Supporting Information for

Pathways to Soot Oxidation: Reaction of OH with Phenanthrene Radicals

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Section 1. Details of Barrierless Reactions: Potential fits

The Morse potential is of the following form

$$E(r) = D_e\left[1 - e^{-\alpha(r-R_e)}\right]^2 \tag{S1}$$

The Varshni potential is of the following form

$$E(r) = D_e\left[1 - \left(\frac{R_e}{r}\right)e^{-\alpha(r^2-R_e^2)}\right]^2 \tag{S2}$$

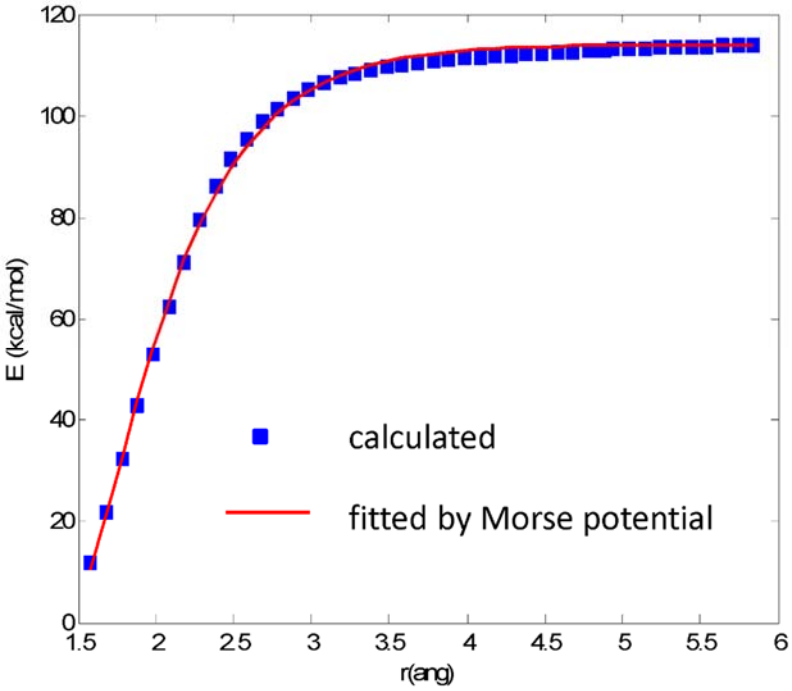

Figure S1. Calculated values and Morse potential for the **2→1** reaction. De = 114.05 kcal/mol, R_e = 1.40 Å, and α = 2.02 $Å^{-1}$.

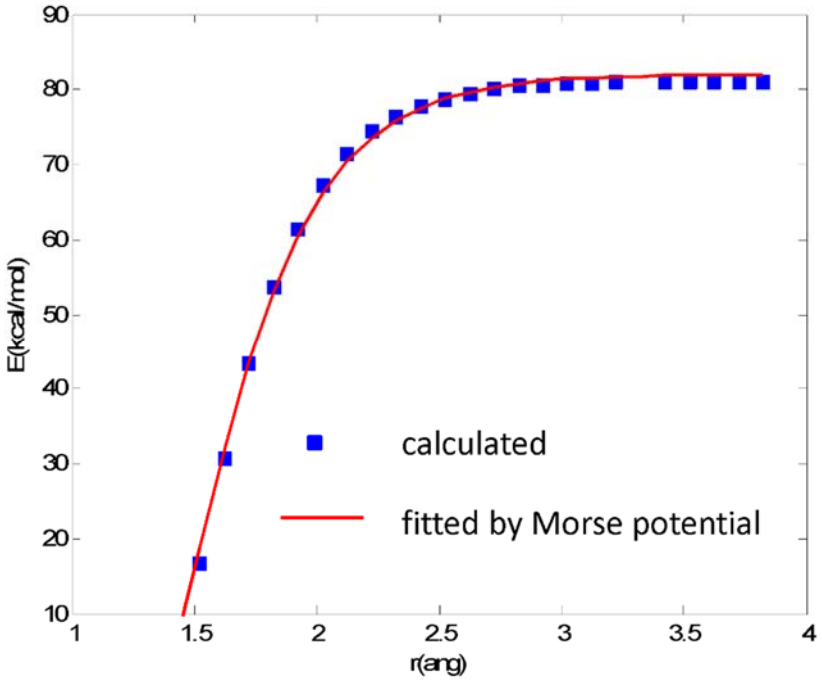

Figure S2. Calculated values and Morse potential for the **20→21** reaction. De = 82.0 kcal/mol, R_e = 1.33 Å, and α = 3.265 $Å^{-1}$.

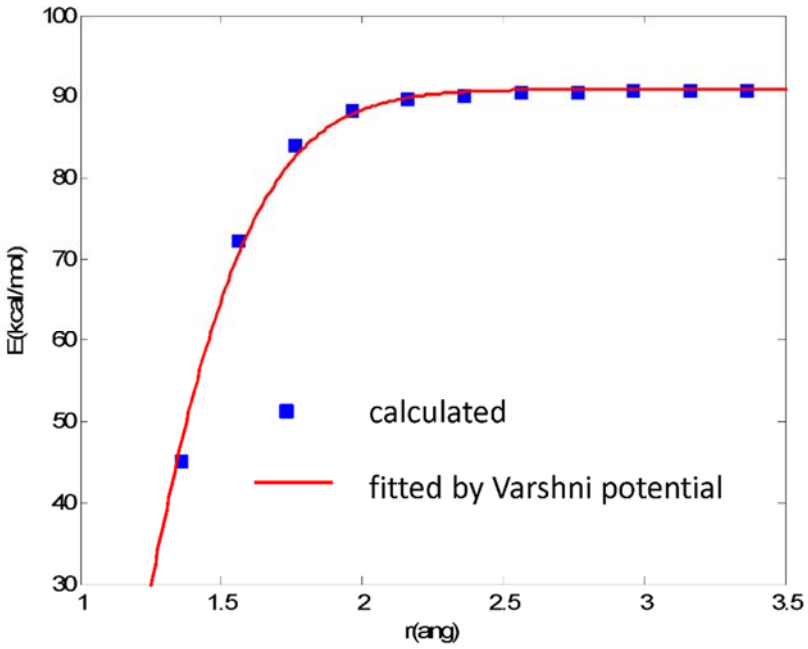

Figure S3. Calculated values and Varshni potential for the **2→4** reaction. De = 90.90 kcal/mol, R_e = 1.02 Å, and α = 1.201 $Å^{-2}$.

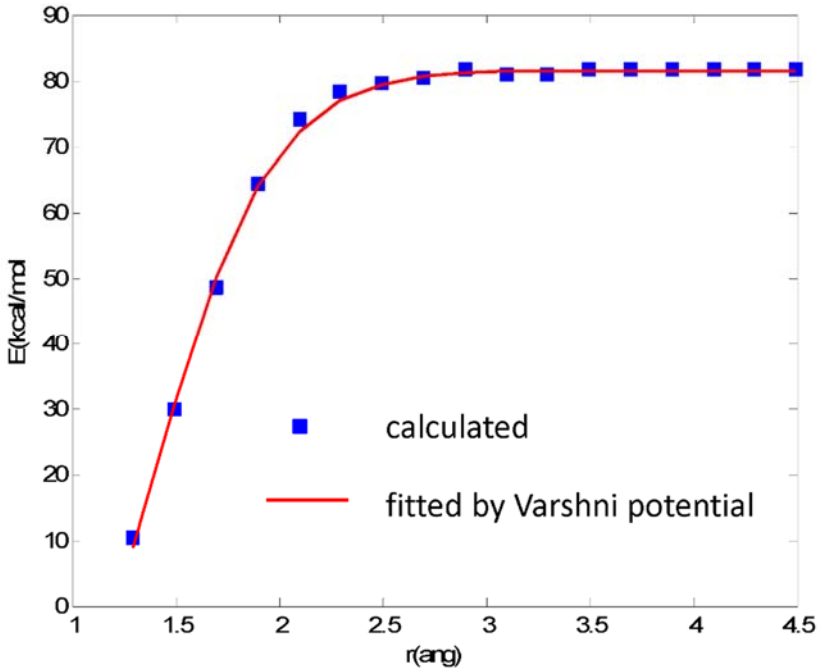

Figure S4. Calculated values and Varshni potential for the **7**→**4** reaction. De = 81.57 kcal/mol, R_e = 1.142 Å, and α = 0.7225 $Å^{-2}$.

Section 2. Supplemental Tables

Table S1. High-pressure rate coefficients (in s^{-1}) of the elementary reactions in the OH + phenanthrene radical reaction system.

Reaction	1500 K	2000 K	2500 K
$k_{2\rightarrow1}$	9.6E+00	7.0E+04	1.3E+07
$k_{2\rightarrow18}$	7.0E-03	1.2E+02	4.2E+04
$k_{2\rightarrow22}$	5.4E-02	3.6E+02	7.5E+04
$k_{2\rightarrow23}$	9.2E+00	1.2E+04	9.3E+05
$k_{2\rightarrow3}$	2.9E-01	8.3E+02	9.9E+04
$k_{2\rightarrow5}$	8.5E+06	2.1E+08	1.5E+09
$k_{2\rightarrow7}$	2.2E+04	3.4E+06	7.2E+07
$k_{2\rightarrow4}$	1.2E+03	1.4E+06	9.5E+07
$k_{5\rightarrow2}$	1.4E+12	2.2E+12	2.9E+12
$k_{5\rightarrow24}$	7.6E+02	1.9E+06	2.1E+08
$k_{5\rightarrow25}$	8.9E+01	1.6E+05	1.5E+07
$k_{5\rightarrow6}$	1.3E+09	1.7E+10	8.1E+10
$k_{6\rightarrow5}$	1.3E+11	4.6E+11	9.9E+11
$k_{6\rightarrow27}$	1.3E+04	1.2E+07	7.1E+08
$k_{6\rightarrow28}$	6.1E+07	1.8E+09	1.3E+10
$k_{7\rightarrow2}$	9.7E+04	7.6E+06	1.1E+08
$k_{7\rightarrow13}$	3.1E+05	1.9E+07	2.3E+08
$k_{7\rightarrow19}$	5.1E+01	1.3E+05	1.5E+07
$k_{7\rightarrow8}$	8.0E+05	4.2E+07	4.5E+08
$k_{7\rightarrow4}$	8.6E+03	5.1E+06	2.2E+08
$k_{8\rightarrow7}$	1.7E+12	2.7E+12	3.5E+12
$k_{8\rightarrow12}$	1.8E+06	3.0E+08	6.5E+09
$k_{8\rightarrow9}$	3.3E+10	1.2E+11	2.6E+11
$k_{9\rightarrow12}$	1.4E+07	1.2E+09	1.8E+10
$k_{9\rightarrow8}$	1.5E+12	2.2E+12	2.8E+12
$k_{9\rightarrow10}$	1.2E+11	5.1E+11	1.2E+12
$k_{10\rightarrow11}$	8.6E+11	3.6E+12	8.6E+12

$k_{10\rightarrow9}$	1.2E+09	2.5E+10	1.6E+11
$k_{12\rightarrow9}$	1.7E+11	3.2E+11	4.8E+11
$k_{12\rightarrow8}$	9.1E+11	1.4E+12	1.9E+12
$k_{13\rightarrow14}$	9.6E+10	3.9E+11	9.2E+11
$k_{13\rightarrow7}$	5.8E+08	7.2E+09	3.3E+10
$k_{14\rightarrow13}$	3.0E+09	8.2E+09	1.5E+10
$k_{14\rightarrow15}$	1.0E+12	1.4E+12	1.7E+12
$k_{15\rightarrow14}$	5.5E+11	9.7E+11	1.4E+12
$k_{15\rightarrow16}$	2.6E+03	3.7E+05	7.3E+06
$k_{16\rightarrow15}$	4.2E+10	2.9E+11	9.1E+11
$k_{16\rightarrow17}$	5.1E+08	9.8E+09	5.8E+10
$k_{24\rightarrow5}$	1.2E+06	9.8E+07	1.4E+09
$k_{25\rightarrow26}$	2.1E+10	1.4E+11	4.5E+11
$k_{25\rightarrow5}$	3.6E+07	1.3E+09	1.2E+10
$k_{27\rightarrow29}$	5.6E+10	1.9E+11	4.0E+11
$k_{6\rightarrow27}$	3.3E+11	8.5E+11	1.5E+12
$k_{28\rightarrow29}$	3.2E+11	1.0E+12	2.1E+12
$k_{6\rightarrow28}$	3.4E+12	4.2E+12	4.7E+12
$k_{20\rightarrow19}$	7.2E+03	1.7E+06	4.4E+07
$k_{20\rightarrow21}$	9.6E+05	5.4E+08	2.2E+10
$k_{19\rightarrow20}$	4.1E+12	5.5E+12	6.5E+12
$k_{4\rightarrow30}$	4.0E+05	4.5E+07	7.7E+08
$k_{4\rightarrow32}$	6.8E+05	2.3E+08	7.7E+09
$k_{30\rightarrow4}$	4.4E+12	4.8E+12	5.1E+12
$k_{30\rightarrow31}$	3.5E+12	4.4E+12	5.1E+12
$k_{30\rightarrow33}$	6.0E+10	2.9E+11	7.5E+11
$k_{31\rightarrow30}$	4.8E+08	4.3E+09	1.7E+10
$k_{31\rightarrow33}$	1.3E+13	1.8E+13	2.2E+13
$k_{31\rightarrow32}$	1.3E+08	3.7E+09	2.8E+10
$k_{32\rightarrow4}$	6.6E+11	1.2E+12	1.8E+12
$k_{32\rightarrow31}$	8.6E+10	1.9E+11	3.0E+11

Table S2. The following are reported for the structures in this study: total energies, zero-point energies, expectation values of S^2, vibrational frequencies, rotational constants, unsymmetrical hindered rotor MultiWell parameters, and Cartesian coordinate geometries. This same information for the structures shown in Figure 3f are reported in our previous work on armchair oxyradicals (See Ref. 8 from main text).

