

Density functional theory simulation of the deoxygenation of
lignite model compounds in the aqueous phase under CO
atmosphere catalyzed by OH⁻ ion

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300072, China.

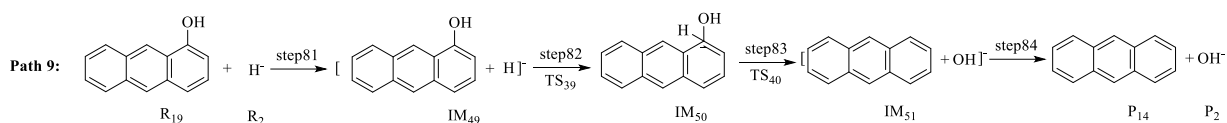
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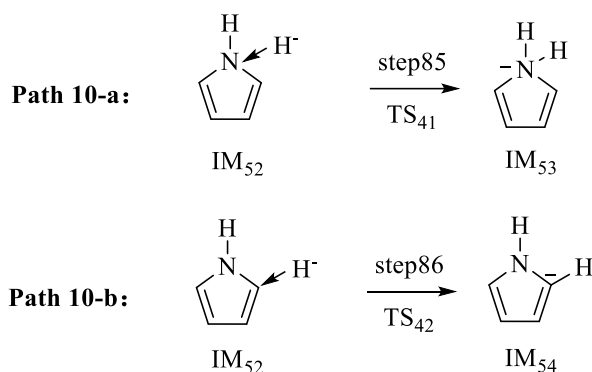
Supplementary Information



Scheme S1: Deoxygenation of 1-anthranol in the presence of H^- to form anthracene

Table S1: Energy barriers of the reaction of H^- with lignite model compound 1-anthranol

No.	Energy Barriers (kJ/mol)
TS ₃₉	80.52
TS ₄₀	21.56



Scheme S2: H^- attacks the reaction paths of two positions on pyrrole

Table S2: Energy barriers of the reaction of H^- attacks the reaction paths of two positions on pyrrole

Path	No.	Energy Barriers (kJ/mol)
Path 10-o	TS ₄₁	287.68
Path 10-p	TS ₄₂	128.52

Table S3: Relationship between energy barrier and LUMO energy for typical arylphenols

Reactant	LUMO	Energy Barriers (kJ/mol)
phenol	0.0055	98.43
1- naphthol	-0.01601	89.24
2- anthracenol	-0.04267	86.79
1- anthracenol	-0.04325	80.52

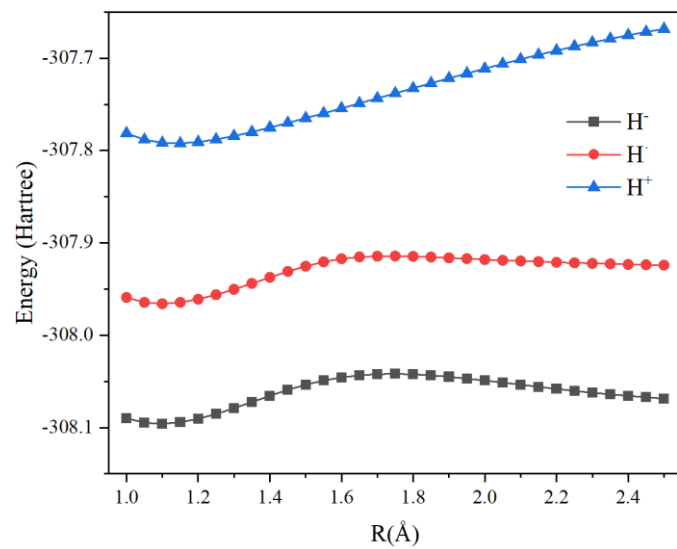
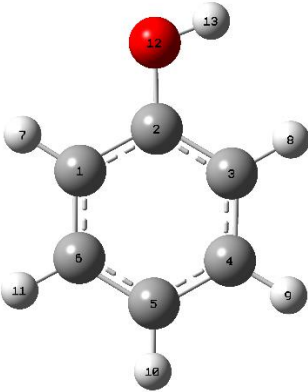

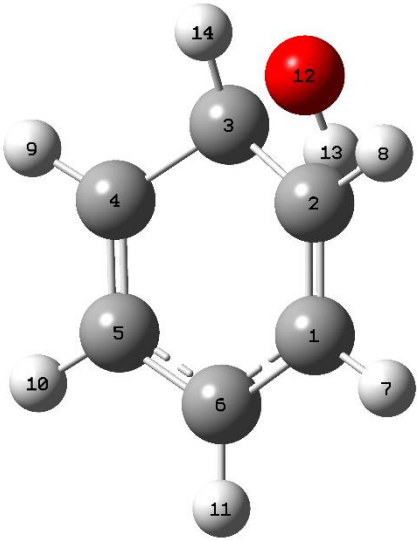
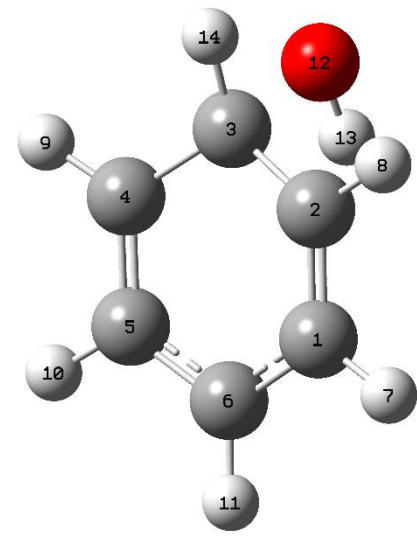


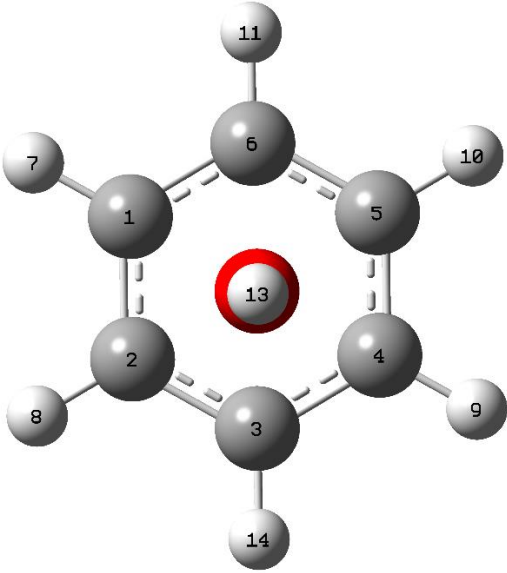
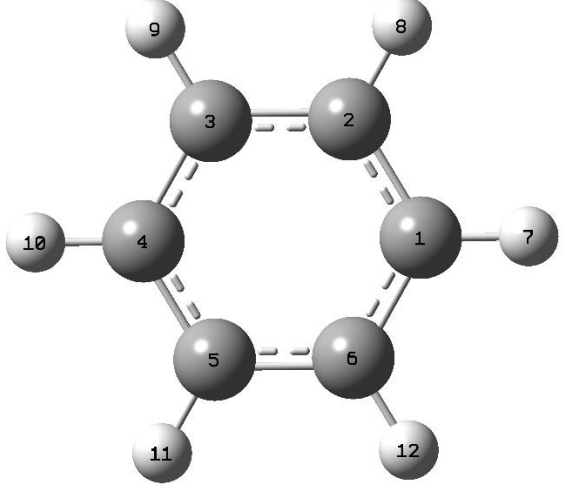
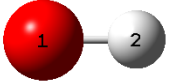

Fig. S1 The scan of the distances between C connected adjacent to O on phenol and H⁻, H[·], and H⁺ (ranged from 1.0 to 2.5 Å, step size 0.05 Å)

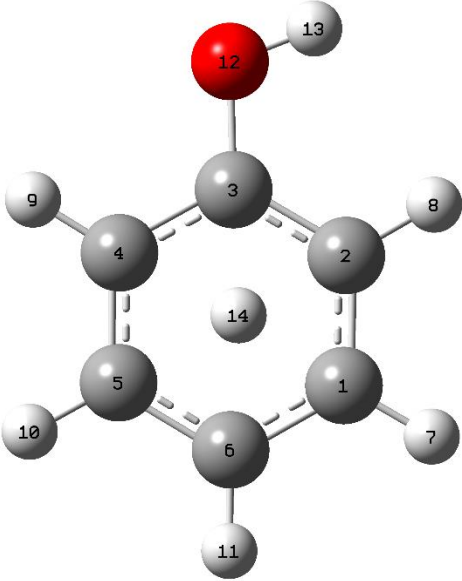
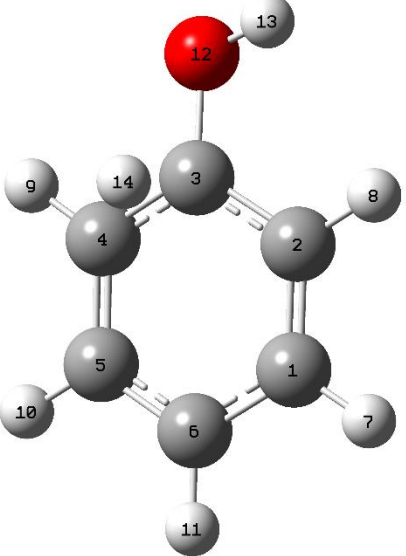
Table S4 Table of all molecular structures and parameters

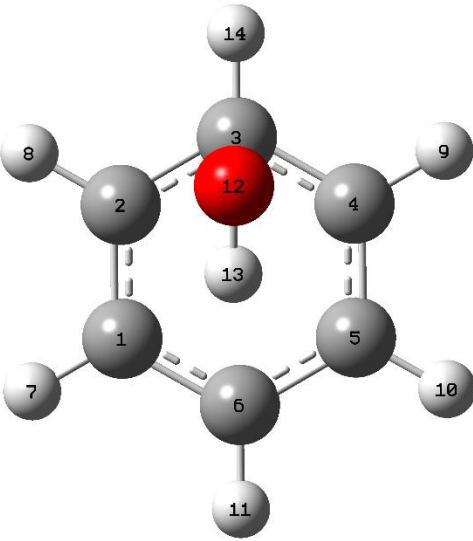
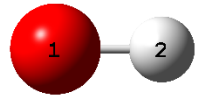

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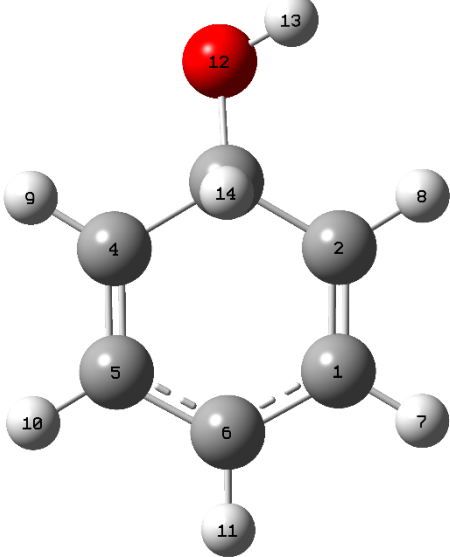
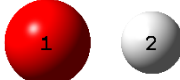
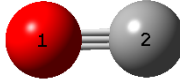

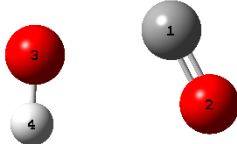
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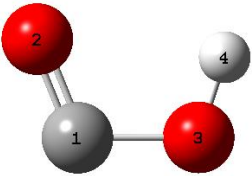
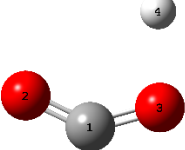
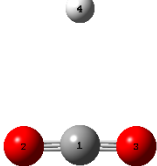
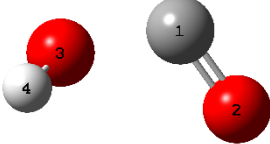
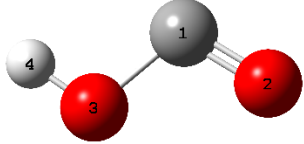
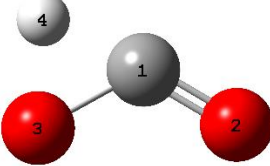
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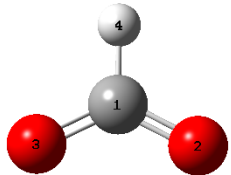
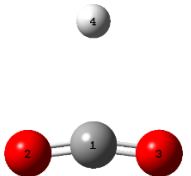



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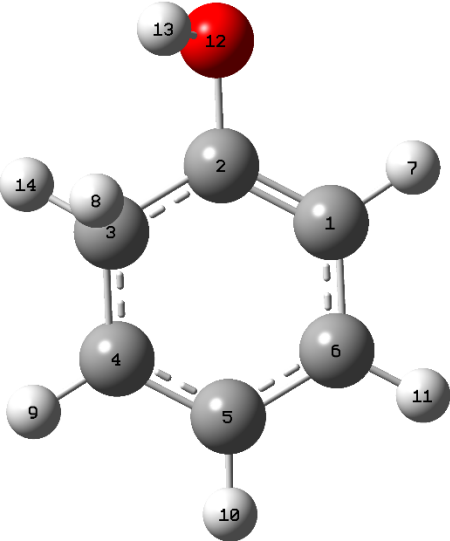
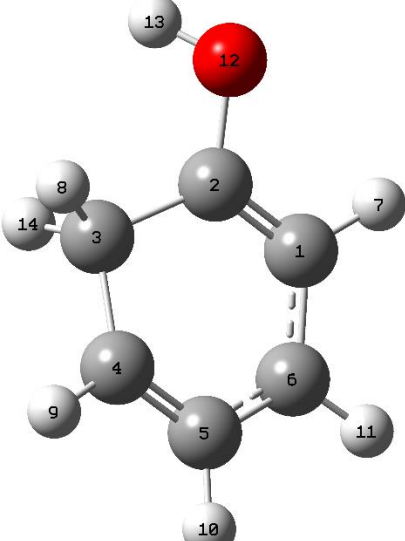
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9	H	-0.737193	-2.169300	-0.075244																																																																													
10	H	1.750109	-2.118579	-0.057433																																																																													
11	H	2.947970	0.052783	0.023929																																																																													
12	O	-2.284056	-0.112644	-0.116152																																																																													
13	H	-2.681544	0.759183	0.004291																																																																													
14	H	-0.890635	-0.015577	1.755182																																																																													

15	IM6		<table border="1"> <thead> <tr> <th>Tag</th> <th>Symbol</th> <th>X</th> <th>Y</th> <th>Z</th> </tr> </thead> <tbody> <tr><td>1</td><td>C</td><td>1.067178</td><td>1.146876</td><td>-0.275030</td></tr> <tr><td>2</td><td>C</td><td>0.012330</td><td>1.262905</td><td>0.626411</td></tr> <tr><td>3</td><td>C</td><td>-0.594565</td><td>0.116444</td><td>1.140658</td></tr> <tr><td>4</td><td>C</td><td>-0.137348</td><td>-1.145527</td><td>0.759037</td></tr> <tr><td>5</td><td>C</td><td>0.918998</td><td>-1.260481</td><td>-0.141577</td></tr> <tr><td>6</td><td>C</td><td>1.519073</td><td>-0.114567</td><td>-0.660355</td></tr> <tr><td>7</td><td>H</td><td>1.536753</td><td>2.036877</td><td>-0.677763</td></tr> <tr><td>8</td><td>H</td><td>-0.342232</td><td>2.242677</td><td>0.925163</td></tr> <tr><td>9</td><td>H</td><td>-0.608845</td><td>-2.035344</td><td>1.160118</td></tr> <tr><td>10</td><td>H</td><td>1.272275</td><td>-2.240500</td><td>-0.440813</td></tr> <tr><td>11</td><td>H</td><td>2.339754</td><td>-0.204001</td><td>-1.362897</td></tr> <tr><td>12</td><td>O</td><td>-2.263326</td><td>0.001185</td><td>-1.079068</td></tr> <tr><td>13</td><td>H</td><td>-1.388517</td><td>-0.048920</td><td>-1.507808</td></tr> <tr><td>14</td><td>H</td><td>-1.416576</td><td>0.205825</td><td>1.841683</td></tr> </tbody> </table>	Tag	Symbol	X	Y	Z	1	C	1.067178	1.146876	-0.275030	2	C	0.012330	1.262905	0.626411	3	C	-0.594565	0.116444	1.140658	4	C	-0.137348	-1.145527	0.759037	5	C	0.918998	-1.260481	-0.141577	6	C	1.519073	-0.114567	-0.660355	7	H	1.536753	2.036877	-0.677763	8	H	-0.342232	2.242677	0.925163	9	H	-0.608845	-2.035344	1.160118	10	H	1.272275	-2.240500	-0.440813	11	H	2.339754	-0.204001	-1.362897	12	O	-2.263326	0.001185	-1.079068	13	H	-1.388517	-0.048920	-1.507808	14	H	-1.416576	0.205825	1.841683	-307.83194	0.111244	0/2
Tag	Symbol	X	Y	Z																																																																													
1	C	1.067178	1.146876	-0.275030																																																																													
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16	P3		<table border="1"> <thead> <tr> <th>Tag</th> <th>Symbol</th> <th>X</th> <th>Y</th> <th>Z</th> </tr> </thead> <tbody> <tr><td>1</td><td>O</td><td>0.000000</td><td>0.000000</td><td>0.108312</td></tr> <tr><td>2</td><td>H</td><td>0.000000</td><td>0.000000</td><td>-0.866497</td></tr> </tbody> </table>	Tag	Symbol	X	Y	Z	1	O	0.000000	0.000000	0.108312	2	H	0.000000	0.000000	-0.866497	-75.727467	0.008538	0/2																																																												
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1	O	0.000000	0.000000	0.108312																																																																													
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1	H	0.000000	0.000000	0.000000																																																																													

