.225928	-0.751486
3	H	0.609949	-2.157734	-1.302559
4	C	0.567855	-1.212663	0.647607
5	H	0.550214	-2.149039	1.191974
6	C	0.554822	-0.000990	1.338396
7	H	0.532639	-0.001355	2.420888
8	C	0.571056	1.211148	0.648493
9	H	0.556005	2.147172	1.193539
10	C	0.604860	1.225340	-0.750592
11	H	0.615655	2.157521	-1.300986
12	H	-2.019694	0.002437	-0.968118
13	O	-2.587316	0.003443	-0.189485
14	H	-1.956007	0.002851	0.539193



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.376	2.159	2.359	3.349	2.714	3.797	2.359	3.349	1.376	2.159	2.670	3.419	3.209
2		1.083	1.400	2.152	2.423	3.401	2.811	3.894	2.451	3.428	2.903	3.464	3.117
3			2.168	2.495	3.410	4.303	3.893	4.977	3.428	4.315	3.420	4.016	3.827
4				1.083	1.395	2.148	2.424	3.404	2.811	3.893	3.284	3.483	2.803
5					2.153	2.474	3.404	4.296	3.894	4.977	3.987	4.048	3.367
6						1.083	1.395	2.153	2.423	3.410	3.457	3.494	2.635
7							2.148	2.474	3.401	4.303	4.243	4.068	3.120
8								1.083	1.400	2.168	3.284	3.484	2.803
9									2.152	2.495	3.988	4.048	3.367
10										1.083	2.904	3.464	3.117
11											3.421	4.017	3.827
12												0.964	1.509
13													0.964

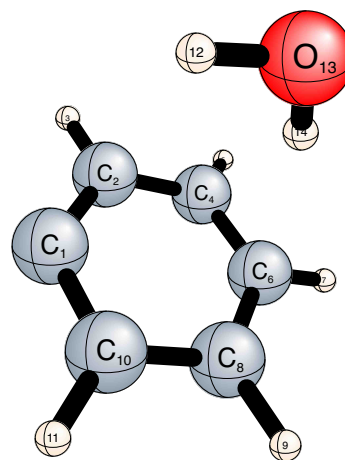
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: M052X

Basis: def2-TZVPP

Energy: -193320.35998525 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.678072	-0.000075	-1.356865
2	C	0.647998	-1.220394	-0.738301
3	H	0.667114	-2.149972	-1.285950
4	C	0.586595	-1.206623	0.655052
5	H	0.555093	-2.139604	1.197530
6	C	0.558701	0.000632	1.341727
7	H	0.510185	0.000878	2.419692
8	C	0.590721	1.207549	0.654681
9	H	0.562656	2.140810	1.196837
10	C	0.652207	1.220569	-0.738639
11	H	0.675124	2.149884	-1.286632
12	H	-2.413883	0.016813	-1.009998
13	O	-2.647093	-0.006291	-0.081913
14	H	-1.802463	-0.012059	0.374382



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.368	2.151	2.348	3.334	2.701	3.780	2.348	3.334	1.369	2.151	3.111	3.561	3.025
2		1.079	1.395	2.145	2.414	3.389	2.800	3.879	2.441	3.415	3.314	3.572	2.950
3			2.160	2.486	3.397	4.287	3.879	4.958	3.415	4.300	3.777	4.127	3.664
4				1.080	1.389	2.140	2.414	3.391	2.800	3.879	3.643	3.527	2.686
5					2.145	2.465	3.391	4.280	3.879	4.958	4.282	4.055	3.281
6						1.079	1.389	2.145	2.413	3.397	3.790	3.508	2.552
7							2.140	2.465	3.389	4.287	4.507	4.028	3.087
8								1.080	1.395	2.160	3.635	3.535	2.701
9									2.145	2.486	4.271	4.068	3.302
10										1.079	3.305	3.581	2.964
11											3.764	4.140	3.684
12												0.957	1.514
13													0.960

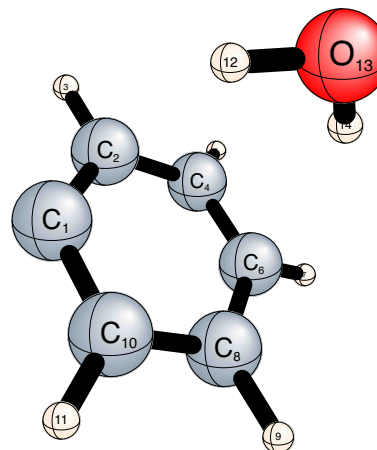
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: M06L

Basis: 6-31G*

Energy: -193230.514307747 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.425431	0.028146	-1.435999
2	C	0.501447	-1.207260	-0.833632
3	H	0.422744	-2.133035	-1.400156
4	C	0.682071	-1.227560	0.554834
5	H	0.744797	-2.180030	1.078760
6	C	0.778178	-0.029772	1.264825
7	H	0.920628	-0.052924	2.343284
8	C	0.694434	1.197377	0.605166
9	H	0.766570	2.126463	1.168338
10	C	0.513779	1.236652	-0.782820
11	H	0.444422	2.186007	-1.310194
12	H	-2.237867	0.030834	-0.652288
13	O	-2.615429	0.018161	0.235811
14	H	-1.827091	-0.007508	0.794167



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.377	2.161	2.368	3.362	2.724	3.812	2.368	3.362	1.377	2.162	2.776	3.470	3.170
2		1.088	1.400	2.159	2.422	3.406	2.809	3.898	2.444	3.427	3.012	3.516	3.084
3			2.170	2.500	3.414	4.311	3.897	4.986	3.427	4.320	3.510	4.066	3.794
4				1.089	1.396	2.153	2.425	3.411	2.809	3.897	3.401	3.539	2.800
5					2.159	2.481	3.411	4.307	3.898	4.986	4.096	4.103	3.379
6						1.088	1.396	2.158	2.422	3.413	3.574	3.547	2.648
7							2.153	2.481	3.406	4.311	4.354	4.117	3.155
8								1.089	1.400	2.170	3.397	3.533	2.801
9									2.159	2.500	4.091	4.093	3.379
10										1.088	3.007	3.509	3.085
11											3.503	4.056	3.795
12												0.965	1.504
13													0.966

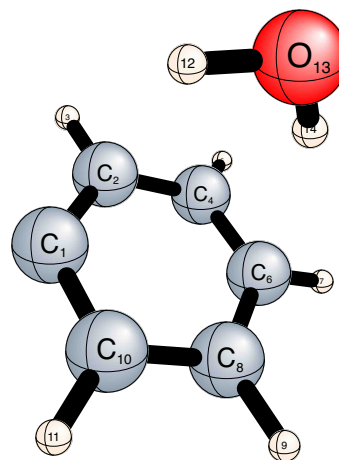
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: M06L

Basis: def2-TZVPP

Energy: -193314.211143785 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.648149	-0.000149	-1.363780
2	C	0.628809	-1.217799	-0.738197
3	H	0.642345	-2.149149	-1.287615
4	C	0.588429	-1.208427	0.656214
5	H	0.569019	-2.143221	1.200322
6	C	0.570078	-0.000616	1.343575
7	H	0.540880	-0.000805	2.424056
8	C	0.591415	1.207437	0.656717
9	H	0.574354	2.142053	1.201217
10	C	0.631817	1.217286	-0.737689
11	H	0.647690	2.148826	-1.286719
12	H	-2.270583	0.002812	-1.017546
13	O	-2.655646	0.002191	-0.140870
14	H	-1.885728	0.001678	0.431918



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.369	2.150	2.355	3.343	2.708	3.789	2.355	3.343	1.369	2.150	2.939	3.523	3.106
2		1.081	1.395	2.149	2.412	3.389	2.798	3.880	2.435	3.411	3.158	3.554	3.030
3			2.160	2.489	3.398	4.290	3.879	4.961	3.411	4.298	3.632	4.101	3.738
4				1.082	1.390	2.141	2.416	3.395	2.798	3.879	3.527	3.553	2.763
5					2.147	2.467	3.395	4.285	3.880	4.961	4.194	4.099	3.349
6						1.081	1.390	2.147	2.412	3.398	3.694	3.551	2.620
7							2.141	2.467	3.389	4.290	4.444	4.098	3.140
8								1.082	1.395	2.160	3.528	3.554	2.764
9									2.149	2.489	4.194	4.100	3.350
10										1.081	3.159	3.555	3.030
11											3.632	4.103	3.739
12												0.958	1.500
13													0.960

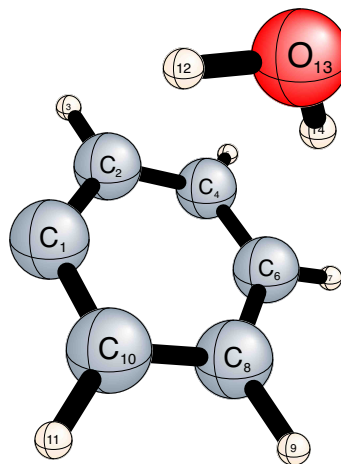
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: M06HF

Basis: 6-31G*

Energy: -193191.351572714 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.605943	0.000294	-1.377044
2	C	0.586864	-1.223654	-0.744589
3	H	0.593756	-2.153009	-1.297929
4	C	0.554320	-1.212950	0.653414
5	H	0.534732	-2.147931	1.197446
6	C	0.543497	-0.001175	1.346460
7	H	0.520445	-0.001736	2.427921
8	C	0.557428	1.211333	0.654804
9	H	0.540274	2.145723	1.199921
10	C	0.590033	1.223557	-0.743193
11	H	0.599451	2.153536	-1.295452
12	H	-2.094043	0.003915	-1.012245
13	O	-2.523581	0.003067	-0.147702
14	H	-1.788090	0.001146	0.479793



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.378	2.155	2.366	3.354	2.724	3.806	2.366	3.354	1.378	2.155	2.725	3.362	3.030
2		1.082	1.398	2.151	2.423	3.400	2.809	3.891	2.447	3.422	2.961	3.396	2.939
3			2.166	2.496	3.410	4.303	3.890	4.972	3.422	4.307	3.458	3.961	3.671
4				1.082	1.396	2.149	2.424	3.403	2.809	3.890	3.357	3.405	2.644
5					2.152	2.474	3.403	4.294	3.891	4.972	4.053	3.974	3.245
6						1.082	1.396	2.152	2.423	3.410	3.538	3.412	2.487
7							2.149	2.474	3.400	4.303	4.321	3.987	3.021
8								1.082	1.398	2.166	3.357	3.405	2.645
9									2.151	2.496	4.052	3.974	3.246
10										1.082	2.960	3.397	2.940
11											3.458	3.962	3.672
12												0.965	1.523
13													0.967

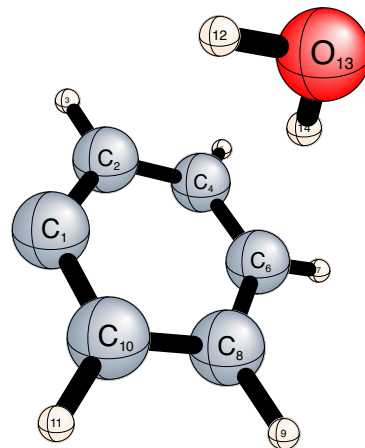
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: M06HF

Basis: def2-TZVPP

Energy: -193294.935609095 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.598161	0.013883	-1.400612
2	C	0.601342	-1.209921	-0.781927
3	H	0.589478	-2.134723	-1.340669
4	C	0.617208	-1.209554	0.612232
5	H	0.614924	-2.147661	1.149049
6	C	0.627641	-0.007327	1.311149
7	H	0.637475	-0.015639	2.391694
8	C	0.621525	1.205667	0.630982
9	H	0.622797	2.135167	1.182548
10	C	0.605628	1.227952	-0.762890
11	H	0.597059	2.161494	-1.306942
12	H	-2.510170	0.009081	-0.864503
13	O	-2.606839	0.002364	0.087966
14	H	-1.711650	-0.004427	0.437527



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.371	2.149	2.356	3.343	2.712	3.793	2.355	3.343	1.371	2.150	3.154	3.534	2.952
2		1.081	1.394	2.147	2.414	3.391	2.799	3.879	2.438	3.412	3.343	3.538	2.879
3			2.161	2.490	3.400	4.292	3.879	4.960	3.412	4.296	3.799	4.102	3.605
4				1.081	1.391	2.143	2.415	3.393	2.799	3.879	3.667	3.484	2.628
5					2.147	2.468	3.393	4.283	3.879	4.960	4.298	4.016	3.242
6						1.081	1.391	2.146	2.414	3.400	3.818	3.458	2.497
7							2.143	2.467	3.391	4.292	4.529	3.979	3.056
8								1.081	1.394	2.161	3.671	3.488	2.635
9									2.147	2.490	4.304	4.022	3.253
10										1.081	3.347	3.542	2.886
11											3.806	4.108	3.614
12												0.957	1.527
13													0.961

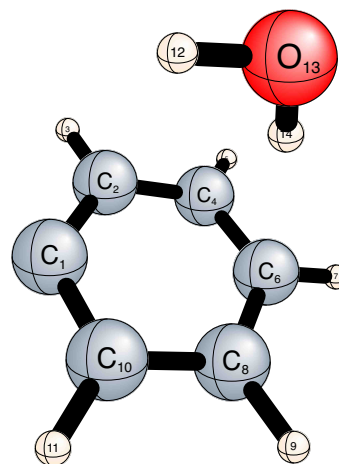
Molecule: $[\text{C}_6\text{H}_5 \cdots \text{H}_2\text{O}]$ (Intermediate 2, over-ring input geometry)

Method: RI-MP2

Basis: def2-TZVPP

Energy: -192945.856722995 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.792710	0.005207	-1.320288
2	C	0.711617	-1.218391	-0.705551
3	H	0.789143	-2.145922	-1.250863
4	C	0.522566	-1.209128	0.679668
5	H	0.447951	-2.143414	1.215742
6	C	0.423804	-0.000542	1.363612
7	H	0.275757	-0.002838	2.432532
8	C	0.513036	1.210971	0.683548
9	H	0.431116	2.142919	1.222619
10	C	0.701995	1.226159	-0.701634
11	H	0.772277	2.156015	-1.243963
12	H	-2.383776	-0.006200	-1.155229
13	O	-2.634240	-0.011514	-0.231005
14	H	-1.788345	-0.008289	0.223755

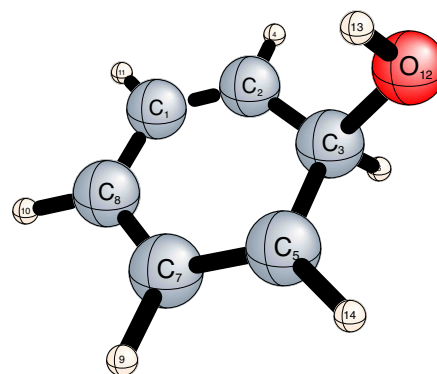


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.372	2.152	2.355	3.342	2.709	3.788	2.355	3.342	1.372	2.152	3.181	3.596	3.008
2		1.079	1.398	2.149	2.418	3.393	2.805	3.885	2.445	3.418	3.355	3.588	2.929
3			2.162	2.490	3.402	4.292	3.884	4.964	3.418	4.302	3.828	4.161	3.659
4				1.080	1.392	2.142	2.420	3.397	2.805	3.884	3.642	3.497	2.644
5					2.148	2.468	3.397	4.286	3.885	4.964	4.267	4.017	3.247
6						1.079	1.392	2.148	2.418	3.402	3.772	3.449	2.489
7							2.142	2.468	3.393	4.292	4.466	3.945	3.023
8								1.080	1.398	2.162	3.641	3.498	2.645
9									2.149	2.490	4.266	4.019	3.248
10										1.079	3.354	3.589	2.930
11											3.827	4.163	3.660
12												0.958	1.502
13													0.960

Molecule: C₆H₆OH (Intermediate 3)
Method: B3LYP
Basis: 6-31G*
Energy: -193274.195642846 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.130066	-1.227506	-0.048178
2	C	-0.204744	-1.252490	0.248355
3	C	-1.018165	-0.000009	0.419973
4	H	-0.741611	-2.192665	0.344750
5	C	-0.204747	1.252471	0.248330
6	H	-1.489011	0.000001	1.416527
7	C	1.130063	1.227485	-0.048203
8	C	1.826925	-0.000011	-0.193010
9	H	1.670777	2.161642	-0.183163
10	H	2.886201	-0.000011	-0.430801
11	H	1.670783	-2.161664	-0.183119
12	O	-2.170083	-0.000019	-0.459953
13	H	-1.815502	-0.000029	-1.365031
14	H	-0.741618	2.192647	0.344705

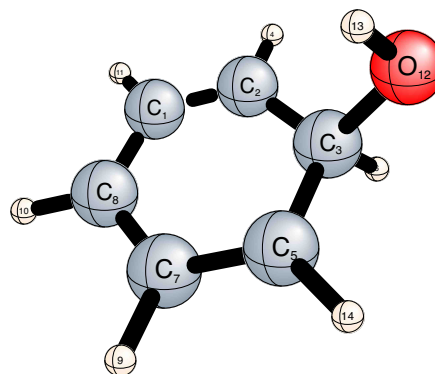


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.368	2.518	2.142	2.832	3.242	2.455	1.419	3.435	2.177	1.088	3.545	3.452	3.919
2		1.503	1.087	2.505	2.141	2.832	2.427	3.919	3.404	2.128	2.436	2.601	3.488
3			2.211	1.503	1.102	2.518	2.910	3.502	3.996	3.502	1.450	1.955	2.211
4				3.488	2.552	3.919	3.420	5.006	4.309	2.470	2.738	2.981	4.385
5					2.141	1.368	2.427	2.128	3.404	3.919	2.436	2.601	1.087
6						3.242	3.686	4.149	4.749	4.149	1.996	2.801	2.552
7							1.419	1.088	2.176	3.435	3.545	3.452	2.142
8								2.167	1.086	2.167	4.006	3.826	3.420
9									2.492	4.323	4.416	4.269	2.470
10										2.492	5.056	4.794	4.309
11											4.416	4.269	5.006
12												0.972	2.738
13													2.981

Molecule: C₆H₆OH (Intermediate 3)
Method: B3LYP
Basis: def2-TZVPP
Energy: -193357.963116317 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.127786	-1.222622	-0.046306
2	C	-0.201224	-1.248812	0.246484
3	C	-1.010381	-0.000009	0.414745
4	H	-0.732957	-2.186202	0.346516
5	C	-0.201228	1.248794	0.246458
6	H	-1.477436	0.000001	1.408565
7	C	1.127782	1.222602	-0.046332
8	C	1.821861	-0.000010	-0.191287
9	H	1.666457	2.153001	-0.177289
10	H	2.876515	-0.000011	-0.427932
11	H	1.666464	-2.153022	-0.177244
12	O	-2.164469	-0.000020	-0.462796
13	H	-1.836870	-0.000029	-1.368872
14	H	-0.732965	2.186184	0.346471



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.361	2.506	2.132	2.821	3.225	2.445	1.413	3.421	2.168	1.083	3.537	3.469	3.903
2		1.498	1.082	2.498	2.130	2.821	2.417	3.904	3.389	2.118	2.432	2.616	3.477
3			2.205	1.498	1.098	2.506	2.896	3.486	3.977	3.486	1.450	1.966	2.205
4				3.477	2.542	3.903	3.405	4.986	4.290	2.456	2.736	2.990	4.372
5					2.130	1.361	2.417	2.118	3.389	3.904	2.432	2.616	1.082
6						3.225	3.667	4.127	4.725	4.127	1.993	2.801	2.542
7							1.413	1.083	2.168	3.421	3.537	3.469	2.132
8								2.159	1.081	2.159	3.996	3.844	3.405
9									2.482	4.306	4.404	4.281	2.456
10										2.482	5.041	4.806	4.290
11											4.404	4.281	4.986
12												0.963	2.736
13													2.990

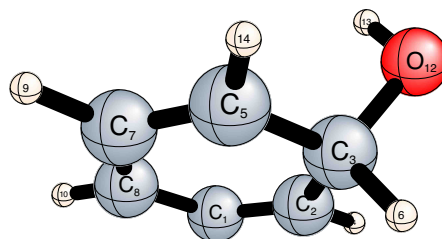
Molecule: C₆H₆OH (Intermediate 3)

Method: ω B97

Basis: 6-31G*

Energy: -193235.540603382 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.125609	-0.048994	1.229483
2	C	-0.207177	0.239722	1.252245
3	C	-1.021366	0.419449	0.000000
4	H	-0.747876	0.329098	2.193703
5	C	-0.207177	0.239722	-1.252245
6	H	-1.470619	1.426125	0.000000
7	C	1.125609	-0.048994	-1.229483
8	C	1.826371	-0.187781	0.000000
9	H	1.666222	-0.183920	-2.165910
10	H	2.889211	-0.419235	0.000000
11	H	1.666222	-0.183920	2.165910
12	O	-2.166061	-0.446395	0.000000
13	H	-1.817245	-1.350166	0.000000
14	H	-0.747876	0.329098	-2.193703

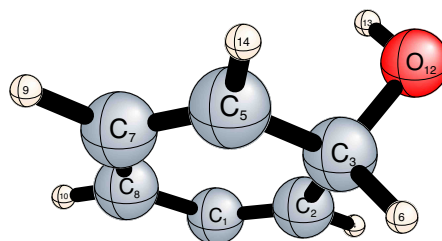


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.364	2.518	2.141	2.832	3.229	2.459	1.422	3.441	2.182	1.090	3.536	3.445	3.921
2		1.504	1.089	2.504	2.138	2.832	2.426	3.921	3.404	2.127	2.424	2.586	3.489
3			2.213	1.504	1.102	2.518	2.912	3.504	4.000	3.504	1.435	1.940	2.213
4				3.489	2.557	3.921	3.421	5.010	4.313	2.468	2.725	2.962	4.387
5					2.138	1.364	2.426	2.127	3.404	3.921	2.424	2.586	1.089
6						3.229	3.671	4.138	4.734	4.138	1.997	2.798	2.557
7							1.422	1.090	2.182	3.441	3.536	3.445	2.141
8								2.172	1.088	2.172	4.001	3.825	3.421
9									2.498	4.332	4.410	4.264	2.468
10										2.498	5.055	4.798	4.313
11											4.410	4.264	5.010
12												0.969	2.725
13													2.962

Molecule: C₆H₆OH (Intermediate 3)
Method: ω B97
Basis: def2-TZVPP
Energy: -193314.473049727 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.123773	-0.047601	1.225777
2	C	-0.203334	0.241098	1.249542
3	C	-1.014795	0.414567	0.000000
4	H	-0.739245	0.335859	2.188345
5	C	-0.203334	0.241098	-1.249542
6	H	-1.468169	1.414962	0.000000
7	C	1.123773	-0.047601	-1.225777
8	C	1.821743	-0.188869	0.000000
9	H	1.662442	-0.178623	-2.158831
10	H	2.879741	-0.421462	0.000000
11	H	1.662442	-0.178623	2.158831
12	O	-2.155533	-0.458600	0.000000
13	H	-1.825762	-1.360949	0.000000
14	H	-0.739245	0.335859	-2.188345

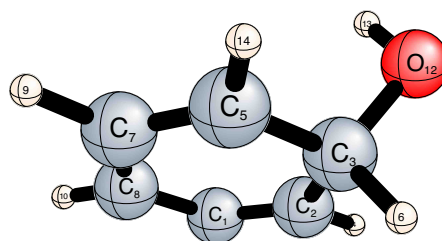


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.358	2.508	2.132	2.823	3.219	2.452	1.418	3.430	2.174	1.085	3.525	3.454	3.908
2		1.500	1.085	2.499	2.131	2.823	2.418	3.908	3.392	2.118	2.421	2.600	3.481
3			2.207	1.500	1.098	2.508	2.900	3.490	3.983	3.490	1.437	1.952	2.207
4				3.481	2.546	3.908	3.409	4.993	4.296	2.456	2.725	2.975	4.377
5					2.131	1.358	2.418	2.118	3.392	3.908	2.421	2.600	1.085
6						3.219	3.660	4.123	4.720	4.123	1.996	2.799	2.546
7							1.418	1.085	2.174	3.430	3.525	3.454	2.132
8								2.165	1.083	2.165	3.986	3.831	3.409
9									2.490	4.318	4.395	4.269	2.456
10										2.490	5.035	4.798	4.296
11											4.395	4.269	4.993
12												0.961	2.725
13													2.975

Molecule: C₆H₆OH (Intermediate 3)
Method: ω B97X
Basis: 6-31G*
Energy: -193221.787931022 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.125051	-0.048608	1.226694
2	C	-0.206165	0.238913	1.250047
3	C	-1.019247	0.417373	0.000000
4	H	-0.745099	0.328663	2.190148
5	C	-0.206165	0.238913	-1.250047
6	H	-1.468194	1.422632	0.000000
7	C	1.125051	-0.048608	-1.226694
8	C	1.823967	-0.187087	0.000000
9	H	1.664978	-0.182625	-2.161348
10	H	2.884970	-0.417787	0.000000
11	H	1.664978	-0.182625	2.161348
12	O	-2.164474	-0.444950	0.000000
13	H	-1.820704	-1.349059	0.000000
14	H	-0.745099	0.328663	-2.190148

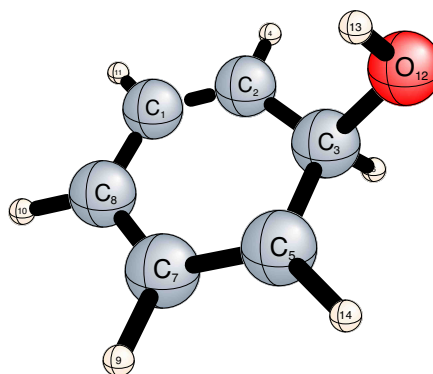


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.362	2.514	2.137	2.826	3.224	2.453	1.419	3.433	2.177	1.088	3.533	3.446	3.913
2		1.502	1.087	2.500	2.135	2.826	2.422	3.914	3.398	2.124	2.422	2.587	3.483
3			2.209	1.502	1.101	2.514	2.907	3.498	3.993	3.498	1.434	1.940	2.209
4				3.483	2.553	3.913	3.415	5.001	4.305	2.464	2.722	2.961	4.380
5					2.135	1.362	2.422	2.124	3.398	3.914	2.422	2.587	1.087
6						3.224	3.665	4.131	4.726	4.131	1.993	2.794	2.553
7							1.419	1.088	2.177	3.433	3.533	3.446	2.137
8								2.167	1.086	2.167	3.997	3.825	3.415
9									2.493	4.323	4.405	4.264	2.464
10										2.493	5.050	4.797	4.305
11											4.405	4.264	5.001
12												0.967	2.722
13													2.961

Molecule: C₆H₆OH (Intermediate 3)
Method: ω B97X
Basis: def2-TZVPP
Energy: -193300.430761256 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.123458	-1.222681	-0.046772
2	C	-0.201956	-1.247032	0.239368
3	C	-1.011964	-0.000009	0.412667
4	H	-0.736208	-2.184713	0.333536
5	C	-0.201960	1.247014	0.239342
6	H	-1.461413	0.000001	1.413655
7	C	1.123454	1.222660	-0.046797
8	C	1.819683	-0.000011	-0.186660
9	H	1.661515	2.154042	-0.177167
10	H	2.876239	-0.000011	-0.417619
11	H	1.661521	-2.154063	-0.177122
12	O	-2.154987	-0.000019	-0.452715
13	H	-1.831833	-0.000029	-1.356026
14	H	-0.736215	2.184695	0.333491



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.356	2.503	2.128	2.817	3.211	2.445	1.414	3.422	2.169	1.084	3.522	3.456	3.900
2		1.497	1.083	2.494	2.126	2.817	2.413	3.900	3.386	2.114	2.418	2.599	3.474
3			2.203	1.497	1.097	2.503	2.894	3.484	3.976	3.484	1.434	1.949	2.203
4				3.474	2.543	3.900	3.402	4.983	4.288	2.452	2.721	2.971	4.369
5					2.126	1.356	2.413	2.114	3.386	3.900	2.418	2.599	1.083
6						3.211	3.651	4.114	4.708	4.114	1.991	2.794	2.543
7							1.414	1.084	2.169	3.422	3.522	3.456	2.128
8								2.160	1.082	2.160	3.984	3.834	3.402
9									2.485	4.308	4.391	4.270	2.452
10										2.485	5.031	4.801	4.288
11											4.391	4.270	4.983
12												0.959	2.721
13													2.971

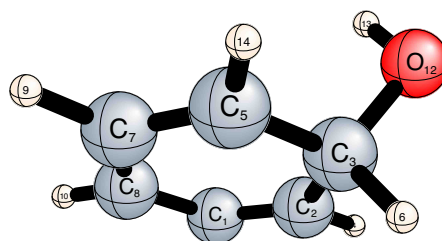
Molecule: C₆H₆OH (Intermediate 3)

Method: ω B97X-D

Basis: 6-31G*

Energy: -193209.229106458 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.125131	-0.049149	1.225824
2	C	-0.205645	0.243257	1.250150
3	C	-1.019606	0.416024	0.000000
4	H	-0.742633	0.336793	2.189753
5	C	-0.205645	0.243257	-1.250150
6	H	-1.475895	1.417587	0.000000
7	C	1.125131	-0.049149	-1.225824
8	C	1.821915	-0.191781	0.000000
9	H	1.665064	-0.183016	-2.159424
10	H	2.880958	-0.426992	0.000000
11	H	1.665064	-0.183016	2.159424
12	O	-2.160084	-0.453184	0.000000
13	H	-1.811551	-1.354770	0.000000
14	H	-0.742633	0.336793	-2.189753

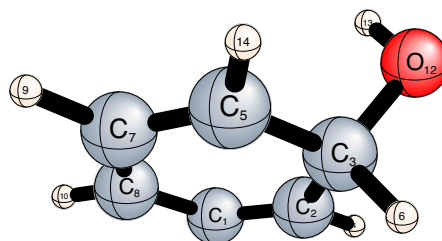


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.363	2.514	2.137	2.826	3.228	2.452	1.417	3.431	2.174	1.087	3.530	3.440	3.912
2		1.502	1.086	2.500	2.134	2.826	2.421	3.912	3.397	2.123	2.422	2.588	3.483
3			2.209	1.502	1.101	2.514	2.906	3.497	3.991	3.497	1.434	1.940	2.209
4				3.483	2.550	3.912	3.413	4.998	4.302	2.463	2.725	2.966	4.380
5					2.134	1.363	2.421	2.123	3.397	3.912	2.422	2.588	1.086
6						3.228	3.670	4.134	4.731	4.134	1.992	2.793	2.550
7							1.417	1.087	2.174	3.431	3.530	3.440	2.137
8								2.165	1.085	2.165	3.991	3.815	3.413
9									2.490	4.319	4.401	4.257	2.463
10										2.490	5.041	4.783	4.302
11											4.401	4.257	4.998
12												0.967	2.725
13													2.966

Molecule: C₆H₆OH (Intermediate 3)
Method: ω B97X-D
Basis: def2-TZVPP
Energy: -193287.983689143 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.122149	-0.046919	1.221291
2	C	-0.202733	0.242065	1.246628
3	C	-1.013291	0.410898	0.000000
4	H	-0.735202	0.338829	2.183908
5	C	-0.202733	0.242065	-1.246628
6	H	-1.466346	1.410171	0.000000
7	C	1.122149	-0.046919	-1.221291
8	C	1.816300	-0.189574	0.000000
9	H	1.660322	-0.177248	-2.151650
10	H	2.871355	-0.423529	0.000000
11	H	1.660322	-0.177248	2.151650
12	O	-2.153218	-0.457306	0.000000
13	H	-1.825841	-1.358356	0.000000
14	H	-0.735202	0.338829	-2.183908