(reaction) Species	Information	Frequencies (unscaled) (cm^{-1})	Cartesian coordinates, (angstroms)			
			Atom	X	Y	Z
(OH + benzene) 2	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0696622 ZPE (hartree): 0.1106050 Relative energy, scaled, w/ZPE (kcal/mol): -2.932 $<S^2>$: 0.755 Rotational constants (GHz): 3.9483 2.2440 1.8373	26.733 65.528 134.63 151.38 409.08 414.72 470.24 620.14 620.39 690.78 716.4 859.24 869.14 976.03 984.47 1005.9 1008.1 1023.1 1054 1059.2 1176 1195.2 1197.2 1331.7 1381.1 1505.7 1509.8 1620.2 1628.6 3162.4 3172.5 3180 3190.7 3191.4 3209.7 3738.5	C	0.089528	1.211186	0.546266
			C	0.694974	0.000029	0.902492
			C	0.089545	-1.211152	0.546314
			C	-1.110978	-1.209919	-0.157810
			C	-1.712761	-0.000015	-0.508102
			C	-1.110995	1.209909	-0.157854
			H	-1.579186	-2.147910	-0.434298
			H	-2.648690	-0.000033	-1.055667
			H	-1.579216	2.147881	-0.434382
			H	0.564477	-2.146721	0.816398
			O	2.459067	0.000036	-0.837824
			H	1.760593	-0.000543	-1.514251
			H	0.564457	2.146768	0.816303
			H	1.609152	0.000045	1.480660
(OH + benzene) 2-3_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0674256 ZPE (hartree): 0.1112250 Relative energy, scaled, w/ZPE (kcal/mol): -1.153 $<S^2>$: 0.781 Rotational constants (GHz): 4.2325	-347.06 124.31 133.17 231.78 390.57 407.21 610.57 612.66 663.92 724.7 809.08 835.73 899.87 965.95 978.16 992.91 1012.6 1029.1 1040 1053.2 1172.5 1181 1194.7 1322.2 1377.2 1487.1 1498.4 1582.8 1605.7 3164.9 3174.1 3184.4 3194.8 3195.5 3211.9 3759.6	C	-0.176667	1.220519	-0.472455
			C	-0.859882	-0.000075	-0.715843
			C	-0.176547	-1.220591	-0.472406
			C	1.087856	-1.214351	0.092340
			C	1.724727	0.000077	0.376901
			C	1.087737	1.214428	0.092293
			H	1.592106	-2.150394	0.304081
			H	2.716848	0.000133	0.814045
			H	1.591889	2.150530	0.304005
			H	-0.676101	-2.154386	-0.698665
			O	-2.175677	0.000012	0.799791
			H	-1.537204	-0.000134	1.529706
			H	-0.676316	2.154254	-0.698747

	2.5527 1.9572		H	-1.729144	-0.000134	-1.357727
(OH + benzene) 2-5_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0598408 ZPE (hartree): 0.1052300 Relative energy, scaled, w/ZPE (kcal/mol): -0.03082 <S^2>: 0.757 Rotational constants (GHz): 5.5830 1.7212 1.3239	-1265.2 77.929 110.62 174.8 358.41 409.79 446.23 613.31 642.39 688.2 726.03 793.03 832.72 917.32 975.46 1001.1 1009.7 1018.5 1032.2 1070.4 1107 1180 1184.5 1322.5 1324.6 1325.5 1468.9 1500.7 1603.6 1623.4 3161.2 3169.2 3180.6 3186.4 3191.7 3762.9	C C C C C C H H H H O H H H	-0.025107 -0.681412 -0.022447 1.373230 2.063444 1.370594 1.916123 3.145996 1.911444 -0.573625 -3.149834 -3.164407 -0.578279 -1.928400	1.216508 -0.001385 -1.217969 -1.209208 0.001522 1.210710 -2.147654 0.002734 2.150335 -2.150534 -0.000028 0.001107 2.147882 -0.004716	-0.053391 -0.096504 -0.053158 0.020609 0.057209 0.020440 0.049063 0.116399 0.048770 -0.082904 -0.019431 0.950521 -0.083442 -0.214188
(OH + benzene) 3	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0912973 ZPE (hartree): 0.1135330 Relative energy, scaled, w/ZPE (kcal/mol): -14.73 <S^2>: 0.786 Rotational constants (GHz): 4.8484 2.6350 1.8517	105.06 286.69 391.56 398.7 442.14 533.17 584.26 617.19 704.33 759.19 809.4 865.94 946.67 972.21 977.59 989.88 1023.3 1030.5 1120.1 1168.4 1190.8 1235 1306.8 1356.6 1399.2 1409.4 1449.7 1541.9 1594.8 2967.1 3154.7 3157.5 3178 3178.4 3194.4 3794.5	C C C C C C H H H H O H H H	0.203406 1.013549 0.203609 -1.128548 -1.825544 -1.128950 -1.667825 -2.882654 -1.668192 0.741769 2.175134 1.838689 0.740731 1.471278	1.251276 0.000266 -1.251391 -1.225779 -0.000276 1.225885 -2.157883 -0.001020 2.158059 -2.188431 -0.000073 0.001049 2.188796 0.000130	0.241056 0.417876 0.241478 -0.049827 -0.190529 -0.049673 -0.185170 -0.425752 -0.184303 0.333341 -0.449752 -1.353825 0.333263 1.418174
(OH + benzene) 3-4_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0855436 ZPE (hartree): 0.1123910	-299.73 96.361 295.87 399.47 441.97 530.48 583.62 615.68 700.79 752.19 806.8 874.98 947.45 968.35 976.85 991.76 1010.2 1024.6 1118.6 1169.8 1193.5 1221.6 1308.6 1330.6 1376.1 1437.2 1453 1545.1 1599.3 2896.2	C C C C C C H	-0.180631 -1.009718 -0.219645 1.112651 1.827657 1.150323 1.638523	-1.260438 -0.024504 1.238779 1.236993 0.024541 -1.212220 2.179061	0.225558 0.415571 0.242771 -0.048357 -0.197838 -0.059366 -0.165053

	Relative energy, scaled, w/ZPE (kcal/mol): -11.81 <S^2>: 0.787 Rotational constants (GHz): 4.8416 2.6485 1.8509	3141.5 3158.7 3166.1 3182.5 3194.6 3823.7	H H H O H H H	2.885082 1.703777 -0.754839 -2.137086 -2.321347 -0.704360 -1.433977	0.043150 -2.135417 2.175074 -0.103461 0.788702 -2.206550 -0.035238	-0.431009 -0.196505 0.376355 -0.497895 -0.808287 0.301487 1.436141
(OH + benzene) 4	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0866183 ZPE (hartree): 0.1128650 Relative energy, scaled, w/ZPE (kcal/mol): -12.2 <S^2>: 0.787 Rotational constants (GHz): 4.9037 2.6275 1.8358	99.747 223.72 301.4 403.23 436.51 530.22 584.6 613.17 703.46 747.66 803.54 873.16 953.17 968.05 975.39 991.73 1016.2 1028.8 1117.5 1166.8 1193.3 1211.1 1310.4 1346 1376.9 1423.9 1456.5 1544.6 1599.1 2874 3147.8 3159.7 3167.5 3183.9 3194.6 3814.3	C C C C C C H H H H O H H H	-0.186882 -1.003918 -0.205770 1.131692 1.842206 1.151482 1.663980 2.904686 1.699642 -0.744375 -2.123741 -2.767743 -0.723325 -1.415806	-1.253087 -0.011826 1.247747 1.234392 0.014770 -1.215246 2.170826 0.022564 -2.143746 2.187064 -0.087239 0.573796 -2.192546 -0.020542	0.207612 0.392423 0.205212 -0.056483 -0.172390 -0.044702 -0.188765 -0.382103 -0.166063 0.287264 -0.523261 -0.247914 0.273430 1.420203
(OH + benzene) 4-7_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0279118 ZPE (hartree): 0.1108650 Relative energy, scaled, w/ZPE (kcal/mol): 23.42 <S^2>: 0.779 Rotational constants (GHz): 4.3601 2.8612 2.4803	-657.33 188.07 221.32 274.74 461.89 509.18 593.42 642.53 683.89 739.09 756.06 796.43 865.17 900.08 911.27 950.99 1030.6 1049.1 1110.5 1122.3 1158 1186.4 1294.4 1318.5 1378.3 1397.5 1409.4 1437.2 1549.5 3041.7 3153.8 3164.3 3172.3 3178.7 3203.7 3814.1	C C C C C C H H H H O H H H	-0.191812 -1.216420 -0.193973 1.025814 1.589496 0.991167 1.576414 2.439690 1.336243 -0.478893 -1.590490 -1.769236 -0.321974 -2.083953	-0.877458 0.009684 1.089758 1.153048 -0.086234 -1.168414 2.085376 -0.145142 -2.188059 1.861178 -0.222910 0.635379 -1.306694 0.118943	0.853777 0.302240 0.602709 -0.087106 -0.531235 0.038460 -0.151302 -1.198228 -0.086820 1.310413 -1.038776 -1.437735 1.841587 0.959209

(OH + benzene) 4-9_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0443806 ZPE (hartree): 0.1062210 Relative energy, scaled, w/ZPE (kcal/mol): 10.27 <S^2>: 0.774 Rotational constants (GHz): 5.3822 2.5557 1.7795	-965.88 208.72 302.72 368.38 420.48 483.96 502.18 529.49 624.59 643.79 682.08 769.11 809.15 827.74 898.67 963.75 983.42 1002.7 1035.1 1094.1 1174 1185 1191.8 1264.5 1337.8 1370.1 1492.8 1510.6 1596.1 1623 3158.5 3170 3178 3193.1 3201.2 3829.1	C C C C C C H H H H O H H H	-0.199051 -0.931307 -0.230267 1.154630 1.872717 1.184174 1.681935 2.955832 1.736973 -0.790922 -2.281217 -2.694111 -0.751117 -0.994239	-1.228564 -0.018576 1.212011 1.219299 0.020762 -1.196589 2.166165 0.034904 -2.128836 2.140922 -0.106445 0.736280 -2.159740 0.011811	-0.021189 0.071558 -0.034681 -0.030785 -0.012847 -0.026426 -0.061173 -0.016495 -0.055147 -0.060174 -0.163697 0.051503 -0.040194 1.817472
(OH + benzene) 5	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0740579 ZPE (hartree): 0.1103620 Relative energy, scaled, w/ZPE (kcal/mol): -5.838 <S^2>: 0.757 Rotational constants (GHz): 5.6535 1.4165 1.1385	42.544 52.264 63.727 118 215.61 307.57 409.08 429.84 600.47 622.83 675.1 730.09 825.66 910.78 977.52 987.63 999.63 1016.4 1050 1073.9 1175.8 1176.2 1302.2 1322.3 1462 1469.3 1573.2 1626.8 1648.4 3157.5 3164.7 3175.7 3184.6 3190.2 3810.2 3895.7	C C C C C C H H H H O H H H	0.403011 0.391730 -0.724055 -1.963630 -2.018810 -0.848909 -2.878490 -2.981651 -0.900374 -0.665566 3.550717 3.128733 1.330282 3.125299	-0.755591 0.619451 1.421611 0.765916 -0.627796 -1.386976 1.349160 -1.125845 -2.470698 2.504267 -0.000964 0.422130 -1.315936 0.424952	-0.000235 -0.000232 -0.000049 0.000148 0.000151 -0.000043 0.000299 0.000302 -0.000050 -0.000060 -0.000205 0.754890 -0.000394 -0.751789
(OH + benzene) 7	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0512091 ZPE (hartree): 0.1122500 Relative energy, scaled, w/ZPE (kcal/mol): 9.645 <S^2>: 0.775	102.26 209.09 245.47 457.56 524.21 575.13 692.99 706.22 736.24 742.04 793.27 820.58 921.49 925.98 947.79 998.17 1019.6 1056.2 1062.6 1091.7 1102.8 1212.8 1285.6 1295.2 1320.9 1333.2 1401.1 1402.3 1473.9 3087.5 3144 3153.4 3188.4 3207.2 3220 3815.4	C C C C C C H H H H	0.130309 1.300889 0.130038 -0.980925 -1.580372 -0.979231 -1.253536 -2.378734 -1.230034 0.342453	0.824952 0.031543 -0.708545 -1.145584 -0.038763 1.136331 -2.179754 -0.088124 2.136747 -1.229773	0.806180 0.251187 0.909295 0.033741 -0.560786 -0.125085 -0.128189 -1.290782 -0.449140 1.836506

	Rotational constants (GHz): 4.4953 2.7937 2.6966		O H H H	1.525279 1.658067 0.329181 2.206120	0.015277 -0.898408 1.466873 0.070623	-1.121851 -1.394189 1.657402 0.856010
(OH + benzene) 7-8_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0328169 ZPE (hartree): 0.1107800 Relative energy, scaled, w/ZPE (kcal/mol): 20.29 <S^2>: 0.785 Rotational constants (GHz): 4.6242 2.6291 2.3729	-453.33 140.51 219.96 362.73 410.47 520.19 540.07 626.55 696.69 735.05 799.01 811.36 823.12 912.2 938.03 940.59 1020 1041 1097.1 1110.9 1159.7 1219.8 1246.4 1293.3 1306.7 1369 1410.8 1452.4 1546.8 3037.9 3167.2 3188.1 3206.7 3223.7 3231 3822.1	C C C C C C H H H H O H H H	-0.187293 -1.404311 0.399499 1.372641 1.506798 0.632601 1.919594 2.188033 0.481757 0.153137 -1.739383 -2.287449 -0.338040 -2.121577	0.130388 0.335498 1.230557 0.679505 -0.716855 -1.067414 1.204446 -1.394134 -2.053270 2.275321 -0.601316 -0.191453 0.305777 1.113774	1.016267 0.169168 0.165736 -0.656150 -0.342684 0.639415 -1.427204 -0.842861 1.054678 0.280255 -0.758392 -1.435532 2.084802 0.402486
(OH + benzene) 8	Theory: B3LYP/6-311G(d,p) Energy (hartree): -308.0478501 ZPE (hartree): 0.1118450 Relative energy, scaled, w/ZPE (kcal/mol): 11.51 <S^2>: 0.753 Rotational constants (GHz): 5.2686 2.1763 1.9587	86.215 117.63 267.08 353.93 366.57 534.43 611.82 643.8 703.65 719.05 808.21 842.3 873.99 949.2 953.74 988.2 1008.2 1021.3 1107.5 1117 1178.6 1194.9 1233.7 1301.2 1316.7 1391.6 1439.7 1557.4 1643 2983 3115.9 3183.6 3196 3215.7 3223.3 3846.1	C C C C C C H H H H O H H H	-0.227010 -1.678594 0.607872 1.686320 1.656819 0.557344 2.466405 2.413546 0.244471 0.339960 -1.953773 -2.898413 -0.179346 -2.372940	0.104253 0.084211 1.211076 0.673324 -0.787614 -1.137512 1.214817 -1.461796 -2.135899 2.257644 -0.204050 -0.102638 0.229987 0.743855	0.778985 0.418711 0.146545 -0.446012 -0.280997 0.406063 -0.966643 -0.661655 0.678255 0.196982 -0.893977 -1.042737 1.872545 0.935291
(OH + benzene) 1 benzene	Theory: B3LYP/6-311G(d,p) Energy (hartree): -232.3085405	412.46 412.97 622.97 623.07 688.81 723.27 862.26 862.67 981.32 981.6 1013.4 1016.6 1023.4 1059.9 1060.4 1174.7 1197.5 1197.6 1335.3 1381.7	C C C C	0.869098 1.378263 0.509165 -0.869066	-1.089673 0.207767 1.297390 1.089697	-0.000036 0.000032 0.000004 -0.000034

	ZPE (hartree): 0.1001780 Relative energy, scaled, w/ZPE (kcal/mol): N/A <S^2>: 0 Rotational constants (GHz): 5.7106 5.7099 2.8551	1512.5 1513.1 1637.2 1637.8 3155.8 3165.3 3165.5 3181.1 3181.3 3191.8	C C H H H H H H	-1.378257 -0.509204 -1.545210 -2.450525 -0.905301 0.905333 1.545199 2.450510	-0.207826 -1.297364 1.937462 -0.369473 -2.306853 2.306842 -1.937472 0.369553	0.000029 0.000005 0.000053 -0.000061 0.000016 0.000005 0.000041 -0.000054
(OH + benzene) H	Theory: B3LYP/6-311G(d,p) Energy (hartree): -0.5021559 ZPE (hartree): 0.0000000 Relative energy, scaled, w/ZPE (kcal/mol): N/A <S^2>: 0.75 Rotational constants (GHz): 0.0000 0.0000 0.0000 CBS-QB3 Energy (hartree): -0.499818	N/A	H	0.000000	0.000000	0.000000
(OH + benzene) H_2O	Theory: B3LYP/6-311G(d,p) Energy (hartree): -76.4474480 ZPE (hartree): 0.0213160 Relative energy, scaled, w/ZPE (kcal/mol): N/A	1638.2 3810.7 3907.9	O H H	0.000000 0.757120 -0.757120	0.118670 -0.474679 -0.474679	0.000000 0.000000 0.000000

	$<S^2>$: 0 Rotational constants (GHz): 801.9134 437.3937 283.0226					
(OH + benzene) OH	Theory: B3LYP/6-311G(d,p) Energy (hartree): -75.7545274 ZPE (hartree): 0.0084400 Relative energy, scaled, w/ZPE (kcal/mol): N/A $<S^2>$: 0.752 Rotational constants (GHz): 0.0000 560.4914 560.4914 CBS-QB3 Energy (hartree): -75.64972	3704.7	O H	0.000000 0.000000	0.000000 0.000000	0.108357 -0.866857
(OH + benzene) 9 phenoxy	Theory: B3LYP/6-311G(d,p) Energy (hartree): -306.9068598 ZPE (hartree): 0.0911780 Relative energy, scaled, w/ZPE (kcal/mol): N/A $<S^2>$: 0.788 Rotational constants (GHz):	190.65 379.51 445.74 483.98 531.37 597.54 656.34 802.12 803.94 805.05 928.12 983.91 987.72 999.85 1008.8 1088.6 1163.2 1164.6 1271.6 1336.6 1418.7 1442.8 1480.2 1546.2 1587.1 3165.5 3171.8 3187.3 3195.1 3198.3	C C C C C C O H H H H H	-0.288981 1.085679 1.782219 1.085679 -0.288981 -1.048571 -2.300041 -0.856681 1.642609 2.866209 1.642609 -0.856681	1.237850 1.223510 0.000000 -1.223510 -1.237850 0.000000 0.000000 2.160890 2.153980 0.000000 -2.153980 -2.160890	0.000129 0.000039 -0.000121 0.000059 0.000139 -0.000461 0.000049 0.000489 0.000109 -0.000181 0.000139 0.000369