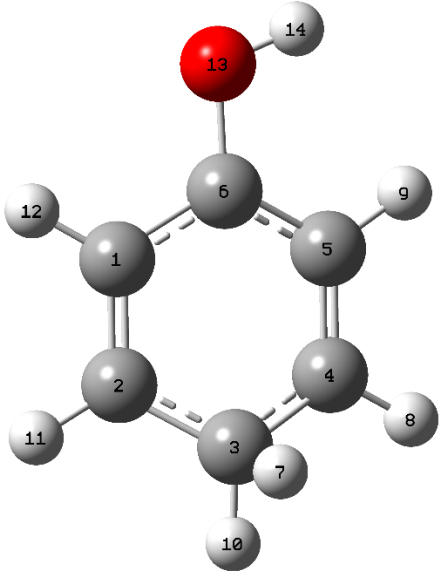
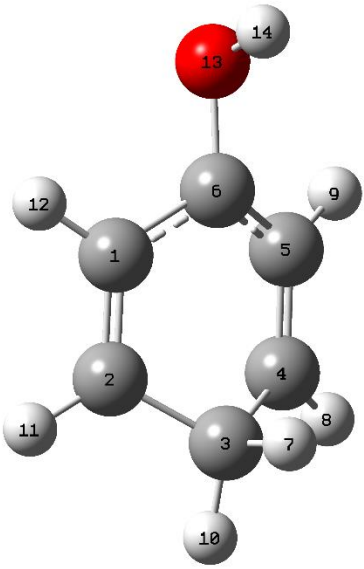
18	IM7		<table border="1"> <thead> <tr> <th>Tag</th> <th>Symbol</th> <th>X</th> <th>Y</th> <th>Z</th> </tr> </thead> <tbody> <tr><td>1</td><td>C</td><td>1.146227</td><td>1.243616</td><td>-0.026729</td></tr> <tr><td>2</td><td>C</td><td>-0.222686</td><td>1.239465</td><td>0.004138</td></tr> <tr><td>3</td><td>C</td><td>-0.938143</td><td>-0.019492</td><td>0.156191</td></tr> <tr><td>4</td><td>C</td><td>-0.185308</td><td>-1.253066</td><td>0.014669</td></tr> <tr><td>5</td><td>C</td><td>1.184782</td><td>-1.214748</td><td>-0.022569</td></tr> <tr><td>6</td><td>C</td><td>1.838477</td><td>0.023747</td><td>-0.054165</td></tr> <tr><td>7</td><td>H</td><td>1.690913</td><td>2.177297</td><td>-0.067610</td></tr> <tr><td>8</td><td>H</td><td>-0.804816</td><td>2.155200</td><td>0.011101</td></tr> <tr><td>9</td><td>H</td><td>-0.741244</td><td>-2.183927</td><td>0.028690</td></tr> <tr><td>10</td><td>H</td><td>1.756957</td><td>-2.131823</td><td>-0.059746</td></tr> <tr><td>11</td><td>H</td><td>2.921622</td><td>0.040919</td><td>-0.103024</td></tr> <tr><td>12</td><td>O</td><td>-2.275434</td><td>-0.103340</td><td>-0.206249</td></tr> <tr><td>13</td><td>H</td><td>-2.741927</td><td>0.683063</td><td>0.107351</td></tr> <tr><td>14</td><td>H</td><td>-0.818123</td><td>-0.031139</td><td>1.304020</td></tr> </tbody> </table>	Tag	Symbol	X	Y	Z	1	C	1.146227	1.243616	-0.026729	2	C	-0.222686	1.239465	0.004138	3	C	-0.938143	-0.019492	0.156191	4	C	-0.185308	-1.253066	0.014669	5	C	1.184782	-1.214748	-0.022569	6	C	1.838477	0.023747	-0.054165	7	H	1.690913	2.177297	-0.067610	8	H	-0.804816	2.155200	0.011101	9	H	-0.741244	-2.183927	0.028690	10	H	1.756957	-2.131823	-0.059746	11	H	2.921622	0.040919	-0.103024	12	O	-2.275434	-0.103340	-0.206249	13	H	-2.741927	0.683063	0.107351	14	H	-0.818123	-0.031139	1.304020	-307.6786	0.11423	1/1
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1	O	0.000000	0.000000	0.114066																																																																													
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1	O	0.000000	0.000000	0.480954																																																																													
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21	IM8		<table border="1"> <thead> <tr> <th>Tag</th> <th>Symbol</th> <th>X</th> <th>Y</th> <th>Z</th> </tr> </thead> <tbody> <tr><td>1</td><td>C</td><td>1.069273</td><td>0.648779</td><td>0.003984</td></tr> <tr><td>2</td><td>O</td><td>1.405347</td><td>-0.422967</td><td>-0.003889</td></tr> <tr><td>3</td><td>O</td><td>-2.042308</td><td>0.013633</td><td>-0.004791</td></tr> <tr><td>4</td><td>H</td><td>-1.319950</td><td>-0.618001</td><td>0.045544</td></tr> </tbody> </table>	Tag	Symbol	X	Y	Z	1	C	1.069273	0.648779	0.003984	2	O	1.405347	-0.422967	-0.003889	3	O	-2.042308	0.013633	-0.004791	4	H	-1.319950	-0.618001	0.045544	-189.22747	0.015573	-1/1																																																		
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22	TS5		<table border="1"> <thead> <tr> <th>Tag</th> <th>Symbol</th> <th>X</th> <th>Y</th> <th>Z</th> </tr> </thead> <tbody> <tr><td>1</td><td>C</td><td>0.469096</td><td>0.611380</td><td>-0.000016</td></tr> <tr><td>2</td><td>O</td><td>1.149457</td><td>-0.328385</td><td>0.000002</td></tr> <tr><td>3</td><td>O</td><td>-1.346261</td><td>-0.009083</td><td>0.000006</td></tr> <tr><td>4</td><td>H</td><td>-1.240139</td><td>-0.968530</td><td>0.000027</td></tr> </tbody> </table>	Tag	Symbol	X	Y	Z	1	C	0.469096	0.611380	-0.000016	2	O	1.149457	-0.328385	0.000002	3	O	-1.346261	-0.009083	0.000006	4	H	-1.240139	-0.968530	0.000027	-189.21603	0.016335	-1/1																																																		
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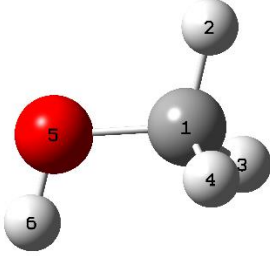
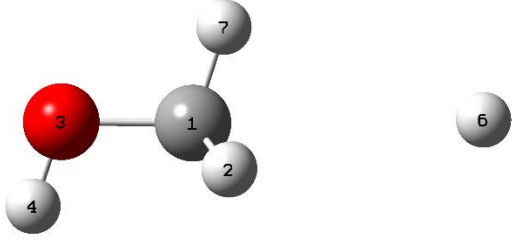
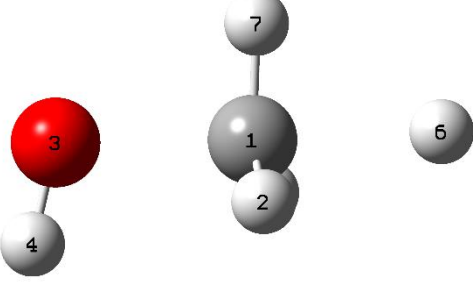
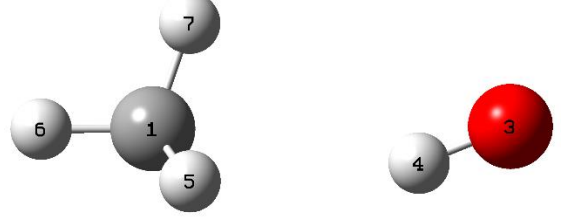
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			3	O	1.097428	0.063147	-0.000011			
			4	H	0.948023	1.028089	0.000047			
24	TS6		Tag	Symbol	X	Y	Z			
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			2	O	-1.156863	0.144273	-0.000002	-189.14993	0.01207	-1/1
			3	O	1.083713	-0.055275	0.000003			
			4	H	1.055479	1.551025	0.000023			
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			2	O	1.120140	-0.262503	-0.009450	-189.21207	0.017121	-1/1
			3	O	-1.123551	-0.113707	-0.121595			
			4	H	-1.399161	-0.375560	0.768218			
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			3	O	-0.926610	-0.522254	0.000000			
			4	H	-1.806890	-0.129647	0.000000			
28	TS8		Tag	Symbol	X	Y	Z			
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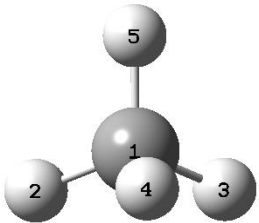
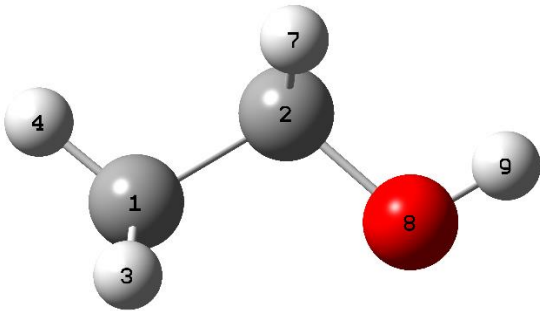
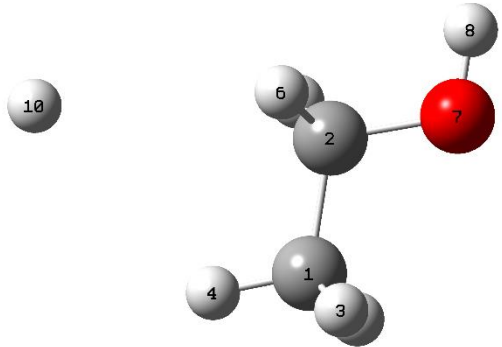
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			3	O	-1.121752	-0.219101	0.000000			
			4	H	0.000195	1.452076	0.000000			
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			2	O	-1.154803	-0.141034	0.000000	-189.20812	0.012571	-1/1
			3	O	1.154983	-0.139638	0.000000			
			4	H	-0.001444	2.178564	0.000000			
31	P5		Tag	Symbol	X	Y	Z			
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			2	O	0.000000	0.000000	1.155082	-188.55970	0.011731	0/1
			3	O	0.000000	0.000000	-1.155082			
32	P6		Tag	Symbol	X	Y	Z			
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			2	O	0.000000	0.000000	1.167784	-188.58912	0.008019	-1/2
			3	O	0.000000	0.000000	-1.167784			
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			2	O	0.000000	0.000000	1.263777	-188.59249	0.00579	-2/3
			3	O	0.000000	0.000000	-1.263777			

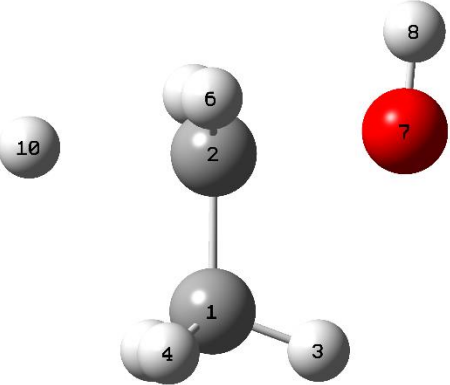
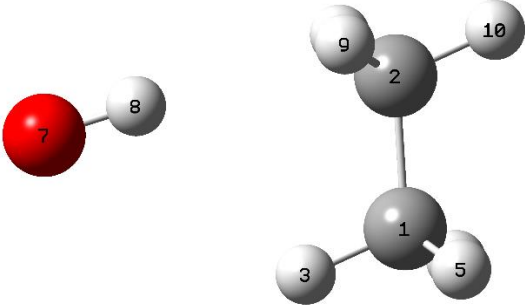
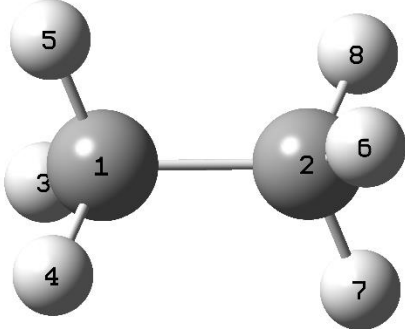
34	TS10		<table border="1"> <thead> <tr> <th>Tag</th> <th>Symbol</th> <th>X</th> <th>Y</th> <th>Z</th> </tr> </thead> <tbody> <tr><td>1</td><td>C</td><td>-0.149704</td><td>-1.265319</td><td>0.002970</td></tr> <tr><td>2</td><td>C</td><td>-0.901104</td><td>-0.125514</td><td>0.116934</td></tr> <tr><td>3</td><td>C</td><td>-0.329596</td><td>1.182577</td><td>-0.012671</td></tr> <tr><td>4</td><td>C</td><td>1.096686</td><td>1.230220</td><td>0.108696</td></tr> <tr><td>5</td><td>C</td><td>1.857771</td><td>0.073094</td><td>-0.005317</td></tr> <tr><td>6</td><td>C</td><td>1.257805</td><td>-1.185570</td><td>-0.082894</td></tr> <tr><td>7</td><td>H</td><td>-0.655546</td><td>-2.225618</td><td>-0.020129</td></tr> <tr><td>8</td><td>H</td><td>-0.913775</td><td>1.567279</td><td>-1.491793</td></tr> <tr><td>9</td><td>H</td><td>1.586881</td><td>2.193637</td><td>0.192247</td></tr> <tr><td>10</td><td>H</td><td>2.941156</td><td>0.148755</td><td>0.008329</td></tr> <tr><td>11</td><td>H</td><td>1.854040</td><td>-2.087520</td><td>-0.142517</td></tr> <tr><td>12</td><td>O</td><td>-2.290624</td><td>-0.192920</td><td>0.103145</td></tr> <tr><td>13</td><td>H</td><td>-2.580649</td><td>0.483070</td><td>-0.537492</td></tr> <tr><td>14</td><td>H</td><td>-0.898262</td><td>2.006824</td><td>0.399882</td></tr> </tbody> </table>	Tag	Symbol	X	Y	Z	1	C	-0.149704	-1.265319	0.002970	2	C	-0.901104	-0.125514	0.116934	3	C	-0.329596	1.182577	-0.012671	4	C	1.096686	1.230220	0.108696	5	C	1.857771	0.073094	-0.005317	6	C	1.257805	-1.185570	-0.082894	7	H	-0.655546	-2.225618	-0.020129	8	H	-0.913775	1.567279	-1.491793	9	H	1.586881	2.193637	0.192247	10	H	2.941156	0.148755	0.008329	11	H	1.854040	-2.087520	-0.142517	12	O	-2.290624	-0.192920	0.103145	13	H	-2.580649	0.483070	-0.537492	14	H	-0.898262	2.006824	0.399882	-307.93733	0.10673	-1/1
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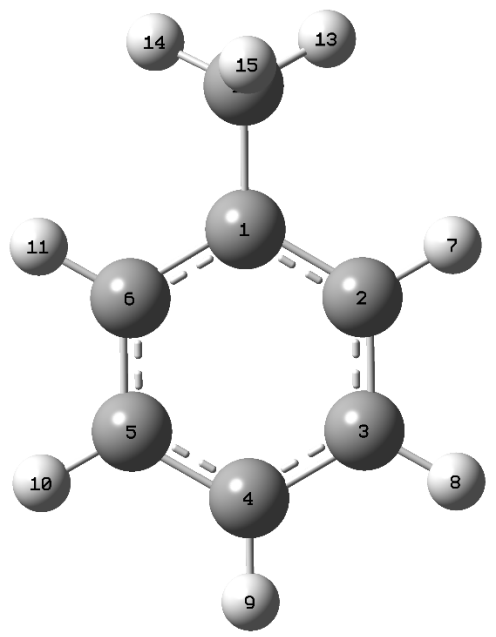
47	TS14		<table border="1"> <thead> <tr> <th>Tag</th> <th>Symbol</th> <th>X</th> <th>Y</th> <th>Z</th> </tr> </thead> <tbody> <tr><td>1</td><td>C</td><td>-1.127476</td><td>-0.530476</td><td>-0.000009</td></tr> <tr><td>2</td><td>C</td><td>-0.175052</td><td>0.649623</td><td>0.000014</td></tr> <tr><td>3</td><td>H</td><td>-0.563130</td><td>-1.464710</td><td>0.000021</td></tr> <tr><td>4</td><td>H</td><td>-1.768393</td><td>-0.519810</td><td>0.881019</td></tr> <tr><td>5</td><td>H</td><td>-1.768329</td><td>-0.519821</td><td>-0.881081</td></tr> <tr><td>6</td><td>H</td><td>0.082196</td><td>1.142911</td><td>0.921249</td></tr> <tr><td>7</td><td>O</td><td>1.401431</td><td>-0.333094</td><td>0.000019</td></tr> <tr><td>8</td><td>H</td><td>2.069884</td><td>0.360002</td><td>-0.000150</td></tr> <tr><td>9</td><td>H</td><td>0.082206</td><td>1.142898</td><td>-0.921224</td></tr> <tr><td>10</td><td>H</td><td>-1.530710</td><td>1.808406</td><td>-0.000017</td></tr> </tbody> </table>	Tag	Symbol	X	Y	Z	1	C	-1.127476	-0.530476	-0.000009	2	C	-0.175052	0.649623	0.000014	3	H	-0.563130	-1.464710	0.000021	4	H	-1.768393	-0.519810	0.881019	5	H	-1.768329	-0.519821	-0.881081	6	H	0.082196	1.142911	0.921249	7	O	1.401431	-0.333094	0.000019	8	H	2.069884	0.360002	-0.000150	9	H	0.082206	1.142898	-0.921224	10	H	-1.530710	1.808406	-0.000017	-155.52926	0.081053	-1/1
Tag	Symbol	X	Y	Z																																																									
1	C	-1.127476	-0.530476	-0.000009																																																									
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9	H	0.082206	1.142898	-0.921224																																																									
10	H	-1.530710	1.808406	-0.000017																																																									
48	IM19		<table border="1"> <thead> <tr> <th>Tag</th> <th>Symbol</th> <th>X</th> <th>Y</th> <th>Z</th> </tr> </thead> <tbody> <tr><td>1</td><td>C</td><td>1.259641</td><td>-0.733725</td><td>-0.000011</td></tr> <tr><td>2</td><td>C</td><td>1.045269</td><td>0.777160</td><td>0.000012</td></tr> <tr><td>3</td><td>H</td><td>0.306034</td><td>-1.266734</td><td>0.003430</td></tr> <tr><td>4</td><td>H</td><td>1.816484</td><td>-1.052429</td><td>-0.884000</td></tr> <tr><td>5</td><td>H</td><td>1.822303</td><td>-1.051595</td><td>0.880587</td></tr> <tr><td>6</td><td>H</td><td>0.484632</td><td>1.097183</td><td>-0.881915</td></tr> <tr><td>7</td><td>O</td><td>-2.404015</td><td>-0.084139</td><td>0.000003</td></tr> <tr><td>8</td><td>H</td><td>-1.513429</td><td>0.277078</td><td>-0.000067</td></tr> <tr><td>9</td><td>H</td><td>0.488513</td><td>1.097635</td><td>0.884221</td></tr> <tr><td>10</td><td>H</td><td>1.998125</td><td>1.311361</td><td>-0.002285</td></tr> </tbody> </table>	Tag	Symbol	X	Y	Z	1	C	1.259641	-0.733725	-0.000011	2	C	1.045269	0.777160	0.000012	3	H	0.306034	-1.266734	0.003430	4	H	1.816484	-1.052429	-0.884000	5	H	1.822303	-1.051595	0.880587	6	H	0.484632	1.097183	-0.881915	7	O	-2.404015	-0.084139	0.000003	8	H	-1.513429	0.277078	-0.000067	9	H	0.488513	1.097635	0.884221	10	H	1.998125	1.311361	-0.002285	-155.65049	0.085841	-1/1
Tag	Symbol	X	Y	Z																																																									
1	C	1.259641	-0.733725	-0.000011																																																									
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49	P9		<table border="1"> <thead> <tr> <th>Tag</th> <th>Symbol</th> <th>X</th> <th>Y</th> <th>Z</th> </tr> </thead> <tbody> <tr><td>1</td><td>C</td><td>-0.762853</td><td>0.000000</td><td>-0.000001</td></tr> <tr><td>2</td><td>C</td><td>0.762789</td><td>0.000000</td><td>0.000005</td></tr> <tr><td>3</td><td>H</td><td>-1.157235</td><td>-0.881736</td><td>-0.509919</td></tr> <tr><td>4</td><td>H</td><td>-1.157203</td><td>-0.000750</td><td>1.018575</td></tr> <tr><td>5</td><td>H</td><td>-1.157235</td><td>0.882487</td><td>-0.508619</td></tr> <tr><td>6</td><td>H</td><td>1.157369</td><td>0.881739</td><td>0.509892</td></tr> <tr><td>7</td><td>H</td><td>1.157369</td><td>-0.882477</td><td>0.508614</td></tr> <tr><td>8</td><td>H</td><td>1.157319</td><td>0.000738</td><td>-1.018565</td></tr> </tbody> </table>	Tag	Symbol	X	Y	Z	1	C	-0.762853	0.000000	-0.000001	2	C	0.762789	0.000000	0.000005	3	H	-1.157235	-0.881736	-0.509919	4	H	-1.157203	-0.000750	1.018575	5	H	-1.157235	0.882487	-0.508619	6	H	1.157369	0.881739	0.509892	7	H	1.157369	-0.882477	0.508614	8	H	1.157319	0.000738	-1.018565	-79.71966	0.074759	0/1										
Tag	Symbol	X	Y	Z																																																									
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3	H	-1.157235	-0.881736	-0.509919																																																									
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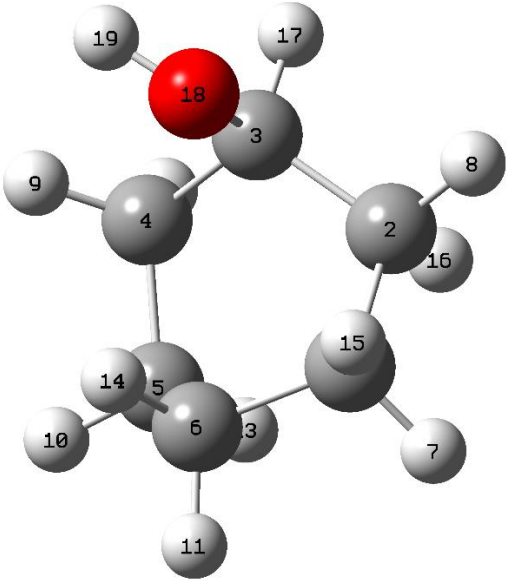
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			3	C	-1.607509	-1.207190	-0.079436			
			4	C	-2.295687	-0.002739	-0.207550			
			5	C	-1.611694	1.204291	-0.082605			
			6	C	-0.242486	1.204913	0.169356			
			7	H	0.299730	-2.139318	0.276445			
			8	H	-2.137515	-2.148087	-0.172502			
			9	H	-3.362283	-0.004865	-0.400424			
			10	H	-2.144806	2.143178	-0.178196			
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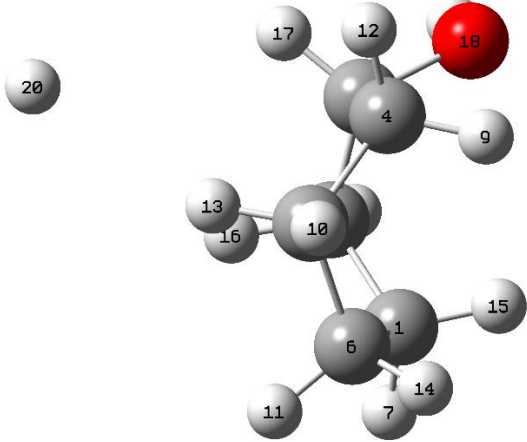
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			2	C	-0.249172	-1.200076	0.126565			
			3	C	-1.624016	-1.211240	-0.091059			
			4	C	-2.318377	-0.010244	-0.218464			
			5	C	-1.633653	1.199563	-0.128861			
			6	C	-0.258692	1.206094	0.088499			
			7	H	0.292899	-2.134113	0.235562			
			8	H	-2.154147	-2.154449	-0.155957			
			9	H	-3.389723	-0.017107	-0.382814			
			10	H	-2.171173	2.136120	-0.222818			
			11	H	0.276022	2.147247	0.168354			
			12	C	1.932724	0.016142	0.423543			
			13	H	2.236227	-0.851926	1.015348			
			14	H	2.234197	0.923663	0.953756			
			15	O	2.559235	-0.028346	-0.866144			
			16	H	3.513594	-0.017621	-0.730129			
17	H	0.937169	0.147843	3.527457						