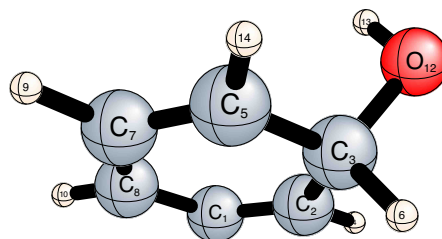


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.356	2.502	2.127	2.816	3.212	2.443	1.412	3.418	2.166	1.083	3.520	3.450	3.898
2		1.497	1.082	2.493	2.125	2.816	2.412	3.898	3.383	2.113	2.418	2.598	3.473
3			2.203	1.497	1.097	2.502	2.893	3.482	3.973	3.482	1.433	1.947	2.203
4				3.473	2.540	3.898	3.400	4.980	4.285	2.451	2.723	2.973	4.368
5					2.125	1.356	2.412	2.113	3.383	3.898	2.418	2.598	1.082
6						3.212	3.652	4.114	4.709	4.114	1.990	2.792	2.540
7							1.412	1.083	2.166	3.418	3.520	3.450	2.127
8								2.157	1.081	2.157	3.979	3.825	3.400
9									2.481	4.303	4.388	4.264	2.451
10										2.481	5.025	4.789	4.285
11											4.388	4.264	4.980
12												0.959	2.723
13													2.973

Molecule: C₆H₆OH (Intermediate 3)
Method: M06
Basis: 6-31G*
Energy: -193136.601051646 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.124964	-0.048040	1.223375
2	C	-0.207269	0.241165	1.246085
3	C	-1.015017	0.417783	0.000000
4	H	-0.750759	0.325369	2.186621
5	C	-0.207269	0.241165	-1.246085
6	H	-1.472977	1.424318	0.000000
7	C	1.124964	-0.048040	-1.223375
8	C	1.822269	-0.184901	0.000000
9	H	1.664285	-0.186914	-2.159922
10	H	2.885026	-0.417872	0.000000
11	H	1.664285	-0.186914	2.159922
12	O	-2.156547	-0.446477	0.000000
13	H	-1.807160	-1.350257	0.000000
14	H	-0.750759	0.325369	-2.186621

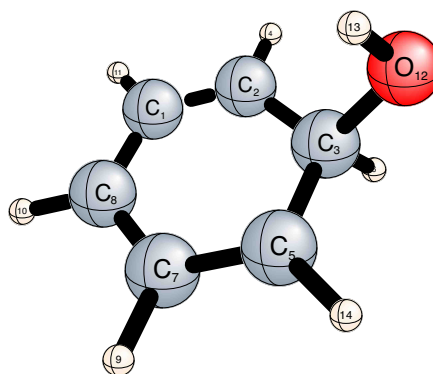


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.363	2.509	2.141	2.821	3.227	2.447	1.415	3.429	2.175	1.090	3.525	3.434	3.910
2		1.495	1.090	2.492	2.134	2.821	2.419	3.910	3.398	2.126	2.414	2.578	3.476
3			2.204	1.495	1.106	2.509	2.901	3.494	3.989	3.494	1.432	1.937	2.204
4				3.476	2.552	3.910	3.415	4.999	4.307	2.469	2.712	2.950	4.373
5					2.134	1.363	2.419	2.126	3.398	3.910	2.414	2.578	1.090
6						3.227	3.667	4.136	4.731	4.136	1.992	2.795	2.552
7							1.415	1.090	2.175	3.429	3.525	3.434	2.141
8								2.166	1.088	2.166	3.987	3.812	3.415
9									2.492	4.320	4.397	4.251	2.469
10										2.492	5.042	4.784	4.307
11											4.397	4.251	4.999
12												0.969	2.712
13													2.950

Molecule: C₆H₆OH (Intermediate 3)
Method: M06
Basis: def2-TZVPP
Energy: -193214.302132688 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.121416	-1.217741	-0.046554
2	C	-0.203213	-1.241841	0.241503
3	C	-1.008401	-0.000009	0.414299
4	H	-0.740247	-2.178622	0.330521
5	C	-0.203217	1.241823	0.241478
6	H	-1.461475	0.000001	1.417289
7	C	1.121413	1.217720	-0.046579
8	C	1.815560	-0.000011	-0.184865
9	H	1.657722	2.149313	-0.182319
10	H	2.871912	-0.000011	-0.418139
11	H	1.657728	-2.149335	-0.182275
12	O	-2.145806	-0.000019	-0.451303
13	H	-1.813807	-0.000030	-1.352350
14	H	-0.740253	2.178604	0.330477

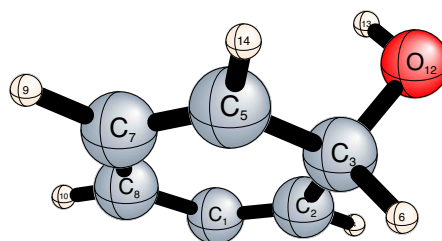


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.356	2.496	2.129	2.808	3.209	2.435	1.408	3.412	2.165	1.083	3.510	3.436	3.891
2		1.490	1.083	2.484	2.123	2.808	2.408	3.891	3.381	2.113	2.407	2.584	3.463
3			2.197	1.490	1.101	2.496	2.887	3.476	3.969	3.476	1.429	1.942	2.197
4				3.463	2.539	3.891	3.398	4.974	4.284	2.452	2.708	2.955	4.357
5					2.123	1.356	2.408	2.113	3.381	3.891	2.407	2.584	1.083
6						3.209	3.648	4.112	4.706	4.112	1.990	2.792	2.539
7							1.408	1.083	2.165	3.412	3.510	3.436	2.129
8								2.155	1.082	2.155	3.970	3.813	3.398
9									2.480	4.299	4.377	4.247	2.452
10										2.480	5.018	4.778	4.284
11											4.377	4.247	4.974
12												0.960	2.708
13													2.955

Molecule: C₆H₆OH (Intermediate 3)
Method: M062X
Basis: 6-31G*
Energy: -193183.94025907 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.124366	-0.049334	1.225912
2	C	-0.205288	0.239800	1.248400
3	C	-1.018148	0.418160	0.000000
4	H	-0.744458	0.329887	2.187038
5	C	-0.205288	0.239800	-1.248400
6	H	-1.471563	1.421420	0.000000
7	C	1.124366	-0.049334	-1.225912
8	C	1.823542	-0.188513	0.000000
9	H	1.662993	-0.184286	-2.159742
10	H	2.882275	-0.420864	0.000000
11	H	1.662993	-0.184286	2.159742
12	O	-2.160026	-0.447412	0.000000
13	H	-1.811737	-1.352272	0.000000
14	H	-0.744458	0.329887	-2.187038

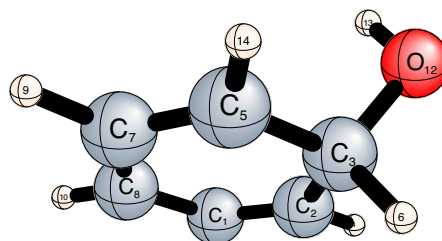


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.361	2.512	2.135	2.824	3.226	2.452	1.418	3.431	2.175	1.086	3.528	3.438	3.910
2		1.500	1.086	2.497	2.135	2.824	2.420	3.910	3.395	2.122	2.419	2.583	3.479
3			2.206	1.500	1.101	2.512	2.906	3.495	3.990	3.495	1.433	1.940	2.206
4				3.479	2.550	3.910	3.413	4.995	4.301	2.462	2.719	2.958	4.374
5					2.135	1.361	2.420	2.122	3.395	3.910	2.419	2.583	1.086
6						3.226	3.667	4.131	4.728	4.131	1.992	2.794	2.550
7							1.418	1.086	2.175	3.431	3.528	3.438	2.135
8								2.166	1.084	2.166	3.992	3.817	3.413
9									2.491	4.319	4.399	4.255	2.462
10										2.491	5.042	4.786	4.301
11											4.399	4.255	4.995
12												0.970	2.719
13													2.958

Molecule: C₆H₆OH (Intermediate 3)
Method: M062X
Basis: def2-TZVPP
Energy: -193267.592627938 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.122496	-0.046952	1.222644
2	C	-0.203026	0.236264	1.245994
3	C	-1.012533	0.412030	0.000000
4	H	-0.738789	0.327450	2.182246
5	C	-0.203026	0.236264	-1.245994
6	H	-1.460899	1.413565	0.000000
7	C	1.122496	-0.046952	-1.222644
8	C	1.819907	-0.183963	0.000000
9	H	1.659813	-0.178420	-2.153201
10	H	2.875432	-0.413097	0.000000
11	H	1.659813	-0.178420	2.153201
12	O	-2.156210	-0.450571	0.000000
13	H	-1.831928	-1.356381	0.000000
14	H	-0.738789	0.327450	-2.182246

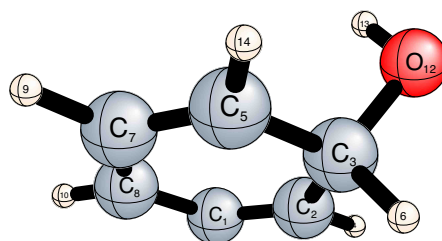


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.356	2.503	2.127	2.816	3.210	2.445	1.414	3.421	2.168	1.083	3.522	3.455	3.898
2		1.496	1.083	2.492	2.126	2.816	2.413	3.898	3.384	2.113	2.416	2.597	3.471
3			2.201	1.496	1.097	2.503	2.894	3.482	3.975	3.482	1.433	1.949	2.201
4				3.471	2.542	3.898	3.402	4.980	4.286	2.452	2.716	2.965	4.364
5					2.126	1.356	2.413	2.113	3.384	3.898	2.416	2.597	1.083
6						3.210	3.649	4.112	4.705	4.112	1.990	2.795	2.542
7							1.414	1.083	2.168	3.421	3.522	3.455	2.127
8								2.159	1.080	2.159	3.985	3.835	3.402
9									2.484	4.306	4.390	4.268	2.452
10										2.484	5.032	4.801	4.286
11											4.390	4.268	4.980
12												0.962	2.716
13													2.965

Molecule: C₆H₆OH (Intermediate 3)
Method: M052X
Basis: 6-31G*
Energy: -193247.770057884 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.121171	-0.049853	1.225307
2	C	-0.206129	0.250912	1.247749
3	C	-1.017709	0.425144	0.000000
4	H	-0.742142	0.347536	2.183645
5	C	-0.206129	0.250912	-1.247749
6	H	-1.483050	1.417523	0.000000
7	C	1.121171	-0.049853	-1.225307
8	C	1.816847	-0.196842	0.000000
9	H	1.657934	-0.185383	-2.156674
10	H	2.870448	-0.437116	0.000000
11	H	1.657934	-0.185383	2.156674
12	O	-2.149246	-0.462878	0.000000
13	H	-1.785110	-1.358447	0.000000
14	H	-0.742142	0.347536	-2.183645

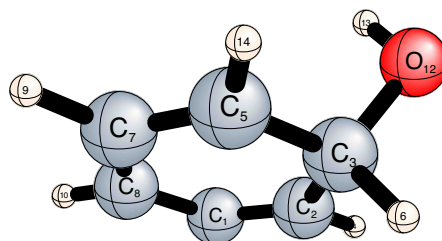


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.361	2.510	2.133	2.823	3.231	2.451	1.417	3.427	2.171	1.083	3.517	3.415	3.905
2		1.499	1.083	2.495	2.133	2.823	2.419	3.906	3.391	2.119	2.417	2.577	3.474
3			2.202	1.499	1.096	2.510	2.902	3.490	3.983	3.490	1.438	1.942	2.202
4				3.474	2.542	3.905	3.408	4.988	4.294	2.459	2.721	2.961	4.367
5					2.133	1.361	2.419	2.119	3.391	3.906	2.417	2.577	1.083
6						3.231	3.674	4.134	4.732	4.134	1.995	2.792	2.542
7							1.417	1.083	2.171	3.427	3.517	3.415	2.133
8								2.163	1.081	2.163	3.975	3.785	3.408
9									2.487	4.313	4.384	4.229	2.459
10										2.487	5.020	4.746	4.294
11											4.384	4.229	4.988
12												0.967	2.721
13													2.961

Molecule: C₆H₆OH (Intermediate 3)
Method: M052X
Basis: def2-TZVPP
Energy: -193332.247632462 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.118611	-0.046969	1.221248
2	C	-0.203649	0.249342	1.244672
3	C	-1.010931	0.419705	0.000000
4	H	-0.736332	0.347690	2.178475
5	C	-0.203649	0.249342	-1.244672
6	H	-1.476989	1.408629	0.000000
7	C	1.118611	-0.046969	-1.221248
8	C	1.811811	-0.193257	0.000000
9	H	1.654147	-0.179340	-2.149716
10	H	2.862268	-0.431831	0.000000
11	H	1.654147	-0.179340	2.149716
12	O	-2.142587	-0.469123	0.000000
13	H	-1.799623	-1.365946	0.000000
14	H	-0.736332	0.347690	-2.178475

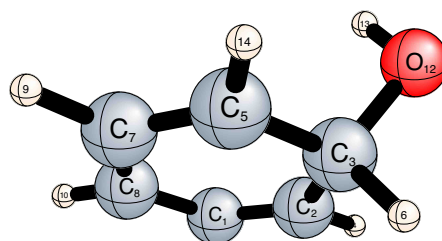


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.355	2.499	2.124	2.814	3.217	2.442	1.412	3.416	2.163	1.080	3.508	3.427	3.893
2		1.493	1.080	2.489	2.125	2.814	2.410	3.893	3.378	2.111	2.413	2.589	3.466
3			2.197	1.493	1.093	2.499	2.889	3.476	3.966	3.476	1.439	1.952	2.197
4				3.466	2.534	3.893	3.396	4.972	4.278	2.448	2.719	2.969	4.357
5					2.125	1.355	2.410	2.111	3.378	3.893	2.413	2.589	1.080
6						3.217	3.658	4.117	4.713	4.117	1.992	2.793	2.534
7							1.412	1.080	2.163	3.416	3.508	3.427	2.124
8								2.156	1.077	2.156	3.964	3.797	3.396
9									2.479	4.299	4.373	4.238	2.448
10										2.479	5.005	4.755	4.278
11											4.373	4.238	4.972
12												0.960	2.719
13													2.969

Molecule: C₆H₆OH (Intermediate 3)
Method: M06L
Basis: 6-31G*
Energy: -193244.288129042 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.125767	-0.047585	1.222900
2	C	-0.207036	0.252209	1.246128
3	C	-1.014461	0.419919	0.000000
4	H	-0.746890	0.342147	2.187531
5	C	-0.207036	0.252209	-1.246128
6	H	-1.495603	1.413663	0.000000
7	C	1.125767	-0.047585	-1.222900
8	C	1.821534	-0.192904	0.000000
9	H	1.663848	-0.188111	-2.159640
10	H	2.881980	-0.435494	0.000000
11	H	1.663848	-0.188111	2.159640
12	O	-2.158084	-0.463248	0.000000
13	H	-1.791985	-1.360990	0.000000
14	H	-0.746890	0.342147	-2.187531

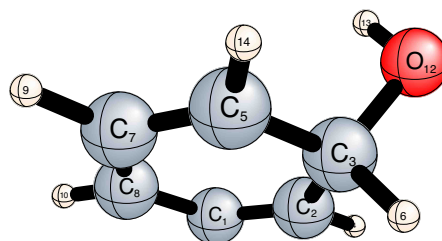


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.366	2.509	2.142	2.822	3.241	2.446	1.414	3.428	2.175	1.089	3.529	3.425	3.910
2		1.494	1.089	2.492	2.136	2.822	2.422	3.911	3.401	2.128	2.423	2.582	3.477
3			2.205	1.494	1.104	2.509	2.901	3.494	3.989	3.494	1.445	1.943	2.205
4				3.477	2.548	3.910	3.416	4.999	4.308	2.469	2.725	2.963	4.375
5					2.136	1.366	2.422	2.128	3.401	3.911	2.423	2.582	1.089
6						3.241	3.686	4.149	4.752	4.149	1.990	2.790	2.548
7							1.414	1.089	2.175	3.428	3.529	3.425	2.142
8								2.165	1.088	2.165	3.989	3.798	3.416
9									2.492	4.319	4.399	4.241	2.469
10										2.492	5.040	4.765	4.308
11											4.399	4.241	4.999
12												0.970	2.725
13													2.963

Molecule: C₆H₆OH (Intermediate 3)
Method: M06L
Basis: def2-TZVPP
Energy: -193322.38600034 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.121679	-0.047550	1.218213
2	C	-0.204571	0.249243	1.242910
3	C	-1.008847	0.415947	0.000000
4	H	-0.738281	0.344179	2.179036
5	C	-0.204571	0.249243	-1.242910
6	H	-1.483872	1.405700	0.000000
7	C	1.121679	-0.047550	-1.218213
8	C	1.814443	-0.192692	0.000000
9	H	1.657025	-0.184038	-2.148642
10	H	2.867874	-0.433252	0.000000
11	H	1.657025	-0.184038	2.148642
12	O	-2.152045	-0.468150	0.000000
13	H	-1.802968	-1.362997	0.000000
14	H	-0.738281	0.344179	-2.179036

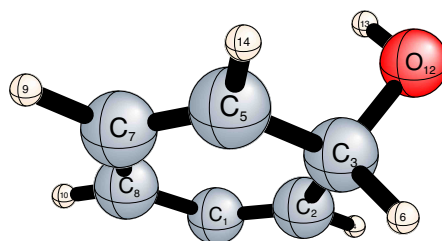


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.359	2.498	2.130	2.811	3.223	2.436	1.409	3.412	2.164	1.082	3.518	3.430	3.893
2		1.490	1.082	2.486	2.126	2.811	2.412	3.893	3.384	2.115	2.419	2.588	3.465
3			2.197	1.490	1.098	2.498	2.888	3.476	3.969	3.476	1.445	1.948	2.197
4				3.465	2.536	3.893	3.399	4.974	4.285	2.453	2.722	2.966	4.358
5					2.126	1.359	2.412	2.115	3.384	3.893	2.419	2.588	1.082
6						3.223	3.665	4.124	4.724	4.124	1.989	2.787	2.536
7							1.409	1.082	2.164	3.412	3.518	3.430	2.130
8								2.154	1.081	2.154	3.976	3.802	3.399
9									2.479	4.297	4.383	4.240	2.453
10										2.479	5.020	4.762	4.285
11											4.383	4.240	4.974
12												0.961	2.722
13													2.966

Molecule: C₆H₆OH (Intermediate 3)
Method: M06HF
Basis: 6-31G*
Energy: -193208.519312831 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.118914	-0.050633	1.229066
2	C	-0.204446	0.247536	1.250764
3	C	-1.023458	0.425669	0.000000
4	H	-0.739793	0.346787	2.186266
5	C	-0.204446	0.247536	-1.250764
6	H	-1.478760	1.420817	0.000000
7	C	1.118914	-0.050633	-1.229066
8	C	1.817830	-0.196302	0.000000
9	H	1.656973	-0.184306	-2.158889
10	H	2.870316	-0.433214	0.000000
11	H	1.656973	-0.184306	2.158889
12	O	-2.145457	-0.460425	0.000000
13	H	-1.789920	-1.361503	0.000000
14	H	-0.739793	0.346787	-2.186266

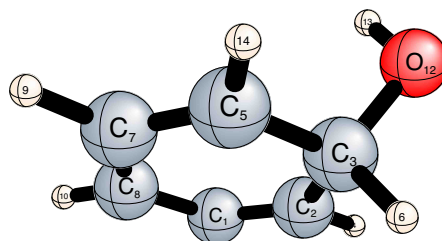


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.357	2.515	2.128	2.827	3.229	2.458	1.421	3.433	2.174	1.083	3.512	3.419	3.909
2		1.506	1.082	2.502	2.137	2.827	2.419	3.909	3.389	2.116	2.415	2.582	3.480
3			2.206	1.506	1.094	2.515	2.909	3.495	3.987	3.495	1.430	1.945	2.206
4				3.480	2.545	3.909	3.408	4.991	4.292	2.455	2.722	2.967	4.373
5					2.137	1.357	2.419	2.116	3.389	3.909	2.415	2.582	1.082
6						3.229	3.672	4.132	4.728	4.132	1.996	2.800	2.545
7							1.421	1.083	2.174	3.433	3.512	3.419	2.128
8								2.165	1.079	2.165	3.972	3.791	3.408
9									2.489	4.318	4.381	4.234	2.455
10										2.489	5.016	4.752	4.292
11											4.381	4.234	4.991
12												0.969	2.722
13													2.967

Molecule: C₆H₆OH (Intermediate 3)
Method: M06HF
Basis: def2-TZVPP
Energy: -193306.163898716 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.118871	-0.046436	1.226372
2	C	-0.202046	0.240481	1.248508
3	C	-1.017437	0.417682	0.000000
4	H	-0.736831	0.335995	2.183874
5	C	-0.202046	0.240481	-1.248508
6	H	-1.466834	1.413854	0.000000
7	C	1.118871	-0.046436	-1.226372
8	C	1.816870	-0.185815	0.000000
9	H	1.657421	-0.177107	-2.155260
10	H	2.870277	-0.415667	0.000000
11	H	1.657421	-0.177107	2.155260
12	O	-2.144906	-0.457891	0.000000
13	H	-1.822514	-1.362449	0.000000
14	H	-0.736831	0.335995	-2.183874

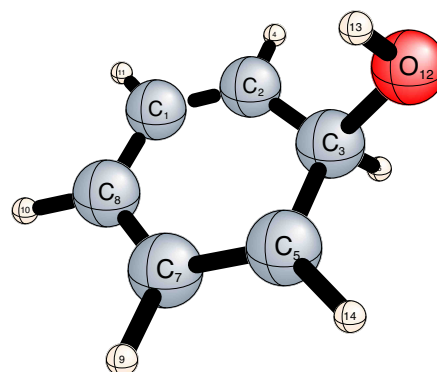


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.352	2.507	2.123	2.820	3.213	2.453	1.418	3.427	2.170	1.082	3.511	3.448	3.901
2		1.502	1.082	2.497	2.130	2.820	2.412	3.901	3.381	2.110	2.413	2.599	3.475
3			2.203	1.502	1.093	2.507	2.898	3.486	3.976	3.486	1.428	1.954	2.203
4				3.475	2.542	3.901	3.400	4.982	4.283	2.449	2.717	2.972	4.368
5					2.130	1.352	2.412	2.110	3.381	3.901	2.413	2.599	1.082
6						3.213	3.653	4.115	4.707	4.115	1.991	2.799	2.542
7							1.418	1.082	2.170	3.427	3.511	3.448	2.123
8								2.161	1.078	2.161	3.971	3.825	3.400
9									2.485	4.311	4.380	4.261	2.449
10										2.485	5.015	4.787	4.283
11											4.380	4.261	4.982
12												0.960	2.717
13													2.972

Molecule: C₆H₆OH (Intermediate 3)
Method: RI-MP2
Basis: def2-TZVPP
Energy: -192953.98416497 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.129870	-1.210743	-0.048633
2	C	-0.209424	-1.238411	0.252370
3	C	-1.013795	-0.000009	0.417724
4	H	-0.733094	-2.177403	0.351858
5	C	-0.209427	1.238393	0.252345
6	H	-1.482590	0.000001	1.406580
7	C	1.129866	1.210722	-0.048657
8	C	1.810553	-0.000011	-0.195672
9	H	1.660135	2.141954	-0.181620
10	H	2.861590	-0.000012	-0.438372
11	H	1.660141	-2.141976	-0.181577
12	O	-2.151550	-0.000019	-0.467557
13	H	-1.789841	-0.000029	-1.359422
14	H	-0.733100	2.177385	0.351814

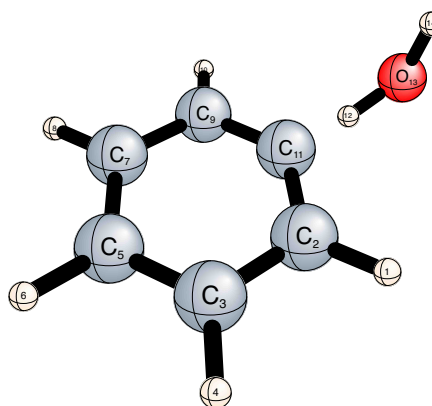


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.373	2.506	2.137	2.808	3.226	2.421	1.397	3.397	2.149	1.080	3.523	3.422	3.887
2		1.486	1.080	2.477	2.118	2.808	2.411	3.887	3.383	2.121	2.413	2.575	3.457
3			2.196	1.486	1.094	2.506	2.890	3.478	3.969	3.478	1.442	1.939	2.196
4				3.457	2.533	3.887	3.393	4.967	4.276	2.452	2.725	2.964	4.355
5					2.118	1.373	2.411	2.121	3.383	3.887	2.413	2.575	1.080
6						3.226	3.662	4.122	4.720	4.122	1.990	2.783	2.533
7							1.397	1.080	2.149	3.397	3.523	3.422	2.137
8								2.147	1.079	2.147	3.971	3.784	3.393
9									2.469	4.284	4.382	4.228	2.452
10										2.469	5.013	4.742	4.276
11											4.382	4.228	4.967
12												0.962	2.725
13													2.964

Molecule: TS₁
Method: B3LYP
Basis: 6-31G*
Energy: -193251.263436883 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.574421	-2.155929	0.077350
2	C	0.022609	-1.220742	0.050039
3	C	-1.376078	-1.211754	-0.022293
4	H	-1.920044	-2.152524	-0.051832
5	C	-2.068077	0.001173	-0.056569
6	H	-3.153194	0.001921	-0.114637
7	C	-1.374642	1.213147	-0.017874
8	H	-1.917493	2.154662	-0.043995
9	C	0.024055	1.220214	0.054487
10	H	0.576982	2.154637	0.085184
11	C	0.679473	-0.000726	0.093096
12	H	1.962202	-0.001675	0.214277
13	O	3.147803	-0.001962	0.019786
14	H	3.168947	-0.000710	-0.956554

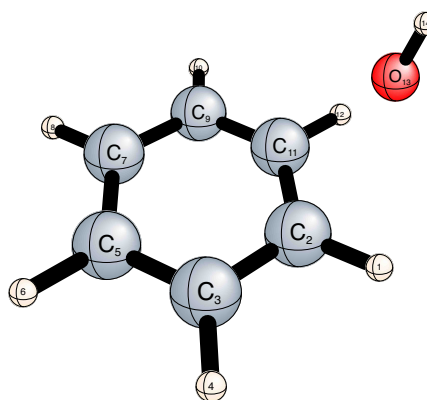


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.086	2.169	2.498	3.414	4.311	3.893	4.981	3.421	4.311	2.158	2.566	3.356	3.528
2		1.401	2.157	2.424	3.407	2.807	3.894	2.441	3.421	1.386	2.297	3.355	3.522
3			1.087	1.397	2.154	2.425	3.410	2.807	3.893	2.389	3.559	4.683	4.795
4				2.159	2.483	3.410	4.307	3.894	4.981	3.378	4.446	5.506	5.599
5					1.087	1.397	2.159	2.424	3.414	2.752	4.039	5.216	5.314
6						2.154	2.483	3.407	4.311	3.838	5.126	6.302	6.378
7							1.087	1.401	2.169	2.389	3.559	4.683	4.796
8								2.157	2.498	3.378	4.446	5.506	5.599
9									1.086	1.386	2.297	3.355	3.522
10										2.158	2.566	3.356	3.528
11											1.288	2.469	2.702
12												1.201	1.681
13													0.977

Molecule: TS₁
Method: B3LYP
Basis: def2-TZVPP
Energy: -193339.189221734 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.566925	-2.146309	0.066011
2	C	0.017599	-1.215134	0.041280
3	C	-1.376078	-1.207204	-0.016679
4	H	-1.916756	-2.144536	-0.039110
5	C	-2.066345	0.000127	-0.046143
6	H	-3.147303	0.000210	-0.093443
7	C	-1.375894	1.207352	-0.016694
8	H	-1.916429	2.144766	-0.039138
9	C	0.017784	1.215069	0.041266
10	H	0.567257	2.146159	0.065982
11	C	0.673044	-0.000081	0.078378
12	H	1.909196	-0.000174	0.175446
13	O	3.162455	-0.000227	0.039880
14	H	3.231510	-0.000285	-0.926572

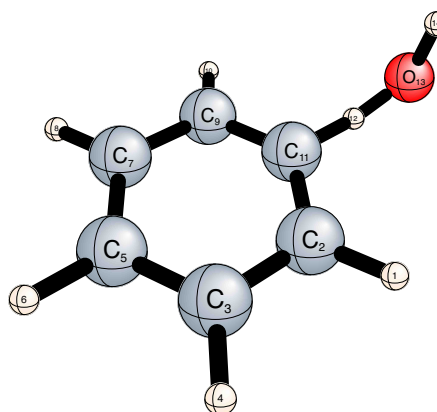


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.081	2.160	2.486	3.399	4.293	3.877	4.959	3.406	4.292	2.149	2.534	3.368	3.562
2		1.395	2.148	2.414	3.393	2.795	3.878	2.430	3.406	1.381	2.252	3.371	3.570
3			1.082	1.391	2.145	2.415	3.395	2.795	3.877	2.380	3.505	4.697	4.849
4				2.150	2.473	3.395	4.289	3.878	4.959	3.364	4.391	5.514	5.647
5					1.082	1.391	2.150	2.414	3.399	2.742	3.982	5.230	5.371
6						2.145	2.473	3.393	4.293	3.824	5.064	6.311	6.433
7							1.082	1.395	2.160	2.380	3.505	4.697	4.849
8								2.148	2.486	3.364	4.391	5.514	5.647
9									1.081	1.381	2.252	3.371	3.570
10										2.149	2.534	3.368	3.562
11											1.240	2.490	2.749
12												1.261	1.721
13													0.969

Molecule: TS₁
Method: ω B97
Basis: 6-31G*
Energy: -193203.115584338 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.584886	-2.154079	0.102602
2	C	0.028765	-1.218968	0.066057
3	C	-1.365267	-1.211079	-0.022567
4	H	-1.911320	-2.152942	-0.056647
5	C	-2.056339	-0.000005	-0.067134
6	H	-3.143054	0.000034	-0.137065
7	C	-1.365137	1.211017	-0.023297
8	H	-1.911085	2.152920	-0.057940
9	C	0.028898	1.218809	0.065336
10	H	0.585093	2.153898	0.101372
11	C	0.685257	-0.000102	0.111757
12	H	1.951161	-0.000235	0.233965
13	O	3.130875	-0.000575	-0.006096
14	H	3.104232	0.001041	-0.979876