	5.5253 2.7889 1.8534					
(OH + benzene) 6 phenyl radical	Theory: B3LYP/6-311G(d,p) Energy (hartree): -231.6194243 ZPE (hartree): 0.0870270 Relative energy, scaled, w/ZPE (kcal/mol): N/A <S^2>: 0.757 Rotational constants (GHz): 6.2967 5.6215 2.9700	400.83 426.76 601.79 620.31 673.26 721.29 812.8 892.18 964.35 988.68 992.85 1016.4 1049.4 1072.8 1175 1175.8 1301.7 1323.6 1462.5 1470.4 1574.7 1629.3 3155.3 3161 3173.5 3175.9 3187.7	C C C C C C H H H H H	-1.223869 -0.000003 1.223873 1.211875 -0.000003 -1.211871 2.150419 0.000008 -2.150425 2.157649 -2.157659	-0.770644 -1.395903 -0.770637 0.631400 1.321976 0.631409 1.176021 2.405944 1.176013 -1.321801 -1.321785	-0.000011 0.000003 0.000009 -0.000010 0.000002 0.000006 -0.000013 0.000006 0.000013 0.000008 -0.000004
OH + Bi-layer						
(OH + Bi-layer) 2	Theory: M062X/6-311G(d,p) Energy (hartree): -539.6196977 ZPE (hartree): 0.2078280 Relative energy, scaled, w/ZPE (kcal/mol): -3.09 <S^2>: 0 Rotational constants (GHz): 1.4347 0.5491 0.5302	25.323 49.562 58.38 69.726 100.61 135.99 238.39 346.11 408.32 412.36 415.72 421.75 515.82 538.27 620.87 622.19 632.85 697.29 700.01 720.71 767.5 836.84 840.06 874.27 882.36 898.84 978.65 998.81 1002.8 1005.6 1015 1016.5 1031.1 1032.5 1062.2 1077.1 1079.9 1109.8 1177.6 1180 1199.7 1207.6 1209.7 1217.3 1311.8 1339.3 1353.9 1375.9 1385.7 1520.7 1527.7 1530.3 1552.8 1673.4 1676.8 1677.5 1693.6 3181.9 3186.6 3193.5 3199.4 3200.9 3206.3 3209.8 3214.7 3217.2 3224.2 3226.7 3912.9	C C C C C C H H H H H H C C H C H C H C	0.456136 0.786114 1.746198 2.383301 2.066090 1.105323 -0.308149 0.279717 2.011376 2.568036 0.856886 -1.454703 -1.727433 -1.071410 -0.283930 -1.414562 -0.896953 -2.409751 -2.674545 -3.060716	1.119122 -0.196786 -0.879157 -0.240856 1.078947 1.752374 1.638553 -0.703519 -1.905382 1.574949 2.776473 -2.588431 -1.572335 -0.925002 -1.433929 0.380467 0.887945 1.042008 2.061360 0.397091	1.345574 1.654742 0.921152 -0.139786 -0.452962 0.293166 1.909264 2.468004 1.144104 -1.278583 0.039118 0.166746 -0.094621 -1.137304 -1.681184 -1.467572 -2.273405 -0.754080 -1.010857 0.291756

			H	-3.835341	0.911991	0.848300
			C	-2.719204	-0.911574	0.621471
			H	-3.227309	-1.415428	1.435752
			O	3.305338	-0.958439	-0.841035
			H	3.681695	-0.402874	-1.528195
(OH + Bi-layer) 2-3_TS	Theory: M062X/6-311G(d,p) Energy (hartree): -539.4595781 ZPE (hartree): 0.2024110 Relative energy, scaled, w/ZPE (kcal/mol): 93.99 <S^2>: 0 Rotational constants (GHz): 1.5503 0.4935 0.4812	-557.24 9.4077 36.774 48.622 51.801 74.325 108.32 185.8 336.53 398.91 407.26 411.61 461.66 511.3 561.12 615.98 617.94 660.33 688.49 719.64 723.71 728.09 811.51 846.76 867.22 876.46 938.36 944.04 986.56 992.07 995.94 999.46 1016.1 1024.8 1034.2 1060 1069.7 1071.8 1118.3 1128 1153 1162.7 1191.8 1199.3 1201.1 1277.7 1334.3 1336.2 1370.9 1409.3 1497.2 1518.9 1521.7 1580 1626.3 1670.2 1676.6 3084.2 3171.9 3177.9 3186.7 3192.9 3195 3202.7 3205.3 3211 3229.1 3235.4 3889.8	C	0.415000	1.526829	0.540726
			C	1.238677	0.913251	1.414258
			C	2.522805	0.423623	0.813966
			C	2.283289	-0.669270	0.009620
			C	2.006334	0.614607	-0.876806
			C	0.961460	1.496243	-0.784958
			H	-0.570774	1.903083	0.784350
			H	1.011063	0.677047	2.445601
			H	3.507138	0.736918	1.175293
			H	2.706050	0.605412	-1.703662
			H	0.622063	2.098961	-1.615354
			H	-2.497274	-1.094960	2.263343
			C	-2.380973	-0.806330	1.225145
			C	-1.329744	-1.320102	0.472808
			H	-0.606811	-1.988625	0.924462
			C	-1.177692	-0.944356	-0.856975
			H	-0.333786	-1.318195	-1.424634
			C	-2.079069	-0.057617	-1.437399
			H	-1.956861	0.238350	-2.473014
			C	-3.128212	0.460735	-0.684852
			H	-3.829267	1.154317	-1.134725
			C	-3.278503	0.086855	0.647602
			H	-4.095882	0.489978	1.234260
			O	3.335978	-1.465786	-0.304596
			H	3.036285	-2.122810	-0.937966
(OH + Bi-layer) 3	Theory: M062X/6-311G(d,p) Energy (hartree): -539.4869670 ZPE (hartree): 0.2049050 Relative energy, scaled, w/ZPE (kcal/mol): 78.37 <S^2>: 0	37.208 49.002 54.388 64.022 71.454 79.852 110.95 140.34 337.06 409.27 414.9 446.76 499.3 569.99 619.9 622.31 692.27 721.47 741.55 747.2 807.77 826.97 837.67 870.63 881.03 951.94 970.31 976.68 994.78 1004.8 1011.9 1015.4 1027.6 1032.6 1033.1 1035.4 1079.3 1081.9 1114.3 1118.5 1175.2 1177 1206.6 1212.7 1257.2 1310.9 1341.4 1343.8 1352.1 1386.8 1413.1	C	0.364834	1.241828	1.041171
			C	1.280393	0.368722	1.491157
			C	2.429977	0.301228	0.528570
			C	2.342165	-0.986641	-0.264345
			C	2.052113	1.330410	-0.511552
			C	0.847293	1.841426	-0.202474
			H	-0.599638	1.448003	1.487210
			H	1.198920	-0.262431	2.364655
			H	3.422010	0.461529	0.966288
			H	2.664169	1.559362	-1.372008

	Rotational constants (GHz): 1.4779 0.4837 0.4502	1529.7 1531.4 1569.4 1662 1675 1678.8 3072.9 3179.2 3189 3193.9 3205.4 3206.5 3209.6 3217.1 3218.2 3236 3247.4 3843	H H C C H C H C H C H C H O H	0.306007 -2.002963 -2.120236 -1.229107 -0.390214 -1.377551 -0.665105 -2.411355 -2.526292 -3.297251 -4.101350 -3.152773 -3.843846 3.577839 3.544576	2.583237 -2.150476 -1.391974 -1.338680 -2.021085 -0.361363 -0.309816 0.565210 1.327339 0.517735 1.240923 -0.463524 -0.502932 -1.369098 -2.167136	-0.775038 1.499336 0.733733 -0.332622 -0.387247 -1.311097 -2.126070 -1.220422 -1.983174 -0.147370 -0.074787 0.829046 1.663145 -0.502787 -1.042780
(OH + Bi-layer) 4	Theory: M062X/6-311G(d,p) Energy (hartree): -539.4833951 ZPE (hartree): 0.2047230 Relative energy, scaled, w/ZPE (kcal/mol): 80.49 <S^2>: 0 Rotational constants (GHz): 1.7312 0.3588 0.3247	16.042 26.592 42.549 51.646 75.193 88.072 96.216 182.05 292.23 413.63 417.15 434.77 541.91 620.24 620.41 666.2 702.03 715.11 726.21 740.75 786.83 821.17 861.38 879.21 888.01 918.97 970.48 984.94 994.73 1004.8 1010.4 1015.7 1017.4 1034.3 1041.2 1043.3 1074.4 1080.4 1108.3 1113.4 1168.2 1172.2 1202.4 1207.1 1230.5 1305.4 1340.1 1358.3 1369.4 1379.7 1406.2 1523.9 1528.1 1585.8 1667.8 1674.4 1679.1 3052.1 3175.9 3183.1 3189.2 3197.8 3203.4 3209.7 3209.9 3221 3240.8 3248.5 3814.8	C C C C C C H H H H H H C C H C H C H C H O H	2.047596 1.709860 2.754532 2.392834 3.746767 3.313652 1.483788 0.821673 3.265453 4.636439 3.815336 -3.353833 -3.133782 -1.839123 -1.043729 -1.555929 -0.542241 -2.571632 -2.352600 -3.866806 -4.657323 -4.148031 -5.156688 1.134765 0.905978	1.554788 0.302838 -0.650921 -1.721572 0.264173 1.528727 2.451047 0.002630 -1.173981 -0.095327 2.403390 -1.884025 -1.023790 -0.809401 -1.500209 0.295657 0.454384 1.185351 2.046665 0.971224 1.664785 -0.133176 -0.298804 -1.555573 -2.209365	0.641656 0.986189 0.480318 -0.528851 -0.209770 -0.105869 0.865017 1.524806 1.302076 -0.704666 -0.497758 1.379087 0.757532 0.295673 0.550475 -0.502079 -0.851042 -0.837659 -1.458056 -0.376964 -0.638598 0.421046 0.780939 -0.856385 -1.528524

(OH + Bi-layer) 1 benzene	Theory: M062X/6-311G(d,p) Energy (hartree): -232.1961506 ZPE (hartree): 0.1009610 Relative energy, scaled, w/ZPE (kcal/mol): N/A <S^2>: 0 Rotational constants (GHz): 5.7316 5.7311 2.8657	407.8 413.39 618.21 618.97 693.43 723.95 870.68 883.02 998.51 1007 1016.1 1032.9 1033.7 1072.2 1074.1 1167.5 1200.2 1200.9 1333.8 1376.8 1523.1 1525.2 1674.2 1676.8 3175.5 3180.1 3194.4 3200.4 3209 3214.7	C C C C C C H H H H H H	0.939731 1.358145 0.418450 -0.939732 -1.358145 -0.418451 1.671620 2.416093 0.744526 -1.671609 -2.416096 -0.744518	1.025713 -0.300902 -1.326573 -1.025711 0.300904 1.326572 1.824870 -0.535647 -2.359951 -1.824880 0.535640 2.359955	-0.000009 -0.000027 -0.000005 -0.000011 -0.000027 -0.000002 0.000104 0.000003 0.000138 0.000105 0.000007 0.000123
(OH + Bi-layer) 1 phenol	Theory: M062X/6-311G(d,p) Energy (hartree): -307.4173554 ZPE (hartree): 0.1056000 Relative energy, scaled, w/ZPE (kcal/mol): N/A <S^2>: 0 Rotational constants (GHz): 5.6955 2.6365 1.8022	233.67 376.67 414.55 422.79 520.02 537.23 630.84 704.39 773.66 840.96 841.77 905.2 983.97 1006.4 1017.5 1059.8 1107.1 1175.2 1193.2 1214.1 1315.1 1355.1 1371.5 1520.1 1550.5 1683.5 1693.1 3174.7 3190.2 3196.2 3211.8 3218.7 3913.4	C C C C C C H H H H H O H	1.849521 1.166292 -0.220153 -0.937423 -0.263482 1.127236 2.931761 1.718869 -0.769202 -0.825166 1.644723 -2.295367 -2.669996	0.027634 -1.186018 -1.218569 -0.023860 1.194458 1.213993 0.046247 -2.118109 -2.151752 2.123542 2.165921 -0.110671 0.773687	0.000014 0.000019 -0.000032 -0.000044 -0.000019 0.000006 0.000045 0.000012 -0.000085 -0.000040 -0.000001 0.000057 -0.000052
OH + phenanthrene radical						
(OH + phen. rad.) 1 phenanthrene rad.	Theory: B3LYP/6-311G(d,p) Energy (hartree): -538.9768311 ZPE (hartree): 0.1806060 <S^2>: 0.758	99.663 116.17 222.14 225.65 247.91 406.89 410.22 447.55 451.16 494.86 500.23 555.45 555.91 588.13 629.11 706.77 720.95 725.21 743.07 770.15 802.63 828.08 835.76 884.47 889.2 889.27 963.08 968.29 981.43 996.58 1012.8 1050.4 1065.2 1099.6 1162.5 1172.1 1179.7 1190 1230.6 1243 1281.7	C C C C C C H H	3.539185 2.858944 1.479556 0.728306 1.414009 2.826567 3.421399 0.952837	-0.319849 -1.551187 -1.583017 -0.389252 0.855603 0.860690 -2.478030 -2.530807	0.000077 0.000037 -0.000070 -0.000039 0.000048 0.000075 0.000067 -0.000095

	Rotational constants (GHz): 1.6504 0.5540 0.4148 CBS-QB3 Energy (hartree): -537.839563	1314.3 1355.2 1367.4 1424 1431.8 1450.2 1476.4 1515.6 1533.5 1585.6 1637.5 1650.6 1655.7 3155.4 3159.1 3159.7 3167.1 3169.8 3174.8 3178.1 3182.5 3189.2	H H C C C C H H C C C C H H H	4.623153 3.345972 -0.719430 -1.441036 -0.700264 0.658181 -1.253453 1.200481 -1.507020 -2.865732 -3.558579 -2.854954 -3.405285 -4.643265 -3.388233	-0.301201 1.813398 -0.394105 0.841191 2.069652 2.075425 3.003200 3.015235 -1.541281 -1.603599 -0.368318 0.818459 -2.544158 -0.363195 1.763080	0.000124 0.000140 -0.000111 -0.000104 -0.000108 -0.000029 -0.000260 0.000028 -0.000120 -0.000027 0.000165 0.000092 0.000076 0.000411 0.000203
(OH + phen. rad.) 2	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.9029022 ZPE (hartree): 0.1979190 <S^2>: 0 Rotational constants (GHz): 1.1839 0.5325 0.3673 CBS-QB3 Energy (hartree): -613.662247	60.272 93.889 194.27 226.58 254.34 288.34 346.56 358.4* 404.33 412.44 489.06 502.37 513.01 525.85 549.99 569.55 581.5 631.29 683.36 714.58 727.96 750.51 771.01 792.85 812.38 823.58 859.27 863.8 884.03 958.83 962.82 983.03 998.57 1011.1 1024.6 1073.4 1115.7 1155.9 1175.9 1189.8 1195.8 1206.6 1235 1250.4 1283 1311.2 1336.6 1362.4 1372.6 1441.6 1450.9 1473.7 1493.4 1536.7 1569.9 1607.8 1643.7 1654.2 1666.3 3141.4 3156.2 3158.9 3168.2 3170.4 3177.8 3185.1 3189.3 3276.2 3825.9	C C C C C C H H C C C C H H H O H	3.646447 2.892586 1.511311 0.800847 1.580994 2.990862 3.395361 0.966673 4.729894 3.552505 -0.657463 -1.249368 -0.411903 0.937438 -0.892543 1.558863 -1.567917 -2.940880 -3.489025 -2.650487 -3.594075 -4.565401 -3.051940 -1.079566 -1.823450	-0.326611 -1.508853 -1.471125 -0.244131 0.954170 0.884449 -2.469756 -2.398812 -0.366157 1.812926 -0.131305 1.171392 2.334512 2.232489 3.306805 3.121930 -1.229389 -1.033889 0.252138 1.342223 -1.902395 0.378589 2.349064 -2.508583 -3.119963	0.000147 0.000413 0.000291 -0.000076 -0.000198 -0.000155 0.000758 0.000526 0.000280 -0.000379 -0.000115 0.000036 -0.000063 -0.000253 0.000011 -0.000325 -0.000208 0.000069 0.000360 0.000267 0.000091 0.000494 0.000414 -0.000613 -0.000060