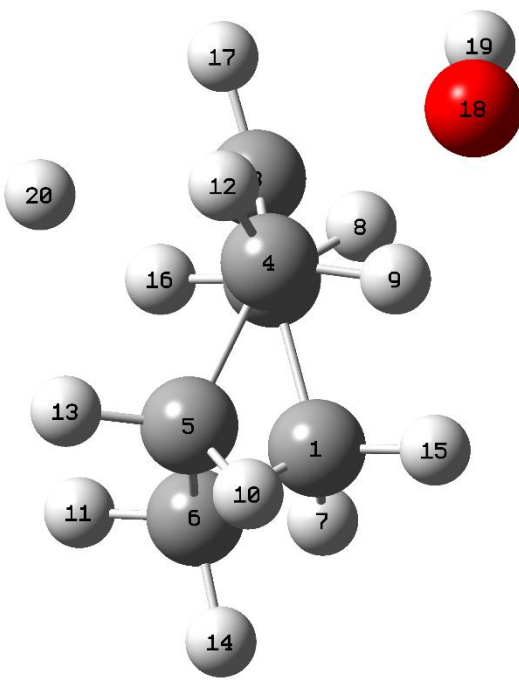
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			3	C	-1.598110	-1.206916	-0.099983			
			4	C	-2.287169	-0.006691	-0.265620			
			5	C	-1.606036	1.200269	-0.116064			
			6	C	-0.251797	1.206040	0.202155			
			7	H	0.290304	-2.135488	0.348637			
			8	H	-2.117167	-2.151228	-0.220567			
			9	H	-3.342544	-0.011858	-0.511733			
			10	H	-2.131421	2.139456	-0.248646			
			11	H	0.275936	2.147120	0.321173			
			12	C	1.897860	0.012841	0.666062			
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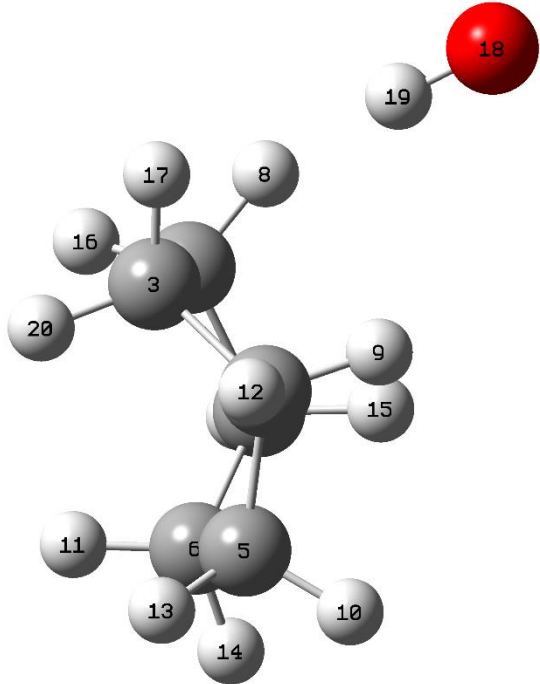
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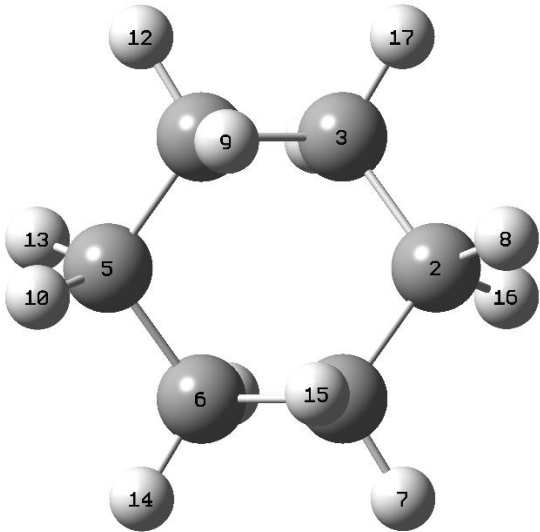
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			4	C	-1.898983	-0.001826	0.008094			
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			6	C	0.193948	1.201142	-0.008755			
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			11	H	0.733915	2.142596	-0.017282			
			12	C	2.416865	0.001009	0.008427			
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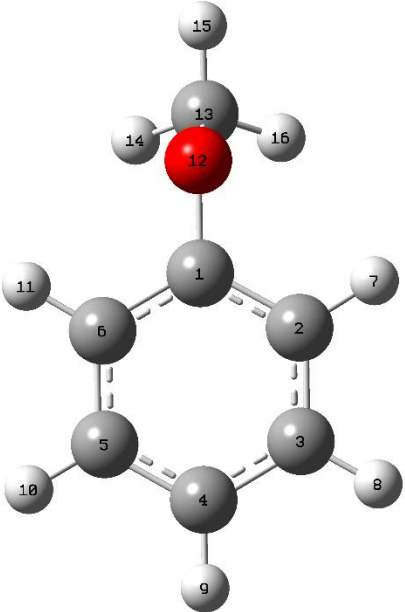
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			10	H	1.739998	1.975513	-0.248456			
			11	H	2.504337	-0.284464	-0.884663			
			12	H	-0.453920	2.006324	1.214359			
			13	H	1.652669	0.929216	1.158430			
			14	H	0.968695	0.036551	-1.673487			
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			16	H	0.011603	-0.753144	1.889836			
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			6	C	-1.852577	0.269134	-0.272740			
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			8	H	1.063021	1.844939	0.787483			
			9	H	0.186519	-1.008614	-1.485565			
			10	H	-1.897742	-1.906621	-0.308313			
			11	H	-2.618719	0.548373	0.455839			
			12	H	0.540547	-2.259067	-0.295299			
			13	H	-1.267127	-1.235614	1.185811			
			14	H	-2.347098	0.211771	-1.246539			
			15	H	-0.310947	1.393675	-1.315846			
			16	H	-0.109999	0.892507	1.688730			
			17	H	1.481714	-0.720576	1.215449			
			18	O	2.173612	0.025941	-0.581838			
			19	H	2.794898	0.598830	-0.117947			
20	H	0.088579	-1.194438	3.606558						

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			4	C	-0.104190	1.328119	-0.070954			
			5	C	1.420388	1.114946	-0.089910			
			6	C	1.835227	-0.374200	-0.105986			
			7	H	1.022187	-2.335363	-0.537787			
			8	H	-1.294128	-1.805978	0.272631			
			9	H	-0.457504	1.308328	-1.104020			
			10	H	1.815112	1.617284	-0.977926			
			11	H	2.188044	-0.666492	0.888154			
			12	H	-0.341190	2.316412	0.326883			
			13	H	1.867698	1.603990	0.777690			
			14	H	2.672769	-0.521432	-0.792125			
			15	H	0.288068	-1.036636	-1.470569			
			16	H	-0.078519	-1.560570	1.515277			
			17	H	-1.653616	0.536311	1.391486			
			18	O	-2.276301	0.163472	-0.649727			
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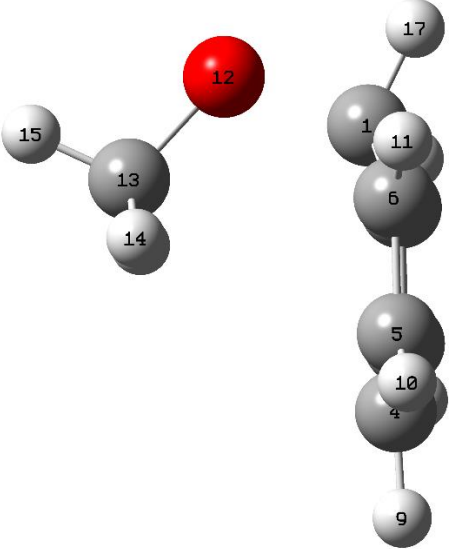
58	IM26		<table border="1"> <thead> <tr> <th>Tag</th> <th>Symbol</th> <th>X</th> <th>Y</th> <th>Z</th> </tr> </thead> <tbody> <tr><td>1</td><td>C</td><td>-0.866040</td><td>1.236109</td><td>-0.600600</td></tr> <tr><td>2</td><td>C</td><td>0.123925</td><td>1.242755</td><td>0.579559</td></tr> <tr><td>3</td><td>C</td><td>0.269809</td><td>-0.157949</td><td>1.209946</td></tr> <tr><td>4</td><td>C</td><td>0.049425</td><td>-1.245241</td><td>0.156560</td></tr> <tr><td>5</td><td>C</td><td>-1.405434</td><td>-1.213644</td><td>-0.350166</td></tr> <tr><td>6</td><td>C</td><td>-1.978821</td><td>0.217639</td><td>-0.350531</td></tr> <tr><td>7</td><td>H</td><td>-1.277241</td><td>2.236975</td><td>-0.752059</td></tr> <tr><td>8</td><td>H</td><td>1.098968</td><td>1.600039</td><td>0.234347</td></tr> <tr><td>9</td><td>H</td><td>0.738594</td><td>-1.072648</td><td>-0.677127</td></tr> <tr><td>10</td><td>H</td><td>-1.446342</td><td>-1.627046</td><td>-1.362060</td></tr> <tr><td>11</td><td>H</td><td>-2.439973</td><td>0.435293</td><td>0.619131</td></tr> <tr><td>12</td><td>H</td><td>0.287566</td><td>-2.232717</td><td>0.559215</td></tr> <tr><td>13</td><td>H</td><td>-2.029037</td><td>-1.855785</td><td>0.278695</td></tr> <tr><td>14</td><td>H</td><td>-2.768643</td><td>0.307001</td><td>-1.100130</td></tr> <tr><td>15</td><td>H</td><td>-0.342837</td><td>0.967400</td><td>-1.524901</td></tr> <tr><td>16</td><td>H</td><td>-0.217935</td><td>1.949671</td><td>1.341244</td></tr> <tr><td>17</td><td>H</td><td>1.251724</td><td>-0.260753</td><td>1.680054</td></tr> <tr><td>18</td><td>O</td><td>3.471374</td><td>-0.085670</td><td>-0.634752</td></tr> <tr><td>19</td><td>H</td><td>2.688690</td><td>0.047192</td><td>-0.092858</td></tr> <tr><td>20</td><td>H</td><td>-0.471710</td><td>-0.287278</td><td>2.005861</td></tr> </tbody> </table>	Tag	Symbol	X	Y	Z	1	C	-0.866040	1.236109	-0.600600	2	C	0.123925	1.242755	0.579559	3	C	0.269809	-0.157949	1.209946	4	C	0.049425	-1.245241	0.156560	5	C	-1.405434	-1.213644	-0.350166	6	C	-1.978821	0.217639	-0.350531	7	H	-1.277241	2.236975	-0.752059	8	H	1.098968	1.600039	0.234347	9	H	0.738594	-1.072648	-0.677127	10	H	-1.446342	-1.627046	-1.362060	11	H	-2.439973	0.435293	0.619131	12	H	0.287566	-2.232717	0.559215	13	H	-2.029037	-1.855785	0.278695	14	H	-2.768643	0.307001	-1.100130	15	H	-0.342837	0.967400	-1.524901	16	H	-0.217935	1.949671	1.341244	17	H	1.251724	-0.260753	1.680054	18	O	3.471374	-0.085670	-0.634752	19	H	2.688690	0.047192	-0.092858	20	H	-0.471710	-0.287278	2.005861	-311.56679	0.180996	-1/1
Tag	Symbol	X	Y	Z																																																																																																											
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12	H	0.287566	-2.232717	0.559215																																																																																																											
13	H	-2.029037	-1.855785	0.278695																																																																																																											
14	H	-2.768643	0.307001	-1.100130																																																																																																											
15	H	-0.342837	0.967400	-1.524901																																																																																																											
16	H	-0.217935	1.949671	1.341244																																																																																																											
17	H	1.251724	-0.260753	1.680054																																																																																																											
18	O	3.471374	-0.085670	-0.634752																																																																																																											
19	H	2.688690	0.047192	-0.092858																																																																																																											
20	H	-0.471710	-0.287278	2.005861																																																																																																											