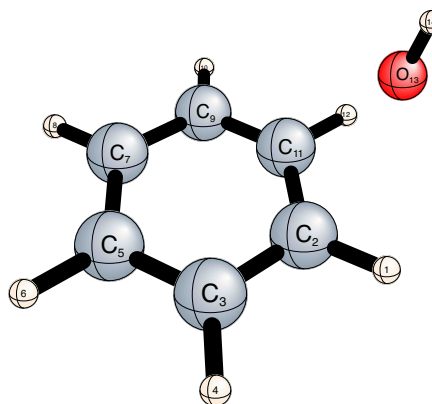


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.089	2.170	2.501	3.412	4.312	3.891	4.981	3.419	4.308	2.156	2.554	3.336	3.488
2		1.397	2.157	2.419	3.404	2.803	3.892	2.438	3.419	1.385	2.282	3.334	3.470
3			1.089	1.395	2.154	2.422	3.408	2.803	3.891	2.385	3.540	4.656	4.729
4				2.158	2.482	3.408	4.306	3.892	4.981	3.377	4.431	5.483	5.536
5					1.089	1.395	2.158	2.419	3.412	2.747	4.019	5.188	5.241
6						2.154	2.482	3.404	4.312	3.836	5.108	6.275	6.304
7							1.089	1.397	2.170	2.385	3.540	4.656	4.728
8								2.157	2.501	3.377	4.432	5.483	5.535
9									1.089	1.385	2.282	3.334	3.469
10										2.156	2.554	3.337	3.486
11											1.272	2.448	2.654
12												1.204	1.674
13													0.974

Molecule: TS₁
Method: ω B97
Basis: def2-TZVPP
Energy: -193285.649757896 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.574523	-2.145549	0.085688
2	C	0.021914	-1.213173	0.054245
3	C	-1.368337	-1.202730	-0.020497
4	H	-1.913829	-2.140076	-0.050076
5	C	-2.055507	0.005446	-0.057549
6	H	-3.138588	0.007341	-0.116733
7	C	-1.364158	1.211215	-0.019945
8	H	-1.906399	2.150459	-0.049090
9	C	0.026124	1.216819	0.054790
10	H	0.581947	2.147267	0.086658
11	C	0.678916	0.000677	0.096451
12	H	1.909998	-0.001540	0.197243
13	O	3.147116	-0.003962	0.018077
14	H	3.168705	-0.003460	-0.948476

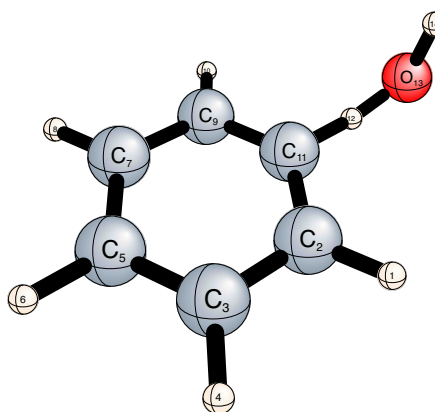


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.084	2.162	2.492	3.401	4.297	3.878	4.963	3.407	4.293	2.149	2.528	3.348	3.520
2		1.392	2.149	2.411	3.392	2.794	3.879	2.430	3.407	1.381	2.248	3.351	3.517
3			1.085	1.390	2.146	2.414	3.396	2.794	3.878	2.378	3.498	4.672	4.784
4				2.150	2.473	3.396	4.291	3.879	4.963	3.366	4.388	5.494	5.586
5					1.085	1.390	2.150	2.411	3.401	2.739	3.974	5.203	5.300
6						2.146	2.473	3.392	4.297	3.823	5.058	6.287	6.362
7							1.085	1.392	2.162	2.378	3.498	4.672	4.784
8								2.149	2.492	3.366	4.388	5.494	5.586
9									1.084	1.381	2.248	3.351	3.517
10										2.149	2.529	3.349	3.520
11											1.235	2.469	2.700
12												1.250	1.702
13													0.967

Molecule: TS₁
Method: ω B97X
Basis: 6-31G*
Energy: -193191.701910361 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.582050	-2.150497	0.099167
2	C	0.027412	-1.216907	0.063912
3	C	-1.364906	-1.209147	-0.022347
4	H	-1.909700	-2.149330	-0.055693
5	C	-2.055104	0.000066	-0.065531
6	H	-3.139827	0.000066	-0.133693
7	C	-1.364891	1.209279	-0.022606
8	H	-1.909676	2.149460	-0.056154
9	C	0.027429	1.217050	0.063661
10	H	0.582039	2.150665	0.098733
11	C	0.682983	0.000071	0.109329
12	H	1.947167	-0.000041	0.230523
13	O	3.130041	-0.000773	-0.003221
14	H	3.111947	-0.000229	-0.975615

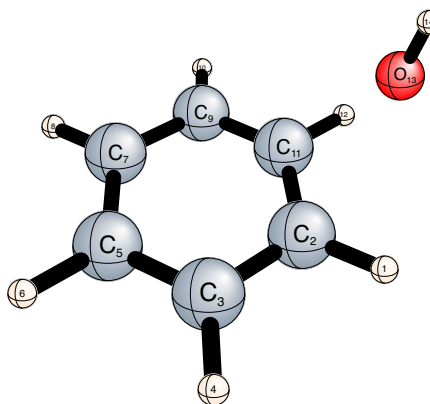


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.086	2.166	2.497	3.407	4.305	3.885	4.972	3.413	4.301	2.153	2.551	3.335	3.490
2		1.395	2.153	2.416	3.399	2.799	3.886	2.434	3.413	1.383	2.279	3.333	3.475
3			1.087	1.393	2.151	2.418	3.403	2.799	3.885	2.382	3.535	4.655	4.734
4				2.154	2.478	3.403	4.299	3.886	4.972	3.372	4.425	5.479	5.539
5					1.087	1.393	2.154	2.416	3.407	2.744	4.013	5.186	5.247
6						2.151	2.478	3.399	4.305	3.831	5.100	6.271	6.308
7							1.087	1.395	2.166	2.382	3.535	4.655	4.734
8								2.153	2.497	3.372	4.425	5.480	5.539
9									1.086	1.383	2.279	3.334	3.475
10										2.153	2.551	3.336	3.490
11											1.270	2.450	2.660
12												1.206	1.677
13													0.973

Molecule: TS₁
Method: ω B97X
Basis: def2-TZVPP
Energy: -193273.986475271 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.571804	-2.143739	0.079993
2	C	0.020112	-1.212985	0.050874
3	C	-1.367904	-1.203967	-0.023181
4	H	-1.911259	-2.140230	-0.054435
5	C	-2.055091	0.001389	-0.057493
6	H	-3.136237	0.002386	-0.116315
7	C	-1.365987	1.205481	-0.017637
8	H	-1.907854	2.142741	-0.044586
9	C	0.022040	1.211944	0.056470
10	H	0.575204	2.141677	0.089923
11	C	0.675490	-0.001137	0.095872
12	H	1.904032	-0.002414	0.197060
13	O	3.144576	-0.002424	0.019997
14	H	3.169897	0.001500	-0.945038

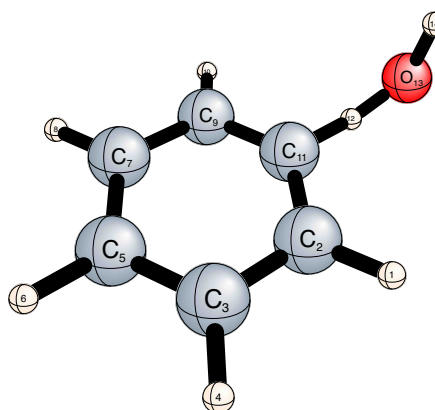


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.082	2.158	2.487	3.394	4.289	3.871	4.954	3.401	4.285	2.145	2.525	3.348	3.522
2		1.390	2.145	2.407	3.386	2.788	3.871	2.425	3.401	1.378	2.244	3.351	3.520
3			1.083	1.388	2.143	2.409	3.390	2.788	3.871	2.374	3.493	4.670	4.785
4				2.146	2.469	3.390	4.283	3.871	4.954	3.360	4.381	5.490	5.586
5					1.083	1.388	2.146	2.407	3.394	2.735	3.967	5.200	5.300
6						2.143	2.469	3.386	4.289	3.818	5.050	6.282	6.360
7							1.083	1.390	2.158	2.374	3.493	4.670	4.784
8								2.145	2.487	3.360	4.381	5.489	5.584
9									1.082	1.378	2.244	3.351	3.518
10										2.145	2.525	3.347	3.519
11											1.233	2.470	2.703
12												1.253	1.705
13													0.965

Molecule: TS₁
Method: ω B97X-D
Basis: 6-31G*
Energy: -193181.472784495 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.581032	-2.151056	0.088822
2	C	0.027722	-1.217859	0.058492
3	C	-1.365408	-1.208522	-0.026098
4	H	-1.910114	-2.147425	-0.062796
5	C	-2.054691	0.001804	-0.063581
6	H	-3.138398	0.003066	-0.130825
7	C	-1.363195	1.210536	-0.016505
8	H	-1.906191	2.150694	-0.045778
9	C	0.029948	1.216658	0.068144
10	H	0.584956	2.148573	0.105840
11	C	0.684176	-0.001382	0.109843
12	H	1.943596	-0.003034	0.229614
13	O	3.134598	-0.003220	-0.003059
14	H	3.121554	0.000782	-0.974812

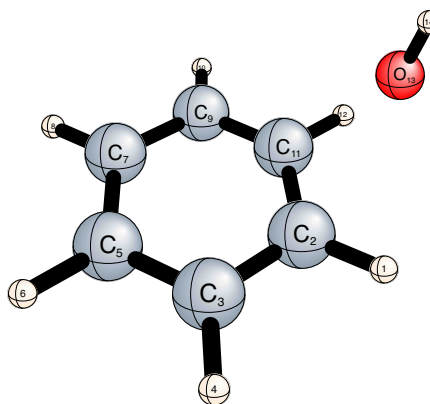


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.085	2.166	2.496	3.407	4.304	3.885	4.971	3.413	4.300	2.152	2.548	3.338	3.495
2		1.396	2.153	2.416	3.399	2.800	3.886	2.435	3.413	1.383	2.275	3.336	3.482
3			1.086	1.393	2.150	2.419	3.403	2.800	3.885	2.383	3.531	4.659	4.743
4				2.154	2.477	3.403	4.298	3.886	4.971	3.371	4.420	5.482	5.547
5					1.086	1.393	2.154	2.416	3.407	2.744	4.009	5.190	5.256
6						2.150	2.477	3.399	4.304	3.830	5.095	6.274	6.317
7							1.086	1.396	2.166	2.383	3.531	4.659	4.743
8								2.153	2.496	3.371	4.420	5.482	5.546
9									1.085	1.383	2.275	3.336	3.482
10										2.152	2.548	3.338	3.495
11											1.265	2.453	2.668
12												1.214	1.685
13													0.972

Molecule: TS₁
Method: ω B97X-D
Basis: def2-TZVPP
Energy: -193263.863250334 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.573779	-2.140536	0.089079
2	C	0.021532	-1.211457	0.056434
3	C	-1.366563	-1.205278	-0.017534
4	H	-1.907413	-2.142040	-0.044703
5	C	-2.055645	-0.001470	-0.057241
6	H	-3.135815	-0.002456	-0.116359
7	C	-1.368472	1.203586	-0.022833
8	H	-1.910798	2.139364	-0.054111
9	C	0.019614	1.212293	0.051103
10	H	0.570392	2.142379	0.079660
11	C	0.675600	0.001030	0.097444
12	H	1.895953	0.002216	0.198366
13	O	3.151429	0.002528	0.018318
14	H	3.175232	0.000065	-0.946115

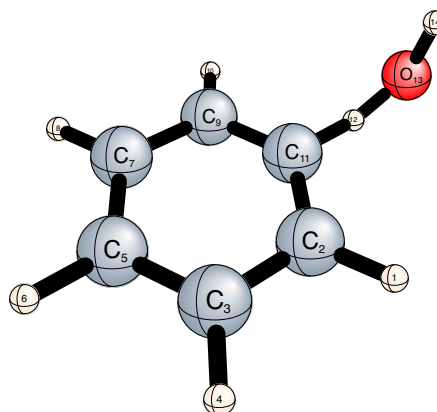


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.081	2.157	2.485	3.393	4.287	3.869	4.951	3.399	4.283	2.144	2.520	3.353	3.524
2		1.390	2.144	2.407	3.385	2.788	3.870	2.424	3.399	1.378	2.238	3.357	3.524
3			1.082	1.388	2.142	2.409	3.389	2.788	3.869	2.375	3.485	4.677	4.790
4				2.146	2.468	3.389	4.281	3.870	4.951	3.359	4.373	5.495	5.589
5					1.082	1.388	2.146	2.407	3.393	2.736	3.960	5.208	5.306
6						2.142	2.468	3.385	4.287	3.817	5.042	6.289	6.365
7							1.082	1.390	2.157	2.375	3.485	4.677	4.790
8								2.144	2.485	3.359	4.373	5.495	5.589
9									1.081	1.378	2.238	3.358	3.524
10										2.144	2.520	3.353	3.525
11											1.225	2.477	2.709
12												1.268	1.717
13													0.965

Molecule: TS₁
Method: M06
Basis: 6-31G*
Energy: -193106.046650109 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.563009	-2.172123	0.098739
2	C	0.018306	-1.230483	0.064642
3	C	-1.374108	-1.210869	-0.022478
4	H	-1.926688	-2.148633	-0.056958
5	C	-2.053870	0.003287	-0.066194
6	H	-3.140137	0.011784	-0.137050
7	C	-1.354622	1.206465	-0.022476
8	H	-1.892113	2.152915	-0.057378
9	C	0.037586	1.202133	0.064474
10	H	0.601807	2.132352	0.097631
11	C	0.682829	-0.019293	0.116755
12	H	1.940100	-0.014454	0.246884
13	O	3.136069	0.060220	-0.012260
14	H	3.108796	0.026431	-0.983865

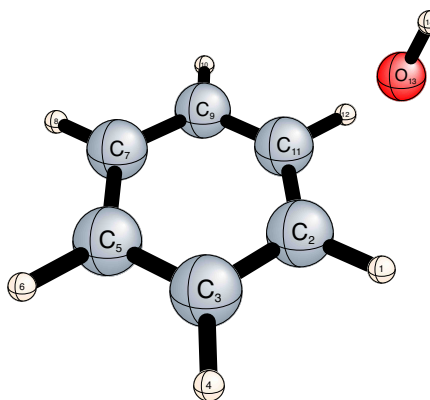


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.088	2.166	2.495	3.407	4.306	3.887	4.976	3.415	4.305	2.156	2.564	3.408	3.534
2		1.395	2.154	2.415	3.400	2.798	3.887	2.433	3.413	1.382	2.281	3.375	3.497
3			1.089	1.392	2.151	2.417	3.404	2.797	3.885	2.381	3.534	4.686	4.749
4				2.156	2.479	3.404	4.302	3.886	4.974	3.373	4.427	5.524	5.563
5					1.089	1.392	2.156	2.414	3.408	2.743	4.006	5.191	5.244
6						2.151	2.480	3.399	4.307	3.832	5.095	6.278	6.306
7							1.089	1.395	2.168	2.382	3.524	4.635	4.716
8								2.155	2.499	3.373	4.413	5.446	5.513
9									1.088	1.382	2.266	3.303	3.452
10										2.153	2.534	3.275	3.448
11											1.264	2.458	2.664
12												1.226	1.698
13													0.973

Molecule: TS₁
Method: M06
Basis: def2-TZVPP
Energy: -193187.511259677 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.524921	-2.161567	0.078888
2	C	-0.007359	-1.219626	0.049777
3	C	-1.394194	-1.183883	-0.018703
4	H	-1.954624	-2.110109	-0.044286
5	C	-2.056741	0.032445	-0.055438
6	H	-3.137586	0.053959	-0.111557
7	C	-1.345912	1.221357	-0.023200
8	H	-1.868879	2.169127	-0.052502
9	C	0.041149	1.201309	0.045716
10	H	0.610987	2.121146	0.072252
11	C	0.668446	-0.022103	0.091573
12	H	1.906290	-0.044934	0.196395
13	O	3.143642	-0.054677	0.040689
14	H	3.196051	-0.021603	-0.921367

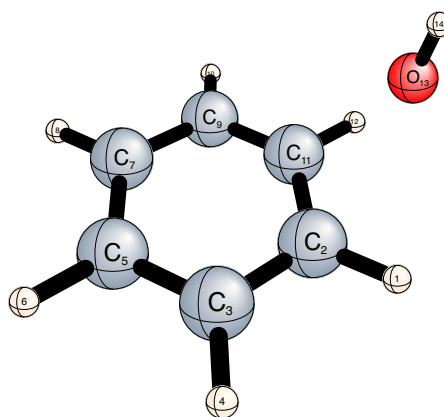


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.082	2.156	2.483	3.391	4.285	3.867	4.950	3.398	4.284	2.144	2.530	3.361	3.566
2		1.389	2.143	2.404	3.383	2.785	3.868	2.421	3.398	1.376	2.250	3.359	3.555
3			1.083	1.386	2.140	2.406	3.387	2.785	3.867	2.370	3.498	4.677	4.820
4				2.145	2.467	3.387	4.280	3.867	4.950	3.355	4.385	5.498	5.627
5					1.083	1.386	2.145	2.404	3.391	2.730	3.972	5.202	5.324
6						2.140	2.467	3.383	4.285	3.812	5.054	6.284	6.386
7							1.083	1.389	2.156	2.370	3.497	4.668	4.794
8								2.143	2.483	3.356	4.384	5.484	5.586
9									1.082	1.376	2.248	3.347	3.519
10										2.144	2.527	3.339	3.502
11											1.242	2.476	2.723
12												1.247	1.707
13													0.964

Molecule: TS₁
Method: M062X
Basis: 6-31G*
Energy: -193156.017591374 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.583224	-2.150424	0.108680
2	C	0.030841	-1.216789	0.071323
3	C	-1.361310	-1.208160	-0.027292
4	H	-1.905314	-2.147088	-0.068955
5	C	-2.050699	0.001790	-0.073135
6	H	-3.133485	0.002736	-0.151593
7	C	-1.359645	1.210533	-0.021057
8	H	-1.902334	2.150427	-0.057804
9	C	0.032532	1.216734	0.077512
10	H	0.586236	2.149394	0.119599
11	C	0.690193	-0.000621	0.128458
12	H	1.923837	-0.001822	0.252333
13	O	3.136643	-0.003082	-0.026896
14	H	3.076246	-0.003895	-1.000708

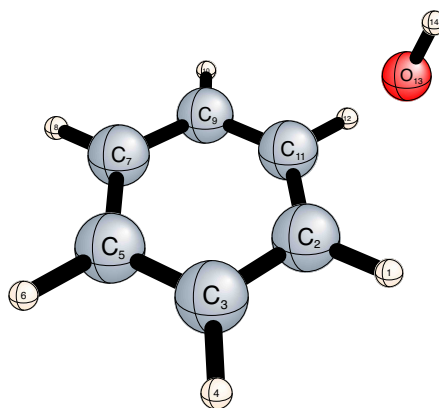


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.085	2.165	2.495	3.406	4.303	3.884	4.970	3.412	4.300	2.153	2.537	3.339	3.472
2		1.396	2.153	2.416	3.399	2.799	3.885	2.434	3.412	1.385	2.257	3.336	3.449
3			1.086	1.393	2.150	2.419	3.402	2.799	3.884	2.386	3.511	4.657	4.700
4				2.154	2.477	3.402	4.298	3.885	4.970	3.374	4.401	5.479	5.502
5					1.086	1.393	2.154	2.416	3.406	2.748	3.988	5.188	5.210
6						2.150	2.477	3.399	4.303	3.834	5.073	6.271	6.268
7							1.086	1.396	2.165	2.386	3.511	4.657	4.702
8								2.153	2.495	3.374	4.401	5.480	5.506
9									1.085	1.385	2.257	3.337	3.452
10										2.153	2.537	3.341	3.477
11											1.240	2.451	2.640
12												1.245	1.702
13													0.976

Molecule: TS₁
Method: M062X
Basis: def2-TZVPP
Energy: -193242.367191589 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.569849	-2.142823	0.086922
2	C	0.022218	-1.210727	0.056850
3	C	-1.366199	-1.198400	-0.028451
4	H	-1.910439	-2.132738	-0.067968
5	C	-2.050710	0.009248	-0.063973
6	H	-3.130342	0.013219	-0.132025
7	C	-1.358165	1.211812	-0.014733
8	H	-1.896089	2.150176	-0.043441
9	C	0.030310	1.213890	0.070586
10	H	0.584196	2.141895	0.111217
11	C	0.684026	-0.000904	0.113219
12	H	1.885161	-0.005590	0.218874
13	O	3.158490	-0.010720	-0.003833
14	H	3.140119	-0.009605	-0.972458



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.081	2.157	2.485	3.394	4.288	3.871	4.953	3.400	4.285	2.145	2.513	3.355	3.504
2		1.391	2.145	2.408	3.387	2.789	3.871	2.425	3.400	1.380	2.225	3.359	3.496
3			1.082	1.389	2.143	2.410	3.390	2.789	3.871	2.379	3.472	4.678	4.755
4				2.147	2.469	3.390	4.283	3.871	4.953	3.363	4.360	5.496	5.553
5					1.082	1.389	2.147	2.408	3.394	2.740	3.946	5.210	5.270
6						2.143	2.469	3.387	4.288	3.822	5.028	6.290	6.327
7							1.082	1.391	2.157	2.379	3.472	4.679	4.759
8								2.145	2.485	3.363	4.361	5.497	5.558
9									1.081	1.380	2.225	3.360	3.501
10										2.145	2.513	3.358	3.512
11											1.206	2.477	2.685
12												1.293	1.730
13													0.969

Molecule: TS₁
Method: M052X
Basis: 6-31G*
Energy: not available kcal/mol

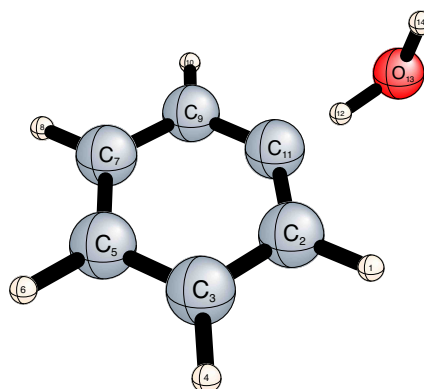
(This calculation failed to converge to a suitable accuracy after multiple attempts)

Molecule: TS₁
Method: M052X
Basis: def2-TZVPP
Energy: not available kcal/mol

(This calculation failed to converge to a suitable accuracy after multiple attempts)

Molecule: TS₁
Method: M06L
Basis: 6-31G*
Energy: -193221.355741729 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.570727	-2.155266	0.072880
2	C	0.018415	-1.218207	0.046279
3	C	-1.377509	-1.208911	-0.020052
4	H	-1.922072	-2.151475	-0.046318
5	C	-2.067015	0.001249	-0.052458
6	H	-3.153879	0.002407	-0.106849
7	C	-1.375113	1.209948	-0.017343
8	H	-1.917790	2.153658	-0.041553
9	C	0.020843	1.216345	0.049251
10	H	0.574707	2.152427	0.078407
11	C	0.673754	-0.001633	0.086865
12	H	1.955928	-0.004244	0.195943
13	O	3.148346	-0.008216	0.028033
14	H	3.197622	0.011650	-0.942619

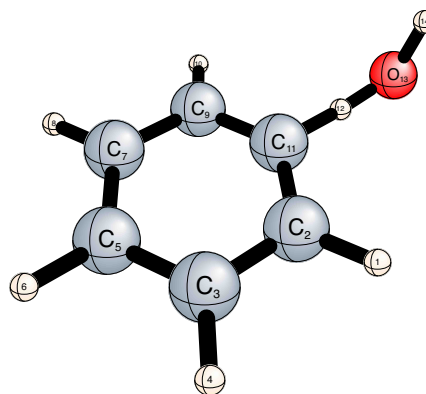


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.088	2.168	2.496	3.409	4.308	3.888	4.977	3.416	4.308	2.156	2.561	3.355	3.553
2		1.398	2.155	2.418	3.402	2.800	3.889	2.435	3.416	1.382	2.291	3.356	3.549
3			1.089	1.393	2.152	2.419	3.406	2.800	3.888	2.383	3.551	4.683	4.824
4				2.158	2.482	3.406	4.305	3.889	4.977	3.373	4.439	5.505	5.630
5					1.088	1.393	2.158	2.418	3.409	2.744	4.031	5.216	5.339
6						2.152	2.482	3.402	4.308	3.833	5.119	6.304	6.406
7							1.089	1.398	2.168	2.383	3.552	4.685	4.817
8								2.155	2.495	3.373	4.441	5.509	5.619
9									1.088	1.382	2.293	3.359	3.539
10										2.156	2.564	3.361	3.536
11											1.287	2.475	2.726
12												1.204	1.685
13													0.972

Molecule: TS₁
Method: M06L
Basis: def2-TZVPP
Energy: -193302.907470881 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.558177	-2.143388	0.043222
2	C	0.011361	-1.211232	0.026669
3	C	-1.379947	-1.198316	-0.021292
4	H	-1.922557	-2.133722	-0.044492
5	C	-2.064449	0.008196	-0.039668
6	H	-3.144742	0.011669	-0.079292
7	C	-1.372680	1.210307	-0.009008
8	H	-1.909635	2.149169	-0.022607
9	C	0.018687	1.214371	0.038993
10	H	0.571088	2.142996	0.065008
11	C	0.664846	-0.000554	0.063552
12	H	1.926918	-0.004998	0.148680
13	O	3.148635	-0.009149	0.059278
14	H	3.256725	-0.006614	-0.898256

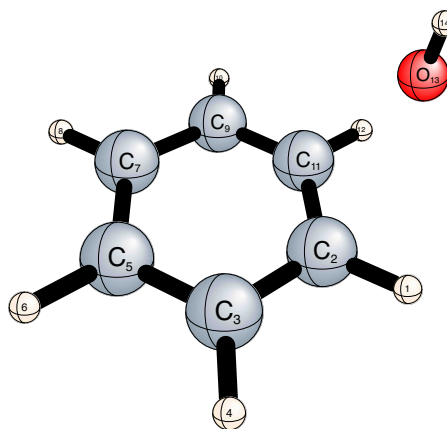


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.081	2.157	2.482	3.393	4.286	3.870	4.952	3.401	4.286	2.146	2.541	3.356	3.569
2		1.392	2.144	2.408	3.386	2.789	3.871	2.426	3.401	1.376	2.267	3.360	3.583
3			1.082	1.387	2.141	2.409	3.389	2.789	3.870	2.371	3.520	4.683	4.867
4				2.147	2.469	3.389	4.283	3.871	4.952	3.355	4.403	5.499	5.664
5					1.081	1.387	2.147	2.408	3.393	2.731	3.996	5.214	5.390
6						2.141	2.469	3.386	4.286	3.812	5.077	6.295	6.454
7							1.082	1.392	2.157	2.371	3.520	4.683	4.869
8								2.144	2.482	3.355	4.403	5.500	5.666
9									1.081	1.376	2.267	3.361	3.585
10										2.146	2.541	3.358	3.572
11											1.265	2.484	2.765
12												1.225	1.692
13													0.964

Molecule: TS₁
Method: M06HF
Basis: 6-31G*
Energy: -193179.6808836 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.572036	-2.158105	0.173423
2	C	0.026840	-1.225634	0.112859
3	C	-1.359960	-1.213632	-0.029687
4	H	-1.905000	-2.146901	-0.082825
5	C	-2.043146	-0.001868	-0.104719
6	H	-3.119380	0.002376	-0.216141
7	C	-1.349139	1.204305	-0.039477
8	H	-1.885630	2.142066	-0.100222
9	C	0.037614	1.204000	0.103010
10	H	0.593733	2.130542	0.155903
11	C	0.695823	-0.013392	0.183180
12	H	1.881276	-0.011720	0.330236
13	O	3.131818	0.049524	-0.089104
14	H	2.955345	0.038399	-1.052450



Distance Matrix

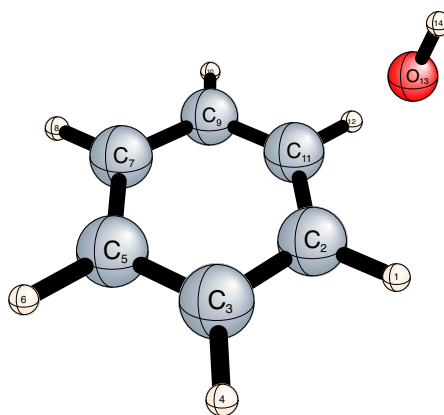
	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.082	2.160	2.490	3.401	4.295	3.878	4.960	3.405	4.289	2.148	2.519	3.390	3.465
2		1.394	2.149	2.414	3.393	2.797	3.879	2.430	3.404	1.386	2.227	3.363	3.396
3			1.082	1.393	2.147	2.418	3.397	2.796	3.877	2.390	3.476	4.666	4.608
4				2.150	2.472	3.397	4.289	3.878	4.960	3.374	4.366	5.495	5.417
5					1.082	1.393	2.150	2.414	3.401	2.754	3.948	5.175	5.088
6						2.147	2.473	3.393	4.296	3.836	5.030	6.253	6.132
7							1.082	1.394	2.161	2.390	3.471	4.628	4.573
8								2.149	2.493	3.375	4.360	5.436	5.364
9									1.082	1.386	2.220	3.308	3.348
10										2.147	2.505	3.291	3.379
11											1.195	2.452	2.576
12												1.320	1.752
13													0.979

Molecule: TS₁
Method: M06HF
Basis: def2-TZVPP
Energy: not available kcal/mol

(This calculation failed to converge to a suitable accuracy after multiple attempts)

Molecule: TS₁
Method: RI-MP2
Basis: def2-TZVPP
Energy: -192925.899067196 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.569168	-2.140955	0.120238
2	C	0.020907	-1.212650	0.076790
3	C	-1.367016	-1.206912	-0.029421
4	H	-1.907671	-2.140328	-0.071779
5	C	-2.055971	-0.000046	-0.083141
6	H	-3.132073	-0.000047	-0.166802
7	C	-1.366999	1.206820	-0.029641
8	H	-1.907641	2.140236	-0.072170
9	C	0.020924	1.212557	0.076568
10	H	0.569205	2.140858	0.119848
11	C	0.685805	-0.000045	0.135993
12	H	1.853583	-0.000039	0.252106
13	O	3.137117	0.000386	-0.006485
14	H	3.069592	0.000241	-0.970476

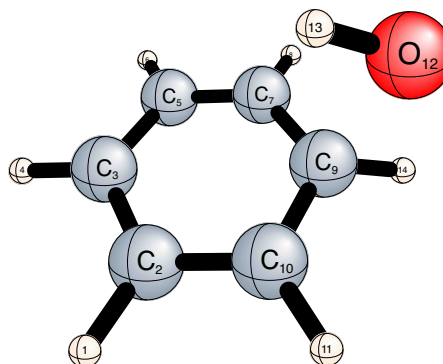


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.079	2.155	2.484	3.394	4.285	3.870	4.950	3.398	4.282	2.144	2.500	3.346	3.468
2		1.392	2.145	2.410	3.387	2.791	3.871	2.425	3.398	1.384	2.205	3.345	3.444
3			1.080	1.391	2.143	2.414	3.391	2.791	3.870	2.387	3.451	4.663	4.693
4				2.145	2.468	3.391	4.281	3.871	4.950	3.369	4.340	5.481	5.492
5					1.079	1.391	2.145	2.410	3.394	2.751	3.924	5.194	5.202
6						2.143	2.468	3.387	4.285	3.830	5.003	6.271	6.254
7							1.080	1.392	2.155	2.387	3.451	4.663	4.693
8								2.145	2.484	3.369	4.340	5.480	5.492
9									1.079	1.384	2.205	3.345	3.444
10										2.144	2.500	3.345	3.467
11											1.174	2.455	2.628
12												1.309	1.724
13													0.966