	*Vibration replaced by unsymmetrical hindered rotor (hrd 2 4 1). The same representation of the hindered rotor potential was also used in VariFlex	Multiwell hindered rotor parameters: Vhrd2 1 0.0 948.0 -948.0 Ihrd1 1 0.0 1.655 -0.4777 -0.4924 0.595662				
(OH + phen. rad.) 2-3_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7500511 ZPE (hartree): 0.1937850 <S^2>: 0 Rotational constants (GHz): 1.0823 0.5910 0.4065	-498.39 99.553 107.48 190.71 211.02 221.62 267.31 313.46 398.78 428.69 450.08 465.1 490.35 516.21 538.69 542.72 567.94 590.56 670.84 674.47 700.19 734.32 761.24 788.06 797.45 818.62 829.95 882.26 920.22 938.68 953.33 970.6 971.43 980.97 993.9 1021.8 1059.8 1112.8 1125.8 1140.2 1166.7 1183.6 1186.6 1231.1 1246.2 1282 1305.9 1337.6 1363.5 1371.6 1397.8 1454.8 1482.6 1513.4 1551.1 1558.5 1600.9 1622.7 1650.5 3047.7 3157.8 3161.4 3169.5 3180.7 3184.9 3187.2 3207.6 3214.9 3795.8	C C C C C C H H H H C C C C C H H H O H	3.483530 2.707639 1.333139 0.661079 1.449577 2.861802 3.192946 0.758208 4.564579 3.448430 -0.781465 -1.349734 -0.542172 0.823322 -1.013342 1.449554 -1.624543 -2.046675 -3.146164 -2.759156 -1.897830 -4.166024 -3.426956 -1.077614 -0.709738	-0.292522 -1.452761 -1.397565 -0.181001 1.006268 0.906156 -2.397671 -2.301868 -0.345737 1.809072 -0.052301 1.253208 2.391564 2.271449 3.367344 3.148052 -1.338972 -1.037221 -0.015265 1.210731 -1.665178 -0.329676 2.049871 -2.552598 -2.544033	-0.212940 -0.401593 -0.312661 -0.044379 0.120899 0.043315 -0.619011 -0.452190 -0.275864 0.178098 0.081788 0.076566 0.250421 0.307667 0.306324 0.428903 0.610421 -0.679240 -0.601820 -0.196524 -1.563432 -0.786056 -0.047935 0.854227 1.745824
(OH + phen. rad.) 2-5_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8375810 ZPE (hartree): 0.1924100 <S^2>: 0 Rotational constants (GHz): 1.1655 0.5590	-1224.8 89.942 140.91 214.59 228.21 270.03 329.27 382.16 410.34 441.42 481.48 496.23 511.77 545.86 563.97 567.39 575.18 626.77 681.99 707 727.65 748.41 773.82 787.91 811.76 841 856.35 881.2 901.69 946.38 980.93 988.65 996.13 997.84 1030.6 1059.7 1086.3 1116.5 1164.1 1184 1187.1 1203 1243.7 1263.4 1293.7 1345.5 1370.4 1384.7 1396 1436.4 1450 1468.8 1475.7 1509 1547.6 1588.2 1594.7 1626.2 1658.3	C C C C C C H H H H C	-3.527189 -2.855549 -1.443340 -0.734362 -1.487812 -2.855969 -3.390913 -1.214015 -4.587039 -3.421812 0.670912	-0.282437 -1.435068 -1.420607 -0.142630 1.059232 0.958386 -2.374903 -1.972058 -0.305211 1.869468 -0.107585	-0.281427 0.033290 0.327643 0.206211 0.004336 -0.236147 0.114851 1.251465 -0.506391 -0.405235 0.176844

	0.3821	1878.1 3000.3 3158 3159.2 3161 3171.3 3177.6 3180.3 3189.4 3195.6	C C C H H C C C C H H H O H	1.353319 0.562428 -0.789687 1.081401 -1.367126 1.410334 2.814339 3.451379 2.739905 3.364880 4.531249 3.261492 0.814346 -0.625122	1.154868 2.357878 2.317412 3.310640 3.231887 -1.348025 -1.237456 -0.014533 1.183180 -2.154942 0.024820 2.133334 -2.481903 -2.163502	0.128708 0.126442 0.026646 0.134034 -0.057280 -0.023100 -0.229052 -0.155407 0.012751 -0.396701 -0.257135 0.007428 -0.047840 -0.208750
(OH + phen. rad.) 2-7_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8028751 ZPE (hartree): 0.1915140 <S^2>: 0 Rotational constants (GHz): 1.2046 0.5236 0.3675	-2165.7 82.512 100.78 195.96 212.02 217.01 288.48 368.47 401.67 406.99 469.76 481.81 496.77 539.55 551.56 561.16 597.78 627.18 679.37 702.04 716.45 752.31 770.46 805.61 817.03 841.15 852.27 866.8 893.86 962 971.81 990.68 998.08 1010.1 1034.1 1061.3 1083.4 1136.6 1154.5 1178.4 1184.4 1184.6 1220.7 1239.2 1258.1 1304.9 1364.8 1381.6 1389.6 1414.1 1452.5 1463.1 1485.3 1517.5 1532.6 1572.5 1617.3 1640.7 1657.6 1807.8 3077 3158.4 3161.2 3165.5 3171.6 3179.1 3184.2 3187.3 3214.5	C C C C C C C H H H H C C C C C H H C C C C H H H O H	-3.656533 -2.873935 -1.496604 -0.837283 -1.632357 -3.042019 -3.359443 -0.902313 -4.738085 -3.632659 0.598655 1.212893 0.373863 -0.984819 0.841244 -1.602623 1.511402 2.930173 3.487655 2.644229 3.317001 4.558214 3.034181 1.301874 2.657573	-0.396678 -1.566897 -1.498082 -0.245837 0.938283 0.834305 -2.536135 -2.401306 -0.467750 1.744288 -0.112931 1.166477 2.318727 2.208171 3.295342 3.099818 -1.213716 -1.049206 0.269738 1.329267 -1.672834 0.420708 2.337209 -2.429812 -2.270577	0.064512 0.081792 0.060974 0.023804 -0.005224 0.018051 0.105581 0.058226 0.080492 -0.001149 0.039126 -0.020872 -0.088222 -0.066767 -0.147949 -0.103078 0.003212 0.221428 0.108073 -0.037468 1.032366 0.193399 -0.122120 -0.381153 -0.461048

(OH + phen. rad.) 2-18_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7158495 ZPE (hartree): 0.1915290 <S^2>: 0 Rotational constants (GHz): 0.9431 0.5772 0.3593	-252.74 45.326 98.014 160.2 169.08 196.36 214.02 254.44 334.94 412.34 420.29 445.19 475.99 488.24 493.96 500.5 548.33 557.04 574.45 578.47 684.99 703.22 719 736.66 760.34 803.41 806.93 822.86 837.23 866.98 896.05 905.04 959.76 969.29 981.15 1001.9 1029.4 1058.5 1093.3 1159.5 1165.6 1179.8 1208.1 1229.3 1250.6 1308.7 1337.7 1353.6 1392.4 1426.9 1438 1479.4 1499.2 1514.7 1531.4 1614 1633.2 1649.1 1660.4 3141.9 3154.5 3156.1 3164.7 3172.1 3173.8 3181.6 3229.9 3250.6 3811.5	C C C C C C H H H H C C C C H H C C C C H H H O H	-3.472334 -2.570320 -1.216482 -0.780256 -1.646755 -3.033387 -2.978986 0.189552 -4.539043 -3.749376 0.609239 1.228737 0.330873 -1.028018 0.757044 -1.666798 1.426642 2.778187 3.385838 2.642052 3.368626 4.468647 3.147891 1.014055 0.965915	0.516933 1.617684 1.380958 0.043833 -1.067553 -0.792838 2.621843 2.823599 0.719119 -1.607373 -0.128250 -1.402987 -2.527644 -2.367256 -3.525274 -3.244300 0.993731 1.008098 -0.284190 -1.445728 1.909917 -0.332339 -2.404965 3.307297 3.312644	-0.059828 -0.110710 -0.082157 -0.008998 0.032771 0.008835 -0.174333 -0.100927 -0.081609 0.039608 0.002151 0.028831 0.078598 0.084721 0.106467 0.121947 -0.059243 -0.117328 -0.094212 -0.016524 -0.175115 -0.133035 0.002197 0.145350 1.110571
(OH + phen. rad.) 2-22_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7300698 ZPE (hartree): 0.1859690 <S^2>: 0 Rotational constants (GHz): 1.1827 0.5691 0.3876	-1247.3 88.026 133.45 166.88 217.84 251.3 297.07 343.33 400.4 425.51 453.72 486.84 489.63 513.98 521.22 547.67 564.56 573.42 600.17 640.71 671.17 701.38 711.86 740.02 757.68 787.25 800.06 812.55 832.32 851.68 875 886.62 944.46 955.09 973.46 981.62 999.31 1050.8 1064.3 1079.4 1147.6 1167.3 1187.4 1198.3 1233.3 1251.6 1313.4 1324.5 1341.3 1375.2 1406.8 1443.6 1450 1453.4 1500.5 1521.2 1557.5 1599.4 1636.1 1646.3 3159.8 3160.5 3172.1 3177.9 3181.6 3188.2 3195.5 3219 3229.9	C C C C C C H H H H C C C C C C H	3.498460 2.774292 1.427611 0.706944 1.476514 2.873219 3.268080 0.545339 4.567301 3.463114 -0.706533 -1.404339 -0.615469 0.745900 -1.131348	-0.248634 -1.446262 -1.284141 -0.102678 1.093952 0.985212 -2.405157 -2.547791 -0.320129 1.888385 -0.067656 1.156933 2.360641 2.331315 3.314969	-0.201207 0.019415 0.127297 0.107575 -0.008027 -0.170964 0.085124 0.962202 -0.365812 -0.279590 0.110775 0.106375 0.111071 0.031961 0.133091

			H	1.308193	3.257771	-0.017421
			C	-1.347176	-1.337958	-0.058867
			C	-2.746608	-1.325952	-0.178620
			C	-3.446304	-0.115277	-0.101633
			C	-2.809361	1.114120	0.028525
			H	-3.269167	-2.265432	-0.309457
			H	-4.529248	-0.140891	-0.165922
			H	-3.382475	2.033962	0.034679
			O	-0.574814	-2.381295	-0.132217
			H	1.195826	-2.447024	1.438773
(OH + phen. rad.) 2-23_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7637731 ZPE (hartree): 0.1929780 <S^2>: 0 Rotational constants (GHz): 1.1420 0.5319 0.3640	-358.89 76.335 97.968 183.39 217.94 228.66 266.66 297.84 406.86 410.62 427.72 473.94 479.96 503.34 530.02 552.25 567.88 594.54 636.95 710.45 718.28 730.91 760.82 793.9 812.6 823.7 857.98 876.85 887.27 892.13 964.62 971.23 977.06 986.81 996.32 1001.1 1064.3 1085.5 1143.2 1168.7 1174.1 1187.1 1229.8 1244.3 1270.1 1310.3 1356.6 1358.4 1401.8 1439.2 1452 1471.7 1494.4 1507.6 1542.8 1586.9 1631.9 1652.8 1664.6 2511 3133.6 3154.6 3159.4 3161.7 3170.6 3179.2 3186.8 3218.6 3679	C	-3.630146	0.369332	-0.007952
			C	-2.855161	1.535310	-0.119713
			C	-1.476556	1.460651	-0.131873
			C	-0.803424	0.219969	-0.028711
			C	-1.596651	-0.964047	0.046860
			C	-3.005130	-0.856202	0.065976
			H	-3.340461	2.500736	-0.208967
			H	-0.910646	2.371641	-0.264843
			H	-4.712151	0.433995	0.005321
			H	-3.592201	-1.766345	0.131476
			C	0.641595	0.085443	-0.018360
			C	1.239370	-1.217933	-0.021009
			C	0.387405	-2.367371	0.027680
			C	-0.963721	-2.248456	0.078800
			H	0.852628	-3.347261	0.033320
			H	-1.592927	-3.130566	0.129460
			C	1.633122	1.071716	0.001565
			C	2.973046	1.053365	-0.028188
			C	3.497359	-0.264748	-0.081865
			C	2.650174	-1.356964	-0.057618
			H	2.318210	2.743771	0.083721
			H	4.570699	-0.429674	-0.123602
			H	3.056723	-2.364424	-0.064804
			O	1.278483	2.629784	0.113536
			H	0.974569	2.829478	1.017088
(OH + phen. rad.) 3	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7840160 ZPE (hartree): 0.1956300	32.259 71.003 109.18 164.1 211.22 242.56 281.04 353.36 403.89 430.18 445.61 488.56 491.74 524.41 552.62 563.46 627.75 680.07 689.52 739.69 756.58 764.48 802.93 822.81 836.41	C	3.426700	-0.879103	-0.034280
			C	2.442733	-1.864563	-0.280163
			C	1.112679	-1.525266	-0.333261
			C	0.696841	-0.180048	-0.141671
			C	1.695357	0.822546	0.103828

	<S^2>: 0 Rotational constants (GHz): 0.9726 0.5761 0.3749	852.13 878.98 895.05 952.41 962.41 972.63 977.29 990.24 995.8 998.9 1045.6 1057.2 1117.1 1157.4 1168.4 1180.7 1186.1 1229.7 1239.8 1250.1 1280.9 1288.8 1346.5 1363.9 1378.2 1399 1410.4 1467 1487.2 1551.1 1579.7 1618 1633.9 1663.4 2996.8 3157.3 3160.4 3167.7 3179.2 3182 3191.7 3194 3224 3757.3	C H H H H C C C C H H C C C C H H H O H	3.058141 2.743996 0.365510 4.472521 3.810753 -0.651810 -0.999827 -0.012802 1.304124 -0.292815 2.078007 -2.139913 -1.913580 -2.986645 -2.447330 -1.893286 -4.035153 -2.988777 -2.181429 -2.317336	0.430983 -2.895522 -2.287525 -1.162081 1.190172 0.245086 1.581718 2.562251 2.177866 3.600872 2.914996 -1.426372 -0.564485 0.506034 1.711319 -1.150540 0.283777 2.645736 -2.685720 -3.241918	0.151897 -0.429322 -0.518931 0.004348 0.338576 -0.193575 -0.020500 0.226782 0.288118 0.363995 0.475616 0.809415 -0.424205 -0.421243 -0.166153 -1.353626 -0.561224 -0.087045 0.399844 1.178937
(OH + phen. rad.) 4	CBS-QB3 Energy (hartree): -613.030277					
(OH + phen. rad.) 5	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8482363 ZPE (hartree): 0.1958870 <S^2>: 0 Rotational constants (GHz): 1.1716 0.5394 0.3701	60.326 112.51 180.66 215.17 234.03 241.86 327.57 363.93 402.22 459.22 486.91 487.64 513.17 518.4 536.69 557.35 582.75 649.63 694.47 716.82 717.04 769.05 791.16 799.84 832.74 853.32 884.8 907.15 939.06 965.54 984.49 987.91 1001.1 1003.9 1033.2 1075.9 1096.4 1155.8 1175.1 1179.6 1189.2 1195.8 1231.8 1262.9 1270.6 1314.8 1369.4 1381.2 1416.2 1436.1 1452.7 1468.1 1497.9 1508.5 1586.6 1610.9 1627.8 1657.4 1680 2963 2987.4 3155.6 3158.6 3161 3169.3 3176.2 3179.5 3187.9 3193.5	C C C C C C H H H H C C C C H H C	3.614606 2.946118 1.465564 0.725606 1.509748 2.889877 3.481386 1.107048 4.698247 3.446425 -0.662736 -1.324060 -0.517272 0.832008 -1.023779 1.433678 -1.499129	-0.270675 -1.444024 -1.508473 -0.197499 1.021732 0.958904 -2.387556 -2.126843 -0.244868 1.890909 -0.128945 1.165790 2.356761 2.292013 3.316144 3.194557 -1.362106	-0.000090 0.000326 0.000224 0.000066 -0.000103 -0.000288 0.000646 -0.837735 -0.000231 -0.000502 0.000051 0.000099 0.000098 -0.000061 0.000207 -0.000175 -0.000058