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			3	C	0.652548	1.214167	-0.395656			
			4	C	-0.655974	1.212514	0.395553			
			5	C	-1.518888	-0.002067	0.000134			
			6	C	-0.652522	-1.214157	-0.395685			
			7	H	1.212921	-2.138532	0.234415			
			8	H	2.170905	0.272746	0.835584			
			9	H	-0.419255	1.170750	1.464335			
			10	H	-2.170885	-0.272725	0.835707			
			11	H	-0.415884	-1.171259	-1.464439			
			12	H	-1.212914	2.138496	0.234148			
			13	H	-2.171801	0.266757	-0.835342			
			14	H	-1.206830	-2.141782	-0.234720			
			15	H	0.419155	-1.170680	1.464359			
			16	H	2.171649	-0.266906	-0.835463			
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18	H	0.415933	1.171440	-1.464415						

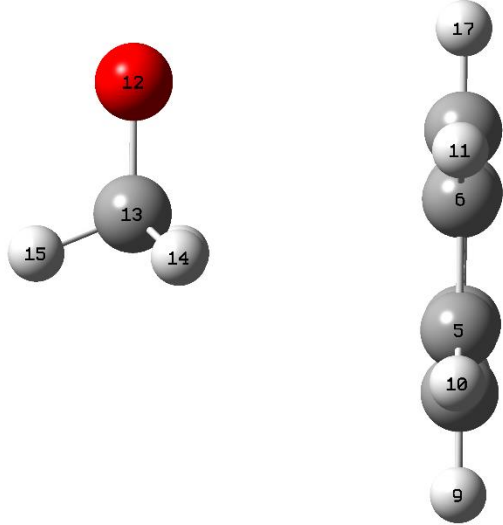
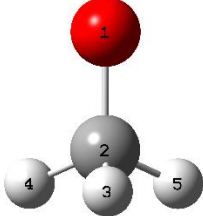
60	R9		<table border="1"> <thead> <tr> <th>Tag</th> <th>Symbol</th> <th>X</th> <th>Y</th> <th>Z</th> </tr> </thead> <tbody> <tr><td>1</td><td>C</td><td>0.466805</td><td>-0.002815</td><td>-0.304847</td></tr> <tr><td>2</td><td>C</td><td>-0.203171</td><td>1.209219</td><td>-0.175157</td></tr> <tr><td>3</td><td>C</td><td>-1.571038</td><td>1.207327</td><td>0.083685</td></tr> <tr><td>4</td><td>C</td><td>-2.258983</td><td>0.003124</td><td>0.215133</td></tr> <tr><td>5</td><td>C</td><td>-1.575774</td><td>-1.204019</td><td>0.086602</td></tr> <tr><td>6</td><td>C</td><td>-0.207848</td><td>-1.211833</td><td>-0.172096</td></tr> <tr><td>7</td><td>H</td><td>0.348756</td><td>2.136276</td><td>-0.283022</td></tr> <tr><td>8</td><td>H</td><td>-2.099531</td><td>2.148634</td><td>0.180384</td></tr> <tr><td>9</td><td>H</td><td>-3.323947</td><td>0.005474</td><td>0.414851</td></tr> <tr><td>10</td><td>H</td><td>-2.107851</td><td>-2.143061</td><td>0.185652</td></tr> <tr><td>11</td><td>H</td><td>0.340552</td><td>-2.141251</td><td>-0.277483</td></tr> <tr><td>12</td><td>O</td><td>1.822041</td><td>-0.006202</td><td>-0.592704</td></tr> <tr><td>13</td><td>C</td><td>2.635763</td><td>0.003416</td><td>0.584252</td></tr> <tr><td>14</td><td>H</td><td>2.437590</td><td>-0.884612</td><td>1.190659</td></tr> <tr><td>15</td><td>H</td><td>3.672149</td><td>-0.001929</td><td>0.251394</td></tr> <tr><td>16</td><td>H</td><td>2.441432</td><td>0.903573</td><td>1.173763</td></tr> </tbody> </table>	Tag	Symbol	X	Y	Z	1	C	0.466805	-0.002815	-0.304847	2	C	-0.203171	1.209219	-0.175157	3	C	-1.571038	1.207327	0.083685	4	C	-2.258983	0.003124	0.215133	5	C	-1.575774	-1.204019	0.086602	6	C	-0.207848	-1.211833	-0.172096	7	H	0.348756	2.136276	-0.283022	8	H	-2.099531	2.148634	0.180384	9	H	-3.323947	0.005474	0.414851	10	H	-2.107851	-2.143061	0.185652	11	H	0.340552	-2.141251	-0.277483	12	O	1.822041	-0.006202	-0.592704	13	C	2.635763	0.003416	0.584252	14	H	2.437590	-0.884612	1.190659	15	H	3.672149	-0.001929	0.251394	16	H	2.441432	0.903573	1.173763	-346.57849	0.133223	0/1
Tag	Symbol	X	Y	Z																																																																																							
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16	H	2.441432	0.903573	1.173763																																																																																							

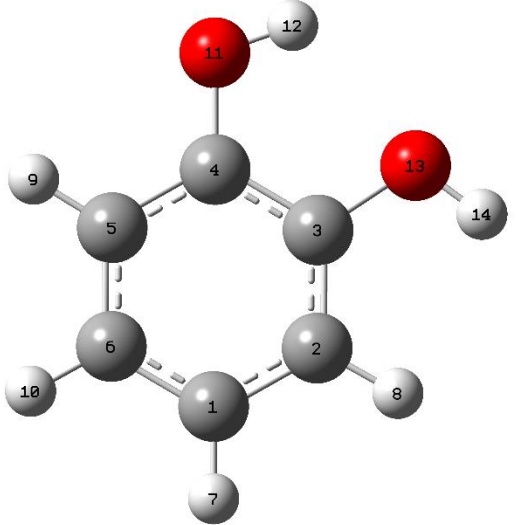
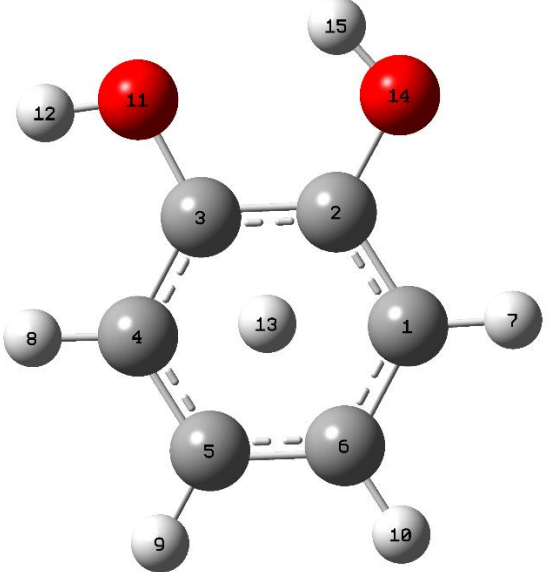
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			4	C	-0.146040	-2.247351	0.000000			
			5	C	-0.144916	-1.549789	-1.205533			
			6	C	-0.144916	-0.157900	-1.210310			
			7	H	-0.152418	0.403002	2.138170			
			8	H	-0.151496	-2.089203	2.145533			
			9	H	-0.152750	-3.330873	0.000000			
			10	H	-0.151496	-2.089203	-2.145533			
			11	H	-0.152418	0.403002	-2.138170			
			12	O	-0.193267	1.911663	0.000000			
			13	C	1.108167	2.504870	0.000000			
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			15	H	0.963815	3.583891	0.000000			
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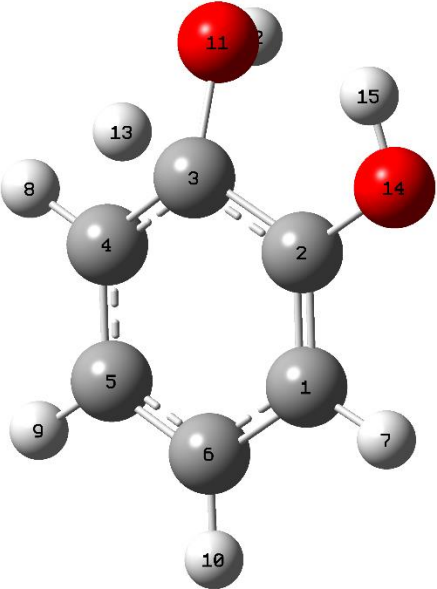
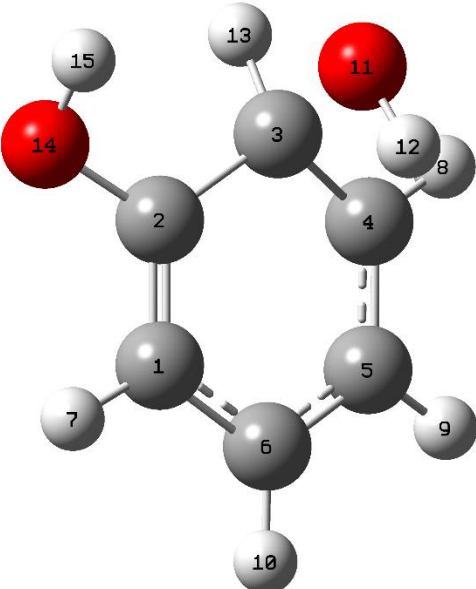
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			4	C	-0.281117	-2.235297	0.000000			
			5	C	-0.230617	-1.516060	-1.201404			
			6	C	-0.230617	-0.133231	-1.209001			
			7	H	-0.209436	0.416444	2.144163			
			8	H	-0.172900	-2.049791	2.145034			
			9	H	-0.279733	-3.318222	0.000000			
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			13	C	1.361775	2.143096	0.000000			
			14	H	1.817593	1.701902	-0.890931			
			15	H	1.531983	3.219528	0.000000			
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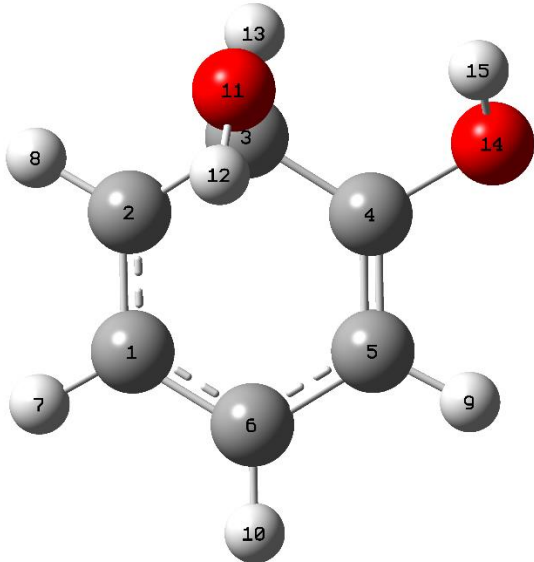
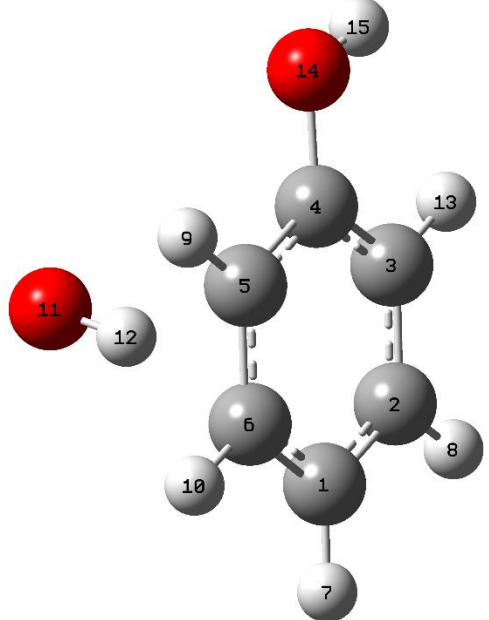
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			3	C	0.686667	1.102757	1.201399			
			4	C	0.619320	1.839040	0.000000			
			5	C	0.686667	1.102757	-1.201399			
			6	C	0.686667	-0.274990	-1.223060			
			7	H	0.809623	-0.805843	2.162750			
			8	H	0.794800	1.638296	2.142990			
			9	H	0.657561	2.921394	0.000000			
			10	H	0.794800	1.638296	-2.142990			
			11	H	0.809623	-0.805843	-2.162750			
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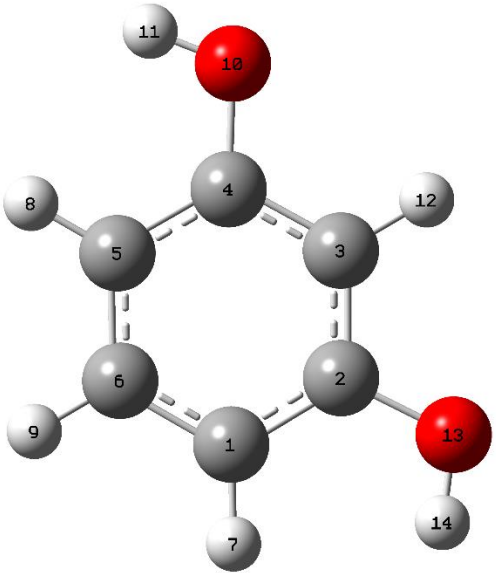
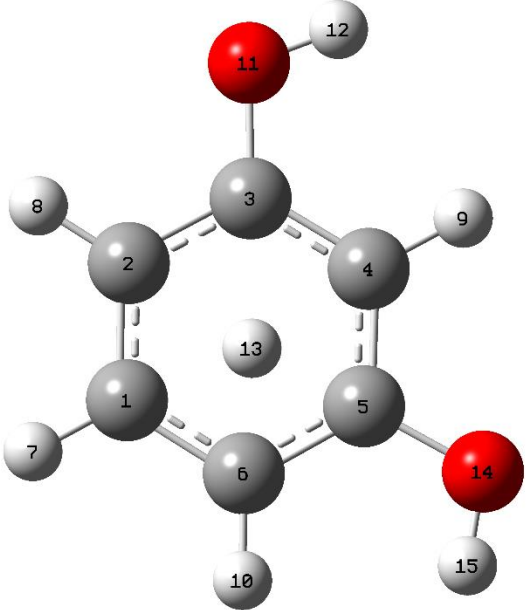
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			6	C	0.708435	-0.270735	-1.214746			
			7	H	0.801705	-0.802496	2.156559			
			8	H	0.790244	1.646694	2.143715			
			9	H	0.688950	2.923923	0.000000			
			10	H	0.790244	1.646694	-2.143715			
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17	H	0.885229	-2.048136	0.000000						