Molecule: TS₂
Method: B3LYP
Basis: 6-31G*
Energy: -193258.276303647 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.596265	-2.154093	-0.270567
2	C	-1.087622	-1.215567	-0.067054
3	C	-1.729883	0.000700	-0.342230
4	H	-2.731897	0.001078	-0.762850
5	C	-1.086587	1.216484	-0.067328
6	H	-1.594434	2.155393	-0.271055
7	C	0.191847	1.221708	0.474648
8	H	0.695235	2.158181	0.694367
9	C	0.877007	-0.000289	0.708059
10	C	0.190813	-1.221755	0.474913
11	H	0.693408	-2.158604	0.694840
12	O	2.168257	-0.001059	-0.854821
13	H	1.500613	-0.000525	-1.568418
14	H	1.769008	-0.000592	1.322228

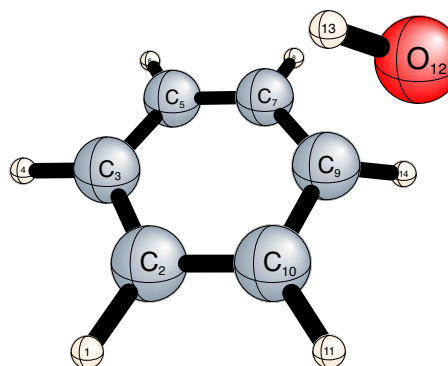


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.087	2.160	2.485	3.415	4.309	3.892	4.978	3.423	2.149	2.485	4.376	3.989	4.301
2		1.403	2.161	2.432	3.415	2.805	3.891	2.437	1.389	2.154	3.563	3.229	3.401
3			1.087	1.403	2.160	2.419	3.407	2.811	2.419	3.407	3.932	3.455	3.875
4				2.161	2.485	3.401	4.304	3.897	3.401	4.304	4.901	4.308	4.960
5					1.087	1.389	2.154	2.437	2.805	3.891	3.563	3.229	3.401
6						2.149	2.485	3.423	3.892	4.978	4.376	3.989	4.301
7							1.086	1.420	2.443	3.424	2.677	2.717	2.168
8								2.166	3.424	4.317	3.038	3.229	2.491
9									1.420	2.166	2.027	2.360	1.083
10										1.086	2.677	2.717	2.168
11											3.038	3.230	2.491
12												0.977	2.213
13													2.903

Molecule: TS₂
Method: B3LYP
Basis: def2-TZVPP
Energy: -193343.565128763 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.595439	-2.145585	-0.300003
2	C	-1.091213	-1.211672	-0.090038
3	C	-1.725582	0.000452	-0.375569
4	H	-2.715604	0.000690	-0.812074
5	C	-1.090439	1.212275	-0.090471
6	H	-1.594074	2.146434	-0.300768
7	C	0.171857	1.218426	0.470789
8	H	0.668274	2.150874	0.699952
9	C	0.852571	-0.000175	0.713781
10	C	0.171080	-1.218426	0.471223
11	H	0.666899	-2.151108	0.700724
12	O	2.186764	-0.000889	-0.795654
13	H	1.570107	-0.000706	-1.542019
14	H	1.722531	-0.000342	1.351056

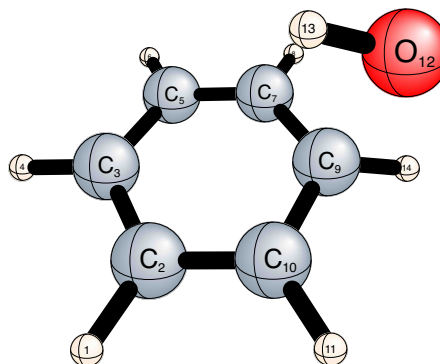


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.082	2.151	2.475	3.402	4.292	3.877	4.958	3.409	2.139	2.474	4.376	4.020	4.282
2		1.398	2.152	2.424	3.402	2.796	3.876	2.427	1.381	2.144	3.565	3.265	3.385
3			1.082	1.398	2.151	2.408	3.393	2.799	2.408	3.393	3.935	3.496	3.856
4				2.152	2.475	3.386	4.285	3.881	3.386	4.285	4.902	4.347	4.937
5					1.082	1.381	2.144	2.427	2.796	3.876	3.565	3.264	3.385
6						2.139	2.474	3.409	3.877	4.958	4.376	4.020	4.282
7							1.081	1.417	2.437	3.413	2.674	2.737	2.160
8								2.159	3.413	4.302	3.029	3.236	2.483
9									1.417	2.159	2.015	2.367	1.078
10										1.081	2.674	2.737	2.160
11											3.029	3.236	2.483
12												0.968	2.196
13													2.897

Molecule: TS₂
Method: ω B97
Basis: 6-31G*
Energy: -193211.992865682 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.579022	-2.155293	-0.281243
2	C	-1.071901	-1.214598	-0.072298
3	C	-1.708710	0.000155	-0.358099
4	H	-2.706666	0.000245	-0.793893
5	C	-1.071677	1.214804	-0.072325
6	H	-1.578639	2.155588	-0.281253
7	C	0.198198	1.220196	0.486998
8	H	0.699313	2.158771	0.714756
9	C	0.881810	-0.000074	0.721493
10	C	0.198007	-1.220211	0.486951
11	H	0.699040	-2.158876	0.714509
12	O	2.110886	-0.000673	-0.876842
13	H	1.406411	0.001146	-1.552268
14	H	1.782452	-0.000118	1.328248

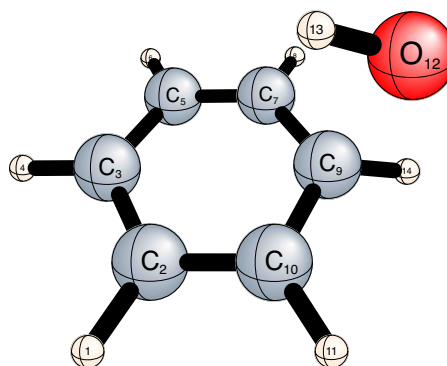


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.089	2.161	2.486	3.414	4.311	3.891	4.979	3.421	2.150	2.486	4.314	3.896	4.305
2		1.401	2.161	2.429	3.414	2.803	3.891	2.434	1.388	2.156	3.500	3.132	3.404
3			1.089	1.401	2.161	2.416	3.407	2.806	2.416	3.407	3.855	3.336	3.877
4				2.161	2.486	3.401	4.305	3.895	3.401	4.305	4.818	4.182	4.965
5					1.089	1.388	2.156	2.434	2.803	3.891	3.500	3.131	3.403
6						2.150	2.486	3.421	3.891	4.979	4.315	3.895	4.305
7							1.088	1.418	2.440	3.424	2.647	2.665	2.169
8								2.167	3.424	4.318	3.031	3.209	2.492
9									1.418	2.167	2.016	2.333	1.086
10										1.088	2.647	2.667	2.170
11											3.030	3.210	2.492
12												0.976	2.229
13													2.905

Molecule: TS₂
Method: ω B97
Basis: def2-TZVPP
Energy: -193292.007130641 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.577746	-2.148033	-0.298234
2	C	-1.074834	-1.211296	-0.084167
3	C	-1.705326	-0.000099	-0.377195
4	H	-2.693554	-0.000221	-0.824411
5	C	-1.074970	1.211251	-0.084534
6	H	-1.577988	2.147868	-0.298873
7	C	0.182887	1.217142	0.488447
8	H	0.679030	2.152126	0.721626
9	C	0.860429	0.000205	0.732902
10	C	0.183028	-1.216878	0.488796
11	H	0.679291	-2.151742	0.722208
12	O	2.127670	0.000240	-0.848825
13	H	1.452525	0.000293	-1.541311
14	H	1.751766	0.000346	1.345722

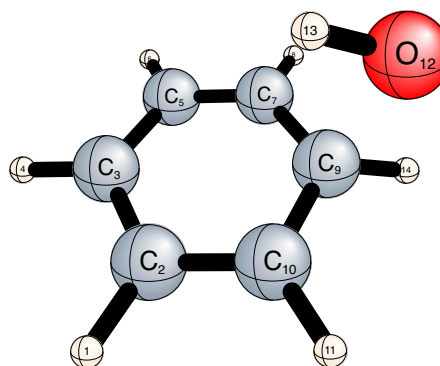


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.085	2.153	2.477	3.403	4.296	3.879	4.962	3.409	2.142	2.477	4.318	3.917	4.290
2		1.397	2.153	2.423	3.403	2.794	3.878	2.425	1.382	2.147	3.508	3.159	3.392
3			1.085	1.397	2.153	2.408	3.395	2.796	2.408	3.395	3.862	3.366	3.863
4				2.153	2.477	3.388	4.289	3.880	3.388	4.289	4.821	4.208	4.947
5					1.085	1.382	2.147	2.425	2.794	3.878	3.508	3.159	3.392
6						2.142	2.477	3.409	3.879	4.962	4.318	3.917	4.290
7							1.084	1.414	2.434	3.413	2.655	2.686	2.163
8								2.160	3.413	4.304	3.032	3.217	2.484
9									1.414	2.160	2.027	2.350	1.082
10										1.084	2.656	2.686	2.163
11											3.033	3.218	2.484
12												0.967	2.227
13													2.902

Molecule: TS₂
Method: ω B97X
Basis: 6-31G*
Energy: -193199.85022203 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.580457	-2.151130	-0.278218
2	C	-1.073342	-1.212384	-0.071356
3	C	-1.710011	0.000525	-0.354195
4	H	-2.707669	0.000744	-0.785480
5	C	-1.072844	1.213165	-0.071269
6	H	-1.579605	2.152124	-0.278031
7	C	0.196691	1.218568	0.482703
8	H	0.697579	2.155265	0.708505
9	C	0.880546	-0.000023	0.714733
10	C	0.196198	-1.218326	0.482629
11	H	0.696751	-2.155234	0.708296
12	O	2.115882	-0.000714	-0.866632
13	H	1.423332	-0.001300	-1.551498
14	H	1.776450	-0.000221	1.324546

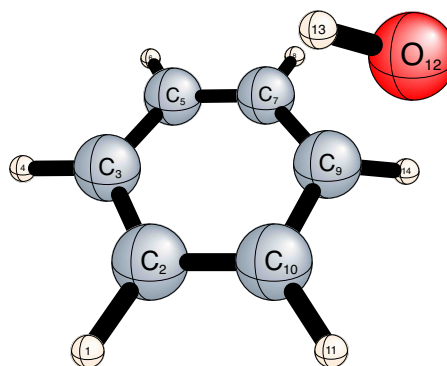


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.087	2.157	2.482	3.409	4.303	3.885	4.971	3.416	2.146	2.482	4.317	3.907	4.297
2		1.399	2.157	2.426	3.409	2.798	3.884	2.430	1.385	2.152	3.503	3.145	3.397
3			1.087	1.399	2.157	2.412	3.401	2.802	2.412	3.401	3.860	3.354	3.870
4				2.157	2.482	3.395	4.298	3.889	3.395	4.298	4.824	4.201	4.956
5					1.087	1.385	2.152	2.430	2.798	3.884	3.503	3.146	3.397
6						2.146	2.482	3.416	3.885	4.971	4.317	3.909	4.297
7							1.086	1.416	2.437	3.418	2.644	2.670	2.166
8								2.163	3.418	4.310	3.023	3.207	2.488
9									1.416	2.163	2.007	2.330	1.084
10										1.086	2.644	2.669	2.166
11											3.023	3.205	2.488
12												0.974	2.217
13													2.898

Molecule: TS₂
Method: ω B97X
Basis: def2-TZVPP
Energy: -193279.561548861 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.578214	-2.144372	-0.295940
2	C	-1.075377	-1.209277	-0.084250
3	C	-1.705778	-0.000497	-0.374928
4	H	-2.693742	-0.000813	-0.818056
5	C	-1.075844	1.208694	-0.084939
6	H	-1.579050	2.143472	-0.297156
7	C	0.181212	1.215043	0.482711
8	H	0.676520	2.148545	0.714474
9	C	0.859560	0.000313	0.724417
10	C	0.181693	-1.214812	0.483379
11	H	0.677368	-2.147993	0.715653
12	O	2.131383	0.000227	-0.835245
13	H	1.469731	0.000034	-1.538179
14	H	1.744800	0.000661	1.342465

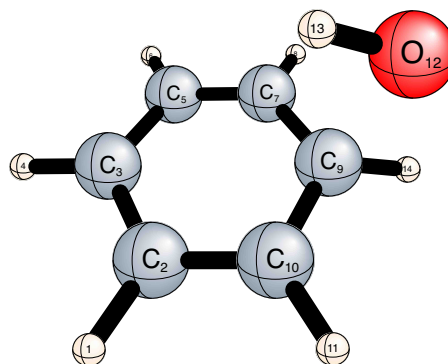


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.083	2.149	2.472	3.397	4.288	3.871	4.953	3.403	2.137	2.472	4.319	3.928	4.281
2		1.394	2.149	2.418	3.397	2.789	3.871	2.421	1.379	2.143	3.509	3.171	3.384
3			1.083	1.394	2.149	2.403	3.388	2.791	2.403	3.388	3.865	3.382	3.854
4				2.149	2.472	3.382	4.281	3.874	3.382	4.281	4.825	4.225	4.936
5					1.083	1.379	2.143	2.421	2.789	3.871	3.509	3.171	3.384
6						2.137	2.472	3.403	3.871	4.953	4.319	3.928	4.281
7							1.082	1.412	2.430	3.407	2.649	2.687	2.158
8								2.156	3.407	4.297	3.022	3.212	2.480
9									1.412	2.156	2.012	2.343	1.080
10										1.082	2.649	2.687	2.158
11											3.022	3.213	2.480
12												0.965	2.212
13													2.894

Molecule: TS₂
Method: ω B97X-D
Basis: 6-31G*
Energy: -193189.080180896 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.575656	-2.153574	-0.304145
2	C	-1.074471	-1.214642	-0.089431
3	C	-1.708569	-0.003214	-0.383746
4	H	-2.697942	-0.005473	-0.831203
5	C	-1.078761	1.211118	-0.092194
6	H	-1.583257	2.147787	-0.309019
7	C	0.181567	1.219719	0.482574
8	H	0.677772	2.156330	0.713137
9	C	0.863122	0.002596	0.727464
10	C	0.185883	-1.217483	0.485336
11	H	0.685398	-2.151808	0.717993
12	O	2.128525	0.002862	-0.838679
13	H	1.449551	0.001708	-1.535468
14	H	1.749548	0.004870	1.348906

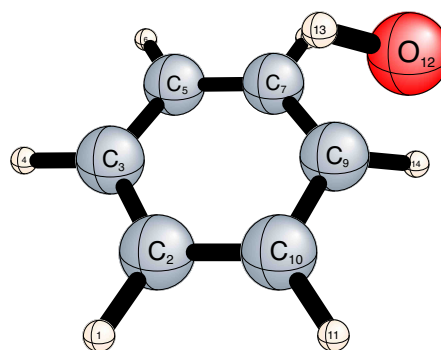


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.086	2.156	2.480	3.408	4.301	3.884	4.969	3.415	2.145	2.481	4.319	3.913	4.295
2		1.399	2.156	2.426	3.408	2.798	3.883	2.430	1.385	2.151	3.508	3.153	3.396
3			1.086	1.399	2.156	2.412	3.400	2.802	2.412	3.400	3.864	3.362	3.868
4				2.156	2.480	3.394	4.296	3.887	3.394	4.296	4.826	4.207	4.953
5					1.086	1.385	2.151	2.430	2.798	3.883	3.508	3.152	3.396
6						2.145	2.481	3.415	3.884	4.969	4.320	3.913	4.295
7							1.085	1.416	2.437	3.417	2.649	2.677	2.164
8								2.162	3.417	4.308	3.025	3.208	2.486
9									1.416	2.162	2.013	2.338	1.083
10										1.085	2.649	2.677	2.164
11											3.025	3.209	2.486
12												0.973	2.220
13													2.900

Molecule: TS₂
Method: ω B97X-D
Basis: def2-TZVPP
Energy: -193268.891409043 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.577888	-2.142369	-0.298878
2	C	-1.075577	-1.208434	-0.085740
3	C	-1.704562	0.000218	-0.377100
4	H	-2.690762	0.000283	-0.821867
5	C	-1.075325	1.208791	-0.085948
6	H	-1.577441	2.142793	-0.299250
7	C	0.180376	1.214793	0.483334
8	H	0.676033	2.146961	0.714600
9	C	0.857613	0.000051	0.725289
10	C	0.180118	-1.214597	0.483555
11	H	0.675585	-2.146823	0.714990
12	O	2.133772	-0.000482	-0.833503
13	H	1.474716	-0.000615	-1.537419
14	H	1.740776	0.000015	1.344461

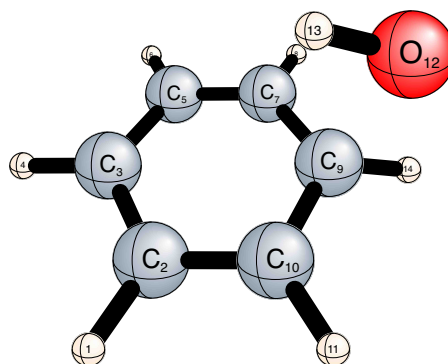


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.082	2.148	2.470	3.395	4.285	3.870	4.950	3.402	2.136	2.471	4.319	3.929	4.278
2		1.393	2.147	2.417	3.395	2.788	3.869	2.420	1.379	2.142	3.510	3.173	3.382
3			1.082	1.393	2.148	2.402	3.386	2.789	2.402	3.386	3.865	3.384	3.852
4				2.147	2.470	3.380	4.278	3.871	3.380	4.278	4.825	4.226	4.933
5					1.082	1.379	2.142	2.420	2.788	3.869	3.510	3.174	3.382
6						2.136	2.471	3.402	3.870	4.950	4.319	3.930	4.278
7							1.081	1.412	2.429	3.406	2.651	2.690	2.157
8								2.155	3.406	4.294	3.022	3.213	2.478
9									1.412	2.155	2.015	2.345	1.079
10										1.081	2.651	2.690	2.157
11											3.022	3.212	2.478
12												0.964	2.213
13													2.894

Molecule: TS₂
Method: M06
Basis: 6-31G*
Energy: -193116.102612356 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.572422	-2.152693	-0.310126
2	C	-1.070298	-1.212414	-0.089723
3	C	-1.701459	-0.000200	-0.384958
4	H	-2.691018	-0.000327	-0.838820
5	C	-1.070713	1.212177	-0.089495
6	H	-1.573163	2.152324	-0.309718
7	C	0.186094	1.218186	0.490679
8	H	0.686748	2.155855	0.721169
9	C	0.863344	0.000136	0.735545
10	C	0.186513	-1.218101	0.490447
11	H	0.687495	-2.155640	0.720750
12	O	2.114411	0.000422	-0.842338
13	H	1.417301	0.000625	-1.522723
14	H	1.754601	0.000235	1.355835

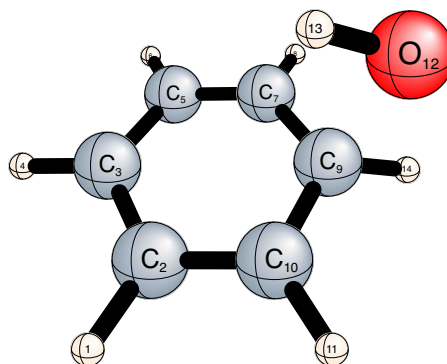


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.088	2.158	2.483	3.409	4.305	3.885	4.973	3.415	2.147	2.484	4.303	3.879	4.299
2		1.398	2.158	2.425	3.409	2.797	3.885	2.427	1.384	2.153	3.490	3.117	3.397
3			1.089	1.398	2.158	2.411	3.402	2.799	2.411	3.402	3.843	3.320	3.870
4				2.158	2.483	3.396	4.300	3.887	3.396	4.300	4.805	4.165	4.958
5					1.088	1.384	2.153	2.427	2.797	3.885	3.490	3.116	3.397
6						2.147	2.484	3.415	3.885	4.973	4.303	3.879	4.299
7							1.088	1.415	2.436	3.419	2.642	2.656	2.166
8								2.163	3.419	4.311	3.021	3.196	2.488
9									1.415	2.163	2.014	2.325	1.086
10										1.088	2.642	2.656	2.166
11											3.021	3.196	2.488
12												0.974	2.227
13													2.898

Molecule: TS₂
Method: M06
Basis: def2-TZVPP
Energy: -193195.14614913 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.571745	-2.141530	-0.297652
2	C	-1.068964	-1.207094	-0.084292
3	C	-1.697247	0.000403	-0.376801
4	H	-2.683435	0.000588	-0.823343
5	C	-1.068295	1.207676	-0.084778
6	H	-1.570561	2.142304	-0.298511
7	C	0.184838	1.214253	0.484416
8	H	0.682785	2.146683	0.713994
9	C	0.863931	-0.000079	0.721227
10	C	0.184165	-1.214136	0.484914
11	H	0.681599	-2.146745	0.714862
12	O	2.104898	-0.001104	-0.836336
13	H	1.434758	-0.000856	-1.530626
14	H	1.744965	-0.000187	1.346057

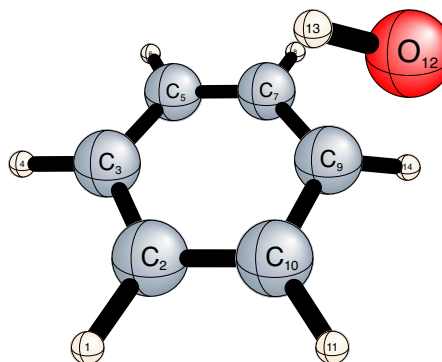


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.082	2.147	2.470	3.394	4.284	3.868	4.949	3.399	2.134	2.470	4.288	3.891	4.276
2		1.392	2.147	2.415	3.394	2.785	3.867	2.417	1.376	2.142	3.478	3.133	3.379
3			1.083	1.392	2.147	2.399	3.385	2.787	2.399	3.385	3.830	3.338	3.849
4				2.147	2.470	3.378	4.278	3.869	3.378	4.278	4.788	4.178	4.931
5					1.082	1.376	2.142	2.417	2.785	3.867	3.478	3.133	3.379
6						2.134	2.470	3.399	3.868	4.949	4.289	3.891	4.276
7							1.082	1.411	2.428	3.405	2.628	2.664	2.157
8								2.154	3.405	4.293	3.006	3.196	2.477
9									1.411	2.154	1.991	2.323	1.080
10										1.082	2.628	2.664	2.157
11											3.006	3.196	2.477
12												0.965	2.212
13													2.893

Molecule: TS₂
Method: M062X
Basis: 6-31G*
Energy: -193162.64243732 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.572589	-2.150483	-0.304283
2	C	-1.070007	-1.212832	-0.088520
3	C	-1.702500	-0.000049	-0.380752
4	H	-2.691734	-0.000079	-0.827941
5	C	-1.070067	1.212777	-0.088553
6	H	-1.572700	2.150395	-0.304341
7	C	0.189944	1.218501	0.486131
8	H	0.688440	2.154042	0.716536
9	C	0.872088	0.000034	0.726037
10	C	0.190009	-1.218474	0.486156
11	H	0.688556	-2.153982	0.716581
12	O	2.100532	-0.000007	-0.829268
13	H	1.412992	0.000270	-1.522653
14	H	1.758728	0.000064	1.347999

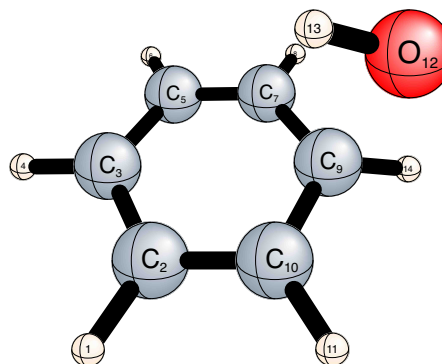


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.086	2.156	2.480	3.407	4.301	3.883	4.968	3.415	2.145	2.481	4.289	3.876	4.296
2		1.399	2.156	2.426	3.407	2.798	3.883	2.430	1.385	2.151	3.474	3.113	3.397
3			1.086	1.399	2.156	2.412	3.400	2.802	2.412	3.400	3.829	3.318	3.869
4				2.156	2.480	3.393	4.295	3.888	3.393	4.295	4.792	4.163	4.954
5					1.086	1.385	2.151	2.430	2.798	3.883	3.475	3.113	3.397
6						2.145	2.481	3.415	3.883	4.968	4.289	3.876	4.296
7							1.085	1.417	2.437	3.417	2.620	2.649	2.165
8								2.162	3.417	4.308	3.004	3.190	2.487
9									1.417	2.162	1.982	2.313	1.083
10										1.085	2.620	2.649	2.165
11											3.004	3.191	2.487
12												0.976	2.204
13													2.891

Molecule: TS₂
Method: M062X
Basis: def2-TZVPP
Energy: -193246.992426768 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.571945	-2.143041	-0.293134
2	C	-1.069883	-1.209013	-0.080257
3	C	-1.700837	0.000291	-0.368561
4	H	-2.688411	0.000254	-0.810298
5	C	-1.070235	1.209624	-0.079660
6	H	-1.572519	2.143621	-0.292128
7	C	0.188289	1.215219	0.485986
8	H	0.685939	2.147561	0.713381
9	C	0.866707	0.000389	0.724910
10	C	0.188616	-1.214539	0.485503
11	H	0.686430	-2.146862	0.712644
12	O	2.101841	0.001449	-0.850627
13	H	1.426898	-0.005093	-1.545004
14	H	1.758991	0.000360	1.331638

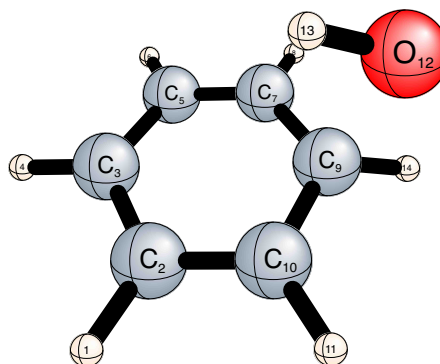


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.082	2.149	2.471	3.397	4.287	3.871	4.952	3.403	2.137	2.472	4.290	3.890	4.281
2		1.394	2.148	2.419	3.397	2.789	3.870	2.421	1.380	2.143	3.481	3.135	3.385
3			1.082	1.394	2.149	2.403	3.388	2.791	2.403	3.388	3.833	3.342	3.855
4				2.148	2.471	3.381	4.280	3.872	3.381	4.280	4.790	4.180	4.936
5					1.082	1.380	2.143	2.421	2.789	3.870	3.481	3.140	3.385
6						2.137	2.472	3.403	3.871	4.952	4.290	3.897	4.281
7							1.081	1.412	2.430	3.406	2.631	2.674	2.158
8								2.155	3.406	4.294	3.009	3.207	2.479
9									1.412	2.155	2.002	2.338	1.079
10										1.081	2.631	2.668	2.158
11											3.010	3.199	2.479
12												0.968	2.209
13													2.896

Molecule: TS₂
Method: M052X
Basis: 6-31G*
Energy: -193226.457251219 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.570374	-2.147424	-0.283474
2	C	-1.066762	-1.212186	-0.074134
3	C	-1.702508	0.000201	-0.357991
4	H	-2.694332	0.000326	-0.791953
5	C	-1.066604	1.212424	-0.073792
6	H	-1.570093	2.147788	-0.282863
7	C	0.199657	1.217932	0.484928
8	H	0.699981	2.150708	0.707946
9	C	0.884493	-0.000123	0.715510
10	C	0.199502	-1.218020	0.484570
11	H	0.699710	-2.150925	0.707302
12	O	2.087889	0.000034	-0.862271
13	H	1.382774	0.000595	-1.533404
14	H	1.776170	-0.000267	1.324361

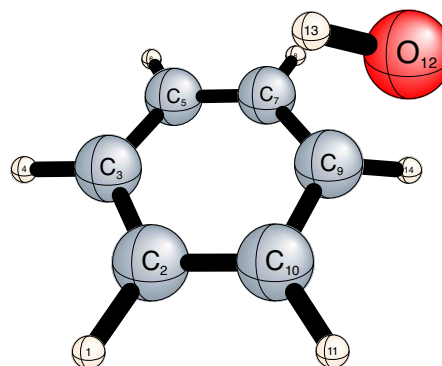


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.083	2.153	2.477	3.404	4.295	3.879	4.961	3.411	2.142	2.477	4.281	3.860	4.289
2		1.398	2.153	2.425	3.404	2.797	3.878	2.429	1.384	2.148	3.470	3.098	3.392
3			1.083	1.398	2.153	2.411	3.396	2.801	2.411	3.396	3.824	3.302	3.864
4				2.153	2.477	3.389	4.289	3.883	3.389	4.289	4.783	4.144	4.946
5					1.083	1.384	2.148	2.429	2.797	3.878	3.470	3.098	3.392
6						2.142	2.477	3.411	3.879	4.961	4.281	3.859	4.289
7							1.082	1.416	2.436	3.413	2.620	2.637	2.162
8								2.159	3.413	4.302	3.003	3.180	2.483
9									1.416	2.159	1.984	2.303	1.080
10										1.082	2.620	2.638	2.162
11											3.003	3.181	2.483
12												0.973	2.209
13													2.885

Molecule: TS₂
Method: M052X
Basis: def2-TZVPP
Energy: -193311.786556313 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.568607	-2.139643	-0.280052
2	C	-1.066636	-1.207690	-0.070647
3	C	-1.699077	0.000406	-0.353547
4	H	-2.687249	0.000428	-0.787405
5	C	-1.066993	1.208464	-0.069684
6	H	-1.569215	2.140442	-0.278363
7	C	0.194270	1.213934	0.486353
8	H	0.692708	2.143947	0.708626
9	C	0.873039	0.000367	0.720530
10	C	0.194601	-1.213241	0.485522
11	H	0.693238	-2.143283	0.707237
12	O	2.094749	0.001147	-0.871892
13	H	1.405818	-0.004476	-1.548980
14	H	1.768856	0.000259	1.317037

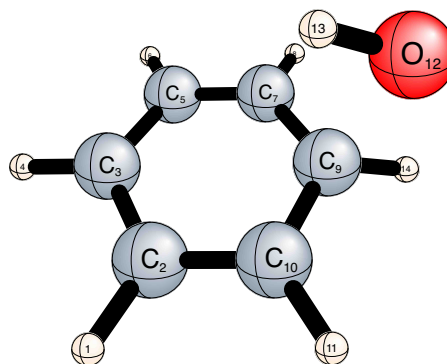


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.079	2.145	2.468	3.392	4.280	3.865	4.944	3.397	2.134	2.468	4.284	3.875	4.274
2		1.393	2.145	2.416	3.392	2.786	3.865	2.418	1.378	2.140	3.478	3.122	3.380
3			1.079	1.393	2.145	2.401	3.383	2.787	2.401	3.383	3.829	3.327	3.849
4				2.145	2.468	3.376	4.273	3.866	3.376	4.273	4.783	4.163	4.928
5					1.079	1.378	2.139	2.418	2.786	3.865	3.478	3.126	3.380
6						2.134	2.468	3.397	3.865	4.944	4.284	3.881	4.274
7							1.078	1.410	2.427	3.401	2.632	2.664	2.155
8								2.151	3.401	4.287	3.009	3.197	2.475
9									1.410	2.151	2.007	2.331	1.076
10										1.078	2.632	2.658	2.155
11											3.009	3.189	2.475
12												0.966	2.213
13													2.889