			C	-2.936815	-1.171348	-0.000178
			C	-3.498551	0.071545	0.000004
			C	-2.701994	1.244880	0.000168
			H	-3.535992	-2.073862	-0.000350
			H	-4.579313	0.173941	-0.000005
			H	-3.179618	2.218097	0.000336
			O	-1.001560	-2.500621	-0.000205
			H	1.106574	-2.126885	0.837899
(OH + phen. rad.) 5-6_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7983302 ZPE (hartree): 0.1920010 <S^2>: 0 Rotational constants (GHz): 1.1872 0.5360 0.3700	-1036.8 76.582 99.09 179.39 213.81 249.51 275.24 364.92 401.82 404.09 461.44 492 510.12 526.89 550.43 559.01 564.39 634.26 672.5 714.01 719.13 751.2 757.41 794.62 813.3 833.46 849.47 857.74 875.36 971.9 983.44 985.88 993.02 994.58 1051.6 1081.2 1089.2 1113.9 1157.7 1170.9 1182.7 1209.1 1228.8 1242.3 1258.9 1267.3 1354.6 1382 1398.7 1417.8 1441 1471.2 1497.2 1509.7 1528.1 1564.3 1596.7 1615 1644.9 2166.5 3104.7 3149.6 3157.3 3166.8 3176.7 3178.8 3181 3185.6 3207.1	C	3.622182	-0.257464	-0.021170
			C	2.879881	-1.469389	-0.023590
			C	1.432262	-1.435972	-0.061670
			C	0.723586	-0.193731	-0.008801
			C	1.519875	1.006596	-0.004847
			C	2.934125	0.934167	-0.010307
			H	3.368615	-2.426182	-0.169399
			H	0.833915	-2.344391	-0.103396
			H	4.703636	-0.287042	-0.021412
			H	3.486953	1.867950	-0.003464
			C	-0.693890	-0.144186	-0.007189
			C	-1.331815	1.151196	-0.001595
			C	-0.509000	2.318937	0.005648
			C	0.854033	2.262848	0.006896
			H	-1.004682	3.284836	0.011862
			H	1.445934	3.171471	0.014700
			C	-1.517874	-1.368533	-0.003873
			C	-2.938499	-1.150737	-0.000639
			C	-3.505601	0.105864	0.001138
			C	-2.721848	1.266126	0.001095
			H	-3.553289	-2.043485	0.000404
			H	-4.587646	0.198439	0.002652
			H	-3.180659	2.247742	0.002303
			O	-1.031383	-2.528116	-0.001340
			H	2.253784	-1.598747	1.049894
(OH + phen. rad.) 5-24_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.6987468 ZPE (hartree): 0.1896640 <S^2>: 0	-179.63 31.763 48.621 79.138 137.69 175.68 182.95 205.42 282.08 300.62 398.74 410.71 428.19 474 480.57 511.3 540.84 547.98 581.45 642.15 674.4 703.29 704.43 723.53 765.67 787.97 811.18 886 898.49 909.62 928.72 961.01 970.05 993.6 996.33 1002.7 1064.7	C	3.771158	-0.926229	0.195297
			C	3.007503	-1.848604	-0.433856
			C	1.544897	-1.656243	-0.647096
			C	1.000071	-0.301904	-0.232155
			C	1.893391	0.658698	0.402132
			C	3.233587	0.347363	0.564864
			H	3.456281	-2.762734	-0.808815

	Rotational constants (GHz): 1.0144 0.3959 0.3051	1128.9 1136.6 1164.4 1181.4 1183.9 1198.3 1239 1250.1 1320.1 1357.3 1375 1406 1422.7 1429.9 1435.2 1448.1 1504.3 1537.7 1618.1 1641.8 1674.4 2207.7 2965.6 2989 3118 3136.7 3137.7 3142.7 3149.5 3160.3 3171.1 3179.9	H H H C C C C H H C C C C H H H O H	1.246161 4.832118 3.928781 -0.262760 -0.756540 0.206593 1.443015 -0.102599 2.126502 -3.242520 -3.118384 -3.221678 -2.175426 -2.924310 -4.221235 -2.399054 -3.362397 1.019089	-1.904147 -1.102483 1.142936 0.101119 1.366185 2.394855 2.023292 3.435549 2.766783 -1.483161 -0.589174 0.871325 1.702045 -0.969461 1.299287 2.754831 -2.276897 -2.402781	-1.678467 0.335607 0.816932 -0.500607 -0.284493 0.034291 0.476694 0.084152 0.873419 0.357523 -0.594313 -0.346410 -0.198221 -1.594162 -0.323131 -0.039295 1.200843 -0.034880
(OH + phen. rad.) 5-25_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7040920 ZPE (hartree): 0.1891570 <S^2>: 0 Rotational constants (GHz): 1.1148 0.5616 0.4161	-476.06 77.11 91.534 119.92 153.7 165.12 222.49 258.15 346.1 400.04 436.94 467.06 494.39 498.13 510.16 540.6 561.58 588.72 629.76 655.89 677.97 700.48 709.39 753.34 767.81 805.71 828.55 854.42 890.72 899.84 909.34 946.21 968.99 973.02 974.79 1018.3 1036.2 1097.9 1105 1133.2 1178.7 1187.6 1201.8 1230.8 1239.5 1259.3 1284.5 1314.8 1379 1386.9 1389.8 1397.1 1430.8 1464.5 1508.7 1556.9 1587.9 1604.3 1904.7 2942.1 2963.2 3059.1 3156.1 3159.5 3177 3181.7 3194.9 3198.3 3222.5	C C C C C C H H C C C C H H C C C C H H	3.512909 2.874879 1.394062 0.672420 1.387276 2.807176 3.413415 0.947415 4.593875 3.354258 -0.762746 -1.480893 -0.724780 0.657486 -1.230002 1.220880 -1.429133 -1.984779 -3.127542 -2.840102 -1.757928 -4.067190	-0.196626 -1.390792 -1.455193 -0.158541 1.042403 0.993368 -2.312779 -2.004746 -0.149018 1.927337 -0.120206 1.159354 2.296267 2.245698 3.249763 3.151300 -1.389385 -1.175082 -0.232793 1.010281 -1.917460 -0.566999	-0.253216 -0.414229 -0.297274 -0.099607 0.129981 0.002178 -0.590738 -1.141619 -0.334909 0.063535 -0.039111 0.059639 0.322297 0.396863 0.442690 0.587683 0.590523 -0.703671 -0.807861 -0.334025 -1.473005 -1.223198

			H	-3.554952	1.823151	-0.306934
			O	-1.224655	-2.111992	1.510170
			H	1.140072	-2.077138	0.580210
(OH + phen. rad.) 6	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8235691 ZPE (hartree): 0.1948880 <S^2>: 0 Rotational constants (GHz): 1.1957 0.5259 0.3660	76.904 82.707 177.3 185.34 238.89 256.37 301.19 363.25 398.82 408.06 474.27 486.92 512.63 520.07 549.65 555.22 618.16 661.64 668.45 712.9 720.65 754.38 801.66 807.12 814.73 841.73 866.9 891.7 917.69 949.05 979.15 983.74 989.04 1007.1 1024.7 1085.1 1099.3 1161.6 1167.1 1174.5 1184.6 1232.9 1240.8 1267.6 1283.7 1352.6 1361.6 1378.1 1388.3 1393.3 1440.1 1455.3 1510.3 1519.9 1525.3 1569.9 1593.2 1606.4 1671.8 2955.4 2958.3 3155.6 3159 3160.8 3168.2 3178.2 3179.9 3181.2 3188.1	C	-3.633697	-0.183837	0.000116
			C	-2.918638	-1.482559	0.000125
			C	-1.441132	-1.416179	0.000145
			C	-0.735478	-0.221563	0.000014
			C	-1.504477	1.007618	-0.000116
			C	-2.949836	0.973610	-0.000022
			H	-3.250299	-2.090538	0.860026
			H	-0.862235	-2.332464	0.000295
			H	-4.718377	-0.189612	0.000272
			H	-3.472542	1.924549	0.000006
			C	0.709672	-0.160929	-0.000045
			C	1.339615	1.121407	-0.000065
			C	0.541486	2.283412	-0.000026
			C	-0.842292	2.237154	-0.000099
			H	1.039892	3.248057	0.000027
			H	-1.419471	3.155042	-0.000078
			C	1.530036	-1.369049	-0.000095
			C	2.953744	-1.137095	0.000223
			C	3.537009	0.123321	0.000232
			C	2.749601	1.263724	-0.000069
			H	3.568832	-2.030423	0.000344
			H	4.618772	0.211649	0.000419
			H	3.186275	2.255091	0.000007
			O	1.068206	-2.536901	-0.000406
			H	-3.250188	-2.090352	-0.859976
(OH + phen. rad.) 6-27_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.6933559 ZPE (hartree): 0.1895880 <S^2>: 0 Rotational constants (GHz): 0.9979 0.4139 0.3282	-92.637 37.492 44.939 102.18 130.3 161.63 191.67 261.9 286.83 350.91 396.44 425.2 437.69 446.72 475.9 495.8 536.65 545.72 595.81 654.26 676.79 688.73 728.08 750.1 776.81 796.16 809.69 847.55 891.66 896.54 932.34 951.07 962.75 982.45 995.3 996.54 1037.4 1124 1127.6 1164.8 1178.2 1191.1 1223.5 1243.8 1267.2 1300 1346.7 1368.1 1384.4 1407.3 1408.1 1425.4 1433.9 1519.7 1559.4 1586 1667.3 1677.6 2202.6 2955 2963.7	C	3.651731	-0.822537	0.367751
			C	2.898531	-1.777248	-0.505738
			C	1.566727	-1.290991	-0.954425
			C	1.044286	-0.083879	-0.573097
			C	1.858361	0.823944	0.231602
			C	3.158234	0.384938	0.692580
			H	3.495705	-2.023576	-1.400562
			H	0.952125	-1.936796	-1.572925
			H	4.617995	-1.142945	0.742002
			H	3.729600	1.054732	1.328732
			C	-0.330621	0.196437	-0.891082
			C	-0.917467	1.299141	-0.249843

		3110.1 3125.6 3133 3148.5 3158 3168.5 3175.2 3176.9	C C H H C C C C H H H O H	-0.058383 1.295922 -0.447459 1.879377 -2.896436 -3.100400 -3.331954 -2.365366 -3.084794 -4.367181 -2.674812 -2.715728 2.786286	2.295403 2.043729 3.297128 2.800964 -1.606031 -0.836783 0.626847 1.546217 -1.321945 0.960772 2.582378 -2.289120 -2.752882	0.254471 0.543128 0.426489 1.056457 0.533888 -0.509328 -0.383345 -0.263652 -1.479789 -0.396987 -0.134921 1.459801 -0.004348
(OH + phen. rad.) 6-28_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7593422 ZPE (hartree): 0.1930520 $<S^2>$: 0 Rotational constants (GHz): 1.1236 0.5502 0.4039	-288.53 70.028 103.26 161.19 164.62 250.31 262.47 278.44 349.12 416.89 435.91 470.21 485.39 495.27 538.75 571.47 612.58 662.09 673.48 699.76 718.94 751.94 778.88 794.7 831.23 849.92 863.52 879.02 910.79 921.66 938.48 964.32 988.51 998.75 999.56 1029.7 1073 1091.4 1121.2 1134.5 1171 1196.1 1203.1 1255.6 1265.6 1279.9 1319.5 1374.3 1383.3 1391.8 1425.2 1434.6 1444 1556.7 1607.3 1632.1 1651.3 1705.2 1845.9 2958.2 2961.4 3113.8 3150.1 3160.9 3168.3 3172 3176.1 3185 3210.3	C C C C C C H H H H C C C H H C C C C H H H O H	3.532775 2.845732 1.355023 0.675773 1.404075 2.852987 3.132681 0.814634 4.616227 3.382729 -0.806113 -1.457558 -0.701560 0.728289 -1.186833 1.288456 -1.491266 -2.154978 -3.196559 -2.850031 -2.067038 -4.164048 -3.508424 -1.243445 3.219649	-0.130940 -1.448123 -1.368809 -0.224817 1.038223 1.001029 -1.893619 -2.300624 -0.116773 1.940148 -0.175514 1.155375 2.264554 2.199158 3.232202 3.115241 -1.374491 -1.142065 -0.103876 1.101522 -1.909429 -0.344147 1.957776 -2.282074 -2.171539	-0.218854 -0.398977 -0.312043 -0.081030 0.109477 0.010187 -1.365246 -0.440525 -0.277177 0.138078 0.065698 0.100161 0.321409 0.359960 0.396111 0.512685 0.580085 -0.688222 -0.761756 -0.267613 -1.456073 -1.185789 -0.204113 1.328388 0.344052
(OH + phen. rad.) 7	Theory: B3LYP/6-311G(d,p)	9.5396 78.386 107 203.38 241.16 245.72 363.92 379.22 396.92 420.61 480.94	C C	3.671178 2.905217	-0.345794 -1.529160	0.000118 0.000035

	Energy (hartree): -614.8880195 ZPE (hartree): 0.1969980 <S^2>: 0 Rotational constants (GHz): 1.2041 0.5198 0.3639	497.83 522.79 534.41 545.26 563.65 626.37 655.79 665.76 711.9 742.21 773.67 794.39 815.32 841.67 853.67 894.6 940.24 960.05 973.74 986.25 999.34 1004.9 1022.9 1025.8 1061.5 1138.4 1174.7 1181.2 1199.7 1206.6 1217.3 1229 1244.4 1301.3 1345 1362.3 1384 1399.8 1416.9 1438.1 1459.7 1496.4 1545.2 1584.8 1632.9 1654.9 1704.1 1725.6 3016.1 3034.4 3153 3158.4 3161 3170.2 3173.6 3179.5 3186.6 3256.3	C C C C H H H H C C C C H H C C C C H H H O H	1.529097 0.827964 1.617141 3.032080 3.407181 0.960019 4.754011 3.600548 -0.610983 -1.203822 -0.391562 0.971301 -0.873661 1.581476 -1.507830 -3.021674 -3.510588 -2.652662 -3.415158 -4.582273 -3.013873 -1.116626 -3.414405	-1.490757 -0.252299 0.946303 0.868711 -2.490506 -2.405431 -0.397740 1.792887 -0.136234 1.137852 2.300880 2.207989 3.272167 3.105443 -1.326261 -1.102482 0.303813 1.326466 -1.649356 0.475270 2.349604 -2.482239 -1.648584	-0.000038 -0.000023 0.000030 0.000110 0.000015 -0.000124 0.000184 0.000155 -0.000040 -0.000088 -0.000096 -0.000014 -0.000153 0.000011 -0.000071 0.000449 0.000082 -0.000157 -0.866004 0.000047 -0.000390 -0.000411 0.867772
(OH + phen. rad.) 7-8_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8114709 ZPE (hartree): 0.1927790 <S^2>: 0 Rotational constants (GHz): 1.1841 0.5308 0.3673	-917.86 57.807 95.598 159.76 219.78 253.45 271.54 359.25 398.62 411.4 452.26 491.55 511.7 529.09 542.29 557.36 564.02 638.38 677.13 703.28 720.98 725.01 767.68 802.01 807.6 818.78 837.63 848.84 895.73 924.13 974.59 985.78 990.02 1023.3 1031.8 1049.5 1068.7 1140.9 1159.2 1180.3 1186.5 1220.2 1233.4 1238.5 1256.8 1303.5 1340.7 1359.6 1368.4 1401.9 1445.1 1454 1488.6 1507.1 1556.9 1577.9 1622.6 1644.8 1659.6 2460.6 3148 3156.8 3159.3 3169.8 3177.6 3185.2 3200.8 3206.8 3242.1	C C C C C C H H H H C C C C H H C	3.650372 2.897903 1.517354 0.812842 1.592912 2.999797 3.404340 0.942876 4.733860 3.565306 -0.632588 -1.240170 -0.410776 0.938603 -0.900804 1.550429 -1.479434	-0.327297 -1.511558 -1.478384 -0.244035 0.957867 0.888867 -2.470441 -2.390496 -0.367896 1.814915 -0.156078 1.142687 2.319302 2.229773 3.286750 3.126018 -1.374980	0.025168 0.013602 -0.006129 -0.008565 0.000182 0.016680 0.016158 -0.023194 0.037380 0.022110 -0.017905 -0.021143 -0.019255 -0.009504 -0.026748 -0.007641 -0.018151