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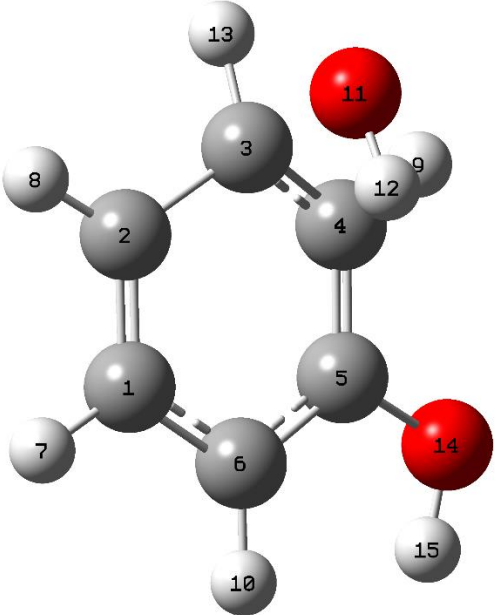
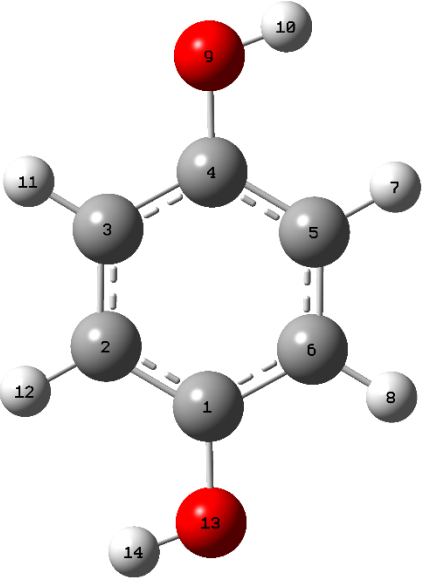
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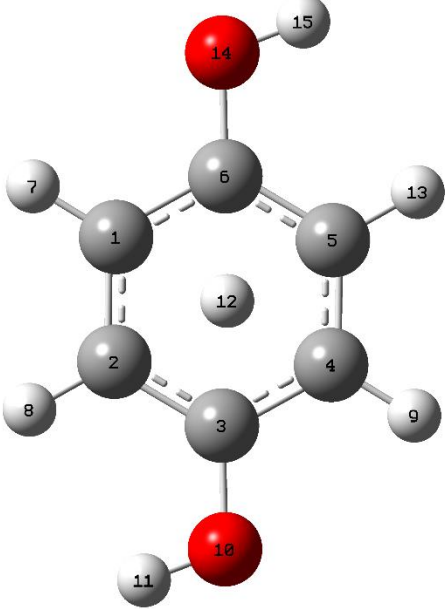
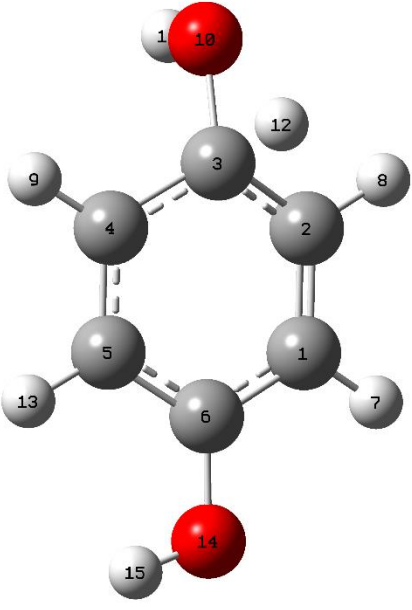
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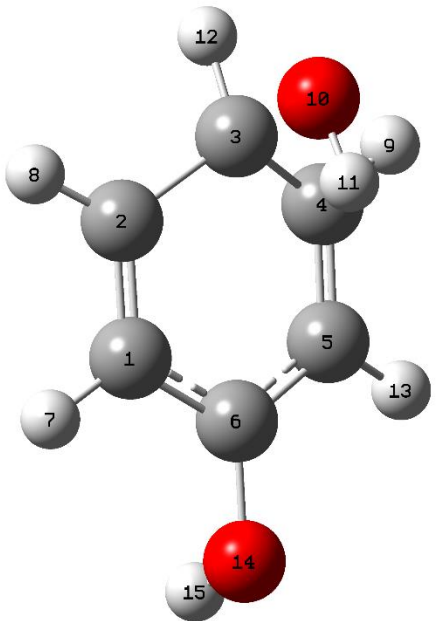
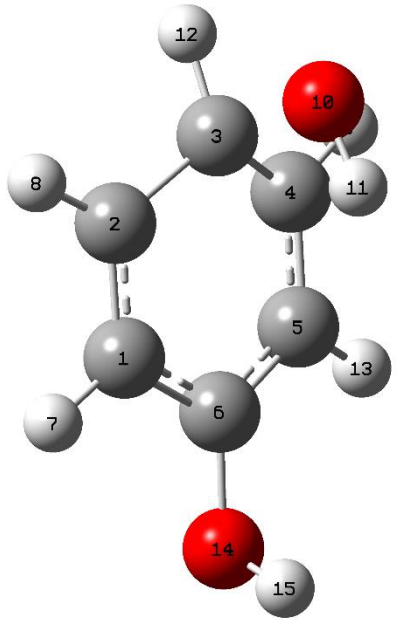
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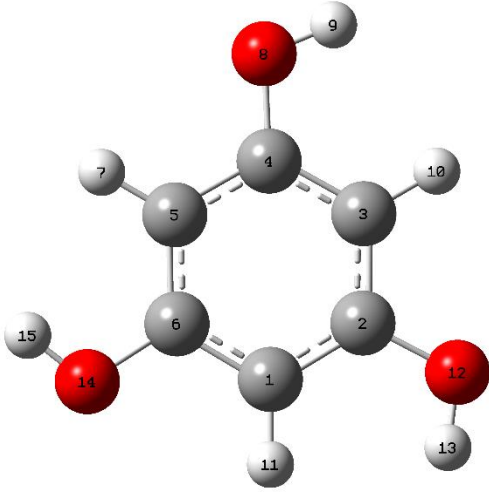
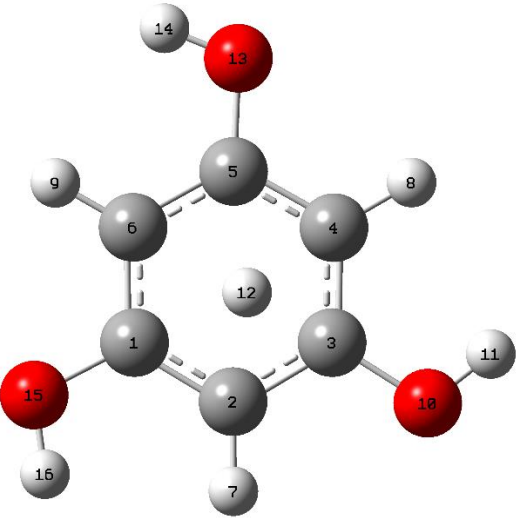
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11	O	-2.436044	-0.895023	-0.038353																																																																																		
12	H	-2.323442	-1.853680	-0.015770																																																																																		
13	H	0.010338	0.351103	3.151429																																																																																		
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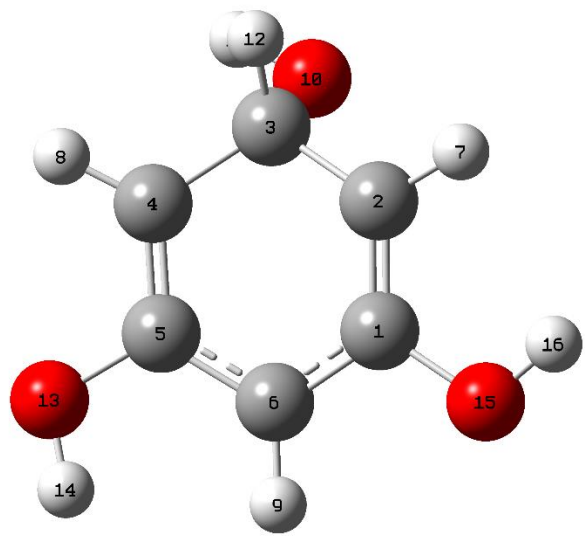
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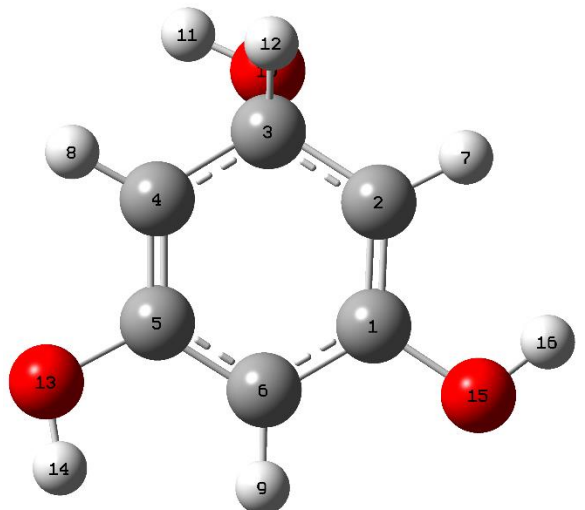
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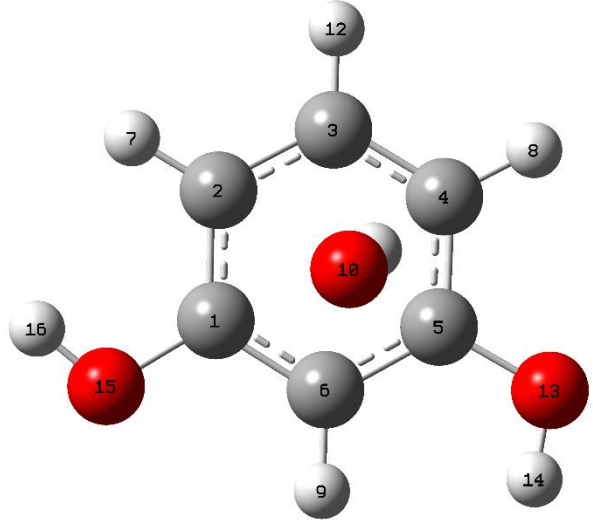
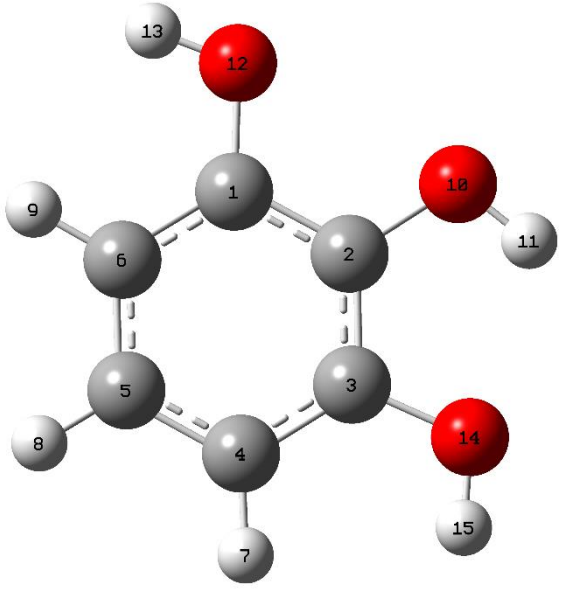
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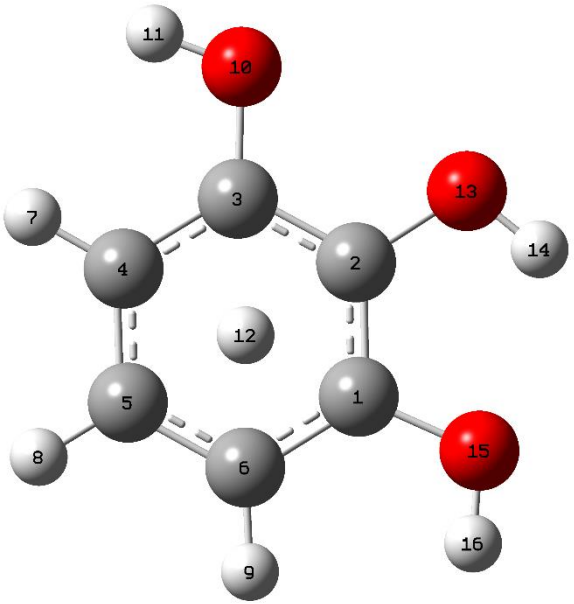
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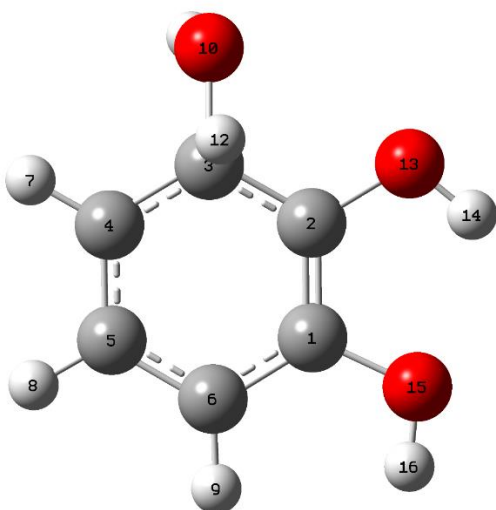
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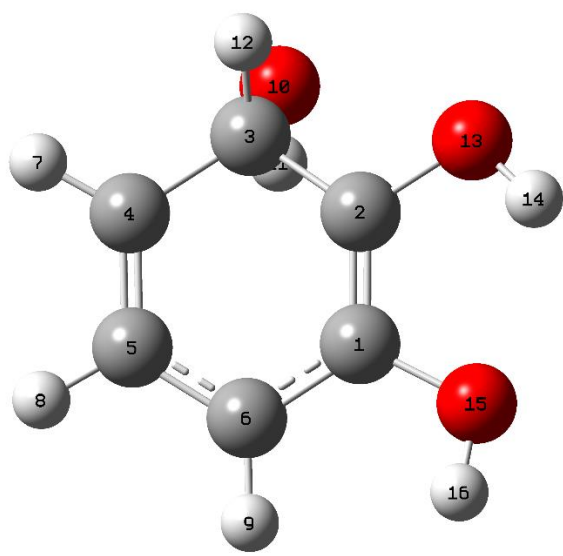
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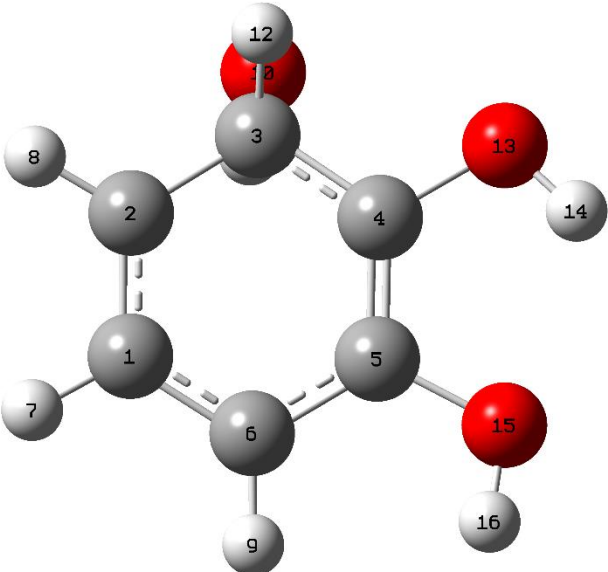
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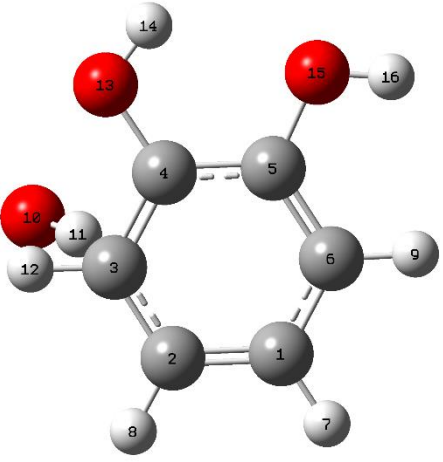
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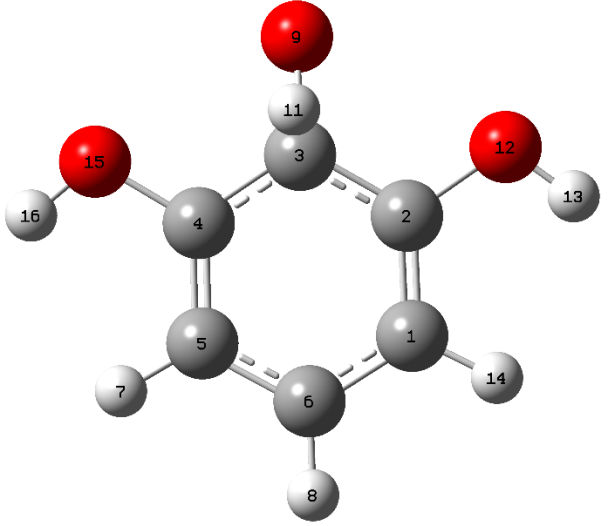
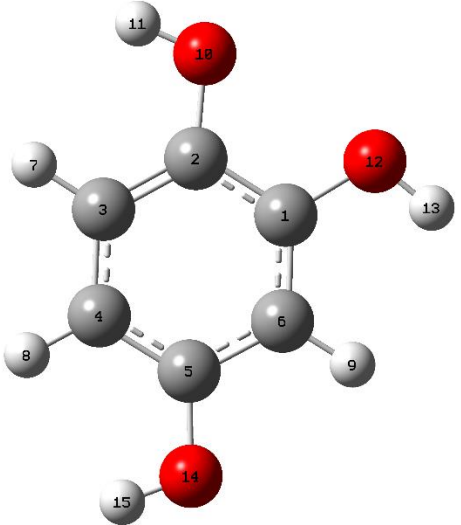
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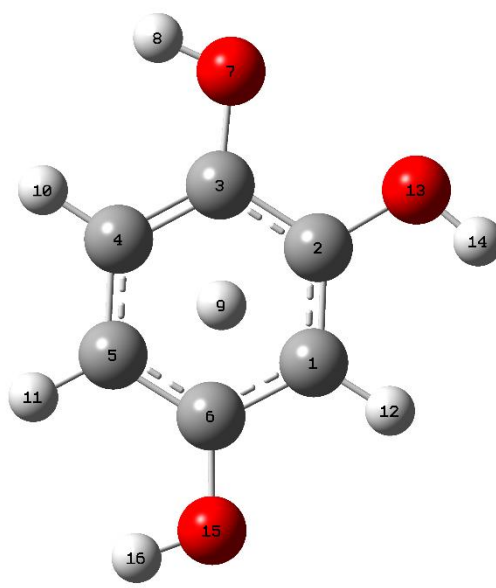
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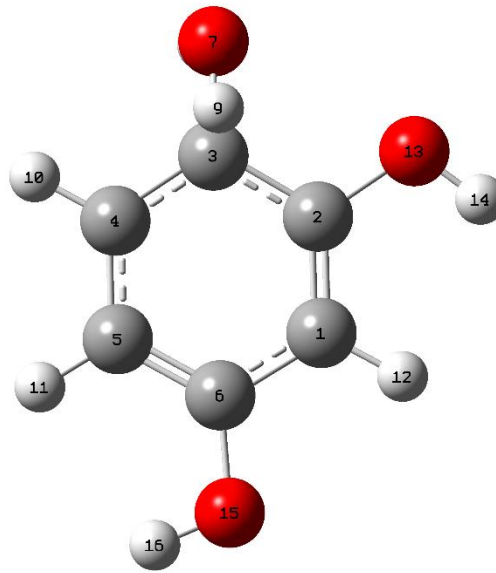
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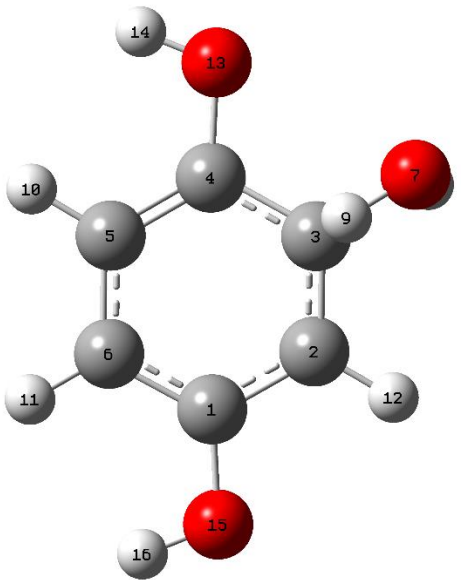
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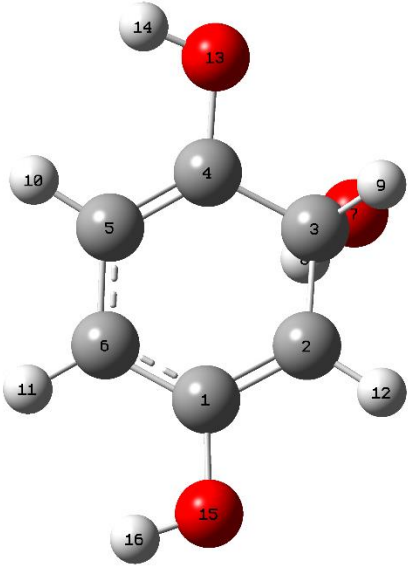
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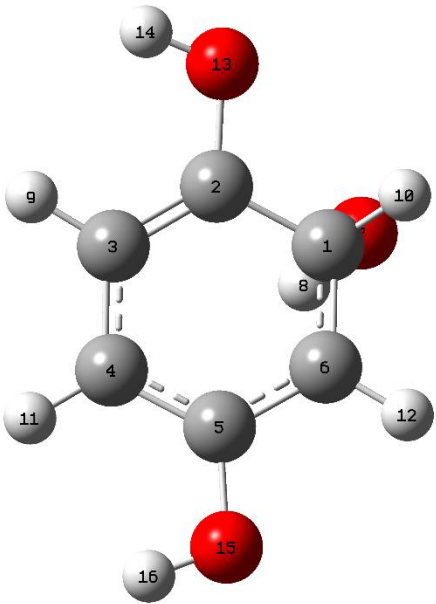
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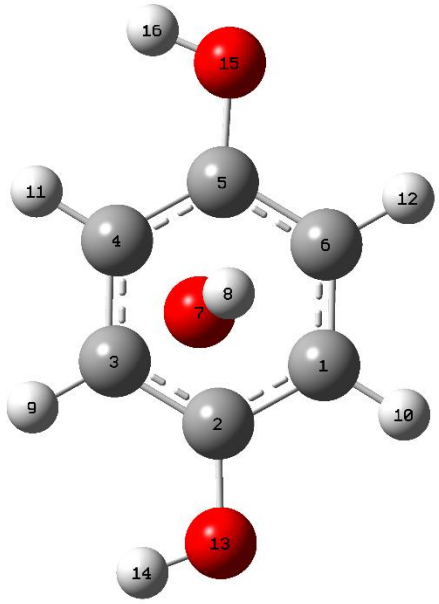
97	IM40		<table border="1"> <thead> <tr> <th>Tag</th> <th>Symbol</th> <th>X</th> <th>Y</th> <th>Z</th> </tr> </thead> <tbody> <tr><td>1</td><td>C</td><td>0.633921</td><td>1.088114</td><td>-0.050113</td></tr> <tr><td>2</td><td>C</td><td>-0.716711</td><td>0.775469</td><td>-0.047240</td></tr> <tr><td>3</td><td>C</td><td>-1.130799</td><td>-0.560763</td><td>-0.055269</td></tr> <tr><td>4</td><td>C</td><td>-0.179551</td><td>-1.566434</td><td>-0.061565</td></tr> <tr><td>5</td><td>C</td><td>1.181810</td><td>-1.263414</td><td>-0.060067</td></tr> <tr><td>6</td><td>C</td><td>1.579605</td><td>0.065967</td><td>-0.053769</td></tr> <tr><td>7</td><td>O</td><td>-2.486813</td><td>-0.797870</td><td>-0.046169</td></tr> <tr><td>8</td><td>H</td><td>-2.642080</td><td>-1.750087</td><td>-0.018923</td></tr> <tr><td>9</td><td>H</td><td>0.147471</td><td>-0.206018</td><td>3.141797</td></tr> <tr><td>10</td><td>H</td><td>-0.509064</td><td>-2.600104</td><td>-0.059938</td></tr> <tr><td>11</td><td>H</td><td>1.923542</td><td>-2.054048</td><td>-0.058260</td></tr> <tr><td>12</td><td>H</td><td>0.949613</td><td>2.125775</td><td>-0.036871</td></tr> <tr><td>13</td><td>O</td><td>-1.697818</td><td>1.729905</td><td>-0.028336</td></tr> <tr><td>14</td><td>H</td><td>-1.297670</td><td>2.608297</td><td>0.006449</td></tr> <tr><td>15</td><td>O</td><td>2.904207</td><td>0.441544</td><td>-0.046967</td></tr> <tr><td>16</td><td>H</td><td>3.461930</td><td>-0.346076</td><td>-0.034341</td></tr> </tbody> </table>	Tag	Symbol	X	Y	Z	1	C	0.633921	1.088114	-0.050113	2	C	-0.716711	0.775469	-0.047240	3	C	-1.130799	-0.560763	-0.055269	4	C	-0.179551	-1.566434	-0.061565	5	C	1.181810	-1.263414	-0.060067	6	C	1.579605	0.065967	-0.053769	7	O	-2.486813	-0.797870	-0.046169	8	H	-2.642080	-1.750087	-0.018923	9	H	0.147471	-0.206018	3.141797	10	H	-0.509064	-2.600104	-0.059938	11	H	1.923542	-2.054048	-0.058260	12	H	0.949613	2.125775	-0.036871	13	O	-1.697818	1.729905	-0.028336	14	H	-1.297670	2.608297	0.006449	15	O	2.904207	0.441544	-0.046967	16	H	3.461930	-0.346076	-0.034341	-458.42864	0.11508	-1/1