Molecule: TS₂
Method: M06L
Basis: 6-31G*
Energy: -193229.526129792 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.579895	-2.156443	-0.304263
2	C	-1.078004	-1.215434	-0.087921
3	C	-1.714849	-0.003212	-0.378640
4	H	-2.708462	-0.005476	-0.822843
5	C	-1.082326	1.211921	-0.090633
6	H	-1.587580	2.150648	-0.309051
7	C	0.180428	1.220663	0.478918
8	H	0.682049	2.158899	0.703230
9	C	0.860178	0.002622	0.726032
10	C	0.184781	-1.218381	0.481633
11	H	0.689761	-2.154312	0.708004
12	O	2.140738	0.002750	-0.828681
13	H	1.467942	0.001647	-1.533017
14	H	1.747949	0.004904	1.348756

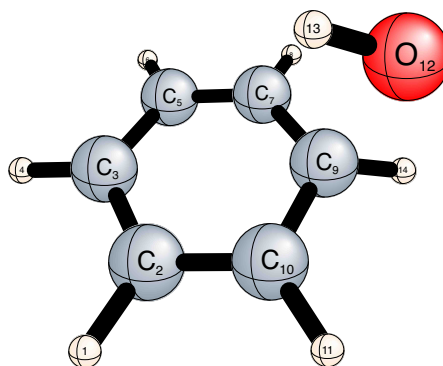


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.088	2.159	2.484	3.412	4.307	3.888	4.975	3.417	2.147	2.485	4.334	3.931	4.299
2		1.400	2.159	2.427	3.412	2.800	3.887	2.430	1.385	2.154	3.520	3.170	3.397
3			1.088	1.400	2.159	2.414	3.404	2.802	2.414	3.404	3.882	3.386	3.870
4				2.159	2.484	3.398	4.302	3.890	3.398	4.302	4.849	4.236	4.957
5					1.088	1.385	2.154	2.430	2.800	3.887	3.521	3.170	3.397
6						2.147	2.485	3.417	3.888	4.975	4.334	3.931	4.299
7							1.087	1.417	2.439	3.421	2.653	2.682	2.166
8								2.164	3.421	4.313	3.021	3.205	2.488
9									1.417	2.164	2.014	2.339	1.084
10										1.087	2.652	2.682	2.166
11											3.020	3.206	2.488
12												0.974	2.213
13													2.895

Molecule: TS₂
Method: M06L
Basis: def2-TZVPP
Energy: -193309.182420946 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.584085	-2.141723	-0.268660
2	C	-1.076199	-1.208953	-0.067364
3	C	-1.712477	0.001215	-0.344713
4	H	-2.708390	0.001878	-0.765571
5	C	-1.074214	1.210532	-0.068224
6	H	-1.580571	2.143986	-0.270184
7	C	0.193427	1.217122	0.470677
8	H	0.695994	2.147952	0.689391
9	C	0.879930	-0.000545	0.694683
10	C	0.191429	-1.217243	0.471536
11	H	0.692469	-2.148737	0.690915
12	O	2.119144	-0.002059	-0.839851
13	H	1.466544	-0.001328	-1.550414
14	H	1.756501	-0.001035	1.322512

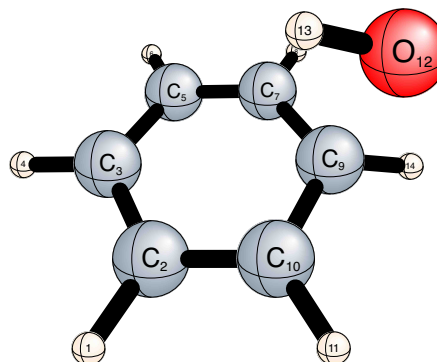


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.081	2.148	2.471	3.397	4.286	3.871	4.952	3.404	2.134	2.471	4.315	3.941	4.275
2		1.395	2.149	2.419	3.397	2.791	3.871	2.422	1.377	2.142	3.502	3.182	3.379
3			1.081	1.395	2.148	2.403	3.388	2.793	2.403	3.388	3.863	3.400	3.849
4				2.149	2.471	3.380	4.279	3.874	3.380	4.279	4.828	4.248	4.929
5					1.081	1.377	2.142	2.422	2.791	3.871	3.502	3.181	3.379
6						2.134	2.471	3.404	3.871	4.952	4.315	3.940	4.275
7							1.080	1.416	2.434	3.410	2.629	2.681	2.157
8								2.156	3.410	4.297	2.998	3.198	2.479
9									1.416	2.156	1.972	2.320	1.078
10										1.080	2.629	2.682	2.157
11											2.998	3.199	2.479
12												0.965	2.193
13													2.888

Molecule: TS₂
Method: M06HF
Basis: 6-31G*
Energy: -193185.823194578 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.562033	-2.146329	-0.288005
2	C	-1.058971	-1.211981	-0.078150
3	C	-1.692082	0.000469	-0.367204
4	H	-2.680188	0.000734	-0.807445
5	C	-1.058474	1.212576	-0.077789
6	H	-1.561153	2.147194	-0.287354
7	C	0.205055	1.217969	0.488430
8	H	0.701555	2.150388	0.718268
9	C	0.891577	-0.000223	0.717935
10	C	0.204555	-1.218066	0.488074
11	H	0.700667	-2.150758	0.717635
12	O	2.049613	-0.000246	-0.857876
13	H	1.333169	-0.000167	-1.524605
14	H	1.786213	-0.000498	1.322820

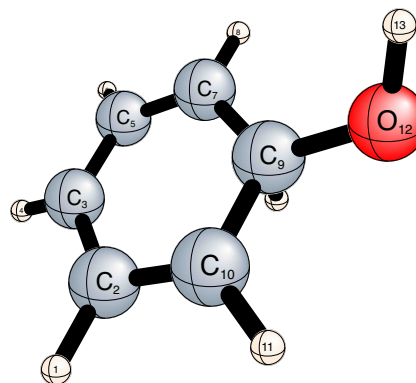


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.082	2.152	2.476	3.403	4.294	3.879	4.960	3.411	2.141	2.476	4.240	3.810	4.291
2		1.398	2.152	2.425	3.403	2.797	3.878	2.430	1.385	2.147	3.426	3.047	3.395
3			1.082	1.398	2.152	2.411	3.396	2.802	2.411	3.396	3.774	3.239	3.867
4				2.152	2.476	3.389	4.288	3.884	3.389	4.288	4.730	4.077	4.948
5					1.082	1.385	2.147	2.430	2.797	3.878	3.426	3.047	3.395
6						2.141	2.476	3.411	3.879	4.960	4.240	3.810	4.291
7							1.081	1.417	2.436	3.413	2.588	2.609	2.164
8								2.159	3.413	4.301	2.988	3.171	2.484
9									1.417	2.159	1.956	2.286	1.080
10										1.081	2.588	2.609	2.164
11											2.988	3.171	2.484
12												0.979	2.197
13													2.883

Molecule: TS₂
Method: M06HF
Basis: def2-TZVPP
Energy: -193136.123059215 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.726022	-2.183070	0.072061
2	C	-1.162438	-1.262538	0.039110
3	C	-1.821591	-0.033626	-0.037640
4	H	-2.903552	-0.023134	-0.052211
5	C	-1.138219	1.189674	-0.078600
6	H	-1.688575	2.117538	-0.129432
7	C	0.229750	1.198973	-0.068933
8	H	0.796735	2.121711	-0.081953
9	C	0.959413	-0.048146	0.073011
10	C	0.209076	-1.288558	0.030153
11	H	0.782203	-2.205947	0.070595
12	O	2.300806	-0.133609	-0.163822
13	H	2.631824	0.559329	-0.742279
14	H	0.772441	-0.008743	1.232612

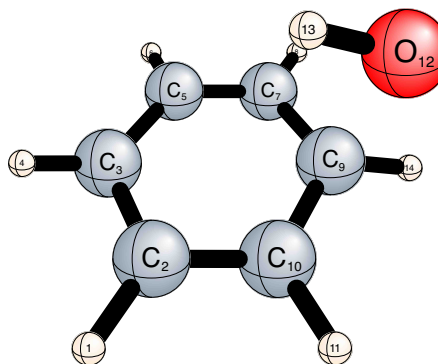


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.080	2.154	2.463	3.427	4.305	3.909	4.992	3.431	2.132	2.508	4.525	5.213	3.510
2		1.397	2.139	2.455	3.425	2.830	3.912	2.445	1.372	2.162	3.648	4.281	2.596
3			1.082	1.402	2.157	2.393	3.392	2.783	2.388	3.393	4.126	4.548	2.888
4				2.142	2.463	3.363	4.277	3.865	3.361	4.285	5.207	5.609	3.894
5					1.080	1.368	2.148	2.440	2.823	3.904	3.686	3.880	2.609
6						2.128	2.486	3.427	3.902	4.984	4.581	4.634	3.526
7							1.083	1.452	2.490	3.452	2.465	2.575	1.857
8								2.181	3.462	4.330	2.712	2.499	2.503
9									1.450	2.165	1.365	1.957	1.175
10										1.082	2.397	3.143	1.844
11											2.580	3.425	2.486
12												0.961	2.074
13													2.771

Molecule: TS₂
Method: RI-MP2
Basis: def2-TZVPP
Energy: -192931.09630695 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	-1.550688	-2.144797	-0.316236
2	C	-1.055292	-1.211408	-0.097625
3	C	-1.683663	-0.003224	-0.393962
4	H	-2.661826	-0.005465	-0.850859
5	C	-1.059501	1.207840	-0.100489
6	H	-1.558147	2.138981	-0.321295
7	C	0.192093	1.213970	0.490222
8	H	0.683259	2.145795	0.722685
9	C	0.870634	0.002555	0.736618
10	C	0.196321	-1.211787	0.493064
11	H	0.690730	-2.141345	0.727708
12	O	2.042290	0.002768	-0.842628
13	H	1.346350	0.002091	-1.513332
14	H	1.750150	0.004822	1.357655

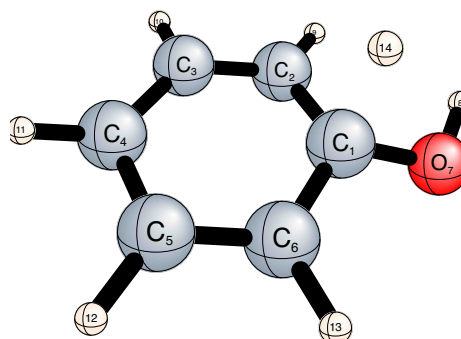


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.079	2.147	2.469	3.395	4.284	3.869	4.948	3.403	2.140	2.473	4.219	3.799	4.280
2		1.394	2.145	2.419	3.395	2.790	3.869	2.425	1.384	2.143	3.409	3.041	3.386
3			1.080	1.394	2.147	2.405	3.386	2.793	2.405	3.386	3.753	3.230	3.855
4				2.145	2.469	3.381	4.277	3.873	3.381	4.277	4.704	4.063	4.934
5					1.079	1.384	2.143	2.425	2.790	3.869	3.409	3.039	3.386
6						2.140	2.473	3.403	3.869	4.948	4.219	3.798	4.280
7							1.079	1.410	2.426	3.400	2.582	2.611	2.155
8								2.151	3.400	4.287	2.982	3.168	2.475
9									1.410	2.151	1.966	2.300	1.077
10										1.079	2.582	2.612	2.155
11											2.982	3.170	2.475
12												0.967	2.220
13													2.899

Molecule: TS₃
Method: B3LYP
Basis: 6-31G*
Energy: -193244.435049607 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.956225	-0.035244	-0.010190
2	C	0.258420	1.205544	0.036045
3	C	-1.126825	1.222039	-0.037955
4	C	-1.854225	0.025647	-0.062988
5	C	-1.175655	-1.198613	0.011176
6	C	0.208259	-1.240811	0.076377
7	O	2.290174	-0.127645	0.313732
8	H	2.719588	0.717855	0.110809
9	H	0.826781	2.132614	0.068622
10	H	-1.648612	2.175264	-0.055725
11	H	-2.938661	0.047457	-0.113487
12	H	-1.738679	-2.127957	0.033012
13	H	0.751523	-2.177417	0.147195
14	H	1.143593	-0.042531	-1.745744

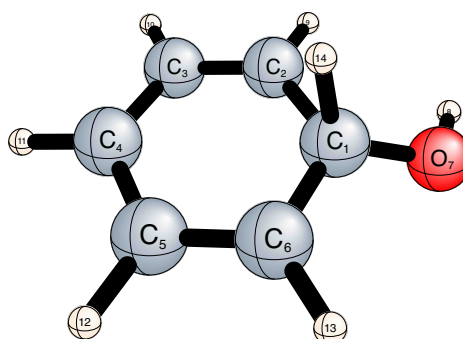


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.424	2.433	2.812	2.429	1.421	1.376	1.921	2.173	3.417	3.897	3.412	2.158	1.746
2		1.387	2.422	2.799	2.447	2.446	2.510	1.088	2.141	3.404	3.886	3.421	2.349
3			1.400	2.422	2.804	3.691	3.882	2.158	1.087	2.161	3.406	3.888	3.110
4				1.402	2.424	4.164	4.629	3.412	2.159	1.086	2.159	3.419	3.438
5					1.386	3.640	4.342	3.887	3.408	2.163	1.087	2.166	3.131
6						2.373	3.185	3.430	3.890	3.406	2.140	1.085	2.373
7							0.970	2.704	4.578	5.249	4.507	2.568	2.359
8								2.363	4.608	5.702	5.290	3.501	2.551
9									2.479	4.308	4.973	4.311	2.850
10										2.489	4.305	4.975	3.946
11											2.489	4.317	4.397
12												2.493	3.977
13													2.880

Molecule: TS₃
Method: B3LYP
Basis: def2-TZVPP
Energy: -193191.663256434 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.968143	-0.045060	-0.103572
2	C	0.246449	1.213082	-0.079746
3	C	-1.148141	1.213527	-0.046490
4	C	-1.836899	0.015645	0.016871
5	C	-1.160125	-1.218899	0.001795
6	C	0.208751	-1.267040	-0.031853
7	O	2.300476	-0.158469	0.081993
8	H	2.741663	0.688081	0.222647
9	H	0.813775	2.132991	-0.155233
10	H	-1.673813	2.157444	-0.065559
11	H	-2.917760	0.025529	0.059465
12	H	-1.725431	-2.139515	0.043313
13	H	0.758731	-2.198151	-0.011219
14	H	0.673514	0.280772	-1.245051

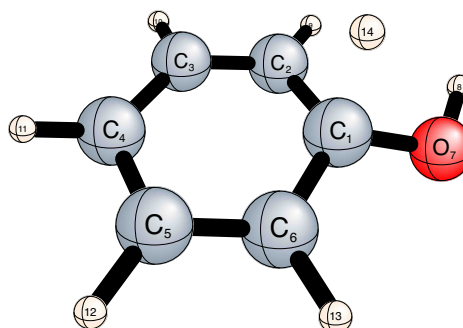


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.451	2.463	2.808	2.433	1.441	1.350	1.947	2.184	3.440	3.890	3.415	2.165	1.223
2		1.395	2.405	2.811	2.481	2.475	2.568	1.083	2.140	3.383	3.891	3.450	1.552
3			1.383	2.433	2.827	3.714	3.934	2.169	1.081	2.134	3.404	3.909	2.372
4				1.408	2.415	4.142	4.632	3.397	2.150	1.082	2.158	3.412	2.822
5					1.370	3.620	4.348	3.893	3.416	2.154	1.081	2.154	2.677
6						2.370	3.210	3.456	3.908	3.384	2.123	1.082	2.021
7							0.965	2.742	4.602	5.222	4.487	2.559	2.145
8								2.439	4.662	5.700	5.290	3.510	2.569
9									2.489	4.291	4.974	4.334	2.154
10										2.471	4.299	4.989	3.228
11											2.472	4.297	3.829
12												2.485	3.643
13													2.770

Molecule: TS₃
Method: ω B97
Basis: 6-31G*
Energy: -193198.328054623 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.934628	-0.020201	-0.074297
2	C	0.236931	1.213091	0.037079
3	C	-1.149354	1.221074	0.029377
4	C	-1.868716	0.022083	0.005618
5	C	-1.181419	-1.198261	0.024349
6	C	0.202486	-1.232311	0.023311
7	O	2.284080	-0.107553	0.154424
8	H	2.682823	0.755427	-0.023628
9	H	0.802069	2.144907	0.069322
10	H	-1.678397	2.172433	0.061198
11	H	-2.956685	0.037585	0.005496
12	H	-1.738836	-2.133340	0.053883
13	H	0.758612	-2.166542	0.049146
14	H	0.977932	0.005894	-1.823890

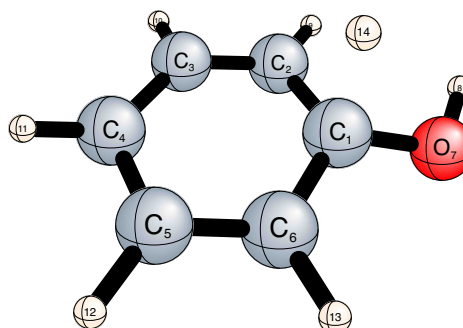


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.421	2.428	2.805	2.424	1.419	1.371	1.913	2.174	3.414	3.893	3.410	2.157	1.750
2		1.386	2.419	2.798	2.446	2.439	2.489	1.090	2.142	3.403	3.886	3.420	2.339
3			1.398	2.420	2.801	3.684	3.861	2.159	1.089	2.160	3.406	3.888	3.072
4				1.401	2.422	4.157	4.610	3.412	2.159	1.088	2.160	3.420	3.384
5					1.384	3.635	4.330	3.888	3.407	2.163	1.089	2.168	3.087
6						2.370	3.179	3.430	3.890	3.405	2.140	1.088	2.355
7							0.967	2.698	4.573	5.245	4.505	2.565	2.373
8								2.340	4.586	5.685	5.282	3.499	2.590
9									2.481	4.310	4.976	4.312	2.862
10										2.489	4.306	4.977	3.912
11											2.490	4.320	4.339
12												2.498	3.935
13													2.877

Molecule: TS₃
Method: ω B97
Basis: def2-TZVPP
Energy: -193277.401352894 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.926639	-0.021914	-0.063947
2	C	0.235312	1.208625	0.038106
3	C	-1.146352	1.218375	0.031165
4	C	-1.864851	0.024409	0.006705
5	C	-1.182005	-1.192595	0.028185
6	C	0.197551	-1.228967	0.028523
7	O	2.277764	-0.107670	0.142737
8	H	2.680921	0.749237	-0.010371
9	H	0.800320	2.135416	0.068364
10	H	-1.672323	2.166577	0.059960
11	H	-2.948449	0.041416	0.005202
12	H	-1.738604	-2.123179	0.056461
13	H	0.748302	-2.161691	0.054984
14	H	0.936404	-0.003536	-1.814500

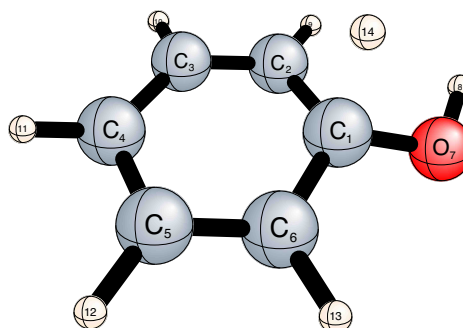


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.415	2.418	2.793	2.414	1.413	1.370	1.917	2.165	3.400	3.876	3.396	2.150	1.751
2		1.382	2.411	2.788	2.438	2.432	2.489	1.086	2.135	3.391	3.873	3.409	2.322
3			1.394	2.411	2.792	3.674	3.856	2.152	1.085	2.153	3.394	3.875	3.039
4				1.396	2.413	4.147	4.603	3.400	2.151	1.084	2.152	3.407	3.341
5					1.380	3.628	4.324	3.874	3.395	2.155	1.085	2.160	3.049
6						2.366	3.175	3.418	3.876	3.393	2.133	1.084	2.333
7							0.959	2.687	4.559	5.230	4.495	2.562	2.375
8								2.338	4.579	5.674	5.271	3.495	2.620
9									2.473	4.294	4.958	4.297	2.853
10										2.479	4.290	4.959	3.877
11											2.480	4.304	4.290
12												2.487	3.892
13													2.861

Molecule: TS₃
Method: ω B97X
Basis: 6-31G*
Energy: -193186.6334844 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.932900	-0.019609	-0.073829
2	C	0.235333	1.211384	0.036894
3	C	-1.148689	1.219126	0.029377
4	C	-1.866535	0.021895	0.006272
5	C	-1.180168	-1.196074	0.024324
6	C	0.201698	-1.229580	0.023014
7	O	2.279038	-0.106885	0.156084
8	H	2.681981	0.750884	-0.028633
9	H	0.798650	2.141917	0.067990
10	H	-1.676922	2.168555	0.060660
11	H	-2.952451	0.037069	0.006317
12	H	-1.736124	-2.129598	0.053178
13	H	0.756095	-2.162422	0.047735
14	H	0.981346	0.007623	-1.817992

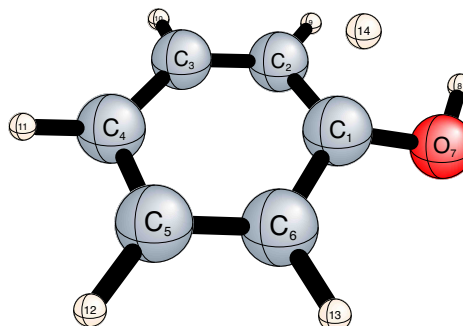


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.419	2.424	2.801	2.420	1.417	1.368	1.912	2.170	3.408	3.887	3.405	2.154	1.745
2		1.384	2.415	2.793	2.441	2.435	2.490	1.088	2.139	3.397	3.879	3.414	2.334
3			1.396	2.415	2.796	3.677	3.860	2.155	1.087	2.157	3.400	3.881	3.069
4				1.398	2.417	4.150	4.607	3.406	2.156	1.086	2.156	3.413	3.382
5					1.382	3.629	4.325	3.881	3.401	2.159	1.087	2.164	3.085
6						2.365	3.174	3.424	3.883	3.399	2.137	1.085	2.351
7							0.966	2.694	4.565	5.236	4.497	2.561	2.365
8								2.343	4.585	5.680	5.275	3.493	2.578
9									2.476	4.302	4.967	4.305	2.854
10										2.485	4.299	4.968	3.907
11											2.485	4.312	4.336
12												2.492	3.931
13													2.871

Molecule: TS₃
Method: ω B97X
Basis: def2-TZVPP
Energy: -193265.769795241 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.925030	-0.021740	-0.063929
2	C	0.234097	1.206215	0.037772
3	C	-1.144936	1.216489	0.031231
4	C	-1.862336	0.025026	0.007600
5	C	-1.180941	-1.189483	0.028852
6	C	0.196123	-1.225869	0.028835
7	O	2.271835	-0.107636	0.142981
8	H	2.676885	0.746666	-0.010706
9	H	0.797397	2.131929	0.066346
10	H	-1.669660	2.163173	0.059526
11	H	-2.944021	0.042143	0.006284
12	H	-1.736493	-2.118423	0.057042
13	H	0.744568	-2.157764	0.054389
14	H	0.936010	-0.003563	-1.807849

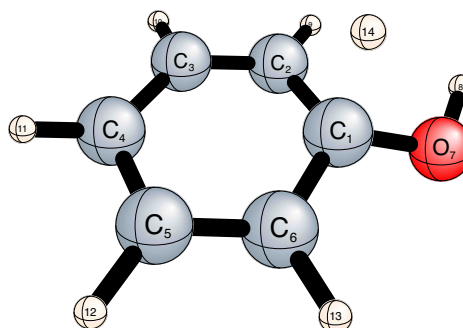


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.413	2.414	2.789	2.410	1.411	1.365	1.914	2.161	3.394	3.870	3.390	2.147	1.744
2		1.379	2.406	2.782	2.432	2.427	2.486	1.084	2.131	3.385	3.865	3.403	2.316
3			1.391	2.406	2.786	3.666	3.851	2.148	1.083	2.149	3.387	3.867	3.033
4				1.393	2.409	4.139	4.596	3.394	2.147	1.082	2.148	3.400	3.336
5					1.378	3.620	4.317	3.866	3.388	2.151	1.083	2.155	3.043
6						2.361	3.170	3.411	3.869	3.387	2.129	1.082	2.327
7							0.958	2.682	4.550	5.220	4.485	2.558	2.367
8								2.336	4.572	5.665	5.262	3.489	2.612
9									2.467	4.286	4.948	4.290	2.845
10										2.475	4.282	4.950	3.869
11											2.476	4.295	4.283
12												2.481	3.885
13													2.854

Molecule: TS₃
Method: ω B97X-D
Basis: 6-31G*
Energy: -193176.110962936 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.933532	-0.018907	-0.071772
2	C	0.234345	1.212171	0.038769
3	C	-1.149656	1.219112	0.029567
4	C	-1.867098	0.021557	0.006677
5	C	-1.180203	-1.195846	0.024682
6	C	0.201951	-1.229033	0.024619
7	O	2.277698	-0.106742	0.159537
8	H	2.685580	0.744898	-0.037590
9	H	0.795424	2.142801	0.067478
10	H	-1.677660	2.167504	0.059557
11	H	-2.951960	0.036272	0.005681
12	H	-1.734958	-2.128883	0.052186
13	H	0.754206	-2.161894	0.046881
14	H	0.984950	0.011276	-1.814883

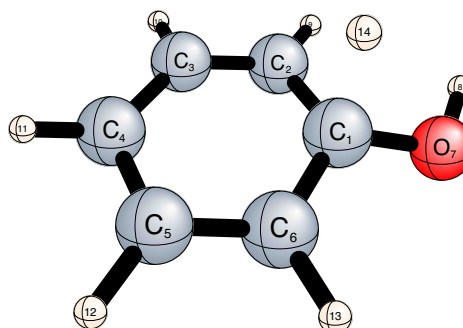


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.420	2.425	2.802	2.421	1.417	1.367	1.912	2.171	3.408	3.887	3.404	2.154	1.744
2		1.384	2.416	2.793	2.441	2.435	2.497	1.087	2.137	3.397	3.878	3.414	2.333
3			1.396	2.415	2.796	3.677	3.865	2.154	1.086	2.156	3.399	3.880	3.069
4				1.398	2.418	4.150	4.610	3.405	2.155	1.085	2.155	3.412	3.384
5					1.383	3.628	4.326	3.880	3.400	2.158	1.086	2.162	3.087
6						2.364	3.173	3.424	3.882	3.398	2.136	1.084	2.353
7							0.965	2.696	4.564	5.234	4.495	2.561	2.363
8								2.353	4.590	5.682	5.273	3.491	2.567
9									2.473	4.299	4.965	4.305	2.850
10										2.484	4.297	4.966	3.905
11											2.484	4.309	4.338
12												2.489	3.932
13													2.871

Molecule: TS₃
Method: ω B97X-D
Basis: def2-TZVPP
Energy: -193255.607718085 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.928382	-0.019719	-0.065681
2	C	0.233822	1.206493	0.036695
3	C	-1.144726	1.214393	0.029918
4	C	-1.860010	0.022271	0.006120
5	C	-1.176509	-1.190194	0.025571
6	C	0.200359	-1.224415	0.025586
7	O	2.272429	-0.103853	0.141998
8	H	2.677542	0.748353	-0.017725
9	H	0.793384	2.133340	0.063378
10	H	-1.670298	2.159517	0.058264
11	H	-2.940755	0.037436	0.004870
12	H	-1.729520	-2.119588	0.052158
13	H	0.747543	-2.155909	0.047891
14	H	0.941608	0.002622	-1.807884

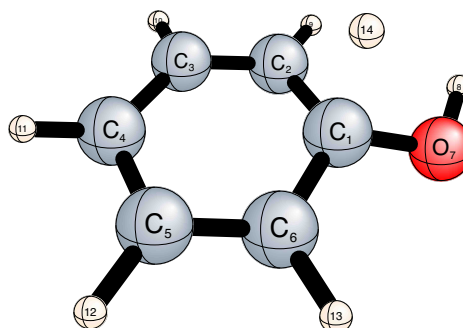


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.413	2.415	2.790	2.410	1.411	1.363	1.911	2.161	3.394	3.870	3.389	2.147	1.742
2		1.379	2.406	2.781	2.431	2.426	2.487	1.083	2.129	3.383	3.862	3.401	2.314
3			1.390	2.405	2.785	3.664	3.851	2.145	1.082	2.147	3.385	3.865	3.033
4				1.392	2.408	4.137	4.595	3.391	2.146	1.081	2.146	3.398	3.338
5					1.377	3.618	4.314	3.864	3.386	2.149	1.082	2.153	3.045
6						2.359	3.167	3.410	3.867	3.385	2.128	1.081	2.327
7							0.957	2.683	4.547	5.217	4.482	2.558	2.363
8								2.340	4.572	5.663	5.259	3.488	2.603
9									2.464	4.283	4.945	4.290	2.840
10										2.474	4.280	4.947	3.867
11											2.474	4.291	4.285
12												2.477	3.886
13													2.853

Molecule: TS₃
Method: M06
Basis: 6-31G*
Energy: -193104.688198546 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.932720	-0.020812	-0.068725
2	C	0.237042	1.209653	0.041010
3	C	-1.146163	1.218465	0.029738
4	C	-1.864204	0.021995	0.007244
5	C	-1.178637	-1.195453	0.025374
6	C	0.202571	-1.229804	0.027686
7	O	2.274637	-0.108243	0.150911
8	H	2.676646	0.755163	-0.017063
9	H	0.804545	2.140499	0.065887
10	H	-1.674965	2.169633	0.057394
11	H	-2.951825	0.037399	0.003969
12	H	-1.735712	-2.130355	0.051286
13	H	0.760409	-2.163042	0.049073
14	H	0.969089	0.009187	-1.832394

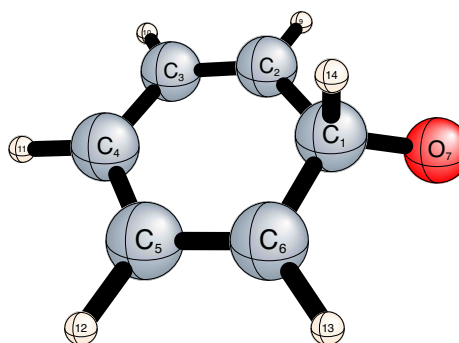


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.418	2.422	2.798	2.418	1.416	1.363	1.909	2.169	3.408	3.886	3.404	2.152	1.764
2		1.383	2.414	2.791	2.440	2.429	2.482	1.090	2.140	3.398	3.879	3.413	2.342
3			1.396	2.414	2.795	3.671	3.851	2.158	1.089	2.158	3.400	3.882	3.067
4				1.397	2.416	4.143	4.600	3.408	2.157	1.088	2.157	3.415	3.378
5					1.382	3.623	4.321	3.881	3.402	2.160	1.089	2.167	3.085
6						2.359	3.172	3.424	3.884	3.399	2.137	1.087	2.363
7							0.967	2.688	4.560	5.231	4.492	2.554	2.377
8								2.330	4.576	5.674	5.273	3.492	2.601
9									2.480	4.305	4.969	4.304	2.859
10										2.486	4.300	4.970	3.903
11											2.486	4.316	4.330
12												2.496	3.930
13													2.881