			C	-2.902675	-1.139761	-0.038900
			C	-3.485128	0.197411	0.020322
			C	-2.630779	1.323387	-0.032004
			H	-3.551190	-2.006485	-0.013174
			H	-4.544062	0.309937	-0.196067
			H	-3.049980	2.320789	-0.042458
			O	-1.062753	-2.546200	-0.039234
			H	-3.418151	-0.216712	1.121115
(OH + phen. rad.) 7-13_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8075593 ZPE (hartree): 0.1914270 $<S^2>$: 0 Rotational constants (GHz): 1.1801 0.5343 0.3765	-1573.4 81.77 97.972 164.99 219.74 222.5 280.2 349.74 401.23 416.29 477.77 488 500.99 530.58 554.85 562.43 604.82 652.67 681.26 703.03 727.1 752.64 782.4 806.85 812.41 840.85 854.53 892.58 918.95 971.65 980.52 990.22 1002 1004.9 1035 1064.4 1078.6 1109 1140.9 1165.1 1179.9 1183.7 1191.7 1239.7 1250.5 1303.9 1320.8 1359.9 1377.4 1406.1 1449.4 1460.9 1477.7 1514.6 1533.4 1569.7 1595.7 1647 1656.2 1773.9 3159.5 3161.7 3161.9 3172.9 3174.2 3179.5 3187.5 3188.5 3227.5	C	-3.623578	-0.337230	0.148728
			C	-2.868947	-1.519647	0.175695
			C	-1.488229	-1.476162	0.112249
			C	-0.807381	-0.243707	0.027416
			C	-1.574888	0.952894	-0.014559
			C	-2.982013	0.880165	0.050760
			H	-3.370519	-2.478575	0.240114
			H	-0.917876	-2.393212	0.106014
			H	-4.705703	-0.381314	0.197740
			H	-3.554157	1.801583	0.022200
			C	0.654165	-0.151828	0.017458
			C	1.272138	1.148692	-0.109172
			C	0.438240	2.312744	-0.196906
			C	-0.912699	2.220718	-0.141533
			H	0.922436	3.278543	-0.291767
			H	-1.524209	3.115420	-0.193515
			C	1.527064	-1.362247	-0.254329
			C	2.813909	-1.093670	0.428864
			C	3.425375	0.168950	0.313920
			C	2.669627	1.270739	-0.034795
			H	1.481775	-0.639793	1.178485
			H	4.475269	0.276476	0.562942
			H	3.122603	2.251408	-0.120373
			O	1.176516	-2.436125	-0.693581
			H	3.401551	-1.963991	0.704034
(OH + phen. rad.) 7-19_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7361361 ZPE (hartree): 0.1844440 $<S^2>$: 0	-216.74 70.659 93.228 125.55 175.39 198.98 229.39 259.42 274.74 336.59 361.15 411.85 425.29 436.27 456.57 492.01 519.73 527.33 540.75 542.74 589.45 654.29 678.11 695.93 732.88 742.93 767.74 811.73 821.6 839.69 844.83 886.94 896.19 940.32 973.49	C	3.646034	-0.454685	-0.032896
			C	2.840835	-1.610058	-0.110622
			C	1.468114	-1.519738	-0.111488
			C	0.821397	-0.255760	-0.038813
			C	1.645085	0.916096	0.042919
			C	3.054691	0.783030	0.041342
			H	3.309751	-2.586046	-0.166516

	Rotational constants (GHz): 1.1856 0.5242 0.3663	986.25 1012.4 1028.1 1057.4 1063 1159.3 1164.8 1179.8 1188.1 1229.6 1240.1 1290.4 1320.9 1339.8 1376.8 1389.2 1410.6 1455.4 1481.9 1516.7 1545 1580.1 1626.5 1643.7 1652.7 3155.4 3160.8 3163.8 3169.6 3172.7 3181.8 3187.9 3242.9 4234.3	H H H C C C C H H C C C C H H H O H	0.860299 4.726235 3.660303 -0.602321 -1.168239 -0.317344 1.038415 -0.767259 1.678734 -1.559805 -2.867999 -3.490127 -2.590838 -4.113199 -4.555950 -2.975052 -1.241196 -3.401683	-2.409983 -0.546127 1.681013 -0.083994 1.203825 2.343331 2.200642 3.328032 3.073758 -1.251446 -0.818218 0.336066 1.396451 -2.665336 0.512814 2.404111 -2.375236 -2.903605	-0.146144 -0.029215 0.103489 -0.110498 -0.016657 0.079649 0.106536 0.139888 0.174255 -0.023433 -0.413353 -0.029743 0.024867 0.371080 -0.127557 -0.100974 0.361038 0.446519
(OH + phen. rad.) 8	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8204367 ZPE (hartree): 0.1941540 $<S^2>$: 0 Rotational constants (GHz): 1.1709 0.5329 0.3670	43.316 90.675 147.88 178.33 217.26 257 289.24 355.31 398.02 404.82 483.38 493.82 508.14 529.32 531.48 560.61 609.13 659.51 673.74 708.05 710.85 752.07 781.53 794.84 807.9 827.54 842.04 878.81 899.52 974.45 980.08 992.57 1008.4 1018.5 1026.4 1063 1088.2 1095.6 1150.4 1179 1184.1 1224.7 1240.1 1261 1300.2 1315.9 1335.1 1339.9 1360.7 1409.7 1417.1 1443.3 1469.1 1498.2 1563.7 1580.7 1611.4 1641.3 1665 2948.1 2948.6 3159.1 3161.4 3172.6 3178.8 3183.7 3186.5 3187.7 3224.7	C C C C C C H H H H C C C C C H H C C C C H H	-3.641421 -2.894587 -1.512950 -0.807857 -1.588451 -2.990048 -3.402599 -0.927451 -4.725239 -3.559000 0.631490 1.240268 0.407694 -0.936876 0.902104 -1.553071 1.477495 2.875545 3.496758 2.606442 3.512094 4.190137	-0.325503 -1.510355 -1.476989 -0.240331 0.966062 0.895273 -2.468089 -2.383411 -0.362829 1.818974 -0.164907 1.151410 2.334822 2.245679 3.300033 3.138558 -1.400503 -1.163735 0.157720 1.314622 -2.041094 0.244586	0.000311 0.000210 -0.000007 -0.000098 -0.000029 0.000176 0.000278 -0.000147 0.000491 0.000218 -0.000170 -0.000167 -0.000296 -0.000204 -0.000415 -0.000246 -0.000191 0.000525 0.000431 0.000126 0.000825 0.858277

			H	3.037475	2.308978	0.000094
			O	1.019358	-2.562410	-0.000644
			H	4.189673	0.243983	-0.857930
(OH + phen. rad.) 8-9_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7960823 ZPE (hartree): 0.1941580 <S^2>: 0 Rotational constants (GHz): 1.1108 0.5527 0.4060	-245.79 92.589 94.05 164.82 204.1 228.07 251.48 309.35 389.25 411.9 432.67 481.32 502.68 532.5 554 571.05 635.65 654.45 674.9 722.34 729.13 757.48 784.87 793.27 813.87 825.65 869.07 886.9 905.38 947.63 956.45 983.43 992.83 1013.9 1031.5 1067.9 1086.9 1123.7 1154.4 1167.1 1187.1 1194.2 1219.8 1236.5 1288.3 1302.3 1309.2 1334.7 1362.4 1373.7 1429.1 1446 1483.9 1506.9 1593 1629.5 1647.3 1669.1 1814.7 2983.1 3019.2 3144.6 3159.9 3162.6 3173.2 3181 3186 3192.8 3196.7	C	3.548562	-0.293628	-0.304628
			C	2.811037	-1.471609	-0.433841
			C	1.427987	-1.446331	-0.302931
			C	0.752460	-0.243704	-0.064649
			C	1.499511	0.953184	0.078185
			C	2.895566	0.903121	-0.042511
			H	3.315419	-2.411408	-0.626535
			H	0.865011	-2.368591	-0.376353
			H	4.628243	-0.313315	-0.399099
			H	3.465081	1.819694	0.071015
			C	-0.707128	-0.177847	0.109836
			C	-1.359490	1.153539	0.107579
			C	-0.524336	2.302863	0.406569
			C	0.818534	2.205418	0.375629
			H	-1.011161	3.257292	0.574246
			H	1.433107	3.083698	0.542768
			C	-1.449671	-1.334456	0.611847
			C	-2.224069	-1.179448	-0.592433
			C	-3.198998	-0.063223	-0.823111
			C	-2.651684	1.212120	-0.273558
			H	-2.185180	-2.008303	-1.294879
			H	-3.428801	0.043652	-1.890492
			H	-3.245584	2.117001	-0.239606
			O	-1.189230	-2.251253	1.358280
			H	-4.151968	-0.329689	-0.339202
(OH + phen. rad.) 8-12_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7228990 ZPE (hartree): 0.1911840 <S^2>: 0 Rotational constants (GHz): 1.0331 0.3869 0.2857	-72.439 32.84 63.9 80.981 148.61 182.29 205.81 217.24 258.76 366.07 391.6 421.55 463.35 485.48 504.27 520.11 541.52 591.08 629.74 640.66 657.97 715.54 737.27 765.01 787.09 808.69 848.56 863.52 897.29 900.18 956.95 979.84 987.28 1010.9 1020.7 1047.2 1065 1120.7 1150.8 1163.8 1176.7 1206.1 1217.8 1238.7 1266.7 1305.9 1341.7 1352.1 1394.1 1428.3 1430.1 1450.6 1454.1 1481.6 1557.5 1574.2 1632.5 1645.3 2219.4 2999.3 3025	C	3.788478	1.147762	-0.050941
			C	2.779327	2.122330	-0.123474
			C	1.454695	1.735521	-0.064534
			C	1.085617	0.368576	0.019037
			C	2.130027	-0.615294	0.056871
			C	3.470769	-0.198369	0.049057
			H	3.044735	3.170385	-0.200782
			H	0.649967	2.461372	-0.079373
			H	4.829679	1.452156	-0.066820
			H	4.261845	-0.939747	0.105402
			C	-0.296583	0.032028	0.159476
			C	-0.581705	-1.374987	0.036603

		3104.1 3137.2 3152.7 3167.4 3169.1 3180.3 3188 3193.7	C C H H C C C C H H H O H	0.474208 1.770879 0.202471 2.565864 -3.471342 -3.331158 -3.138154 -1.860543 -3.245548 -3.958852 -1.980279 -3.597122 -3.239992	-2.388020 -2.013378 -3.439122 -2.752050 1.390873 0.148410 -1.009999 -1.790455 -0.010089 -1.726411 -2.848908 2.496407 -0.668824	0.065322 0.094436 0.014449 0.104280 0.173664 0.561964 -0.386236 -0.259214 1.629676 -0.250485 -0.494961 -0.166202 -1.423945
(OH + phen. rad.) 9	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8035619 ZPE (hartree): 0.1952330 $<S^2>$: 0 Rotational constants (GHz): 1.1229 0.5380 0.4296	70.332 86.34 139.89 177.97 213.12 238.65 269.63 380.13 393.87 427.98 455.52 508.31 513.69 550.73 569.53 618.36 664.8 685.46 695.44 732.74 756.75 763.73 785.99 813.13 832.48 857.57 879.3 895.45 914.95 950.56 950.87 983.33 991.78 1007 1029 1044.5 1062.8 1080.8 1143.3 1157.2 1170.3 1185.8 1191.5 1232 1254.1 1288.3 1303.1 1327.2 1333.1 1354.1 1427.3 1482.5 1486.9 1508.1 1596.5 1632.9 1645.5 1679 1913.5 3002.3 3032.6 3136.6 3157.4 3159.8 3163.9 3176.7 3178.6 3190.8 3193.5	C C C C C C H H H H C C C C H H H C C C C H H H O H	3.550444 2.828466 1.435228 0.748526 1.475778 2.875206 3.346556 0.882408 4.633866 3.433967 -0.727146 -1.373157 -0.569054 0.768604 -1.048771 1.373981 -1.495035 -1.870822 -3.024035 -2.615329 -1.624064 -3.166101 -3.262093 -1.581086 -3.967095	-0.318846 -1.474996 -1.456422 -0.286672 0.894386 0.853866 -2.392960 -2.364601 -0.330910 1.758563 -0.219849 1.136506 2.269591 2.138620 3.230210 2.997247 -1.180352 -1.192886 -0.291642 1.093517 -2.081832 -0.342494 1.954354 -1.699755 -0.618461	-0.219791 -0.506237 -0.462428 -0.142794 0.142741 0.102287 -0.759191 -0.678051 -0.247908 0.318979 -0.008546 -0.080535 0.328044 0.443757 0.480617 0.715758 0.840572 -0.572128 -1.034074 -0.593008 -1.146260 -2.121046 -0.709810 1.912523 -0.580430
(OH + phen. rad.) 9-10_TS	Theory: B3LYP/6-311G(d,p)	-564.3 62.535 72.67 142.16 163.74 226.32 248.43 262.52 343.9 405.02	C C	3.565189 2.864640	-0.306205 -1.474420	-0.062583 -0.386761