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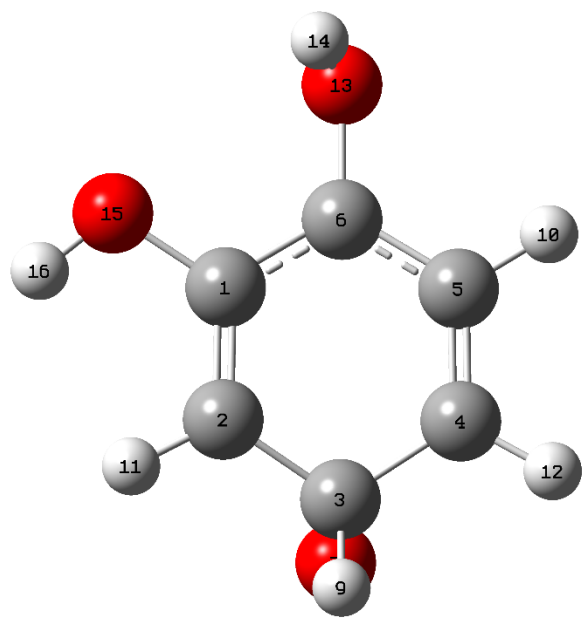
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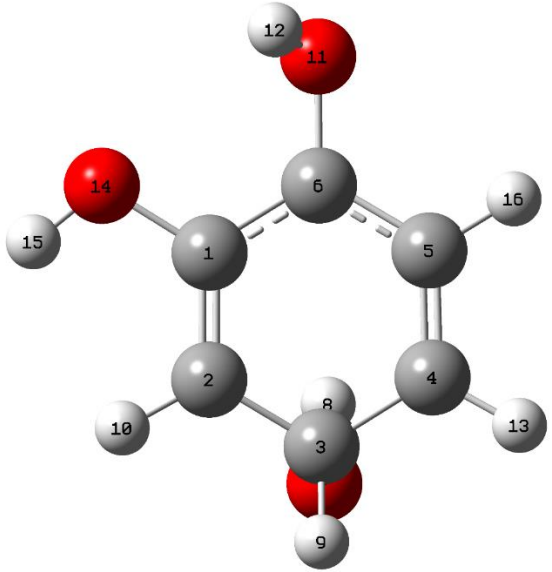
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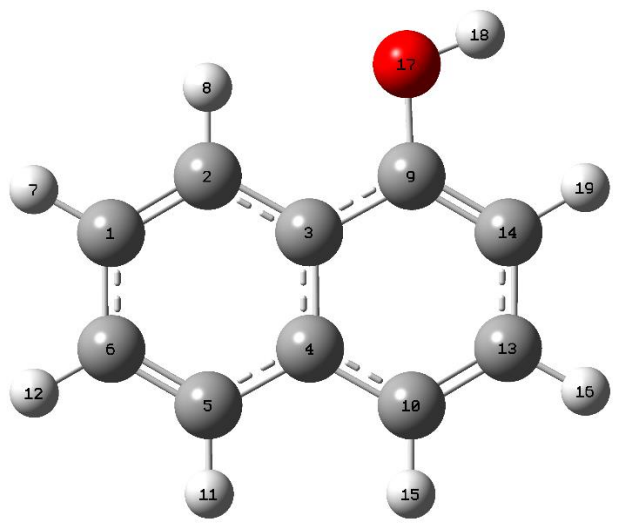
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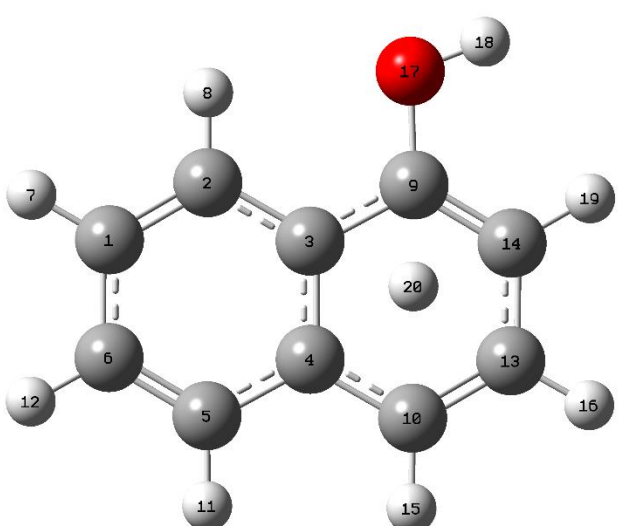
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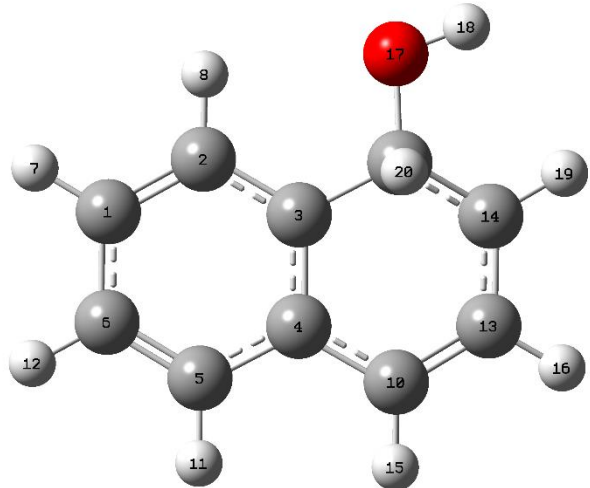
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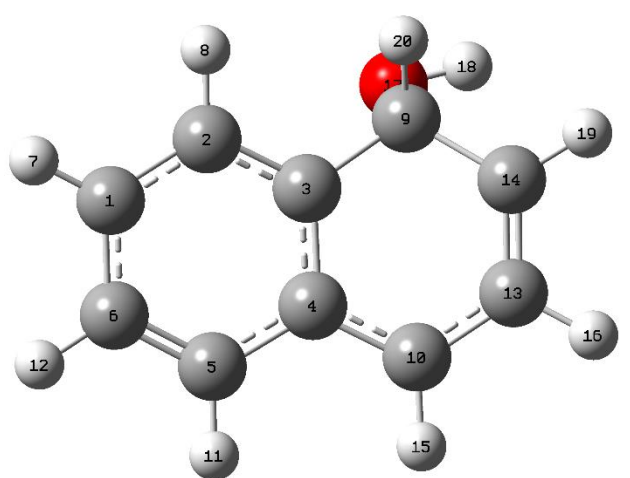
104	IM43		<table border="1"> <thead> <tr> <th>Tag</th> <th>Symbol</th> <th>X</th> <th>Y</th> <th>Z</th> </tr> </thead> <tbody> <tr><td>1</td><td>C</td><td>0.703994</td><td>0.732959</td><td>0.113989</td></tr> <tr><td>2</td><td>C</td><td>-0.566709</td><td>1.135835</td><td>0.473566</td></tr> <tr><td>3</td><td>C</td><td>-1.702035</td><td>0.194546</td><td>0.388814</td></tr> <tr><td>4</td><td>C</td><td>-1.249842</td><td>-1.210218</td><td>0.523809</td></tr> <tr><td>5</td><td>C</td><td>0.039758</td><td>-1.566544</td><td>0.184656</td></tr> <tr><td>6</td><td>C</td><td>1.027847</td><td>-0.615156</td><td>-0.094736</td></tr> <tr><td>7</td><td>O</td><td>-2.470576</td><td>0.376375</td><td>-0.940102</td></tr> <tr><td>8</td><td>H</td><td>-1.830836</td><td>0.151499</td><td>-1.627056</td></tr> <tr><td>9</td><td>H</td><td>-2.509932</td><td>0.451116</td><td>1.077549</td></tr> <tr><td>10</td><td>H</td><td>0.326083</td><td>-2.615681</td><td>0.167338</td></tr> <tr><td>11</td><td>H</td><td>-0.748545</td><td>2.184438</td><td>0.691547</td></tr> <tr><td>12</td><td>H</td><td>-1.979030</td><td>-1.973030</td><td>0.774867</td></tr> <tr><td>13</td><td>O</td><td>2.332225</td><td>-1.000556</td><td>-0.461746</td></tr> <tr><td>14</td><td>H</td><td>2.919671</td><td>-0.878856</td><td>0.293133</td></tr> <tr><td>15</td><td>O</td><td>1.751746</td><td>1.639676</td><td>0.018969</td></tr> <tr><td>16</td><td>H</td><td>1.397351</td><td>2.528016</td><td>0.145059</td></tr> </tbody> </table>	Tag	Symbol	X	Y	Z	1	C	0.703994	0.732959	0.113989	2	C	-0.566709	1.135835	0.473566	3	C	-1.702035	0.194546	0.388814	4	C	-1.249842	-1.210218	0.523809	5	C	0.039758	-1.566544	0.184656	6	C	1.027847	-0.615156	-0.094736	7	O	-2.470576	0.376375	-0.940102	8	H	-1.830836	0.151499	-1.627056	9	H	-2.509932	0.451116	1.077549	10	H	0.326083	-2.615681	0.167338	11	H	-0.748545	2.184438	0.691547	12	H	-1.979030	-1.973030	0.774867	13	O	2.332225	-1.000556	-0.461746	14	H	2.919671	-0.878856	0.293133	15	O	1.751746	1.639676	0.018969	16	H	1.397351	2.528016	0.145059	-458.42967	0.121436	-1/1
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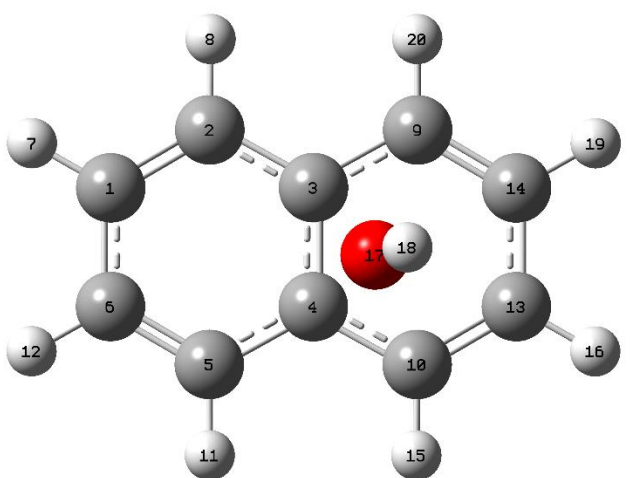
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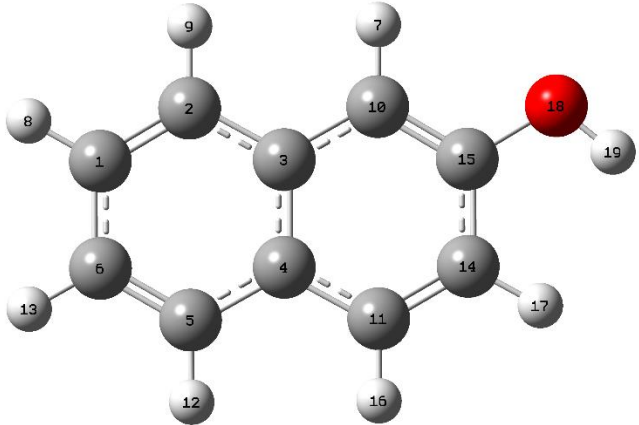
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			3	C	0.046466	-0.419908	0.018323			
			4	C	0.428767	0.946802	0.060472			
			5	C	1.812894	1.253340	0.027447			
			6	C	2.761310	0.258138	-0.041205			
			7	H	3.121152	-1.875063	-0.133969			
			8	H	0.726008	-2.463425	-0.056032			
			9	C	-1.363843	-0.736435	0.159885			
			10	C	-0.574881	1.960415	0.087912			
			11	H	2.113665	2.295954	0.053882			
			12	H	3.814483	0.514866	-0.066899			
			13	C	-1.893787	1.602164	-0.124946			
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			16	H	-2.644366	2.377560	-0.243288			
			17	O	-1.679712	-2.068962	-0.064547			
			18	H	-2.636490	-2.169900	0.008803			
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			20	H	-1.416628	-0.782933	1.923089			