Molecule: TS₃
Method: M06
Basis: def2-TZVPP
Energy: -193051.261297272 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.958151	0.005339	-0.280636
2	C	0.226609	1.256474	-0.132819
3	C	-1.133144	1.246249	-0.024123
4	C	-1.811870	0.025602	0.048847
5	C	-1.152233	-1.204000	0.007834
6	C	0.210863	-1.231086	-0.076570
7	O	2.303940	-0.044731	-0.056574
8	H	2.574600	0.552109	0.644298
9	H	0.789178	2.181357	-0.200196
10	H	-1.684650	2.175146	0.025243
11	H	-2.891710	0.035814	0.144792
12	H	-1.715075	-2.123949	0.087963
13	H	0.779476	-2.154060	-0.082098
14	H	0.795196	-0.020328	-1.418598

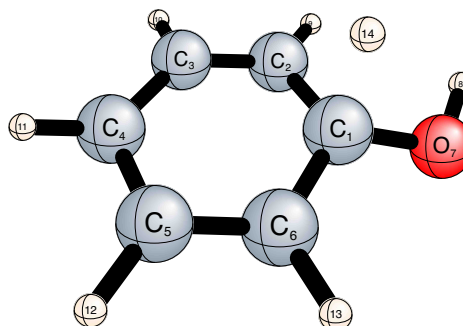


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.457	2.445	2.790	2.449	1.459	1.365	1.941	2.184	3.433	3.873	3.437	2.176	1.150
2		1.364	2.388	2.824	2.488	2.452	2.572	1.085	2.126	3.360	3.905	3.455	1.899
3			1.399	2.451	2.819	3.672	3.831	2.145	1.081	2.142	3.422	3.902	2.696
4				1.396	2.385	4.118	4.458	3.387	2.153	1.084	2.152	3.389	2.992
5					1.366	3.646	4.169	3.908	3.421	2.140	1.081	2.155	2.689
6						2.406	3.047	3.463	3.899	3.359	2.129	1.084	1.900
7							0.960	2.696	4.565	5.200	4.527	2.603	2.033
8								2.560	4.600	5.513	5.086	3.328	2.784
9									2.484	4.274	4.989	4.337	2.516
10										2.459	4.300	4.983	3.613
11											2.460	4.281	4.005
12												2.501	3.605
13													2.518

Molecule: TS₃
Method: M062X
Basis: 6-31G*
Energy: -193154.551842046 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.931121	-0.018639	-0.088855
2	C	0.233273	1.212120	0.039486
3	C	-1.149954	1.219626	0.029492
4	C	-1.868091	0.022056	0.000255
5	C	-1.180803	-1.195868	0.022563
6	C	0.200372	-1.229389	0.023188
7	O	2.279201	-0.106719	0.141473
8	H	2.685418	0.751390	-0.045667
9	H	0.798422	2.140327	0.071483
10	H	-1.677695	2.167771	0.065993
11	H	-2.952586	0.036871	-0.002962
12	H	-1.735989	-2.128328	0.055402
13	H	0.756750	-2.159933	0.048094
14	H	0.986711	0.003001	-1.768556

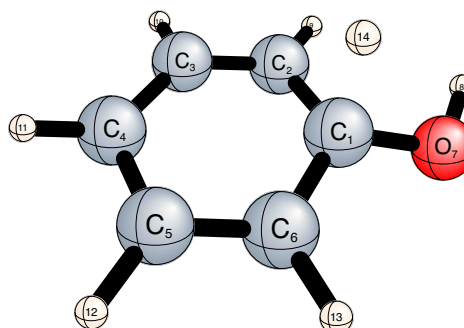


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.421	2.424	2.801	2.420	1.419	1.370	1.916	2.169	3.407	3.885	3.404	2.153	1.681
2		1.383	2.415	2.793	2.442	2.436	2.497	1.087	2.137	3.396	3.878	3.412	2.302
3			1.397	2.416	2.797	3.678	3.865	2.155	1.086	2.156	3.399	3.880	3.046
4				1.399	2.418	4.152	4.612	3.406	2.155	1.085	2.155	3.414	3.358
5					1.382	3.629	4.329	3.879	3.400	2.159	1.086	2.164	3.057
6						2.366	3.179	3.423	3.882	3.398	2.135	1.084	2.312
7							0.968	2.692	4.565	5.236	4.496	2.558	2.309
8								2.346	4.589	5.683	5.277	3.493	2.533
9									2.476	4.301	4.964	4.301	2.827
10										2.484	4.297	4.965	3.892
11											2.484	4.311	4.317
12												2.493	3.909
13													2.834

Molecule: TS₃
Method: M062X
Basis: def2-TZVPP
Energy: -193238.522989879 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.926973	-0.019222	-0.071458
2	C	0.234074	1.208219	0.048040
3	C	-1.144446	1.216271	0.030354
4	C	-1.860040	0.022594	-0.006784
5	C	-1.176245	-1.191613	0.026569
6	C	0.200511	-1.225797	0.036983
7	O	2.276646	-0.103681	0.134691
8	H	2.683434	0.750189	-0.032341
9	H	0.798299	2.132199	0.081750
10	H	-1.670771	2.160854	0.061856
11	H	-2.940635	0.037712	-0.019239
12	H	-1.730243	-2.120273	0.056903
13	H	0.752863	-2.154259	0.066789
14	H	0.933456	-0.005241	-1.747866

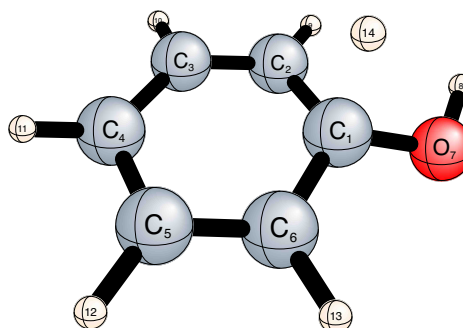


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.415	2.414	2.788	2.410	1.413	1.368	1.918	2.161	3.394	3.868	3.390	2.147	1.676
2		1.379	2.407	2.784	2.434	2.429	2.493	1.083	2.130	3.384	3.865	3.402	2.277
3			1.392	2.408	2.788	3.668	3.857	2.148	1.082	2.149	3.388	3.868	2.995
4				1.394	2.410	4.141	4.601	3.395	2.148	1.081	2.148	3.402	3.292
5					1.377	3.622	4.321	3.866	3.389	2.151	1.082	2.156	3.001
6						2.362	3.174	3.411	3.869	3.386	2.128	1.081	2.283
7							0.960	2.681	4.551	5.221	4.486	2.556	2.315
8								2.340	4.578	5.669	5.266	3.489	2.564
9									2.469	4.287	4.947	4.287	2.817
10										2.475	4.282	4.949	3.840
11											2.475	4.296	4.242
12												2.483	3.850
13													2.818

Molecule: TS₃
Method: M052X
Basis: 6-31G*
Energy: -193215.650775658 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.924567	-0.019833	-0.066933
2	C	0.228644	1.210292	0.045204
3	C	-1.154430	1.217595	0.033746
4	C	-1.871733	0.020653	0.010187
5	C	-1.185019	-1.196067	0.032915
6	C	0.196175	-1.229188	0.035139
7	O	2.272995	-0.104147	0.161790
8	H	2.677840	0.749107	-0.035792
9	H	0.791312	2.136520	0.075734
10	H	-1.680755	2.163451	0.063526
11	H	-2.953414	0.035111	0.006630
12	H	-1.738309	-2.126379	0.063562
13	H	0.751068	-2.157027	0.061571
14	H	0.980563	0.002606	-1.792372

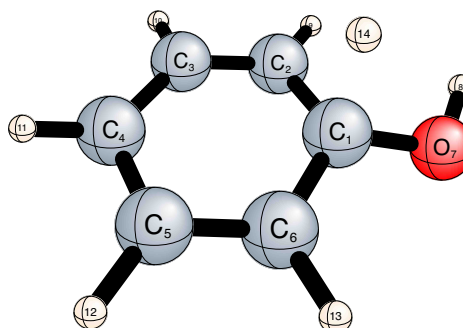


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.418	2.421	2.798	2.417	1.415	1.370	1.915	2.165	3.402	3.879	3.398	2.148	1.726
2		1.383	2.414	2.791	2.440	2.433	2.494	1.084	2.134	3.392	3.873	3.408	2.324
3			1.396	2.414	2.795	3.676	3.861	2.152	1.083	2.153	3.395	3.876	3.061
4				1.397	2.416	4.149	4.608	3.402	2.152	1.082	2.152	3.409	3.374
5					1.382	3.629	4.326	3.875	3.396	2.155	1.083	2.162	3.075
6						2.365	3.174	3.418	3.877	3.394	2.133	1.081	2.339
7							0.965	2.688	4.559	5.231	4.493	2.557	2.345
8								2.344	4.583	5.676	5.271	3.488	2.554
9									2.472	4.295	4.957	4.294	2.842
10										2.480	4.290	4.958	3.898
11											2.480	4.305	4.326
12												2.490	3.920
13													2.855

Molecule: TS₃
Method: M052X
Basis: def2-TZVPP
Energy: -193300.526840414 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.920734	-0.019596	-0.058816
2	C	0.229935	1.206019	0.045870
3	C	-1.147879	1.213434	0.032967
4	C	-1.862019	0.020868	0.004606
5	C	-1.178525	-1.191250	0.031267
6	C	0.197677	-1.224589	0.037184
7	O	2.270302	-0.100085	0.149023
8	H	2.675006	0.751287	-0.024910
9	H	0.792077	2.128233	0.076615
10	H	-1.673108	2.155863	0.060364
11	H	-2.940171	0.035316	-0.002635
12	H	-1.730380	-2.118334	0.058955
13	H	0.749099	-2.150566	0.064242
14	H	0.936756	-0.003904	-1.779825

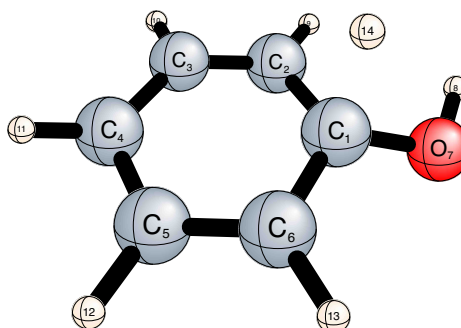


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.411	2.410	2.784	2.406	1.409	1.368	1.916	2.156	3.387	3.862	3.383	2.141	1.721
2		1.378	2.405	2.780	2.431	2.425	2.488	1.080	2.127	3.380	3.859	3.397	2.301
3			1.390	2.405	2.785	3.664	3.851	2.145	1.079	2.145	3.382	3.862	3.019
4				1.392	2.407	4.137	4.596	3.390	2.144	1.078	2.144	3.397	3.319
5					1.377	3.619	4.316	3.861	3.384	2.147	1.079	2.153	3.027
6						2.361	3.169	3.405	3.864	3.382	2.125	1.078	2.310
7							0.959	2.675	4.544	5.214	4.482	2.555	2.347
8								2.335	4.570	5.661	5.258	3.484	2.583
9									2.465	4.280	4.939	4.279	2.831
10										2.471	4.275	4.941	3.855
11											2.471	4.289	4.265
12												2.480	3.869
13													2.836

Molecule: TS₃
Method: M06L
Basis: 6-31G*
Energy: -193214.254577546 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.930487	-0.021056	-0.075979
2	C	0.229804	1.211315	0.033778
3	C	-1.154201	1.218718	0.032539
4	C	-1.873098	0.020851	0.020632
5	C	-1.185153	-1.196979	0.035038
6	C	0.196803	-1.231561	0.027773
7	O	2.273480	-0.111356	0.167382
8	H	2.669756	0.757667	0.012832
9	H	0.793839	2.143596	0.053103
10	H	-1.682208	2.169979	0.063327
11	H	-2.960239	0.035905	0.028742
12	H	-1.740746	-2.132198	0.069315
13	H	0.750732	-2.166281	0.051142
14	H	0.990251	0.004093	-1.824716

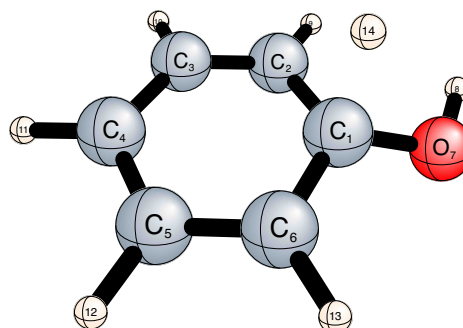


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.422	2.428	2.806	2.423	1.419	1.368	1.908	2.173	3.413	3.893	3.408	2.156	1.750
2		1.384	2.417	2.793	2.443	2.438	2.482	1.090	2.139	3.400	3.881	3.418	2.343
3			1.397	2.416	2.798	3.679	3.852	2.157	1.088	2.159	3.402	3.884	3.086
4				1.399	2.419	4.151	4.602	3.409	2.158	1.087	2.158	3.416	3.407
5					1.382	3.627	4.322	3.883	3.404	2.161	1.088	2.165	3.104
6						2.364	3.174	3.428	3.886	3.402	2.137	1.087	2.364
7							0.968	2.699	4.568	5.238	4.495	2.560	2.372
8								2.333	4.576	5.676	5.273	3.498	2.601
9									2.476	4.305	4.971	4.310	2.853
10										2.488	4.303	4.972	3.924
11											2.488	4.315	4.364
12												2.492	3.951
13													2.879

Molecule: TS₃
Method: M06L
Basis: def2-TZVPP
Energy: -193292.651551636 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.925707	-0.020634	-0.070786
2	C	0.228709	1.206561	0.029016
3	C	-1.149729	1.214072	0.032059
4	C	-1.865516	0.021118	0.021043
5	C	-1.180609	-1.191429	0.033826
6	C	0.196132	-1.226459	0.025470
7	O	2.267493	-0.106255	0.157537
8	H	2.660872	0.758760	0.031618
9	H	0.790940	2.131314	0.048482
10	H	-1.674611	2.158776	0.061980
11	H	-2.945395	0.035953	0.030940
12	H	-1.732610	-2.120440	0.066998
13	H	0.743456	-2.157049	0.048800
14	H	0.974666	-0.001595	-1.822077

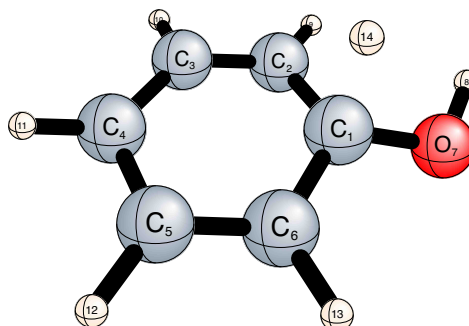


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.415	2.417	2.793	2.412	1.413	1.364	1.905	2.159	3.395	3.873	3.390	2.148	1.752
2		1.378	2.406	2.781	2.433	2.428	2.473	1.082	2.128	3.383	3.862	3.403	2.333
3			1.391	2.406	2.787	3.666	3.838	2.147	1.081	2.148	3.385	3.866	3.071
4				1.393	2.410	4.137	4.586	3.393	2.147	1.080	2.146	3.399	3.386
5					1.377	3.617	4.308	3.864	3.387	2.150	1.081	2.153	3.083
6						2.359	3.165	3.410	3.868	3.386	2.126	1.080	2.349
7							0.959	2.683	4.547	5.216	4.480	2.557	2.367
8								2.320	4.556	5.653	5.253	3.490	2.619
9									2.466	4.284	4.944	4.289	2.843
10										2.474	4.280	4.947	3.903
11											2.474	4.292	4.336
12												2.476	3.923
13													2.863

Molecule: TS₃
Method: M06HF
Basis: 6-31G*
Energy: -193179.281952284 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.922268	-0.015640	-0.075408
2	C	0.224854	1.214852	0.058318
3	C	-1.156840	1.219109	0.034952
4	C	-1.872304	0.020332	-0.008486
5	C	-1.184399	-1.196902	0.029466
6	C	0.195327	-1.228224	0.042818
7	O	2.274489	-0.098818	0.146837
8	H	2.699925	0.732419	-0.103385
9	H	0.788718	2.138769	0.102847
10	H	-1.685566	2.162412	0.069819
11	H	-2.952833	0.033520	-0.027327
12	H	-1.737326	-2.126301	0.061282
13	H	0.755511	-2.151937	0.076024
14	H	0.967679	-0.000898	-1.712851

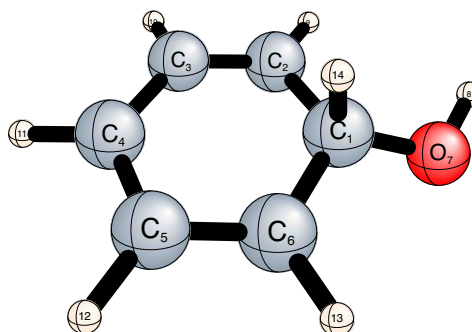


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.421	2.421	2.796	2.418	1.419	1.373	1.929	2.166	3.401	3.876	3.398	2.148	1.638
2		1.382	2.414	2.793	2.443	2.436	2.527	1.083	2.133	3.391	3.875	3.408	2.273
3			1.397	2.416	2.796	3.677	3.890	2.153	1.082	2.153	3.396	3.876	3.009
4				1.399	2.416	4.151	4.628	3.403	2.152	1.081	2.152	3.410	3.312
5					1.380	3.631	4.339	3.876	3.397	2.155	1.082	2.163	3.016
6						2.368	3.184	3.419	3.877	3.392	2.131	1.081	2.277
7							0.967	2.686	4.561	5.232	4.496	2.555	2.275
8								2.382	4.616	5.696	5.281	3.483	2.476
9									2.475	4.295	4.957	4.291	2.812
10										2.479	4.289	4.957	3.860
11											2.480	4.306	4.268
12												2.493	3.871
13													2.806

Molecule: TS₃
Method: M06HF
Basis: def2-TZVPP
Energy: -193136.642491085 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.952296	0.002088	-0.129085
2	C	0.222324	1.254906	-0.012911
3	C	-1.142362	1.246269	-0.007071
4	C	-1.827804	0.019095	0.003876
5	C	-1.171193	-1.210379	-0.021993
6	C	0.201703	-1.234489	-0.029036
7	O	2.272804	-0.100617	0.194378
8	H	2.790118	0.677356	-0.035719
9	H	0.786469	2.179336	-0.004888
10	H	-1.695182	2.173609	0.017953
11	H	-2.909673	0.031466	0.024952
12	H	-1.733059	-2.132236	-0.010119
13	H	0.776709	-2.151458	-0.043245
14	H	0.770161	-0.071270	-1.287378

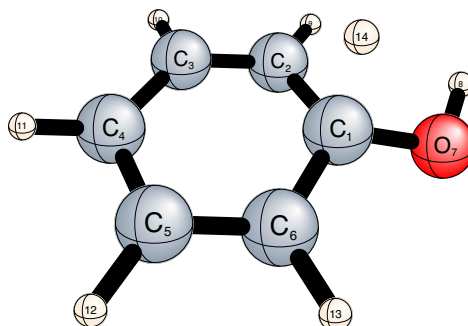


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.455	2.439	2.783	2.448	1.450	1.363	1.960	2.187	3.427	3.865	3.432	2.162	1.175
2		1.365	2.394	2.832	2.490	2.467	2.632	1.083	2.126	3.363	3.911	3.451	1.919
3			1.406	2.457	2.822	3.677	3.974	2.143	1.080	2.145	3.430	3.902	2.652
4				1.394	2.386	4.107	4.665	3.391	2.159	1.082	2.153	3.391	2.903
5					1.373	3.625	4.388	3.914	3.425	2.137	1.080	2.163	2.582
6						2.372	3.218	3.464	3.901	3.359	2.133	1.082	1.805
7							0.962	2.729	4.577	5.187	4.496	2.550	2.111
8								2.504	4.729	5.737	5.325	3.472	2.491
9									2.482	4.275	4.994	4.331	2.590
10										2.462	4.306	4.982	3.581
11											2.463	4.285	3.908
12												2.510	3.485
13													2.424

Molecule: TS₃
Method: RI-MP2
Basis: def2-TZVPP
Energy: -192927.706565455 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	0.931077	-0.017933	-0.084635
2	C	0.236764	1.206389	0.045153
3	C	-1.144822	1.217145	0.025447
4	C	-1.859364	0.022038	-0.005556
5	C	-1.175598	-1.192143	0.017936
6	C	0.204744	-1.221918	0.028545
7	O	2.282210	-0.107515	0.126628
8	H	2.677232	0.749893	-0.051698
9	H	0.797204	2.129986	0.074700
10	H	-1.669247	2.159820	0.060223
11	H	-2.937695	0.036726	-0.018604
12	H	-1.725851	-2.120096	0.048394
13	H	0.754980	-2.149261	0.050069
14	H	0.934519	0.001154	-1.725212



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13	14
1	1.413	2.418	2.792	2.414	1.411	1.370	1.908	2.158	3.395	3.870	3.391	2.143	1.641
2		1.382	2.408	2.784	2.429	2.432	2.485	1.081	2.131	3.384	3.862	3.395	2.252
3			1.393	2.409	2.788	3.676	3.851	2.146	1.079	2.147	3.388	3.866	2.978
4				1.394	2.410	4.146	4.595	3.392	2.147	1.079	2.147	3.399	3.281
5					1.381	3.626	4.315	3.864	3.388	2.149	1.079	2.155	2.986
6						2.360	3.163	3.404	3.866	3.385	2.129	1.079	2.259
7							0.961	2.686	4.556	5.224	4.486	2.551	2.293
8								2.336	4.571	5.660	5.257	3.480	2.529
9									2.467	4.283	4.943	4.280	2.791
10										2.474	4.280	4.944	3.825
11											2.475	4.292	4.232
12												2.481	3.837
13													2.794

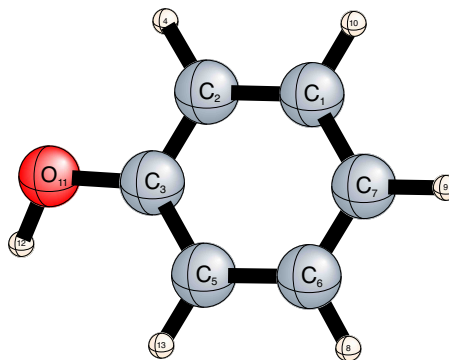
Molecule: phenol

Method: B3LYP

Basis: 6-31G*

Energy: -192936.966257687 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.172172	-1.190784	-0.000001
2	C	-0.220228	-1.223089	-0.000002
3	C	-0.939015	-0.022455	-0.000002
4	H	-0.766545	-2.161115	-0.000003
5	C	-0.260761	1.200833	-0.000001
6	C	1.135081	1.219062	0.000000
7	C	1.859309	0.026828	0.000000
8	H	1.654183	2.173959	0.000000
9	H	2.945139	0.044558	0.000001
10	H	1.725294	-2.126436	-0.000001
11	O	-2.305361	-0.108308	-0.000003
12	H	-2.675981	0.787819	-0.000007
13	H	-0.822420	2.133767	-0.000001

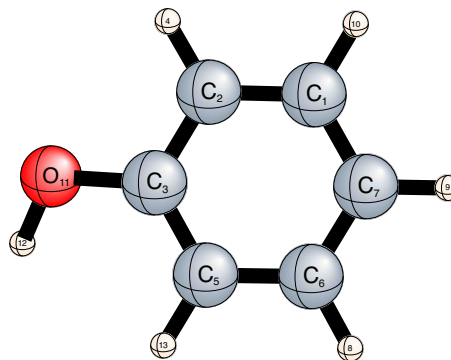


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.393	2.413	2.168	2.788	2.410	1.398	3.399	2.161	1.087	3.642	4.327	3.877
2		1.399	1.086	2.424	2.793	2.426	3.880	3.410	2.145	2.364	3.174	3.410
3			2.146	1.399	2.417	2.799	3.398	3.885	3.395	1.369	1.917	2.159
4				3.400	3.878	3.418	4.965	4.318	2.492	2.566	3.513	4.295
5					1.396	2.423	2.148	3.408	3.875	2.428	2.450	1.089
6						1.395	1.087	2.158	3.397	3.688	3.835	2.161
7							2.157	1.086	2.157	4.167	4.599	3.410
8								2.490	4.301	4.570	4.547	2.477
9									2.490	5.253	5.670	4.308
10										4.508	5.279	4.964
11											0.970	2.688
12												2.291

Molecule: phenol
Method: B3LYP
Basis: def2-TZVPP
Energy: -193019.774215931 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.168362	-1.185138	0.000000
2	C	-0.218977	-1.218093	0.000000
3	C	-0.935450	-0.023500	0.000000
4	H	-0.759890	-2.154310	0.000000
5	C	-0.260713	1.195095	0.000000
6	C	1.129647	1.214736	0.000000
7	C	1.851854	0.027733	0.000000
8	H	1.646550	2.165426	0.000000
9	H	2.932884	0.046130	0.000000
10	H	1.719767	-2.116293	0.000000
11	O	-2.299809	-0.107132	-0.000001
12	H	-2.678795	0.776511	-0.000002
13	H	-0.820382	2.123622	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.388	2.403	2.158	2.776	2.400	1.392	3.385	2.152	1.082	3.632	4.318	3.860
2		1.393	1.081	2.414	2.782	2.417	3.864	3.396	2.137	2.359	3.167	3.395
3			2.138	1.393	2.408	2.788	3.385	3.869	3.381	1.367	1.918	2.150
4				3.386	3.863	3.403	4.945	4.299	2.480	2.562	3.503	4.278
5					1.390	2.414	2.140	3.394	3.858	2.419	2.454	1.084
6						1.389	1.082	2.149	3.383	3.675	3.834	2.151
7							2.148	1.081	2.148	4.154	4.592	3.396
8								2.479	4.282	4.554	4.543	2.467
9									2.479	5.235	5.659	4.290
10										4.494	5.265	4.943
11											0.961	2.677
12												2.295

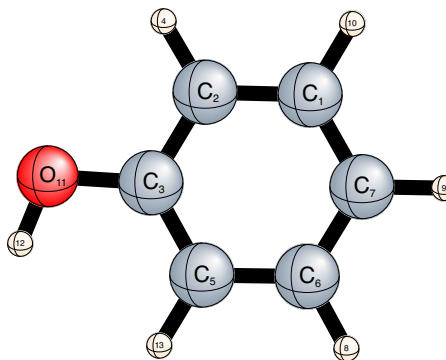
Molecule: phenol

Method: ω B97

Basis: 6-31G*

Energy: -192896.527813799 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.168148	-1.189673	0.000000
2	C	-0.221512	-1.223168	0.000000
3	C	-0.939638	-0.024826	0.000000
4	H	-0.770852	-2.162323	0.000000
5	C	-0.265204	1.197068	0.000000
6	C	1.128975	1.215820	0.000000
7	C	1.853545	0.027090	0.000000
8	H	1.648612	2.173168	0.000000
9	H	2.941603	0.046083	0.000000
10	H	1.723851	-2.126598	0.000000
11	O	-2.303037	-0.110767	0.000000
12	H	-2.669519	0.784123	0.000000
13	H	-0.828842	2.131441	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.390	2.408	2.169	2.784	2.406	1.397	3.397	2.162	1.089	3.635	4.316	3.875
2		1.397	1.088	2.421	2.788	2.423	3.877	3.408	2.145	2.360	3.166	3.409
3			2.144	1.396	2.412	2.794	3.396	3.882	3.393	1.366	1.910	2.159
4				3.397	3.876	3.418	4.965	4.320	2.495	2.561	3.505	4.294
5					1.394	2.420	2.148	3.407	3.873	2.421	2.440	1.091
6						1.392	1.089	2.157	3.395	3.679	3.823	2.161
7							2.156	1.088	2.158	4.159	4.586	3.409
8								2.489	4.300	4.564	4.536	2.478
9									2.491	5.247	5.659	4.309
10										4.503	5.270	4.965
11											0.967	2.683
12												2.281

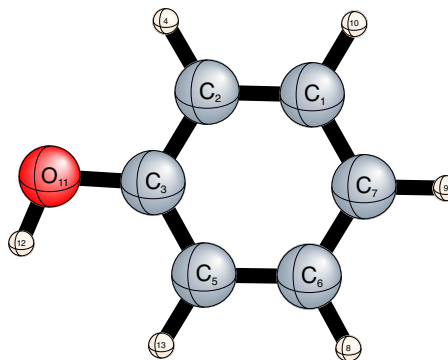
Molecule: phenol

Method: ω B97

Basis: def2-TZVPP

Energy: -192974.026004866 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.167211	-1.183961	0.000000
2	C	-0.218452	-1.218083	0.000000
3	C	-0.933460	-0.024132	0.000000
4	H	-0.763169	-2.155349	0.000000
5	C	-0.262301	1.194229	0.000000
6	C	1.127210	1.213639	0.000000
7	C	1.849787	0.028744	0.000000
8	H	1.645260	2.166955	0.000000
9	H	2.933478	0.047959	0.000000
10	H	1.721218	-2.116908	0.000000
11	O	-2.296461	-0.106930	0.000000
12	H	-2.670887	0.776065	0.000000
13	H	-0.825140	2.123932	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.386	2.400	2.161	2.775	2.398	1.392	3.385	2.153	1.085	3.627	4.310	3.862
2		1.392	1.084	2.413	2.779	2.415	3.864	3.397	2.138	2.356	3.161	3.397
3			2.138	1.391	2.404	2.784	3.384	3.868	3.380	1.366	1.913	2.151
4				3.387	3.863	3.406	4.948	4.303	2.485	2.559	3.498	4.280
5					1.390	2.412	2.141	3.395	3.860	2.415	2.445	1.087
6						1.388	1.085	2.150	3.383	3.670	3.823	2.154
7							2.148	1.084	2.150	4.148	4.582	3.398
8								2.480	4.285	4.551	4.535	2.471
9									2.481	5.232	5.651	4.294
10										4.492	5.259	4.947
11											0.959	2.672
12												2.286

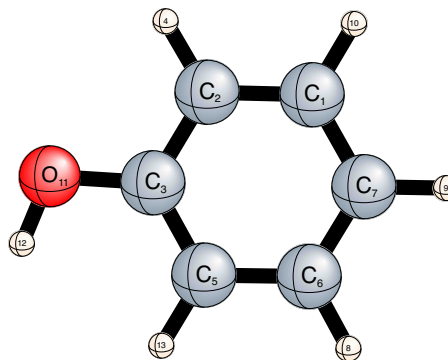
Molecule: phenol

Method: ω B97X

Basis: 6-31G*

Energy: -192883.853097735 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.166819	-1.187779	0.000000
2	C	-0.221040	-1.220819	0.000000
3	C	-0.938238	-0.024480	0.000000
4	H	-0.768632	-2.158560	0.000000
5	C	-0.264124	1.195432	0.000000
6	C	1.127900	1.214284	0.000000
7	C	1.851116	0.026972	0.000000
8	H	1.646626	2.169685	0.000000
9	H	2.937111	0.045753	0.000000
10	H	1.721138	-2.123022	0.000000
11	O	-2.298554	-0.110183	0.000000
12	H	-2.667868	0.781744	0.000000
13	H	-0.826124	2.128409	0.000000