	Energy (hartree): -614.7754758 ZPE (hartree): 0.1931210 <S^2>: 0 Rotational constants (GHz): 1.1647 0.5303 0.4350	423.83 455.62 469.91 513.59 532.18 545.12 592.04 651.86 680.55 687.1 722.97 750.58 766.94 775.09 823.91 845.52 859.53 872.54 932.22 939.11 973.15 975.52 984.08 989.95 1016.1 1054.5 1075.2 1125.8 1154.1 1162 1180.6 1182 1201.9 1229.8 1250.7 1289.4 1304.3 1345.3 1350.9 1417.4 1429.9 1478.4 1490.5 1495.9 1568.2 1582.1 1635.5 1649 2067.2 2930.4 3089.8 3113.5 3150.2 3151.3 3156.9 3170.7 3177.7 3188.7 3214.6	C C C C H H H H C C H H C C C C H H H O H	1.483385 0.749770 1.463888 2.862625 3.406739 0.963388 4.645362 3.395400 -0.669543 -1.394318 -0.620783 0.728652 -1.123790 1.307853 -1.672072 -1.763621 -3.010453 -2.743515 -1.543544 -3.031475 -3.472514 -1.461359 -3.919628	-1.462578 -0.277306 0.914857 0.871126 -2.398534 -2.377959 -0.322229 1.782690 -0.165321 1.077299 2.235762 2.139920 3.178454 3.018346 -1.199036 -1.206981 -0.456505 0.917750 -2.189457 -0.441973 1.715430 -1.333171 -0.949571	-0.501493 -0.289825 0.048686 0.148955 -0.556276 -0.765552 0.020631 0.401676 -0.379334 -0.182117 0.192706 0.289718 0.377317 0.558532 0.939016 -0.510683 -0.995008 -0.398726 -0.927371 -2.098660 -0.399218 2.070262 -0.648473
(OH + phen. rad.) 10	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8343711 ZPE (hartree): 0.1970580 <S^2>: 0 Rotational constants (GHz): 1.3287 0.4644 0.3915	69.713 106.17 146.3 206.88 237.76 257.09 405.75 413.82 436.78 463.22 482.71 513.54 538.52 569.17 579.37 626.64 678.69 706.67 730.12 755.78 796.21 809.24 819.63 837.33 843.55 866.96 880.2 910.27 958.61 967.19 968.75 995.03 1003.2 1031.9 1041 1051.2 1066.9 1117 1158.6 1165.5 1169.5 1175.1 1181.2 1226 1236.6 1245.7 1269.5 1290.4 1379.5 1388.1 1415.6 1471 1482.9 1491.4 1559.5 1606.5 1624.9 1665.6 1891.1 3050.7 3120.8 3148.7 3153.8 3158.9 3163.5 3167.8 3179.3 3182.2 3189.8	C C C C C C H H H H C C C C H H C	3.713122 2.968137 1.602923 0.913074 1.664985 3.076403 3.483187 1.037492 4.791061 3.647568 -0.481864 -1.105857 -0.377344 0.994177 -0.873231 1.589586 -2.578981	-0.464025 -1.654497 -1.607198 -0.366157 0.845844 0.751506 -2.608094 -2.521539 -0.517322 1.663838 -0.226973 1.016039 2.193801 2.096758 3.155417 2.991469 -0.545161	0.157711 -0.018976 -0.155107 -0.117586 0.071546 0.200097 -0.049089 -0.294807 0.260036 0.337705 -0.266397 -0.198860 0.022171 0.136752 0.091235 0.284770 0.682782

			C	-1.635229	-1.202296	-0.400064
			C	-2.558891	-0.423979	-1.401479
			C	-2.582092	0.690531	-0.298479
			H	-1.459757	-2.272340	-0.459765
			H	-2.093302	-0.140118	-2.346620
			H	-3.324982	1.482556	-0.258651
			O	-3.117997	-0.869593	1.688428
			H	-3.529025	-0.902295	-1.556902
(OH + phen. rad.) 10-11_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8067428 ZPE (hartree): 0.1939430 $<S^2>$: 0 Rotational constants (GHz): 1.2095 0.4739 0.4160	-437.49 40.01 69.672 130.77 136 241.73 252.42 279.75 410.3 425.01 462.55 474.31 504.41 519.34 529.14 556.29 599.22 617.83 688.88 706.6 755.46 761.25 801.22 822.65 823.42 843.99 882.82 885.56 897.42 958.97 977.34 980.41 987.27 990.33 993.47 1016.3 1054 1099.3 1138 1168.5 1181.8 1196.6 1210.4 1232.2 1265.5 1281 1325.9 1344.4 1363.5 1407 1445 1472.1 1480.2 1492.4 1558.6 1581.4 1635.3 1654.5 1995.5 3011.2 3108.9 3158.4 3161.1 3167.4 3178.6 3178.7 3180.5 3189.1 3192.1	C	3.663595	-0.325057	0.224510
			C	2.999877	-1.544644	0.000917
			C	1.638146	-1.563372	-0.224316
			C	0.887911	-0.369076	-0.226176
			C	1.557894	0.869699	0.005773
			C	2.953703	0.857641	0.223454
			H	3.561455	-2.472028	0.000905
			H	1.135007	-2.505923	-0.407726
			H	4.733977	-0.316562	0.396279
			H	3.463694	1.799731	0.396341
			C	-0.527476	-0.321494	-0.469445
			C	-1.224822	0.920511	-0.446649
			C	-0.535202	2.134625	-0.170125
			C	0.813476	2.099929	0.027460
			H	-1.077671	3.072892	-0.133549
			H	1.360232	3.018684	0.212734
			C	-2.493305	-0.577047	1.086416
			C	-1.509913	-1.348507	-0.568524
			C	-2.713536	-0.713040	-1.234765
			C	-2.619588	0.621917	-0.523667
			H	-1.281287	-2.405672	-0.631922
			H	-2.535676	-0.587895	-2.312320
			H	-3.388742	1.385403	-0.567500
			O	-2.458045	-0.524429	2.236638
			H	-3.651184	-1.245702	-1.075517
(OH + phen. rad.) 11	Theory: B3LYP/6-311G(d,p) Energy (hartree): -501.5008044 ZPE (hartree): 0.1856260 $<S^2>$: 0	104.5 117.57 235.81 251.61 263.57 362.61 420.07 427.43 453.46 518.97 534.55 553.45 608.07 683.59 691.98 699.96 739.25 755.67 768.57 807.32 827.77 836.83 874.71 885.81 906.34 946.86 952.52 981.76 982.91 991.86 1006.7 1062.7 1111.3 1119.1 1163	C	-3.341189	-0.150714	0.000042
			C	-2.762853	-1.422092	-0.000026
			C	-1.380282	-1.556043	-0.000061
			C	-0.544943	-0.432273	-0.000005
			C	-1.130825	0.861528	0.000027
			C	-2.529765	0.975237	0.000058
			H	-3.391073	-2.305678	-0.000061

	Rotational constants (GHz): 1.8159 0.6615 0.4863	1183.8 1201.9 1225.7 1233.6 1270.2 1276.8 1321.1 1334 1382.2 1405.2 1427.7 1484.7 1503.6 1575 1592 1625.8 1647.2 1678.2 2999.2 3016.4 3154.5 3158.7 3166.4 3176.2 3178.1 3189.3 3210.8 3213.9	H H H C C C C H H C C C H H H H	-0.939097 -4.419847 -2.975949 0.914078 1.721877 1.057733 -0.291409 1.650757 -0.798684 1.752415 3.172000 3.039493 1.482785 3.729186 3.874750 3.729206	-2.546387 -0.042364 1.964485 -0.520575 0.720216 2.001377 2.054342 2.909588 3.013928 -1.586068 -1.096663 0.397547 -2.632974 -1.459990 1.084470 -1.460005	-0.000136 0.000068 0.000086 -0.000006 -0.000064 -0.000075 -0.000014 -0.000109 0.000027 0.000021 0.000026 0.000061 0.000051 0.875770 0.000100 -0.875702
(OH + phen. rad.) 12	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7309444 ZPE (hartree): 0.1911350 <S^2>: 0 Rotational constants (GHz): 1.1607 0.3222 0.2526	21.552 57.374 64.211 108.6 166.28 189.21 195.24 245.6 260.56 392.58 406.82 428.45 465.61 491.55 520.21 559.73 603.96 634.81 638.44 668.58 679.34 730.03 758.5 773.67 783.19 809.74 828.21 898.27 898.75 931.65 978.09 985.98 993.31 994.26 1012.2 1048.4 1075.5 1129.3 1146.3 1168.9 1180 1206.1 1213.4 1238.4 1272.3 1308.5 1315.3 1353.4 1396.2 1413.8 1433.6 1443 1459.3 1492.2 1561.2 1584.6 1635.6 1651.9 2195.7 2781.9 2950 2951.2 3108.2 3137.6 3155.1 3168.7 3170.6 3181.7 3195.7	C C C C C C H H H H C C C C H H C C C C H H H O	-3.936058 -2.920826 -1.599135 -1.238190 -2.290002 -3.627925 -3.179031 -0.791081 -4.975226 -4.423824 0.150997 0.417852 -0.651983 -1.945462 -0.392434 -2.747201 4.098314 3.039596 3.026080 1.712294 2.032293 3.570931 1.826354 5.011765	-1.243458 -2.214075 -1.814134 -0.441956 0.534166 0.108312 -3.266652 -2.536189 -1.555146 0.846384 -0.102788 1.323546 2.320546 1.934907 3.375870 2.666089 -1.157093 -0.396563 1.104257 1.794347 -0.861981 1.521059 2.879341 -1.886236	-0.000047 -0.000066 -0.000011 0.000029 0.000010 -0.000007 -0.000113 0.000009 -0.000059 0.000016 0.000179 0.000052 0.000030 0.000023 0.000045 0.000023 0.000079 0.000143 0.000018 -0.000291 0.000317 0.864492 -0.000630 -0.000136

			H	3.571804	1.521029	-0.863855
(OH + phen. rad.) 12-9_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7185980 ZPE (hartree): 0.1908100 <S^2>: 0 Rotational constants (GHz): 0.9355 0.5020 0.3360	-166.66 43.939 60.467 94.503 155.39 192.49 217.5 244.42 291.5 376.18 406.63 440.88 466.44 506.82 518.21 527.11 573.57 619.57 628.87 636.07 675.06 708.67 737.87 746.48 762.71 774.46 814.17 870.19 874.8 883.61 951.06 968.64 971.71 988.07 1004.1 1045.4 1053.2 1118.4 1125.2 1157.1 1177.9 1192.1 1212.5 1231.1 1261.7 1299.8 1313.1 1327.5 1388.2 1392.5 1417.2 1456.5 1462.4 1483 1532.7 1560.6 1628.2 1632.9 2171.3 2981.1 3020 3150.8 3153.8 3165.4 3171.9 3175.2 3179.9 3189.7 3195.5	C C C C C C C H H H H C C C C C C H H C C C C H H H O H	3.506058 2.487060 1.192301 0.847775 1.885068 3.205950 2.725206 0.412615 4.527317 3.991766 -0.416861 -0.822754 0.248082 1.531142 -0.023938 2.318675 -2.637961 -2.636596 -3.106104 -2.129556 -2.611100 -4.101783 -2.433477 -2.561950 -3.231300	1.079546 2.022044 1.606662 0.232356 -0.723353 -0.272094 3.079846 2.331657 1.411770 -0.999916 -0.276454 -1.565577 -2.534058 -2.119863 -3.564567 -2.831516 1.706614 0.497451 -0.733661 -1.856694 0.482684 -1.025931 -2.856051 2.758831 -0.476129	-0.172696 0.048186 0.285008 0.241927 -0.039040 -0.198707 0.058577 0.488136 -0.320078 -0.376173 0.625797 0.187503 -0.045193 -0.141965 -0.250635 -0.367872 -0.052035 0.493582 -0.269882 -0.112586 1.575167 0.087246 -0.403067 -0.532558 -1.330226
(OH + phen. rad.) 13	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8574617 ZPE (hartree): 0.1966200 <S^2>: 0 Rotational constants (GHz): 1.1839 0.5271 0.3684	40.531 86.533 151.56 213.53 242.63 267.7 336.23 385.41 407.4 453.02 483.34 488.96 517.99 523.66 552.68 564.39 614.43 670.11 712.5 730.59 753.06 775.7 795.59 818.53 827.81 868.9 890.36 905.77 957.45 968.13 976.87 994.06 1005.2 1014.2 1061.3 1073.5 1131.2 1139.6 1161.6 1177.3 1183.2 1193.1 1211.9 1231.7 1241.1 1265.4 1316.9 1336.3 1376.1 1426.6 1446.1 1486.5 1503.2 1561.7 1599.5 1635.5 1646.5 1666.7 1732.5 2884.4 3155 3156.4 3160.1 3171.7 3173.3 3176.5 3187.5 3193.3 3248	C C C C C C H H H H C C C C C C	-3.641264 -2.915700 -1.530434 -0.832943 -1.573073 -2.968994 -3.426437 -0.982253 -4.719048 -3.517823 0.670757 1.298132 0.444932 -0.899624	-0.326491 -1.502343 -1.466905 -0.255721 0.940245 0.885602 -2.458421 -2.386569 -0.356334 1.813066 -0.169504 1.183539 2.337022 2.223128	-0.139370 0.037214 0.187286 0.144240 -0.020931 -0.162764 0.060896 0.314876 -0.251882 -0.289417 0.378709 0.086447 0.011339 -0.040005

			H	0.917657	3.311358	-0.055008
			H	-1.515501	3.112311	-0.127841
			C	1.549708	-1.380167	-0.042358
			C	2.988583	-1.126508	-0.073223
			C	3.490806	0.133893	-0.086649
			C	2.650513	1.291750	-0.045295
			H	0.799814	-0.254048	1.479070
			H	4.562471	0.279675	-0.182962
			H	3.097765	2.272165	-0.166049
			O	1.097110	-2.492505	-0.248124
			H	3.618081	-1.998414	-0.204546
(OH + phen. rad.) 13-14_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8303822 ZPE (hartree): 0.1940800 $<S^2>$: 0 Rotational constants (GHz): 1.1312 0.5190 0.3710	-501.72 80.245 84.414 144.85 186.55 212.84 286.93 319.33 368.93 415.67 441.62 471.64 503.02 504.83 523.32 561.58 577.76 613.41 674.45 703.2 718 743.5 760.81 785.48 800.16 811.13 832.09 858.61 883.48 942.07 960.39 978.74 986.3 991.71 997.37 1026.5 1054.3 1120 1148.8 1175.5 1182.7 1201.7 1215.6 1245.2 1260.6 1293 1347.2 1369 1403.7 1427.2 1460.6 1475.6 1520.8 1537.1 1556.6 1595.8 1635.1 1653.3 1949.2 3082 3139.5 3156.7 3157.6 3160.9 3171.6 3176 3179 3187 3201.7	C	-3.613609	-0.360957	-0.153333
			C	-2.895793	-1.466159	0.334561
			C	-1.536105	-1.375913	0.568591
			C	-0.841265	-0.176491	0.314497
			C	-1.573126	0.949646	-0.158557
			C	-2.959608	0.830512	-0.391849
			H	-3.412632	-2.399637	0.527032
			H	-0.991269	-2.236706	0.934272
			H	-4.678786	-0.444923	-0.335573
			H	-3.507073	1.694336	-0.754627
			C	0.583121	-0.048232	0.523315
			C	1.233686	1.196177	0.303886
			C	0.449345	2.322384	-0.091991
			C	-0.887322	2.195037	-0.330474
			H	0.945235	3.275591	-0.239517
			H	-1.462051	3.054659	-0.660959
			C	1.701765	-1.565898	-0.368399
			C	3.005114	-1.109532	-0.311097
			C	3.433493	0.179092	0.069713
			C	2.649296	1.271193	0.367782
			H	1.003962	-0.653100	1.327710
			H	4.505525	0.341693	0.011025
			H	3.122456	2.242265	0.458777
			O	1.033745	-2.519263	-0.564160
			H	3.710706	-1.765221	-0.814734
(OH + phen. rad.) 14	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8500507	31.996 44.73 80.924 119.53 149.91 187.85 239.06 291.18 381.91 403.31 425.28 467.48 488.92 501.03 524.42 540.82 585.83 604.95 641.65 667.61	C	3.797090	-0.569201	0.124023
			C	3.060710	-1.586112	-0.527193
			C	1.722826	-1.415916	-0.788330
			C	1.053894	-0.221929	-0.410158