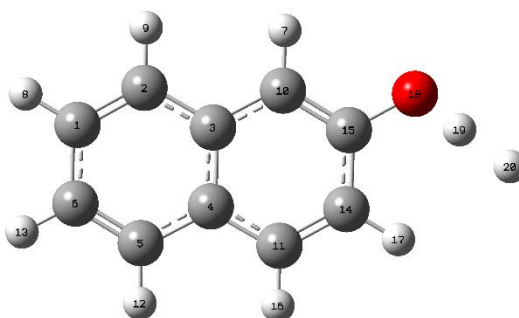
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			4	C	0.326566	0.883974	-0.123131			
			5	C	1.676844	1.295943	-0.306903			
			6	C	2.731728	0.425233	-0.125366			
			7	H	3.335794	-1.587584	0.413110			
			8	H	0.997398	-2.375794	0.690811			
			9	C	-1.292900	-1.020146	0.248643			
			10	C	-0.772241	1.784439	-0.180021			
			11	H	1.870400	2.330199	-0.577527			
			12	H	3.747838	0.778850	-0.268244			
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			3	C	-0.091924	-0.449571	-0.284872			
			4	C	-0.339659	0.897737	0.103953			
			5	C	-1.689282	1.286018	0.329811			
			6	C	-2.727224	0.399269	0.160965			
			7	H	-3.298375	-1.620674	-0.385904			
			8	H	-0.963718	-2.357607	-0.757072			
			9	C	1.283205	-0.920092	-0.427719			
			10	C	0.743472	1.816405	0.192888			
			11	H	-1.890254	2.309811	0.631095			
			12	H	-3.747500	0.723338	0.335997			
			13	C	2.003093	1.404815	-0.216328			
			14	C	2.269800	0.091510	-0.614549			
			15	H	0.550349	2.844710	0.476813			
			16	H	2.805487	2.136696	-0.261880			
			17	O	1.568819	-1.733251	1.183182			
			18	H	2.532464	-1.725966	1.230505			
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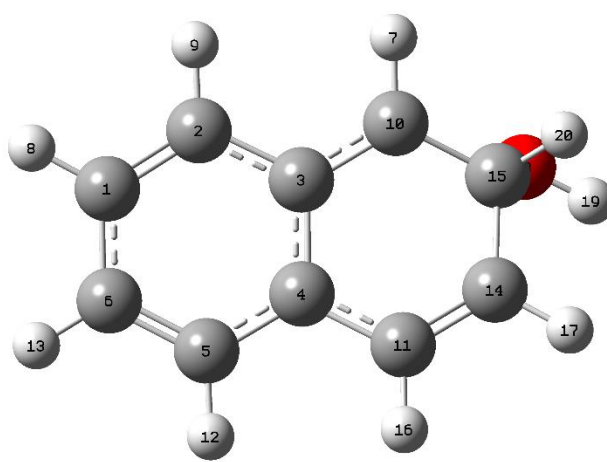
111	IM46		<table border="1"> <thead> <tr> <th>Tag</th> <th>Symbol</th> <th>X</th> <th>Y</th> <th>Z</th> </tr> </thead> <tbody> <tr><td>1</td><td>C</td><td>2.519223</td><td>0.701310</td><td>-0.155655</td></tr> <tr><td>2</td><td>C</td><td>1.343053</td><td>1.382461</td><td>-0.332049</td></tr> <tr><td>3</td><td>C</td><td>0.110393</td><td>0.683259</td><td>-0.428023</td></tr> <tr><td>4</td><td>C</td><td>0.112857</td><td>-0.736625</td><td>-0.342034</td></tr> <tr><td>5</td><td>C</td><td>1.348009</td><td>-1.414867</td><td>-0.163605</td></tr> <tr><td>6</td><td>C</td><td>2.521834</td><td>-0.713398</td><td>-0.070985</td></tr> <tr><td>7</td><td>H</td><td>3.455178</td><td>1.242294</td><td>-0.078411</td></tr> <tr><td>8</td><td>H</td><td>1.333461</td><td>2.465628</td><td>-0.395171</td></tr> <tr><td>9</td><td>C</td><td>-1.127541</td><td>1.362493</td><td>-0.586545</td></tr> <tr><td>10</td><td>C</td><td>-1.122331</td><td>-1.434833</td><td>-0.417249</td></tr> <tr><td>11</td><td>H</td><td>1.342139</td><td>-2.497816</td><td>-0.096462</td></tr> <tr><td>12</td><td>H</td><td>3.459788</td><td>-1.237906</td><td>0.069672</td></tr> <tr><td>13</td><td>C</td><td>-2.301711</td><td>-0.752613</td><td>-0.567154</td></tr> <tr><td>14</td><td>C</td><td>-2.304362</td><td>0.662483</td><td>-0.652214</td></tr> <tr><td>15</td><td>H</td><td>-1.113123</td><td>-2.517601</td><td>-0.347631</td></tr> <tr><td>16</td><td>H</td><td>-3.240098</td><td>-1.292353</td><td>-0.619003</td></tr> <tr><td>17</td><td>O</td><td>-0.791837</td><td>0.195449</td><td>2.897358</td></tr> <tr><td>18</td><td>H</td><td>-1.131262</td><td>0.201741</td><td>1.997144</td></tr> <tr><td>19</td><td>H</td><td>-3.244804</td><td>1.188571</td><td>-0.768036</td></tr> <tr><td>20</td><td>H</td><td>-1.123130</td><td>2.445831</td><td>-0.647888</td></tr> </tbody> </table>	Tag	Symbol	X	Y	Z	1	C	2.519223	0.701310	-0.155655	2	C	1.343053	1.382461	-0.332049	3	C	0.110393	0.683259	-0.428023	4	C	0.112857	-0.736625	-0.342034	5	C	1.348009	-1.414867	-0.163605	6	C	2.521834	-0.713398	-0.070985	7	H	3.455178	1.242294	-0.078411	8	H	1.333461	2.465628	-0.395171	9	C	-1.127541	1.362493	-0.586545	10	C	-1.122331	-1.434833	-0.417249	11	H	1.342139	-2.497816	-0.096462	12	H	3.459788	-1.237906	0.069672	13	C	-2.301711	-0.752613	-0.567154	14	C	-2.304362	0.662483	-0.652214	15	H	-1.113123	-2.517601	-0.347631	16	H	-3.240098	-1.292353	-0.619003	17	O	-0.791837	0.195449	2.897358	18	H	-1.131262	0.201741	1.997144	19	H	-3.244804	1.188571	-0.768036	20	H	-1.123130	2.445831	-0.647888	-461.60513	0.158761	-1/1
Tag	Symbol	X	Y	Z																																																																																																											
1	C	2.519223	0.701310	-0.155655																																																																																																											
2	C	1.343053	1.382461	-0.332049																																																																																																											
3	C	0.110393	0.683259	-0.428023																																																																																																											
4	C	0.112857	-0.736625	-0.342034																																																																																																											
5	C	1.348009	-1.414867	-0.163605																																																																																																											
6	C	2.521834	-0.713398	-0.070985																																																																																																											
7	H	3.455178	1.242294	-0.078411																																																																																																											
8	H	1.333461	2.465628	-0.395171																																																																																																											
9	C	-1.127541	1.362493	-0.586545																																																																																																											
10	C	-1.122331	-1.434833	-0.417249																																																																																																											
11	H	1.342139	-2.497816	-0.096462																																																																																																											
12	H	3.459788	-1.237906	0.069672																																																																																																											
13	C	-2.301711	-0.752613	-0.567154																																																																																																											
14	C	-2.304362	0.662483	-0.652214																																																																																																											
15	H	-1.113123	-2.517601	-0.347631																																																																																																											
16	H	-3.240098	-1.292353	-0.619003																																																																																																											
17	O	-0.791837	0.195449	2.897358																																																																																																											
18	H	-1.131262	0.201741	1.997144																																																																																																											
19	H	-3.244804	1.188571	-0.768036																																																																																																											
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			4	C	0.000062	0.711157	-0.000002			
			5	C	1.242315	1.401210	-0.000004			
			6	C	2.425014	0.708708	0.000002			
			7	H	-1.234651	-2.486188	-0.000010			
			8	H	3.368516	-1.241949	0.000011			
			9	H	1.234618	-2.486210	0.000003			
			10	C	-1.242324	-1.401196	-0.000003			
			11	C	-1.242285	1.401211	0.000001			
			12	H	1.234708	2.486200	-0.000005			
			13	H	3.368574	1.241864	0.000008			
			14	C	-2.424967	0.708778	0.000004			
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			16	H	-1.234668	2.486207	-0.000009			
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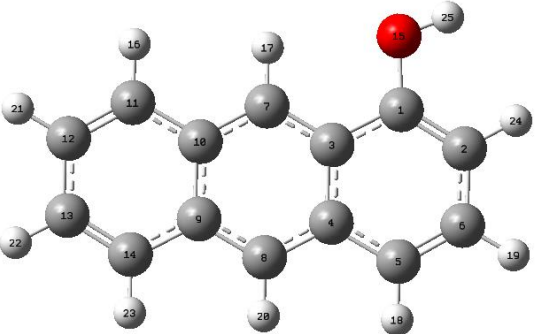
113	R18		<table border="1"> <thead> <tr> <th>Tag</th> <th>Symbol</th> <th>X</th> <th>Y</th> <th>Z</th> </tr> </thead> <tbody> <tr><td>1</td><td>C</td><td>-2.690867</td><td>-0.997380</td><td>0.000000</td></tr> <tr><td>2</td><td>C</td><td>-1.414602</td><td>-1.498036</td><td>0.000000</td></tr> <tr><td>3</td><td>C</td><td>-0.293473</td><td>-0.624010</td><td>0.000000</td></tr> <tr><td>4</td><td>C</td><td>-0.522382</td><td>0.780356</td><td>0.000000</td></tr> <tr><td>5</td><td>C</td><td>-1.855255</td><td>1.268609</td><td>0.000000</td></tr> <tr><td>6</td><td>C</td><td>-2.917048</td><td>0.401611</td><td>0.000000</td></tr> <tr><td>7</td><td>H</td><td>1.219293</td><td>-2.184942</td><td>0.000000</td></tr> <tr><td>8</td><td>H</td><td>-3.537411</td><td>-1.674423</td><td>0.000000</td></tr> <tr><td>9</td><td>H</td><td>-1.240062</td><td>-2.568801</td><td>0.000000</td></tr> <tr><td>10</td><td>C</td><td>1.036479</td><td>-1.115902</td><td>0.000000</td></tr> <tr><td>11</td><td>C</td><td>0.597204</td><td>1.653322</td><td>0.000000</td></tr> <tr><td>12</td><td>H</td><td>-2.014710</td><td>2.341968</td><td>0.000000</td></tr> <tr><td>13</td><td>H</td><td>-3.932117</td><td>0.780775</td><td>0.000000</td></tr> <tr><td>14</td><td>C</td><td>1.873682</td><td>1.160961</td><td>0.000000</td></tr> <tr><td>15</td><td>C</td><td>2.090378</td><td>-0.239558</td><td>0.000000</td></tr> <tr><td>16</td><td>H</td><td>0.426208</td><td>2.724542</td><td>0.000000</td></tr> <tr><td>17</td><td>H</td><td>2.730163</td><td>1.827153</td><td>0.000000</td></tr> <tr><td>18</td><td>O</td><td>3.365118</td><td>-0.745672</td><td>0.000000</td></tr> <tr><td>19</td><td>H</td><td>4.002993</td><td>-0.020729</td><td>0.000000</td></tr> </tbody> </table>	Tag	Symbol	X	Y	Z	1	C	-2.690867	-0.997380	0.000000	2	C	-1.414602	-1.498036	0.000000	3	C	-0.293473	-0.624010	0.000000	4	C	-0.522382	0.780356	0.000000	5	C	-1.855255	1.268609	0.000000	6	C	-2.917048	0.401611	0.000000	7	H	1.219293	-2.184942	0.000000	8	H	-3.537411	-1.674423	0.000000	9	H	-1.240062	-2.568801	0.000000	10	C	1.036479	-1.115902	0.000000	11	C	0.597204	1.653322	0.000000	12	H	-2.014710	2.341968	0.000000	13	H	-3.932117	0.780775	0.000000	14	C	1.873682	1.160961	0.000000	15	C	2.090378	-0.239558	0.000000	16	H	0.426208	2.724542	0.000000	17	H	2.730163	1.827153	0.000000	18	O	3.365118	-0.745672	0.000000	19	H	4.002993	-0.020729	0.000000	-460.90039	0.152131	0/1
Tag	Symbol	X	Y	Z																																																																																																						
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2	C	-1.414602	-1.498036	0.000000																																																																																																						
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6	C	-2.917048	0.401611	0.000000																																																																																																						
7	H	1.219293	-2.184942	0.000000																																																																																																						
8	H	-3.537411	-1.674423	0.000000																																																																																																						
9	H	-1.240062	-2.568801	0.000000																																																																																																						
10	C	1.036479	-1.115902	0.000000																																																																																																						
11	C	0.597204	1.653322	0.000000																																																																																																						
12	H	-2.014710	2.341968	0.000000																																																																																																						
13	H	-3.932117	0.780775	0.000000																																																																																																						
14	C	1.873682	1.160961	0.000000																																																																																																						
15	C	2.090378	-0.239558	0.000000																																																																																																						
16	H	0.426208	2.724542	0.000000																																																																																																						
17	H	2.730163	1.827153	0.000000																																																																																																						
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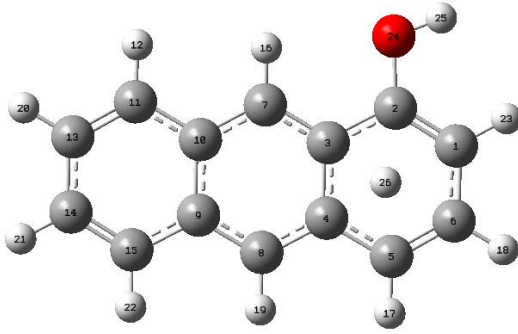
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			4	C	0.579760	0.779213	-0.007860			
			5	C	1.905883	1.284642	0.010815			
			6	C	2.980275	0.432557	0.030992			
			7	H	-1.117241	-2.208704	-0.009323			
			8	H	3.626843	-1.635684	0.047864			
			9	H	1.342341	-2.559423	0.014127			
			10	C	-0.955410	-1.135791	-0.019630			
			11	C	-0.554273	1.633870	-0.034093			
			12	H	2.051489	2.360163	0.008923			
			13	H	3.990261	0.824970	0.045743			
			14	C	-1.824223	1.124997	-0.060068			
			15	C	-2.040257	-0.285908	-0.046070			
			16	H	-0.397456	2.707718	-0.044471			
			17	H	-2.682663	1.784275	-0.099472			
			18	O	-3.294176	-0.787728	-0.080698			
			19	H	-4.014800	-0.093779	0.341244			
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			2	C	1.439465	-1.499098	-0.010389			
			3	C	0.317919	-0.622270	-0.001478			
			4	C	0.574691	0.781624	-0.000487			
			5	C	1.902780	1.254837	-0.000702			
			6	C	2.969796	0.381129	0.001007			
			7	H	-1.197317	-2.166152	0.006557			
			8	H	3.562046	-1.699821	-0.005807			
			9	H	1.261863	-2.569986	-0.015105			
			10	C	-1.014168	-1.097103	-0.005439			
			11	C	-0.552956	1.666543	-0.055145			
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			13	H	3.987037	0.754030	0.003793			
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			15	C	-2.091242	-0.222328	0.165929			
			16	H	-0.371133	2.733583	-0.141022			
			17	H	-2.671530	1.864735	-0.049738			
			18	O	-3.335881	-0.701488	-0.293387			
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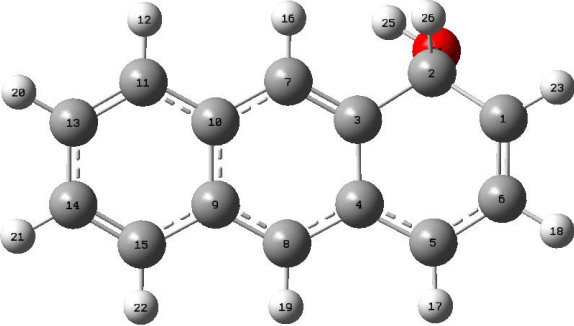
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			3	C	-0.284270	-0.650464	-0.219511			
			4	C	-0.460943	0.771100	-0.031636			
			5	C	-1.737757	1.304787	0.215781			
			6	C	-2.862984	0.503934	0.290751			
			7	H	1.077723	-2.244399	-0.676771			
			8	H	-3.585981	-1.532385	0.126866			
			9	H	-1.395116	-2.518295	-0.323513			
			10	C	0.976837	-1.180511	-0.481275			
			11	C	0.692042	1.604522	-0.227678			
			12	H	-1.826743	2.381323	0.342253			
			13	H	-3.839249	0.928877	0.489771			
			14	C	1.923488	1.085891	-0.454919			
			15	C	2.199304	-0.375464	-0.309363			
			16	H	0.544761	2.682172	-0.247832			
			17	H	2.762008	1.743455	-0.667540			
			18	O	2.770319	-0.626316	1.074459			
			19	H	3.577995	-0.098587	1.143892			
			20	H	3.008423	-0.696044	-0.973030			