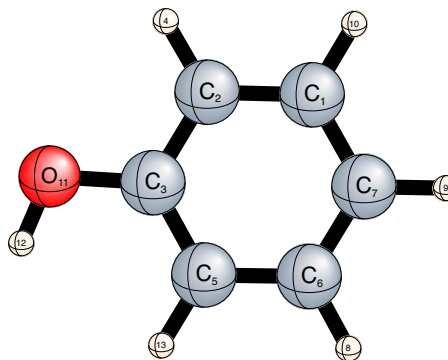


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.388	2.405	2.165	2.780	2.402	1.394	3.392	2.158	1.087	3.629	4.311	3.869
2		1.395	1.086	2.417	2.784	2.419	3.871	3.403	2.142	2.356	3.162	3.403
3			2.141	1.394	2.409	2.790	3.391	3.876	3.388	1.363	1.908	2.156
4				3.392	3.869	3.412	4.957	4.312	2.490	2.557	3.500	4.287
5					1.392	2.417	2.145	3.401	3.867	2.417	2.439	1.089
6						1.390	1.087	2.154	3.390	3.674	3.820	2.157
7							2.152	1.086	2.154	4.152	4.582	3.403
8								2.485	4.293	4.557	4.532	2.473
9									2.486	5.238	5.653	4.301
10										4.495	5.263	4.956
11											0.965	2.679
12												2.282

Molecule: phenol
Method: ω B97X
Basis: def2-TZVPP
Energy: -192961.322713925 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.165105	-1.181832	0.000000
2	C	-0.218307	-1.215588	0.000000
3	C	-0.932947	-0.024198	0.000000
4	H	-0.761040	-2.151795	0.000000
5	C	-0.261805	1.191681	0.000000
6	C	1.125178	1.211495	0.000000
7	C	1.846409	0.028534	0.000000
8	H	1.642191	2.163104	0.000000
9	H	2.928179	0.047639	0.000000
10	H	1.717866	-2.113193	0.000000
11	O	-2.291778	-0.106742	0.000000
12	H	-2.667552	0.774097	0.000000
13	H	-0.822939	2.120268	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.384	2.396	2.157	2.769	2.394	1.389	3.379	2.149	1.083	3.620	4.303	3.854
2		1.389	1.082	2.408	2.774	2.411	3.857	3.391	2.134	2.351	3.156	3.390
3			2.135	1.389	2.401	2.780	3.379	3.862	3.375	1.361	1.909	2.147
4				3.381	3.856	3.399	4.939	4.295	2.479	2.554	3.492	4.273
5					1.387	2.408	2.137	3.389	3.852	2.410	2.442	1.085
6						1.385	1.083	2.146	3.377	3.662	3.818	2.150
7							2.144	1.082	2.146	4.140	4.575	3.391
8								2.476	4.277	4.542	4.528	2.466
9									2.477	5.222	5.643	4.286
10										4.484	5.251	4.937
11											0.958	2.668
12												2.284

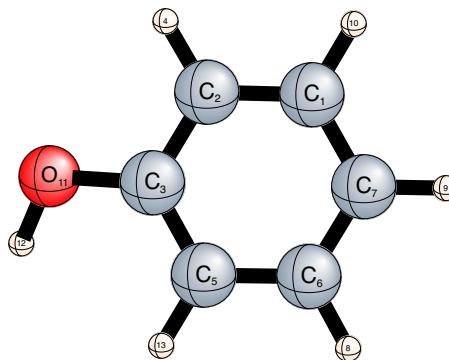
Molecule: phenol

Method: ω B97X-D

Basis: 6-31G*

Energy: -192871.313611116 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.168060	-1.186831	0.000000
2	C	-0.220360	-1.220139	0.000000
3	C	-0.938802	-0.023798	0.000000
4	H	-0.765155	-2.158312	0.000000
5	C	-0.263611	1.196812	0.000000
6	C	1.128620	1.215749	0.000000
7	C	1.852254	0.028095	0.000000
8	H	1.646513	2.170357	0.000000
9	H	2.937186	0.047049	0.000000
10	H	1.721561	-2.121271	0.000000
11	O	-2.297120	-0.111038	-0.000001
12	H	-2.670797	0.778108	-0.000002
13	H	-0.823301	2.130004	0.000000

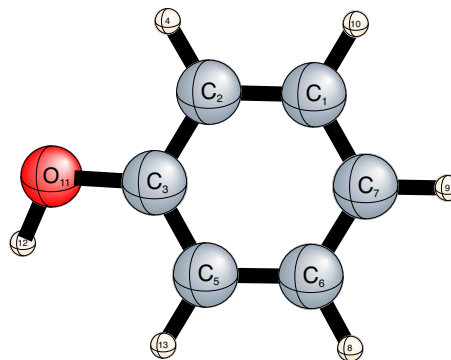


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.389	2.407	2.164	2.781	2.403	1.394	3.391	2.157	1.086	3.628	4.313	3.869
2		1.395	1.085	2.417	2.784	2.419	3.870	3.402	2.141	2.354	3.162	3.404
3			2.142	1.395	2.411	2.792	3.391	3.877	3.388	1.361	1.909	2.157
4				3.392	3.869	3.410	4.955	4.309	2.487	2.557	3.501	4.289
5					1.392	2.417	2.144	3.401	3.867	2.418	2.443	1.088
6						1.391	1.086	2.153	3.389	3.674	3.825	2.155
7							2.152	1.085	2.153	4.152	4.585	3.402
8								2.485	4.292	4.556	4.536	2.470
9									2.486	5.237	5.655	4.299
10										4.493	5.263	4.955
11											0.964	2.682
12												2.289

Molecule: phenol
Method: ω B97X-D
Basis: def2-TZVPP
Energy: -192949.199313463 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.164731	-1.181530	0.000000
2	C	-0.218647	-1.214727	0.000000
3	C	-0.934186	-0.023521	0.000000
4	H	-0.758899	-2.151235	0.000000
5	C	-0.260737	1.191855	0.000000
6	C	1.125860	1.211182	0.000000
7	C	1.846552	0.028000	0.000000
8	H	1.642528	2.161847	0.000000
9	H	2.927357	0.046573	0.000000
10	H	1.716117	-2.112551	0.000000
11	O	-2.290039	-0.105918	-0.000001
12	H	-2.666543	0.773727	-0.000002
13	H	-0.819046	2.121083	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.384	2.397	2.154	2.769	2.393	1.388	3.377	2.148	1.082	3.618	4.301	3.853
2		1.390	1.081	2.407	2.774	2.410	3.856	3.389	2.133	2.349	3.154	3.389
3			2.135	1.389	2.402	2.781	3.379	3.862	3.375	1.358	1.907	2.148
4				3.380	3.855	3.397	4.937	4.292	2.475	2.555	3.492	4.273
5					1.387	2.407	2.136	3.388	3.851	2.409	2.442	1.084
6						1.385	1.082	2.145	3.376	3.661	3.818	2.147
7							2.144	1.081	2.145	4.139	4.574	3.389
8								2.475	4.275	4.540	4.527	2.462
9									2.476	5.220	5.641	4.282
10										4.481	5.248	4.935
11											0.957	2.669
12												2.287

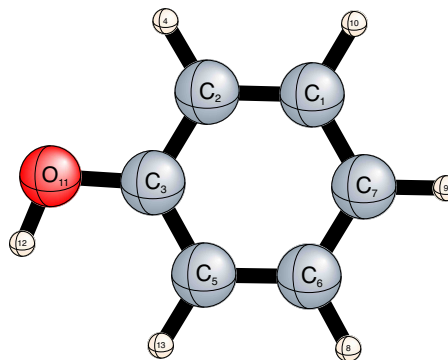
Molecule: phenol

Method: M06

Basis: 6-31G*

Energy: -192800.678135205 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.167220	-1.186627	0.000000
2	C	-0.220157	-1.221019	0.000000
3	C	-0.937969	-0.025334	0.000000
4	H	-0.770634	-2.159384	0.000000
5	C	-0.264308	1.194829	0.000000
6	C	1.126779	1.214930	0.000000
7	C	1.850483	0.027934	0.000000
8	H	1.645878	2.172007	0.000000
9	H	2.938154	0.047052	0.000000
10	H	1.722614	-2.123141	0.000000
11	O	-2.294027	-0.110862	0.000000
12	H	-2.665196	0.782044	0.000000
13	H	-0.830532	2.127877	0.000000

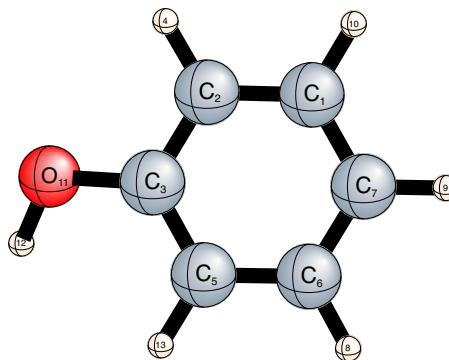


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.388	2.404	2.168	2.779	2.402	1.394	3.393	2.158	1.089	3.625	4.308	3.870
2		1.395	1.088	2.416	2.784	2.418	3.872	3.403	2.142	2.352	3.161	3.404
3			2.141	1.394	2.409	2.789	3.392	3.877	3.388	1.359	1.907	2.156
4				3.392	3.871	3.414	4.960	4.315	2.494	2.553	3.499	4.288
5					1.391	2.415	2.146	3.402	3.867	2.413	2.436	1.091
6						1.390	1.089	2.155	3.391	3.669	3.817	2.160
7							2.154	1.088	2.155	4.147	4.578	3.406
8								2.487	4.296	4.553	4.530	2.477
9									2.487	5.235	5.651	4.305
10										4.493	5.262	4.959
11											0.967	2.675
12												2.275

Molecule: phenol
Method: M06
Basis: def2-TZVPP
Energy: -192877.709519817 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.163717	-1.180152	0.000000
2	C	-0.217754	-1.213974	0.000000
3	C	-0.932942	-0.024326	0.000000
4	H	-0.761446	-2.149563	0.000000
5	C	-0.260384	1.189542	0.000000
6	C	1.124180	1.209976	0.000000
7	C	1.844352	0.028172	0.000000
8	H	1.641301	2.161171	0.000000
9	H	2.925810	0.046973	0.000000
10	H	1.716042	-2.111417	0.000000
11	O	-2.285028	-0.105339	-0.000001
12	H	-2.658635	0.776989	-0.000002
13	H	-0.824164	2.116732	0.000000

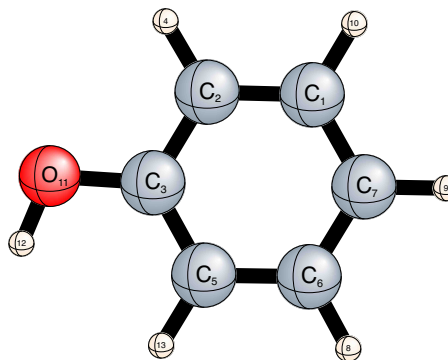


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.382	2.394	2.155	2.765	2.390	1.387	3.375	2.147	1.083	3.612	4.294	3.850
2		1.388	1.082	2.404	2.771	2.407	3.853	3.387	2.132	2.346	3.150	3.385
3			2.132	1.388	2.399	2.778	3.377	3.859	3.372	1.355	1.903	2.144
4				3.376	3.853	3.396	4.935	4.292	2.478	2.550	3.488	4.267
5					1.385	2.404	2.136	3.385	3.847	2.403	2.433	1.085
6						1.384	1.083	2.144	3.374	3.654	3.808	2.149
7							2.143	1.082	2.143	4.132	4.565	3.389
8								2.474	4.273	4.534	4.517	2.466
9									2.474	5.213	5.632	4.283
10										4.476	5.242	4.933
11											0.958	2.659
12												2.272

Molecule: phenol
Method: M062X
Basis: 6-31G*
Energy: -192852.141534462 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.168292	-1.186888	0.000000
2	C	-0.219948	-1.220976	0.000000
3	C	-0.937866	-0.024507	0.000000
4	H	-0.768204	-2.157022	0.000000
5	C	-0.264406	1.196239	0.000000
6	C	1.127809	1.216384	0.000000
7	C	1.851806	0.028792	0.000000
8	H	1.644755	2.171204	0.000000
9	H	2.936445	0.048208	0.000000
10	H	1.722540	-2.120619	0.000000
11	O	-2.297375	-0.112238	0.000000
12	H	-2.672636	0.779441	0.000000
13	H	-0.828521	2.126514	0.000000

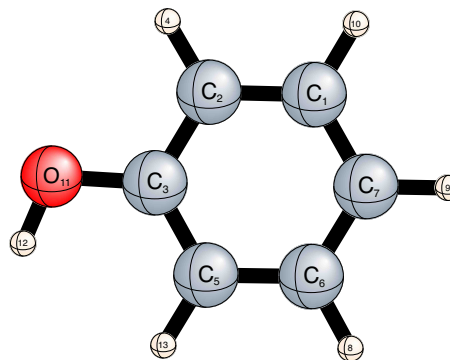


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.389	2.406	2.166	2.781	2.404	1.395	3.392	2.157	1.086	3.628	4.315	3.869
2		1.395	1.085	2.418	2.785	2.420	3.871	3.402	2.141	2.355	3.165	3.402
3			2.139	1.394	2.410	2.790	3.390	3.875	3.387	1.362	1.912	2.154
4				3.391	3.870	3.412	4.955	4.311	2.491	2.553	3.500	4.284
5					1.392	2.417	2.144	3.401	3.866	2.418	2.444	1.088
6						1.391	1.086	2.153	3.390	3.674	3.825	2.158
7							2.152	1.085	2.153	4.152	4.586	3.404
8								2.485	4.293	4.556	4.536	2.474
9									2.485	5.236	5.657	4.301
10										4.494	5.266	4.954
11											0.967	2.678
12												2.284

Molecule: phenol
Method: M062X
Basis: def2-TZVPP
Energy: -192934.349762902 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.164916	-1.183930	0.000000
2	C	-0.219318	-1.216338	0.000000
3	C	-0.933049	-0.023587	0.000000
4	H	-0.764250	-2.150116	0.000000
5	C	-0.260505	1.192231	0.000000
6	C	1.127136	1.211353	0.000000
7	C	1.847481	0.026666	0.000000
8	H	1.643990	2.161791	0.000000
9	H	2.928276	0.044718	0.000000
10	H	1.716186	-2.114887	0.000000
11	O	-2.291957	-0.106041	0.000000
12	H	-2.670377	0.776375	0.000000
13	H	-0.822401	2.119202	0.000000

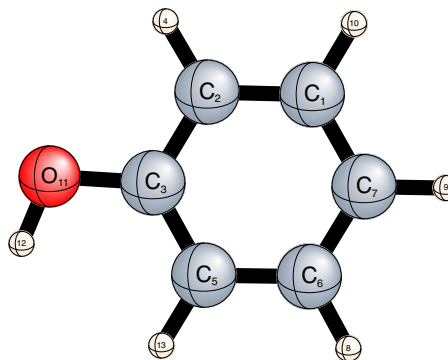


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.385	2.397	2.158	2.771	2.396	1.390	3.380	2.149	1.082	3.621	4.307	3.855
2		1.390	1.081	2.409	2.776	2.412	3.858	3.391	2.134	2.351	3.159	3.390
3			2.133	1.389	2.402	2.781	3.379	3.862	3.375	1.361	1.913	2.146
4				3.380	3.857	3.400	4.939	4.296	2.481	2.552	3.493	4.270
5					1.388	2.409	2.137	3.389	3.853	2.411	2.445	1.084
6						1.386	1.082	2.146	3.378	3.664	3.822	2.151
7							2.145	1.081	2.146	4.142	4.580	3.392
8								2.476	4.277	4.543	4.531	2.467
9									2.477	5.222	5.646	4.286
10										4.483	5.254	4.937
11											0.960	2.667
12												2.284

Molecule: phenol
Method: M052X
Basis: 6-31G*
Energy: -192913.312320992 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.167359	-1.187503	0.000000
2	C	-0.220328	-1.220994	0.000000
3	C	-0.935804	-0.024904	0.000000
4	H	-0.767742	-2.154237	0.000000
5	C	-0.263355	1.195031	0.000000
6	C	1.128141	1.214149	0.000000
7	C	1.851339	0.026882	0.000000
8	H	1.644405	2.166143	0.000000
9	H	2.933271	0.045471	0.000000
10	H	1.719578	-2.119168	0.000000
11	O	-2.297311	-0.108731	0.000000
12	H	-2.668494	0.781688	0.000000
13	H	-0.824931	2.123610	0.000000

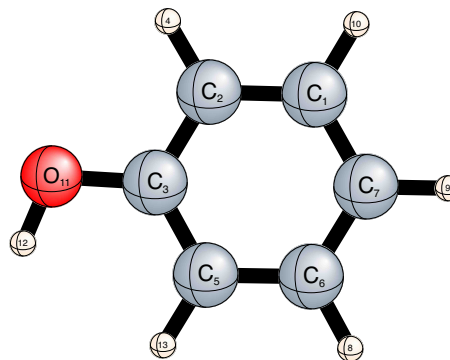


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.388	2.403	2.163	2.779	2.402	1.394	3.387	2.154	1.083	3.629	4.312	3.864
2		1.394	1.082	2.416	2.784	2.418	3.867	3.398	2.138	2.356	3.163	3.399
3			2.136	1.393	2.407	2.788	3.385	3.870	3.382	1.364	1.911	2.151
4				3.387	3.865	3.408	4.948	4.305	2.488	2.554	3.498	4.278
5					1.392	2.416	2.141	3.397	3.862	2.416	2.440	1.085
6						1.390	1.083	2.150	3.385	3.672	3.821	2.154
7							2.149	1.082	2.150	4.151	4.582	3.400
8								2.482	4.286	4.551	4.530	2.470
9									2.482	5.233	5.650	4.295
10										4.492	5.260	4.947
11											0.965	2.674
12												2.280

Molecule: phenol
Method: M052X
Basis: def2-TZVPP
Energy: -192996.497628636 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.165452	-1.181055	0.000000
2	C	-0.217547	-1.215898	0.000000
3	C	-0.930423	-0.025568	0.000000
4	H	-0.759936	-2.148224	0.000000
5	C	-0.262537	1.190333	0.000000
6	C	1.123681	1.211659	0.000000
7	C	1.845249	0.029313	0.000000
8	H	1.638044	2.160631	0.000000
9	H	2.923584	0.049004	0.000000
10	H	1.717197	-2.108840	0.000000
11	O	-2.291280	-0.106831	0.000000
12	H	-2.666911	0.774771	0.000000
13	H	-0.825050	2.114023	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.383	2.393	2.155	2.768	2.393	1.388	3.375	2.146	1.079	3.620	4.303	3.850
2		1.387	1.079	2.407	2.773	2.409	3.853	3.386	2.131	2.352	3.156	3.385
3			2.129	1.387	2.398	2.776	3.373	3.855	3.369	1.363	1.912	2.142
4				3.375	3.852	3.395	4.931	4.289	2.477	2.552	3.490	4.263
5					1.386	2.406	2.134	3.384	3.848	2.408	2.440	1.081
6						1.385	1.079	2.143	3.373	3.661	3.816	2.148
7							2.141	1.079	2.142	4.139	4.573	3.388
8								2.472	4.270	4.537	4.523	2.464
9									2.472	5.217	5.637	4.280
10										4.481	5.247	4.929
11											0.958	2.661
12												2.277

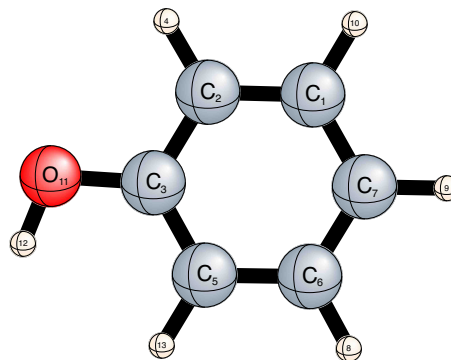
Molecule: phenol

Method: M06L

Basis: 6-31G*

Energy: -192909.907502966 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.167223	-1.187280	0.000000
2	C	-0.221509	-1.222121	0.000000
3	C	-0.941218	-0.025159	0.000000
4	H	-0.768013	-2.162095	0.000000
5	C	-0.265133	1.196680	0.000000
6	C	1.127084	1.216517	0.000000
7	C	1.851562	0.028200	0.000000
8	H	1.645258	2.173833	0.000000
9	H	2.938750	0.047595	0.000000
10	H	1.722011	-2.123882	0.000000
11	O	-2.301382	-0.113258	0.000000
12	H	-2.664901	0.783411	0.000000
13	H	-0.829271	2.130231	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.389	2.407	2.167	2.781	2.404	1.395	3.395	2.159	1.089	3.631	4.309	3.872
2		1.397	1.087	2.419	2.787	2.421	3.875	3.406	2.143	2.357	3.161	3.407
3			2.144	1.396	2.412	2.793	3.395	3.881	3.391	1.363	1.904	2.158
4				3.396	3.874	3.415	4.962	4.315	2.490	2.559	3.503	4.293
5					1.392	2.418	2.146	3.404	3.870	2.421	2.435	1.091
6						1.392	1.089	2.156	3.393	3.677	3.817	2.159
7							2.156	1.087	2.156	4.155	4.579	3.407
8								2.489	4.298	4.561	4.529	2.475
9									2.489	5.243	5.652	4.305
10										4.498	5.263	4.960
11											0.968	2.683
12												2.277

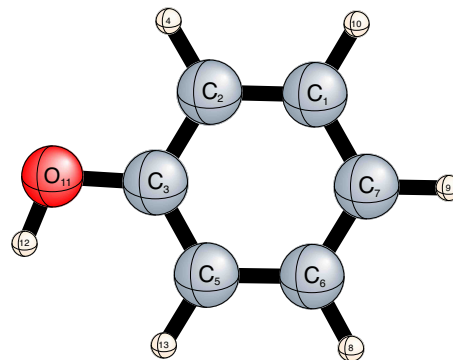
Molecule: phenol

Method: M06L

Basis: def2-TZVPP

Energy: -192986.727962978 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.163541	-1.183013	0.000000
2	C	-0.220110	-1.216758	0.000000
3	C	-0.935393	-0.024096	0.000000
4	H	-0.761034	-2.151962	0.000000
5	C	-0.260930	1.192042	0.000000
6	C	1.125567	1.211357	0.000000
7	C	1.845889	0.026803	0.000000
8	H	1.642169	2.161263	0.000000
9	H	2.925834	0.045003	0.000000
10	H	1.714433	-2.113538	0.000000
11	O	-2.292894	-0.106985	0.000000
12	H	-2.657397	0.779440	0.000000
13	H	-0.823547	2.117882	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.384	2.398	2.155	2.769	2.395	1.389	3.378	2.148	1.081	3.620	4.295	3.853
2		1.391	1.080	2.409	2.776	2.411	3.857	3.390	2.132	2.351	3.150	3.389
3			2.135	1.391	2.403	2.782	3.379	3.862	3.375	1.360	1.900	2.145
4				3.381	3.856	3.398	4.938	4.292	2.476	2.555	3.491	4.270
5					1.387	2.408	2.136	3.387	3.851	2.412	2.432	1.083
6						1.386	1.081	2.145	3.377	3.664	3.808	2.150
7							2.144	1.080	2.144	4.141	4.566	3.391
8								2.475	4.275	4.542	4.516	2.466
9									2.475	5.221	5.631	4.284
10										4.482	5.242	4.934
11											0.958	2.666
12												2.270

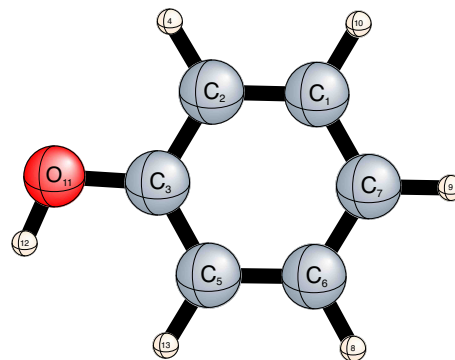
Molecule: phenol

Method: M06HF

Basis: 6-31G*

Energy: -192878.435548357 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.168313	-1.188313	0.000000
2	C	-0.219108	-1.219943	0.000000
3	C	-0.933683	-0.022780	0.000000
4	H	-0.769922	-2.150201	0.000000
5	C	-0.261383	1.196503	0.000000
6	C	1.130868	1.214310	0.000000
7	C	1.852924	0.026617	0.000000
8	H	1.647200	2.165051	0.000000
9	H	2.933954	0.044583	0.000000
10	H	1.719717	-2.119189	0.000000
11	O	-2.294647	-0.108343	0.000000
12	H	-2.685738	0.774965	0.000000
13	H	-0.822365	2.124176	0.000000

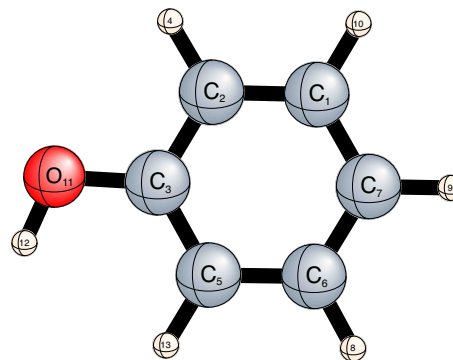


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.388	2.404	2.164	2.781	2.403	1.395	3.387	2.153	1.082	3.627	4.325	3.865
2		1.394	1.081	2.417	2.784	2.418	3.865	3.397	2.137	2.354	3.172	3.398
3			2.134	1.392	2.407	2.787	3.383	3.868	3.382	1.364	1.925	2.150
4				3.385	3.864	3.408	4.946	4.305	2.490	2.548	3.497	4.275
5					1.392	2.416	2.140	3.397	3.862	2.416	2.461	1.084
6						1.390	1.082	2.149	3.385	3.672	3.842	2.155
7							2.148	1.081	2.150	4.150	4.600	3.400
8								2.480	4.285	4.550	4.550	2.470
9									2.481	5.231	5.667	4.294
10										4.490	5.271	4.947
11											0.966	2.674
12												2.301

Molecule: phenol
Method: M06HF
Basis: def2-TZVPP
Energy: -192973.516492031 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.165529	-1.183781	0.000000
2	C	-0.217999	-1.215117	0.000000
3	C	-0.929898	-0.023030	0.000000
4	H	-0.764698	-2.146660	0.000000
5	C	-0.259430	1.191732	0.000000
6	C	1.128096	1.210277	0.000000
7	C	1.848142	0.026465	0.000000
8	H	1.644205	2.160031	0.000000
9	H	2.928128	0.044354	0.000000
10	H	1.716010	-2.114052	0.000000
11	O	-2.290083	-0.102693	0.000000
12	H	-2.682668	0.771453	0.000000
13	H	-0.819205	2.118458	0.000000

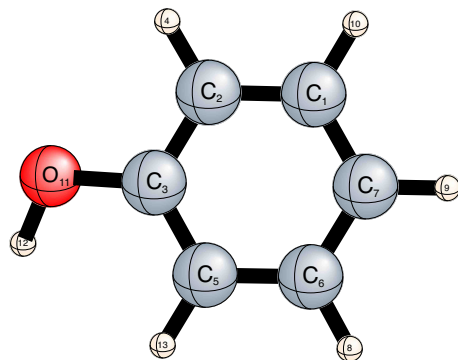


Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.384	2.395	2.157	2.770	2.394	1.389	3.378	2.148	1.081	3.621	4.316	3.853
2		1.388	1.080	2.407	2.774	2.410	3.855	3.389	2.133	2.352	3.166	3.387
3			2.130	1.388	2.399	2.778	3.375	3.859	3.372	1.363	1.924	2.144
4				3.376	3.854	3.398	4.935	4.294	2.481	2.550	3.492	4.265
5					1.388	2.408	2.136	3.388	3.851	2.408	2.459	1.083
6						1.386	1.081	2.145	3.376	3.662	3.836	2.149
7							2.143	1.080	2.145	4.140	4.592	3.390
8								2.475	4.275	4.539	4.544	2.464
9									2.475	5.220	5.658	4.283
10										4.483	5.261	4.934
11											0.958	2.664
12												2.299

Molecule: phenol
Method: RI-MP2
Basis: def2-TZVPP
Energy: -192624.681452791 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	C	1.167394	-1.184423	0.000000
2	C	-0.219588	-1.215281	0.000000
3	C	-0.935449	-0.023852	0.000000
4	H	-0.761115	-2.148283	0.000000
5	C	-0.261977	1.192426	0.000000
6	C	1.127584	1.214629	0.000000
7	C	1.848728	0.027993	0.000000
8	H	1.642165	2.163453	0.000000
9	H	2.927066	0.046999	0.000000
10	H	1.716573	-2.113690	0.000000
11	O	-2.296132	-0.111180	-0.000001
12	H	-2.659010	0.777990	-0.000002
13	H	-0.821191	2.118004	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11	12	13
1	1.387	2.402	2.156	2.774	2.399	1.391	3.381	2.148	1.079	3.626	4.300	3.855
2		1.390	1.079	2.408	2.778	2.413	3.858	3.390	2.134	2.352	3.150	3.387
3			2.132	1.390	2.406	2.785	3.381	3.863	3.376	1.363	1.901	2.145
4				3.378	3.857	3.398	4.936	4.292	2.478	2.551	3.488	4.267
5					1.390	2.411	2.137	3.389	3.853	2.416	2.433	1.081
6						1.389	1.079	2.145	3.380	3.671	3.812	2.148
7							2.145	1.079	2.146	4.147	4.570	3.391
8								2.476	4.278	4.548	4.519	2.464
9									2.477	5.226	5.634	4.282
10										4.485	5.245	4.934
11											0.960	2.673
12												2.274

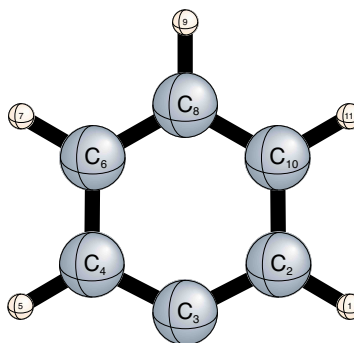
Molecule: phenyl radical

Method: B3LYP

Basis: 6-31G*

Energy: -145306.784007298 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.162793	1.322043	0.000000
2	C	1.226238	0.770601	0.000000
3	C	-0.000006	1.399082	0.000000
4	C	-1.226244	0.770591	0.000000
5	H	-2.162803	1.322026	0.000000
6	C	-1.214141	-0.633858	0.000000
7	H	-2.154548	-1.180335	0.000000
8	C	0.000005	-1.326010	0.000000
9	H	0.000010	-2.412631	0.000000
10	C	1.214146	-0.633848	0.000000
11	H	2.154558	-1.180318	0.000000

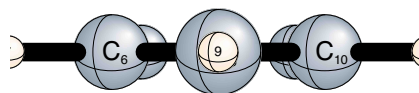


Distance Matrix

	2	3	4	5	6	7	8	9	10	11
1	1.087	2.164	3.434	4.326	3.902	4.990	3.419	4.316	2.174	2.502
2		1.378	2.452	3.434	2.816	3.903	2.429	3.411	1.405	2.161
3			1.378	2.164	2.368	3.361	2.725	3.812	2.368	3.361
4				1.087	1.405	2.161	2.429	3.411	2.816	3.903
5					2.174	2.502	3.419	4.316	3.902	4.990
6						1.088	1.398	2.154	2.428	3.413
7							2.159	2.482	3.413	4.309
8								1.087	1.398	2.159
9									2.154	2.482
10										1.088

Molecule: phenyl radical
Method: B3LYP
Basis: def2-TZVPP
Energy: -145362.96743199 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.153690	0.000000	-1.319104
2	C	1.221410	0.000000	-0.769633
3	C	0.000000	0.000000	-1.391757
4	C	-1.221410	0.000000	-0.769633
5	H	-2.153690	0.000000	-1.319104
6	C	-1.209366	0.000000	0.629688
7	H	-2.145894	0.000000	1.173308
8	C	0.000000	0.000000	1.318518
9	H	0.000000	0.000000	2.400379
10	C	1.209366	0.000000	0.629688
11	H	2.145894	0.000000	1.173308