117	TS38		Tag	Symbol	X	Y	Z	-461.55714	0.158637	-1/1
			1	C	-2.710498	-0.908191	0.107112			
			2	C	-1.477923	-1.450501	-0.161189			
			3	C	-0.302016	-0.637839	-0.232763			
			4	C	-0.475325	0.773575	-0.040949			
			5	C	-1.757042	1.299289	0.229035			
			6	C	-2.865764	0.484679	0.313085			
			7	H	1.068246	-2.224718	-0.717574			
			8	H	-3.579763	-1.555533	0.161506			
			9	H	-1.376878	-2.520624	-0.317259			
			10	C	0.969426	-1.161431	-0.521928			
			11	C	0.670388	1.611340	-0.220453			
			12	H	-1.854923	2.373027	0.365549			
			13	H	-3.843991	0.899579	0.524644			
			14	C	1.900632	1.090157	-0.474133			
			15	C	2.142173	-0.351304	-0.429429			
			16	H	0.529461	2.688707	-0.192181			
			17	H	2.744889	1.749485	-0.650460			
			18	O	2.877968	-0.633248	1.158764			
			19	H	3.713679	-0.148796	1.130370			
			20	H	3.011233	-0.693777	-0.985038			

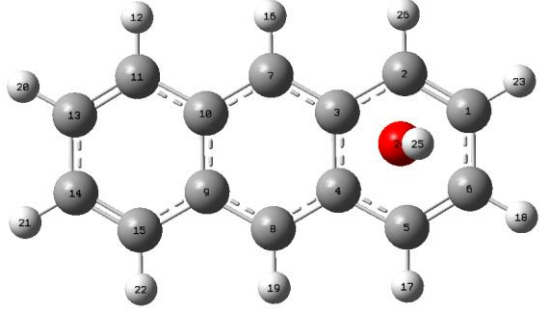
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			1	C	2.396424	0.914064	-0.000041			
			2	C	3.486815	0.094688	0.000211			
			3	C	1.063586	0.376746	-0.000068			
			4	C	0.910221	-1.05072	-0.000067			
			5	C	2.07566	-1.882061	-0.000028			
			6	C	3.316474	-1.320835	0.000138			
			7	C	-0.063955	1.197455	-0.000042			
			8	C	-0.377754	-1.590242	-0.000099			
			9	C	-1.510882	-0.773848	-0.000049			
			10	C	-1.350178	0.651158	-0.000016			
			11	C	-2.518772	1.477724	0.000074			
			12	C	-3.763112	0.922524	0.000108			
			13	C	-3.923494	-0.497178	0.000029			
			14	C	-2.835469	-1.317468	-0.000051			
			15	O	2.484917	2.277681	0.000015			
			16	H	-2.388114	2.554693	0.000112			
			17	H	0.050556	2.275178	-0.000034			
			18	H	1.946038	-2.958303	-0.000121			
			19	H	4.199827	-1.948751	0.00022			
			20	H	-0.499931	-2.669103	-0.00012			
			21	H	-4.64303	1.555149	0.000216			
			22	H	-4.922734	-0.916843	0.000024			
			23	H	-2.950568	-2.396192	-0.000092			
			24	H	4.482164	0.525803	0.000346			
			25	H	3.41307	2.544867	-0.001265			
26	H	3.41307	2.544867	-0.001265						

119	IM49		Tag	Symbol	X	Y	Z	-615.1151	0.200888	-1/1
			1	C	3.466633	0.102899	-0.057773			
			2	C	2.375322	0.92066	-0.049738			
			3	C	1.043856	0.38126	-0.051182			
			4	C	0.892591	-1.045825	-0.054419			
			5	C	2.059021	-1.875367	-0.060256			
			6	C	3.298843	-1.312182	-0.062477			
			7	C	-0.083961	1.200462	-0.033706			
			8	C	-0.393906	-1.587307	-0.041497			
			9	C	-1.528474	-0.772487	-0.023272			
			10	C	-1.369844	0.652612	-0.019445			
			11	C	-2.539153	1.477303	0.000097			
			12	H	-2.410218	2.554511	0.0035			
			13	C	-3.782932	0.920413	0.014149			
			14	C	-3.941271	-0.49916	0.010353			
			15	C	-2.851914	-1.317885	-0.00755			
			16	H	0.029052	2.278365	-0.027293			
			17	H	1.931101	-2.951873	-0.058665			
			18	H	4.183313	-1.938503	-0.063254			
			19	H	-0.514433	-2.66637	-0.04172			
			20	H	-4.663466	1.552028	0.028721			
			21	H	-4.939718	-0.920602	0.022261			
			22	H	-2.96571	-2.396784	-0.0099			
			23	H	4.461259	0.535682	-0.052039			
			24	O	2.462582	2.284553	-0.034657			
			25	H	3.390662	2.550986	-0.015237			
26	H	1.928635	-0.346229	3.111175						

120	TS39		Tag	Symbol	X	Y	Z	-615.08443	0.201007	-1/1
			1	C	3.448067	0.070219	-0.278139			
			2	C	2.393363	0.886797	0.14969			
			3	C	1.035209	0.357715	0.048128			
			4	C	0.881204	-1.071636	0.085163			
			5	C	2.056133	-1.895197	0.067403			
			6	C	3.278021	-1.322027	-0.208975			
			7	C	-0.072328	1.180373	-0.009713			
			8	C	-0.40875	-1.598617	0.078486			
			9	C	-1.543371	-0.773518	0.030456			
			10	C	-1.37561	0.645869	-0.023617			
			11	C	-2.531506	1.477757	-0.080394			
			12	H	-2.392487	2.553396	-0.120251			
			13	C	-3.786572	0.934715	-0.082838			
			14	C	-3.955607	-0.477875	-0.029799			
			15	C	-2.869355	-1.305413	0.024428			
			16	H	0.049828	2.25771	-0.027348			
			17	H	1.940029	-2.971942	0.113457			
			18	H	4.141028	-1.96178	-0.365559			
			19	H	-0.542569	-2.676335	0.102302			
			20	H	-4.659483	1.575651	-0.124578			
			21	H	-4.95657	-0.894083	-0.032696			
			22	H	-2.995024	-2.38261	0.063994			
			23	H	4.43178	0.506332	-0.411577			
			24	O	2.480048	2.259338	0.025347			
			25	H	3.411571	2.51131	0.031474			
26	H	2.438116	0.752688	1.946328						

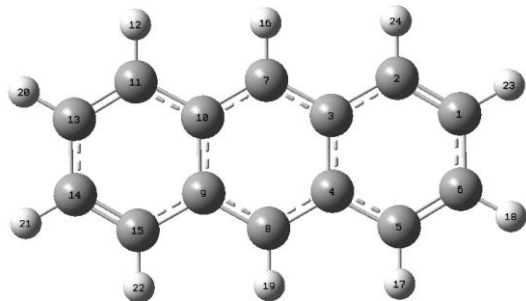
121	IM50		Tag	Symbol	X	Y	Z	-615.13691	0.207486	-1/1
			1	C	3.45378	0.213023	0.596813			
			2	C	2.36545	1.118655	0.150834			
			3	C	1.01654	0.444487	0.176532			
			4	C	0.930087	-0.985553	-0.052334			
			5	C	2.120621	-1.755468	-0.024922			
			6	C	3.318775	-1.139641	0.393708			
			7	C	-0.122375	1.199879	0.318545			
			8	C	-0.355995	-1.53065	-0.216664			
			9	C	-1.519825	-0.755663	-0.106985			
			10	C	-1.417469	0.641512	0.19011			
			11	C	-2.597235	1.419418	0.320381			
			12	H	-2.496325	2.477443	0.54386			
			13	C	-3.838116	0.854821	0.167234			
			14	C	-3.947514	-0.531684	-0.128727			
			15	C	-2.829954	-1.310559	-0.261337			
			16	H	-0.03342	2.267684	0.50868			
			17	H	2.063284	-2.831733	-0.140814			
			18	H	4.173466	-1.781033	0.601599			
			19	H	-0.457177	-2.596774	-0.403682			
			20	H	-4.73363	1.456245	0.269466			
			21	H	-4.930599	-0.973585	-0.249674			
			22	H	-2.920874	-2.368735	-0.48642			
			23	H	4.382649	0.642234	0.954003			
			24	O	2.654934	1.533254	-1.243039			
			25	H	1.926193	2.102398	-1.525333			
			26	H	2.326336	2.04436	0.733486			

122	TS40		Tag	Symbol	X	Y	Z	-615.1287	0.205637	-1/1
			1	C	3.443877	-0.167758	-0.592354			
			2	C	2.354339	-1.038244	-0.354965			
			3	C	1.030357	-0.416893	-0.253786			
			4	C	0.926235	0.991831	0.031959			
			5	C	2.116359	1.781175	0.058741			
			6	C	3.318064	1.198532	-0.29476			
			7	C	-0.117735	-1.183912	-0.378703			
			8	C	-0.350678	1.537151	0.213601			
			9	C	-1.510195	0.761351	0.10189			
			10	C	-1.398418	-0.632578	-0.212118			
			11	C	-2.585422	-1.415839	-0.329857			
			12	H	-2.486334	-2.471074	-0.564452			
			13	C	-3.817251	-0.853683	-0.148713			
			14	C	-3.932022	0.534031	0.160599			
			15	C	-2.818562	1.314476	0.281142			
			16	H	-0.026764	-2.245675	-0.594711			
			17	H	2.043295	2.843318	0.26269			
			18	H	4.199429	1.829665	-0.375249			
			19	H	-0.447451	2.597241	0.431961			
			20	H	-4.713497	-1.456281	-0.23847			
			21	H	-4.916236	0.966855	0.29995			
			22	H	-2.905529	2.370598	0.515681			
			23	H	4.402156	-0.574818	-0.892162			
			24	O	2.59175	-1.752557	1.350246			
			25	H	1.796316	-2.282623	1.485128			
26	H	2.366943	-2.01461	-0.828388						

123	IM51		Tag	Symbol	X	Y	Z	-615.17024	0.205692	-1/1
			1	C	-3.437133	0.698633	-0.601078			
			2	C	-2.267893	1.393581	-0.517613			
			3	C	-1.015817	0.707805	-0.403611			
			4	C	-1.014075	-0.727702	-0.382356			
			5	C	-2.264414	-1.41967	-0.475678			
			6	C	-3.435363	-0.730518	-0.579805			
			7	C	0.194306	1.396118	-0.29844			
			8	C	0.197722	-1.409637	-0.257132			
			9	C	1.408167	-0.721221	-0.149267			
			10	C	1.406423	0.714122	-0.170455			
			11	C	2.655038	1.406095	-0.057991			
			12	H	2.646652	2.490911	-0.073647			
			13	C	3.82387	0.717182	0.066295			
			14	C	3.825603	-0.711468	0.087305			
			15	C	2.658437	-1.406552	-0.016636			
			16	H	0.192631	2.482028	-0.311412			
			17	H	-2.2562	-2.504424	-0.456025			
			18	H	-4.377305	-1.262379	-0.645805			
			19	H	0.198683	-2.495459	-0.238269			
			20	H	4.764162	1.249332	0.151392			
			21	H	4.767198	-1.238619	0.187775			
			22	H	2.652664	-2.491382	-0.000622			
			23	H	-4.38038	1.226029	-0.682633			
			24	O	-1.999197	0.068832	2.892118			
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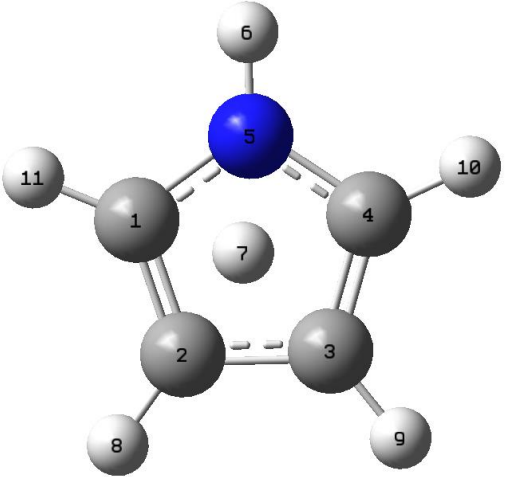
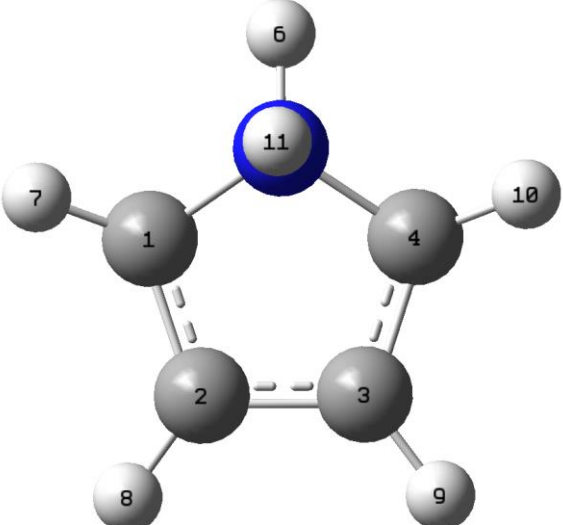


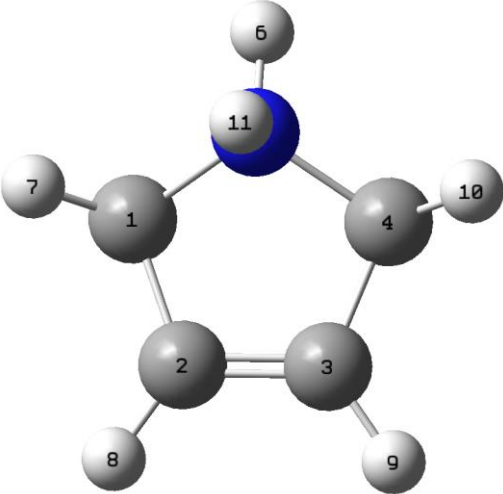
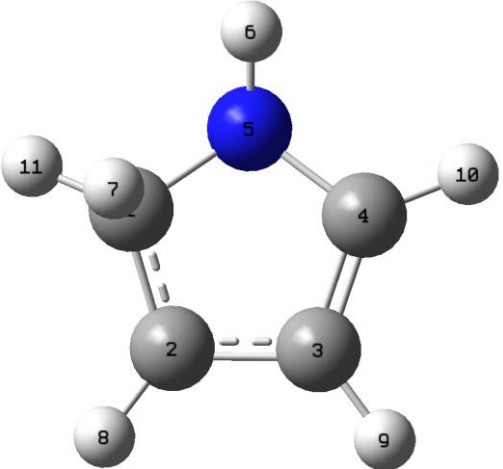
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6	C	-3.646114	0.714465	0.000216
7	C	-0.000035	-1.402836	0.000109
8	C	-0.000009	1.402869	0.000037
9	C	1.217017	0.717818	-0.000059
10	C	1.216998	-0.717807	0.000084
11	C	2.472567	-1.406626	0.00016
12	H	2.465656	-2.491585	0.00042
13	C	3.646149	-0.714471	0.000144
14	C	3.646164	0.714434	-0.000139
15	C	2.472596	1.406608	-0.000259
16	H	-0.000037	-2.488837	0.000042
17	H	-2.465674	2.49161	0.000446
18	H	-4.591611	1.244145	0.000322
19	H	-0.000004	2.488872	-0.000009
20	H	4.591557	-1.244311	0.000163
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22	H	2.465698	2.491568	-0.000425
23	H	-4.591606	-1.244233	-0.000002
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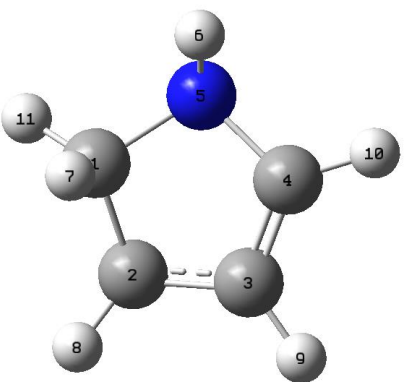
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2	C	-0.994239	0.711622	-0.047734																																																														
3	C	-0.993305	-0.712928	-0.047747																																																														
4	C	0.320886	-1.118872	-0.098848																																																														
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9	H	-1.853211	-1.364223	-0.009862																																																														
10	H	0.758632	-2.104121	-0.111461																																																														
11	H	0.755765	2.105177	-0.111526																																																														
126	TS41		<table border="1"> <thead> <tr> <th>Tag</th> <th>Symbol</th> <th>X</th> <th>Y</th> <th>Z</th> </tr> </thead> <tbody> <tr><td>1</td><td>C</td><td>0.295308</td><td>1.138754</td><td>-0.229045</td></tr> <tr><td>2</td><td>C</td><td>-1.025174</td><td>0.698511</td><td>0.057412</td></tr> <tr><td>3</td><td>C</td><td>-1.024736</td><td>-0.69914</td><td>0.057414</td></tr> <tr><td>4</td><td>C</td><td>0.29605</td><td>-1.138508</td><td>-0.228998</td></tr> <tr><td>5</td><td>N</td><td>1.108501</td><td>0.000295</td><td>0.078962</td></tr> <tr><td>6</td><td>H</td><td>2.055931</td><td>0.000573</td><td>-0.275867</td></tr> <tr><td>7</td><td>H</td><td>0.694616</td><td>2.100983</td><td>0.060031</td></tr> <tr><td>8</td><td>H</td><td>-1.892843</td><td>1.340972</td><td>0.127491</td></tr> <tr><td>9</td><td>H</td><td>-1.891994</td><td>-1.342156</td><td>0.127449</td></tr> <tr><td>10</td><td>H</td><td>0.69596</td><td>-2.100547</td><td>0.059857</td></tr> <tr><td>11</td><td>H</td><td>1.33013</td><td>0.000412</td><td>1.407607</td></tr> </tbody> </table>	Tag	Symbol	X	Y	Z	1	C	0.295308	1.138754	-0.229045	2	C	-1.025174	0.698511	0.057412	3	C	-1.024736	-0.69914	0.057414	4	C	0.29605	-1.138508	-0.228998	5	N	1.108501	0.000295	0.078962	6	H	2.055931	0.000573	-0.275867	7	H	0.694616	2.100983	0.060031	8	H	-1.892843	1.340972	0.127491	9	H	-1.891994	-1.342156	0.127449	10	H	0.69596	-2.100547	0.059857	11	H	1.33013	0.000412	1.407607	-210.59912	0.085541	-1/1
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