Distance Matrix

	2	3	4	5	6	7	8	9	10	11
1	1.082	2.155	3.420	4.307	3.887	4.970	3.405	4.298	2.166	2.492
2		1.371	2.443	3.420	2.805	3.888	2.419	3.397	1.399	2.152
3			1.371	2.155	2.356	3.344	2.710	3.792	2.356	3.344
4				1.082	1.399	2.152	2.419	3.397	2.805	3.888
5					2.166	2.492	3.405	4.298	3.887	4.970
6						1.083	1.392	2.144	2.419	3.399
7							2.151	2.472	3.399	4.292
8								1.082	1.392	2.151
9									2.144	2.472
10										1.083

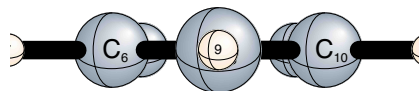
Molecule: phenyl radical

Method: ω B97

Basis: 6-31G*

Energy: -145270.902519963 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.163570	0.000000	-1.324752
2	C	1.225995	0.000000	-0.771099
3	C	0.000000	0.000000	-1.399201
4	C	-1.225995	0.000000	-0.771099
5	H	-2.163570	0.000000	-1.324752
6	C	-1.212261	0.000000	0.629520
7	H	-2.153874	0.000000	1.178156
8	C	0.000000	0.000000	1.321196
9	H	0.000000	0.000000	2.410011
10	C	1.212261	0.000000	0.629520
11	H	2.153874	0.000000	1.178156



Distance Matrix

	2	3	4	5	6	7	8	9	10	11
1	1.089	2.165	3.434	4.327	3.901	4.990	3.418	4.316	2.174	2.503
2		1.378	2.452	3.434	2.812	3.902	2.425	3.409	1.401	2.159
3			1.378	2.165	2.363	3.359	2.720	3.809	2.363	3.359
4				1.089	1.401	2.159	2.425	3.409	2.812	3.902
5					2.174	2.503	3.418	4.316	3.901	4.990
6						1.090	1.396	2.154	2.425	3.411
7							2.159	2.481	3.411	4.308
8								1.089	1.396	2.159
9									2.154	2.481
10										1.090

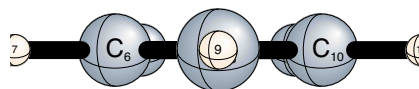
Molecule: phenyl radical

Method: ω B97

Basis: def2-TZVPP

Energy: -145131.801205608 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.180441	0.000000	-1.377816
2	C	1.271247	0.000000	-0.792044
3	C	0.000000	0.000000	-1.147905
4	C	-1.271247	0.000000	-0.792044
5	H	-2.180441	0.000000	-1.377816
6	C	-1.210067	0.000000	0.628789
7	H	-2.164003	0.000000	1.146445
8	C	0.000000	0.000000	1.311649
9	H	0.000000	0.000000	2.394624
10	C	1.210067	0.000000	0.628789
11	H	2.164003	0.000000	1.146445



Distance Matrix

	2	3	4	5	6	7	8	9	10	11
1	1.082	2.193	3.501	4.361	3.940	5.025	3.462	4.357	2.229	2.524
2		1.320	2.542	3.501	2.859	3.944	2.458	3.431	1.422	2.134
3			1.320	2.193	2.150	3.154	2.460	3.543	2.150	3.154
4				1.082	1.422	2.134	2.458	3.431	2.859	3.944
5					2.229	2.524	3.462	4.357	3.940	5.025
6						1.085	1.389	2.141	2.420	3.414
7							2.170	2.498	3.414	4.328
8								1.083	1.389	2.170
9									2.141	2.498
10										1.085

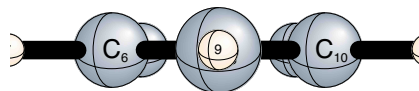
Molecule: phenyl radical

Method: ω B97X

Basis: 6-31G*

Energy: -145262.656227784 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.159461	0.000000	-1.322265
2	C	1.223633	0.000000	-0.769635
3	C	0.000000	0.000000	-1.397843
4	C	-1.223633	0.000000	-0.769635
5	H	-2.159461	0.000000	-1.322265
6	C	-1.210523	0.000000	0.629070
7	H	-2.150308	0.000000	1.176597
8	C	0.000000	0.000000	1.319607
9	H	0.000000	0.000000	2.406356
10	C	1.210523	0.000000	0.629070
11	H	2.150308	0.000000	1.176597



Distance Matrix

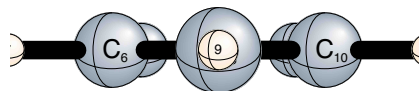
	2	3	4	5	6	7	8	9	10	11
1	1.087	2.161	3.428	4.319	3.894	4.982	3.412	4.309	2.170	2.499
2		1.375	2.447	3.428	2.807	3.895	2.421	3.404	1.399	2.156
3			1.375	2.161	2.361	3.354	2.717	3.804	2.361	3.354
4				1.087	1.399	2.156	2.421	3.404	2.807	3.895
5					2.170	2.499	3.412	4.309	3.894	4.982
6						1.088	1.394	2.150	2.421	3.405
7							2.155	2.477	3.405	4.301
8								1.087	1.394	2.155
9									2.150	2.477
10										1.088

Energy: -145314.288686124 kcal/mol

A diagram showing a linear chain of three carbon clusters. From left to right, the clusters are labeled C_6 , C_9 , and C_{10} . Each cluster is represented by a blue sphere with a grid of lines. The C_9 cluster has a yellow circle in the center with the number 9. The clusters are connected by thick black horizontal lines. The chain is part of a larger structure, with a yellow sphere visible on the far left and a yellow sphere on the far right.

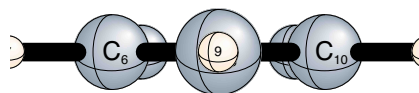
[illegible]

Energy: -145252.567337003 kcal/mol

[illegible]

Molecule: phenyl radical
Method: ω B97X-D
Basis: def2-TZVPP
Energy: -145304.733978694 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.150721	0.000000	-1.316652
2	C	1.218924	0.000000	-0.766806
3	C	0.000000	0.000000	-1.389111
4	C	-1.218924	0.000000	-0.766806
5	H	-2.150721	0.000000	-1.316652
6	C	-1.206182	0.000000	0.627791
7	H	-2.141921	0.000000	1.172167
8	C	0.000000	0.000000	1.315072
9	H	0.000000	0.000000	2.396696
10	C	1.206182	0.000000	0.627791
11	H	2.141921	0.000000	1.172167



Distance Matrix

	2	3	4	5	6	7	8	9	10	11
1	1.082	2.152	3.414	4.301	3.879	4.962	3.399	4.291	2.162	2.489
2		1.369	2.438	3.414	2.798	3.880	2.412	3.390	1.395	2.147
3			1.369	2.152	2.350	3.339	2.704	3.786	2.350	3.339
4				1.082	1.395	2.147	2.412	3.390	2.798	3.880
5					2.162	2.489	3.399	4.291	3.879	4.962
6						1.083	1.388	2.141	2.412	3.392
7							2.147	2.467	3.392	4.284
8								1.082	1.388	2.147
9									2.141	2.467
10										1.083

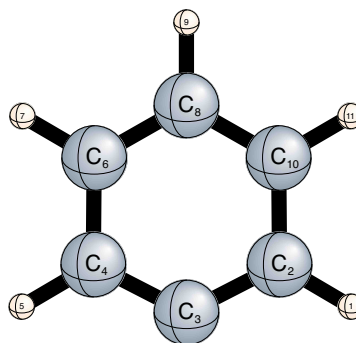
Molecule: phenyl radical

Method: M06

Basis: 6-31G*

Energy: -145188.234643691 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.160370	1.319736	0.000000
2	C	1.221862	0.767349	0.000000
3	C	-0.000006	1.395476	0.000000
4	C	-1.221868	0.767339	0.000000
5	H	-2.160380	1.319719	0.000000
6	C	-1.210459	-0.630989	0.000000
7	H	-2.151348	-1.180391	0.000000
8	C	0.000005	-1.320486	0.000000
9	H	0.000010	-2.409057	0.000000
10	C	1.210464	-0.630980	0.000000
11	H	2.151357	-1.180373	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11
1	1.089	2.162	3.427	4.321	3.895	4.984	3.411	4.309	2.170	2.500
2		1.374	2.444	3.427	2.806	3.895	2.419	3.403	1.398	2.158
3			1.374	2.162	2.360	3.356	2.716	3.805	2.360	3.356
4				1.089	1.398	2.158	2.419	3.403	2.806	3.895
5					2.170	2.500	3.411	4.309	3.895	4.984
6						1.090	1.393	2.151	2.421	3.406
7							2.156	2.477	3.406	4.303
8								1.089	1.393	2.156
9									2.151	2.477
10										1.090

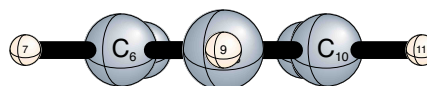
Molecule: phenyl radical

Method: M06

Basis: def2-TZVPP

Energy: -145241.565251198 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.149559	0.000000	-1.315512
2	C	1.216370	0.000000	-0.765823
3	C	0.000000	0.000000	-1.387262
4	C	-1.216370	0.000000	-0.765823
5	H	-2.149559	0.000000	-1.315512
6	C	-1.204973	0.000000	0.626581
7	H	-2.140722	0.000000	1.172629
8	C	0.000000	0.000000	1.312383
9	H	0.000000	0.000000	2.394784
10	C	1.204973	0.000000	0.626581
11	H	2.140722	0.000000	1.172629



Distance Matrix

	2	3	4	5	6	7	8	9	10	11
1	1.083	2.151	3.411	4.299	3.876	4.960	3.395	4.288	2.160	2.488
2		1.366	2.433	3.411	2.793	3.877	2.408	3.387	1.392	2.148
3			1.366	2.151	2.347	3.337	2.700	3.782	2.347	3.337
4				1.083	1.392	2.148	2.408	3.387	2.793	3.877
5					2.160	2.488	3.395	4.288	3.876	4.960
6						1.083	1.386	2.140	2.410	3.390
7							2.145	2.465	3.390	4.281
8								1.082	1.386	2.145
9									2.140	2.465
10										1.083

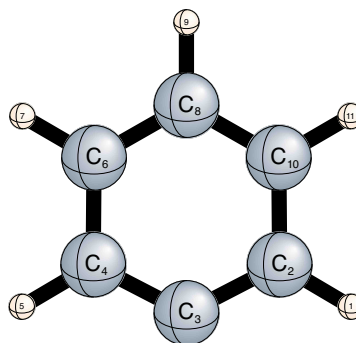
Molecule: phenyl radical

Method: M062X

Basis: 6-31G*

Energy: -145238.017440187 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.156691	1.319096	0.000000
2	C	1.221876	0.766794	0.000000
3	C	-0.000006	1.399398	0.000000
4	C	-1.221882	0.766784	0.000000
5	H	-2.156702	1.319078	0.000000
6	C	-1.210563	-0.632129	0.000000
7	H	-2.149394	-1.178705	0.000000
8	C	0.000005	-1.323332	0.000000
9	H	0.000010	-2.408834	0.000000
10	C	1.210568	-0.632120	0.000000
11	H	2.149403	-1.178688	0.000000

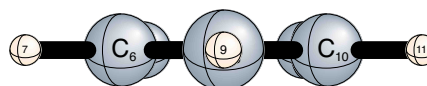


Distance Matrix

	2	3	4	5	6	7	8	9	10	11
1	1.086	2.158	3.423	4.313	3.892	4.978	3.411	4.307	2.169	2.498
2		1.376	2.444	3.423	2.806	3.892	2.421	3.403	1.399	2.155
3			1.376	2.158	2.365	3.357	2.723	3.808	2.365	3.357
4				1.086	1.399	2.155	2.421	3.403	2.806	3.892
5					2.168	2.498	3.411	4.307	3.892	4.978
6						1.086	1.394	2.150	2.421	3.404
7							2.154	2.477	3.404	4.299
8								1.086	1.394	2.154
9									2.150	2.477
10										1.086

Molecule: phenyl radical
Method: M062X
Basis: def2-TZVPP
Energy: -145293.999793424 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.149393	0.000000	-1.317110
2	C	1.218042	0.000000	-0.766527
3	C	0.000000	0.000000	-1.393777
4	C	-1.218042	0.000000	-0.766527
5	H	-2.149393	0.000000	-1.317110
6	C	-1.206692	0.000000	0.628315
7	H	-2.142339	0.000000	1.172486
8	C	0.000000	0.000000	1.316727
9	H	0.000000	0.000000	2.398377
10	C	1.206692	0.000000	0.628315
11	H	2.142339	0.000000	1.172486



Distance Matrix

	2	3	4	5	6	7	8	9	10	11
1	1.082	2.151	3.412	4.299	3.879	4.962	3.400	4.292	2.162	2.490
2		1.370	2.436	3.412	2.797	3.880	2.413	3.391	1.395	2.148
3			1.370	2.151	2.355	3.343	2.711	3.792	2.355	3.343
4				1.082	1.395	2.148	2.413	3.391	2.797	3.880
5					2.162	2.490	3.400	4.292	3.879	4.962
6						1.082	1.389	2.142	2.413	3.393
7							2.147	2.468	3.393	4.285
8								1.082	1.389	2.147
9									2.142	2.468
10										1.082

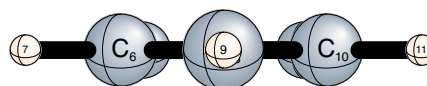
Molecule: phenyl radical

Method: M052X

Basis: 6-31G*

Energy: -145286.950467132 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.156548	0.000000	-1.320373
2	C	1.224293	0.000000	-0.769614
3	C	0.000000	0.000000	-1.394425
4	C	-1.224293	0.000000	-0.769614
5	H	-2.156548	0.000000	-1.320373
6	C	-1.210290	0.000000	0.629425
7	H	-2.146658	0.000000	1.174742
8	C	0.000000	0.000000	1.319519
9	H	0.000000	0.000000	2.402203
10	C	1.210290	0.000000	0.629425
11	H	2.146658	0.000000	1.174742



Distance Matrix

	2	3	4	5	6	7	8	9	10	11
1	1.083	2.158	3.425	4.313	3.891	4.974	3.409	4.302	2.167	2.495
2		1.375	2.449	3.425	2.808	3.892	2.421	3.400	1.399	2.152
3			1.375	2.158	2.358	3.348	2.714	3.797	2.358	3.348
4				1.083	1.399	2.152	2.421	3.400	2.808	3.892
5					2.167	2.495	3.409	4.302	3.891	4.974
6						1.084	1.393	2.147	2.421	3.401
7							2.152	2.473	3.401	4.293
8								1.083	1.393	2.152
9									2.147	2.473
10										1.084

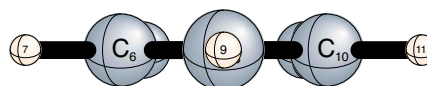
Molecule: phenyl radical

Method: M052X

Basis: def2-TZVPP

Energy: -145343.430817788 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.149073	0.000000	-1.314581
2	C	1.219622	0.000000	-0.766140
3	C	0.000000	0.000000	-1.385716
4	C	-1.219622	0.000000	-0.766140
5	H	-2.149073	0.000000	-1.314581
6	C	-1.205725	0.000000	0.628179
7	H	-2.139242	0.000000	1.171199
8	C	0.000000	0.000000	1.315230
9	H	0.000000	0.000000	2.394399
10	C	1.205725	0.000000	0.628179
11	H	2.139242	0.000000	1.171199

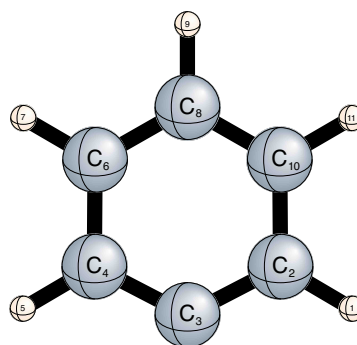


Distance Matrix

	2	3	4	5	6	7	8	9	10	11
1	1.079	2.150	3.413	4.298	3.877	4.957	3.396	4.287	2.160	2.486
2		1.368	2.439	3.413	2.798	3.878	2.412	3.388	1.394	2.145
3			1.368	2.150	2.347	3.334	2.701	3.780	2.347	3.334
4				1.079	1.394	2.145	2.412	3.388	2.798	3.878
5					2.160	2.486	3.396	4.287	3.877	4.957
6						1.080	1.388	2.139	2.411	3.389
7							2.144	2.464	3.389	4.278
8								1.079	1.388	2.144
9									2.139	2.464
10										1.080

Molecule: phenyl radical
Method: M06L
Basis: 6-31G*
Energy: -145285.28614823 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.159082	1.319880	0.000000
2	C	1.220951	0.767562	0.000000
3	C	-0.000006	1.401456	0.000000
4	C	-1.220957	0.767552	0.000000
5	H	-2.159093	1.319863	0.000000
6	C	-1.211171	-0.632229	0.000000
7	H	-2.152538	-1.180493	0.000000
8	C	0.000005	-1.322698	0.000000
9	H	0.000010	-2.410856	0.000000
10	C	1.211176	-0.632219	0.000000
11	H	2.152547	-1.180475	0.000000



Distance Matrix

	2	3	4	5	6	7	8	9	10	11
1	1.089	2.161	3.425	4.318	3.895	4.984	3.412	4.310	2.170	2.500
2		1.376	2.442	3.425	2.806	3.896	2.421	3.405	1.400	2.159
3			1.376	2.161	2.367	3.362	2.724	3.812	2.367	3.362
4				1.089	1.400	2.159	2.421	3.405	2.806	3.896
5					2.170	2.500	3.412	4.310	3.895	4.984
6						1.089	1.394	2.152	2.422	3.408
7							2.157	2.479	3.408	4.305
8								1.088	1.394	2.157
9									2.152	2.479
10										1.089

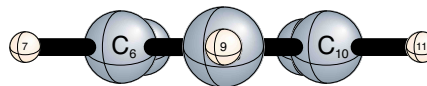
Molecule: phenyl radical

Method: M06L

Basis: def2-TZVPP

Energy: -145339.223054306 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.148080	0.000000	-1.315929
2	C	1.216497	0.000000	-0.766338
3	C	0.000000	0.000000	-1.393017
4	C	-1.216497	0.000000	-0.766338
5	H	-2.148080	0.000000	-1.315929
6	C	-1.206526	0.000000	0.628308
7	H	-2.141546	0.000000	1.173040
8	C	0.000000	0.000000	1.315317
9	H	0.000000	0.000000	2.396230
10	C	1.206526	0.000000	0.628308
11	H	2.141546	0.000000	1.173040



Distance Matrix

	2	3	4	5	6	7	8	9	10	11
1	1.082	2.149	3.409	4.296	3.877	4.959	3.397	4.289	2.160	2.489
2		1.368	2.433	3.409	2.796	3.878	2.411	3.388	1.395	2.149
3			1.368	2.149	2.354	3.342	2.708	3.789	2.354	3.342
4				1.082	1.395	2.149	2.411	3.388	2.796	3.878
5					2.160	2.489	3.397	4.289	3.877	4.959
6						1.082	1.388	2.140	2.413	3.392
7							2.146	2.466	3.392	4.283
8								1.081	1.388	2.146
9									2.140	2.466
10										1.082

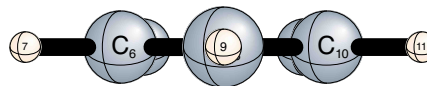
Molecule: phenyl radical

Method: M06HF

Basis: 6-31G*

Energy: -145263.069502074 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.151946	0.000000	-1.320707
2	C	1.222087	0.000000	-0.767795
3	C	0.000000	0.000000	-1.401698
4	C	-1.222087	0.000000	-0.767795
5	H	-2.151946	0.000000	-1.320707
6	C	-1.210104	0.000000	0.629897
7	H	-2.145123	0.000000	1.174878
8	C	0.000000	0.000000	1.321529
9	H	0.000000	0.000000	2.403280
10	C	1.210104	0.000000	0.629897
11	H	2.145123	0.000000	1.174878



Distance Matrix

	2	3	4	5	6	7	8	9	10	11
1	1.082	2.153	3.419	4.304	3.887	4.969	3.408	4.301	2.166	2.496
2		1.377	2.444	3.419	2.805	3.887	2.420	3.398	1.398	2.151
3			1.377	2.153	2.365	3.353	2.723	3.805	2.365	3.353
4				1.082	1.398	2.151	2.420	3.398	2.805	3.887
5					2.166	2.496	3.408	4.301	3.887	4.969
6						1.082	1.394	2.147	2.420	3.399
7							2.150	2.472	3.399	4.290
8								1.082	1.394	2.150
9									2.147	2.472
10										1.082

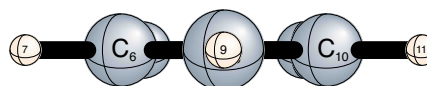
Molecule: phenyl radical

Method: M06HF

Basis: def2-TZVPP

Energy: -145327.302901499 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.147144	0.000000	-1.316679
2	C	1.217990	0.000000	-0.764903
3	C	0.000000	0.000000	-1.393746
4	C	-1.217990	0.000000	-0.764903
5	H	-2.147144	0.000000	-1.316679
6	C	-1.206135	0.000000	0.628737
7	H	-2.140452	0.000000	1.172702
8	C	0.000000	0.000000	1.317712
9	H	0.000000	0.000000	2.398461
10	C	1.206135	0.000000	0.628737
11	H	2.140452	0.000000	1.172702

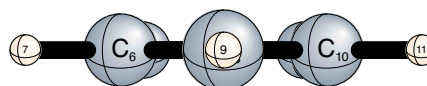


Distance Matrix

	2	3	4	5	6	7	8	9	10	11
1	1.081	2.149	3.410	4.294	3.877	4.958	3.399	4.291	2.161	2.489
2		1.371	2.436	3.410	2.796	3.877	2.413	3.390	1.394	2.146
3			1.371	2.149	2.355	3.342	2.711	3.792	2.355	3.342
4				1.081	1.394	2.146	2.413	3.390	2.796	3.877
5					2.161	2.489	3.399	4.291	3.877	4.958
6						1.081	1.389	2.142	2.412	3.391
7							2.145	2.467	3.391	4.281
8								1.081	1.389	2.145
9									2.142	2.467
10										1.081

Molecule: phenyl radical
Method: RI-MP2
Basis: def2-TZVPP
Energy: -145038.215228709 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	2.150143	0.000000	-1.316042
2	C	1.221573	0.000000	-0.766987
3	C	0.000000	0.000000	-1.390010
4	C	-1.221573	0.000000	-0.766987
5	H	-2.150143	0.000000	-1.316042
6	C	-1.208724	0.000000	0.630735
7	H	-2.142300	0.000000	1.173590
8	C	0.000000	0.000000	1.318814
9	H	0.000000	0.000000	2.397884
10	C	1.208724	0.000000	0.630735
11	H	2.142300	0.000000	1.173590

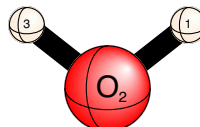


Distance Matrix

	2	3	4	5	6	7	8	9	10	11
1	1.079	2.151	3.416	4.300	3.882	4.962	3.401	4.291	2.162	2.490
2		1.371	2.443	3.416	2.804	3.883	2.417	3.392	1.398	2.148
3			1.371	2.151	2.355	3.341	2.709	3.788	2.355	3.341
4				1.079	1.398	2.148	2.417	3.392	2.804	3.883
5					2.162	2.490	3.401	4.291	3.882	4.962
6						1.080	1.391	2.141	2.417	3.395
7							2.147	2.467	3.395	4.285
8								1.079	1.391	2.147
9									2.141	2.467
10										1.080

Molecule: water
Method: B3LYP
Basis: 6-31G*
Energy: -47947.305932178 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.761537	-0.461399	0.000000
2	O	-0.000003	0.137359	0.000000
3	H	-0.761574	-0.461358	0.000000



Distance Matrix

	2	3
1	0.969	1.523
2		0.969

Molecule: water
Method: B3LYP
Basis: def2-TZVPP
Energy: -47983.5252207854 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.761711	0.000000	0.470103
2	O	0.000000	0.000000	-0.115431
3	H	-0.761711	0.000000	0.470103



Distance Matrix

	2	3
1	0.961	1.523
2		0.961

Molecule: water

Method: ω B97

Basis: 6-31G*

Energy: -47937.4932796433 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.760426	0.000000	0.473191
2	O	0.000000	0.000000	-0.121606
3	H	-0.760426	0.000000	0.473191



Distance Matrix

	2	3
1	0.965	1.521
2		0.965

Molecule: water

Method: ω B97

Basis: def2-TZVPP

Energy: -47972.2115529175 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.760401	0.000000	0.471822
2	O	0.000000	0.000000	-0.110927
3	H	-0.760401	0.000000	0.471822



Distance Matrix

	2	3
1	0.958	1.521
2		0.958

Molecule: water

Method: ω B97X

Basis: 6-31G*

Energy: -47934.3158828017 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.759972	0.000000	0.472534
2	O	0.000000	0.000000	-0.120293
3	H	-0.759972	0.000000	0.472534



Distance Matrix

	2	3
1	0.964	1.520
2		0.964

Molecule: water

Method: ω B97X

Basis: def2-TZVPP

Energy: -47968.7159814025 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.759379	0.000000	0.470610
2	O	0.000000	0.000000	-0.111262
3	H	-0.759379	0.000000	0.470610



Distance Matrix

	2	3
1	0.957	1.519
2		0.957

Molecule: water

Method: ω B97X-D

Basis: 6-31G*

Energy: -47933.5758388477 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.759924	0.000000	0.476683
2	O	0.000000	0.000000	-0.115133
3	H	-0.759924	0.000000	0.476683



Distance Matrix

	2	3
1	0.963	1.520
2		0.963

Molecule: water

Method: ω B97X–D

Basis: def2–TZVPP

Energy: -47967.7196822257 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.758504	0.000000	0.468933
2	O	0.000000	0.000000	-0.113090
3	H	-0.758504	0.000000	0.468933



Distance Matrix

	2	3
1	0.956	1.517
2		0.956

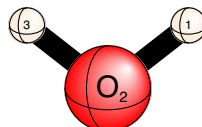
Molecule: water

Method: M06

Basis: 6-31G*

Energy: -47926.5605354662 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.760027	-0.459527	0.000000
2	O	-0.000003	0.133616	0.000000
3	H	-0.760065	-0.459487	0.000000



Distance Matrix

	2	3
1	0.964	1.520
2		0.964

Molecule: water

Method: M06

Basis: def2-TZVPP

Energy: -47958.369893507 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.757290	0.000000	0.469434
2	O	0.000000	0.000000	-0.114092
3	H	-0.757290	0.000000	0.469434



Distance Matrix

	2	3
1	0.956	1.515
2		0.956

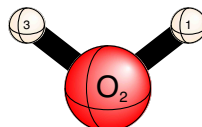
Molecule: water

Method: M062X

Basis: 6-31G*

Energy: -47924.9946281723 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.762393	-0.459302	0.000000
2	O	-0.000003	0.133164	0.000000
3	H	-0.762431	-0.459261	0.000000



Distance Matrix

	2	3
1	0.966	1.525
2		0.966

Molecule: water
Method: M062X
Basis: def2-TZVPP
Energy: -47960.0032065627 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.760945	0.000000	0.469330
2	O	0.000000	0.000000	-0.113885
3	H	-0.760945	0.000000	0.469330



Distance Matrix

	2	3
1	0.959	1.522
2		0.959

Molecule: water

Method: M052X

Basis: 6-31G*

Energy: -47937.8853673468 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.761912	0.000000	0.471073
2	O	0.000000	0.000000	-0.117372
3	H	-0.761912	0.000000	0.471073



Distance Matrix

	2	3
1	0.963	1.524
2		0.963

Molecule: water
Method: M052X
Basis: def2-TZVPP
Energy: -47973.0686040822 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.761118	0.000000	0.468264
2	O	0.000000	0.000000	-0.111753
3	H	-0.761118	0.000000	0.468264

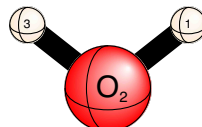


Distance Matrix

	2	3
1	0.957	1.522
2		0.957

Molecule: water
Method: M06L
Basis: 6-31G*
Energy: -47941.706671881 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.757193	-0.460905	0.000000
2	O	-0.000003	0.136372	0.000000
3	H	-0.757230	-0.460865	0.000000



Distance Matrix

	2	3
1	0.964	1.514
2		0.964

Molecule: water
Method: M06L
Basis: def2-TZVPP
Energy: -47972.0119787001 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.753228	0.000000	0.471500
2	O	0.000000	0.000000	-0.118225
3	H	-0.753228	0.000000	0.471500



Distance Matrix

	2	3
1	0.957	1.506
2		0.957

Molecule: water

Method: M06HF

Basis: 6-31G*

Energy: -47922.9306243145 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.769073	0.000000	0.469452
2	O	0.000000	0.000000	-0.114130
3	H	-0.769073	0.000000	0.469452



Distance Matrix

	2	3
1	0.965	1.538
2		0.965

Molecule: water
Method: M06HF
Basis: def2-TZVPP
Energy: -47963.6269787939 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.767798	0.000000	0.465556
2	O	0.000000	0.000000	-0.106336
3	H	-0.767798	0.000000	0.465556



Distance Matrix

	2	3
1	0.957	1.536
2		0.957

Molecule: water
Method: RI-MP2
Basis: def2-TZVPP
Energy: -47903.1489490223 kcal/mol

Cartesian Geometry (Angstroms)				
#	Atom	X	Y	Z
1	H	0.754101	0.000000	0.474069
2	O	0.000000	0.000000	-0.115056
3	H	-0.754101	0.000000	0.474069



Distance Matrix

	2	3
1	0.957	1.508
2		0.957

4 Frequency Shifts

Table 8: Calculated harmonic frequency shifts for the OH stretch in **I1a** and **I1b** for the methods that geometry and frequency calculations could be sufficiently converged. Note that some of the **I1b** starting geometries converged to **I1a**, and vice versa (see geometry details given above). All calculations use the def2-TZVPP basis set, cited in the main paper. Shifts are given in cm^{-1} relative to hydroxyl radical monomer.

Method	Shift for I1a	Shift for I1b
B3LYP	-17	34
M06	-70	7
M062X	-23	-19
M06L	22	21
M06HF	-43	-37

Table 9: Calculated harmonic frequency shifts for the OH stretch in **I2a** and **I2b** for the methods that geometry and frequency calculations could be sufficiently converged. Note that some of the **I2b** starting geometries converged to **I2a**, and vice versa (see geometry details given above). All calculations use the def2-TZVPP basis set, cited in the main paper. Shifts are given in cm^{-1} relative to hydroxyl radical monomer.

Method	Shift for I2a	Shift for I2b
B3LYP	-14	-118
RI-MP2	-32	-88
M06	-34	-29
M062X	-23	-13
M06L	-40	-83
M06HF	-39	-17
M052X	-29	-74
ω B97	-20	-151
ω B97X-D	-12	-137

References

- [1] K. P. Huber and G. Herzberg, *Molecular Spectra and Molecular Structure. IV. Constants of Diatomic Molecules*, Van Nostrand Reinhold Co., 1979.
- [2] A. R. Hoy and P. R. Bunker, *J. Mol. Spec.*, 1979, **74**, 1–8.
- [3] G. Herzberg, *Electronic Spectra and Electronic Structure of Polyatomic Molecules*, Van Nostrand, 1966.