	ZPE (hartree): 0.1942780 <S^2>: 0 Rotational constants (GHz): 1.1285 0.4213 0.3354	691.15 744.41 764.69 781.34 785.67 812.88 840.6 876.53 914.46 928.99 934.83 963.6 974.74 979 980.27 994.92 1042.2 1132.8 1155.1 1173 1179.5 1191.9 1228.8 1265 1273.4 1289.8 1383.5 1394.9 1405.5 1435.3 1447.4 1467.5 1503 1539.1 1606 1641.6 1658.2 1675.6 2201.5 3133.9 3154.3 3156.1 3158 3162.7 3166.9 3169.7 3175.4 3175.9 3188.1	C C H H H H C C C C C H H C C C C H H H O H	1.800716 3.179663 3.558316 1.156276 4.852162 3.742422 -0.324955 -0.972850 -0.206077 1.127514 -0.702474 1.689507 -2.641176 -3.538581 -3.443693 -2.395607 -0.866089 -4.410415 -2.632329 -1.900951 -4.496612	0.806702 0.599808 -2.504331 -2.197500 -0.716643 1.382393 -0.017371 1.146196 2.171265 2.004595 3.094023 2.794432 -1.554550 -0.821403 0.554627 1.395385 -0.788009 0.955162 2.414054 -2.257660 -1.324882	0.244766 0.499993 -0.818403 -1.283549 0.325289 0.998484 -0.666458 -0.291318 0.339201 0.603252 0.620376 1.091200 0.641314 0.005826 -0.468228 -0.565503 -1.204392 -0.756131 -0.861408 1.190428 -0.082006
(OH + phen. rad.) 14-15_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8435038 ZPE (hartree): 0.1937470 <S^2>: 0 Rotational constants (GHz): 1.1116 0.3542 0.2842	-78.784 22.532 65.789 120.9 161.76 185.91 205.73 264.92 365.73 394.2 426.01 438.81 479.06 484.17 526.03 543.16 561.15 626.31 634.5 669.78 684.78 733.62 767.99 780.08 787.22 798.57 835.19 876.53 915 925.18 960.62 964.91 975.13 994.51 996.8 1007.1 1041.4 1127.2 1145.6 1172.7 1174.2 1187.7 1229.7 1273.4 1277.5 1291.1 1381.9 1389.3 1397.3 1407.2 1438.9 1468.5 1501.9 1540.4 1605.5 1641.4 1660.5 1684.8 2218 3109.8 3133.4 3140.8 3157 3158.7 3163.7 3175.1 3176.4 3188.6 3205.6	C C C C C C H H H C C C C H H C C C	3.922547 3.014661 1.682881 1.189909 2.110113 3.479406 3.377371 0.985547 4.971682 4.173918 -0.179004 -0.656568 0.278744 1.609124 -0.083213 2.297949 -3.614295 -3.339312 -3.186140	-0.963083 -1.966084 -1.672993 -0.363405 0.648573 0.313382 -2.969573 -2.441303 -1.208006 1.083734 -0.039123 1.238786 2.236287 1.953318 3.242041 2.730444 -1.307012 -0.506063 0.966439	0.105546 -0.310227 -0.468919 -0.219574 0.199694 0.354078 -0.502212 -0.786067 0.227113 0.672904 -0.373574 -0.130143 0.278628 0.441545 0.465261 0.756029 0.328974 -0.674580 -0.499298

			C	-2.057224	1.658386	-0.279233
			H	-0.858880	-0.818291	-0.690105
			H	-4.104540	1.544784	-0.576360
			H	-2.192142	2.734680	-0.190425
			O	-3.846472	-2.015644	1.221136
			H	-3.324957	-0.957812	-1.662722
(OH + phen. rad.) 15	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.8543838 ZPE (hartree): 0.1944450 <S^2>: 0 Rotational constants (GHz): 1.2582 0.3001 0.2495	35.931 52.044 104.09 125.05 172.7 187.24 212.11 269.08 375.12 402.05 425.73 455.02 485.59 523.83 526.39 542.01 596.76 635.46 640.67 684.41 693.33 731.04 745.11 772.58 781.98 790.63 837.69 876.12 911.8 921.96 963.11 970.13 975.83 980.55 994.95 1041.7 1063.6 1136.2 1149.8 1172.7 1176.5 1189.1 1227.9 1272.8 1278.3 1290.6 1348 1383.9 1395.2 1405.3 1458.6 1472.6 1504.7 1539.5 1605.1 1640.2 1655.9 1675.4 2207.8 3137.4 3156.1 3157.2 3160.8 3161.5 3171.6 3174.7 3175.7 3179.4 3187.6	C	4.045740	-1.058927	-0.252777
			C	3.155221	-2.049461	0.223167
			C	1.840600	-1.738895	0.473145
			C	1.348845	-0.424025	0.257215
			C	2.252790	0.577740	-0.216626
			C	3.603046	0.224760	-0.465551
			H	3.516530	-3.057911	0.390709
			H	1.157903	-2.498623	0.839711
			H	5.080668	-1.317154	-0.446743
			H	4.284881	0.987727	-0.826984
			C	-0.002424	-0.075183	0.504703
			C	-0.476849	1.208987	0.294163
			C	0.447484	2.200834	-0.151757
			C	1.758439	1.895381	-0.405011
			H	0.089871	3.214053	-0.301913
			H	2.440080	2.665171	-0.752127
			C	-4.261795	-1.058915	-0.369809
			C	-3.116570	-0.410524	-0.261011
			C	-2.999674	0.909225	0.337692
			C	-1.867169	1.610817	0.545422
			H	-0.660828	-0.835715	0.908683
			H	-3.936285	1.388588	0.604896
			H	-1.993219	2.626123	0.911272
			O	-5.261131	-1.641324	-0.464453
			H	-2.256657	-0.912541	-0.689671
(OH + phen. rad.) 15-16_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7586416 ZPE (hartree): 0.1919670 <S^2>: 0 Rotational constants (GHz):	-203.33 45.508 88.638 117.88 163.77 219.32 259.59 266.52 357 404.33 422.07 458.61 468.39 498.42 522.86 552.22 613.12 640.59 655.33 673.91 725.77 749.08 756.07 783.81 803.35 860.06 875.1 893.7 923.22 930.78 952.35 953.72 961 987.38 989.24 1058.1 1078.7 1107.5 1132.1 1157.9 1183.5 1218.6 1237.1 1244.2 1266.9 1283.6 1296.5 1323 1342	C	-3.451062	-0.845670	0.218803
			C	-2.504942	-1.876317	0.172797
			C	-1.160327	-1.568530	0.007087
			C	-0.731230	-0.242812	-0.104501
			C	-1.686703	0.809121	-0.078735
			C	-3.047083	0.471015	0.090833
			H	-2.818171	-2.910277	0.259631
			H	-0.433748	-2.372820	-0.052797
			H	-4.501860	-1.079412	0.349088

	0.9847 0.5644 0.3722	1350.2 1403.7 1443.8 1472.4 1499.2 1548.2 1558.2 1609.4 1642.1 2009.3 2859.6 2915.5 3155.5 3156.2 3160.5 3174.2 3180.3 3188.5 3188.8 3245.9	H C C C C H H C C C C H H H O H	-3.781133 0.708688 1.056665 0.053857 -1.272407 0.341949 -2.038349 2.416857 1.815575 2.936452 2.426085 1.022139 3.901503 2.981776 2.318691 1.413810	1.269529 0.098487 1.547766 2.532493 2.182708 3.579105 2.949712 -1.669457 -0.564701 0.474266 1.663435 -0.251917 0.308062 2.593362 -2.672450 -0.776562	0.124351 -0.348447 -0.205941 -0.239869 -0.208951 -0.227820 -0.204978 -0.041660 0.635410 0.565073 0.102143 -1.351179 1.016273 0.074691 -0.626838 1.643184
(OH + phen. rad.) 16	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7959041 ZPE (hartree): 0.1953070 $<S^2>$: 0 Rotational constants (GHz): 1.2868 0.4509 0.3570	69.635 80.322 130.51 158.56 227.47 247.02 344.21 395.21 410.69 443.98 484.16 506.78 531.83 539.13 564.99 620.19 654.71 691.43 729.68 735.65 750.07 764.21 801.94 819.38 854.19 878.49 884.69 900.73 920.13 949.72 958.1 981.72 992.06 1000 1031.1 1051.6 1065.1 1073.5 1132.5 1160 1185.4 1200.3 1207.3 1229 1237.1 1241.1 1269.9 1307 1321 1331.8 1348.7 1425.7 1481.5 1506.4 1594.4 1630.3 1643.1 1669 1919.9 2946 3130.5 3150.5 3156.7 3159.5 3165.2 3176.2 3177.6 3189.5 3194.1	C C C C C C H H H H C C C C H H H C C C C H H H O	-3.679890 -2.810443 -1.435154 -0.912803 -1.791607 -3.171228 -3.198486 -0.769627 -4.749493 -3.845588 0.557905 0.972430 0.049240 -1.263157 0.399355 -1.981077 3.000601 1.625194 2.676816 2.141772 0.682073 3.132039 2.646837 3.823869	-0.776357 -1.861175 -1.661428 -0.386481 0.721119 0.502145 -2.862092 -2.516796 -0.926262 1.350589 -0.118545 1.281405 2.361262 2.074822 3.387864 2.873968 -0.887021 -1.028594 -0.067069 1.299102 -0.179315 -0.300032 2.191479 -1.222258	0.129622 0.208126 0.082586 -0.108404 -0.188088 -0.070014 0.359079 0.123581 0.222214 -0.125341 -0.361900 0.062297 -0.211024 -0.351359 -0.213961 -0.504947 -0.211166 0.285879 0.986264 0.727543 -1.455595 1.945125 1.076403 -1.008613

			H	1.334970	-1.960440	0.760182
(OH + phen. rad.) 16-17_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7389947 ZPE (hartree): 0.1923240 <S^2>: 0 Rotational constants (GHz): 1.3281 0.4377 0.3591	-605.54 60.847 74.413 115.92 153.35 232.59 250.56 308.12 380.15 400.67 416.34 436.49 455.41 504.13 531.49 552.73 564.7 625.22 667.32 709.33 743.53 749.15 771.63 794.87 813.22 834.09 861.82 877.67 902.26 929.2 953.22 959.92 987.56 994.45 1015 1059.6 1083.8 1121.9 1155.7 1179 1184.1 1214.2 1226.5 1234.7 1241.8 1262.4 1298.6 1307.8 1316.4 1331.6 1364 1427.4 1480.9 1505.9 1594.4 1627.8 1644.4 1664.7 2000.8 2771.8 3025 3154.4 3157.8 3166.4 3176.5 3179.8 3189.2 3214.4 3229.4	C C C C C C H H H H C C C C C C H H H O H	3.750445 2.948508 1.558601 0.954212 1.762952 3.158193 3.402735 0.941216 4.830463 3.777037 -0.547502 -1.027713 -0.174366 1.145305 -0.581930 1.806031 -3.346431 -1.487081 -2.645753 -2.218696 -0.708151 -3.216201 -2.827178 -3.614486 -1.492178	-0.622204 -1.751426 -1.633640 -0.394817 0.757034 0.623193 -2.725026 -2.516935 -0.711502 1.509122 -0.232292 1.156041 2.287245 2.076345 3.292203 2.919737 -0.701028 -1.123780 -0.330237 1.114823 -0.306416 -0.549090 1.950910 -1.001522 -2.202371	-0.012266 -0.162141 -0.122779 0.059391 0.195990 0.164056 -0.309105 -0.238918 -0.038410 0.265273 0.220767 -0.170209 0.115900 0.311879 0.098355 0.487673 0.255340 -0.550607 -0.990023 -0.794409 1.323602 -1.897085 -1.110247 1.352259 -0.524543
(OH + phen. rad.) 17	Theory: B3LYP/6-311G(d,p) Energy (hartree): -501.4849628 ZPE (hartree): 0.1859080 <S^2>: 0 Rotational constants (GHz): 1.7442 0.6857 0.5033	99.433 111.53 226.13 247.33 273.21 411.69 417.34 437.09 497.97 516.51 554.3 578.65 604.26 665.18 696.2 725.88 749.52 753.92 805.14 830.02 834.34 859.73 879.04 893.3 945.44 951.22 954.69 976.82 988.6 1010.6 1028.6 1061.2 1101.5 1128.9 1158.5 1174.1 1183.9 1189.5 1229 1239.2 1269.8 1304.3 1322.1 1336.5 1389 1421.2 1480.1 1505.4 1548 1590.2 1619 1639.7 1655.1 2903.5 3154.7 3157.6 3165.3 3174.4 3176.3 3188.4 3188.9 3202.6 3222.4	C C C C C H H H H C C C C H	3.277367 2.693765 1.318752 1.094598 2.482078 3.304894 0.872410 4.346836 2.932467 -0.960472 -1.743990 -1.095363 0.256632 -1.686616	-0.161124 -1.424280 -1.544983 0.871154 0.973486 -2.314185 -2.531054 -0.061613 1.958705 -0.489106 0.724120 2.006522 2.067071 2.910973	-0.219613 -0.148878 0.052949 0.072278 -0.109370 -0.248815 0.118009 -0.366778 -0.175874 0.500922 0.057315 0.059619 0.102829 -0.040183

			H	0.759883	3.028054	0.076179
			C	-1.862362	-1.638211	0.133649
			C	-3.035979	-1.135891	-0.309761
			C	-2.972576	0.319360	-0.360722
			H	-1.635112	-2.679690	0.312700
			H	-3.907667	-1.717652	-0.581992
			H	-3.775103	0.962596	-0.698685
			H	-1.004979	-0.465357	1.609276
			C	0.513048	-0.416583	0.168144
(OH + phen. rad.) 18	Theory: B3LYP/6-311G(d,p) Energy (hartree): -538.3059580 ZPE (hartree): 0.1696910 $<S^2>$: 0 Rotational constants (GHz): 1.4012 0.7556 0.5143	109.25 183.83 216.07 308.96 315.33 448.74 464.08 474.28 493.5 499.62 560.83 569.31 630.49 641.76 660.87 696.14 702.82 755.73 770.22 800.86 805.22 823.02 891.5 894.71 897.7 908.79 969 972.46 974.99 994.85 1004.9 1042.4 1108.3 1164.3 1171.4 1203.5 1210.6 1215.2 1243.8 1311.3 1341.2 1358.1 1401 1424 1449.7 1463.3 1485.7 1501.8 1604.7 1609.5 1659.2 1725.7 3152.4 3156.7 3156.8 3170 3173.1 3173.5 3183.7 3184.7	C	2.968237	-0.793968	-0.382212
			C	1.961590	-1.808449	-0.158445
			C	0.794641	-1.374810	0.412546
			C	0.700502	0.021714	0.652276
			C	1.472831	1.046989	0.171619
			C	2.756844	0.573249	-0.271607
			H	2.138526	-2.819168	-0.507422
			H	3.934568	-1.126632	-0.747078
			H	3.540348	1.255615	-0.584062
			C	-0.700502	0.021716	0.652276
			C	-1.472829	1.046992	0.171616
			C	-0.695137	2.254538	-0.061292
			C	0.695142	2.254537	-0.061289
			H	-1.200263	3.174559	-0.338785
			H	1.200271	3.174558	-0.338780
			C	-0.794644	-1.374809	0.412551
			C	-1.961595	-1.808448	-0.158434
			C	-2.968238	-0.793964	-0.382211
			C	-2.756841	0.573253	-0.271614
			H	-2.138534	-2.819167	-0.507409
			H	-3.934570	-1.126627	-0.747077
			H	-3.540343	1.255620	-0.584071
(OH + phen. rad.) 19	Theory: B3LYP/6-311G(d,p) Energy (hartree): -613.5563657 ZPE (hartree): 0.1717820 $<S^2>$: 0 Rotational constants (GHz):	71.343 101.53 171.06 218.64 224.12 258.37 324.22 357.35 410.56 419.69 434.03 502.14 514.65 529.61 538.32 598.39 617.53 658.6 687.81 731.71 752.74 767.42 824.28 838.2 846.18 855.97 892.79 915.46 951.06 975 987.08 1015.6 1034.3 1057.2 1090.6 1167 1169.1 1184 1191.5 1231.1 1241.3 1296.8 1330.4 1353.7 1376.5 1392.1	C	-3.604389	-0.277498	-0.007956
			C	-2.874973	-1.485428	0.038622
			C	-1.500233	-1.482061	0.061758
			C	-0.778336	-0.256868	0.034286
			C	-1.523598	0.968973	-0.016091
			C	-2.938980	0.924072	-0.031834
			H	-3.406807	-2.430015	0.057005
			H	-0.945173	-2.407526	0.080658
			H	-4.688086	-0.301591	-0.024019

	1.2445 0.5363 0.3767	1408.2 1455.6 1484.1 1512.1 1546.4 1585.2 1619.4 1633.9 1654.3 3136.9 3155.3 3161.4 3163.8 3174 3180.7 3188.4 3237	H C C C C H H C C C C H H O	-3.489027 0.647430 1.298836 0.534076 -0.831022 1.049783 -1.409901 1.550748 2.932543 3.575613 2.733886 4.653758 3.189605 1.214530	1.858446 -0.183095 1.060274 2.259707 2.209900 3.213144 3.126692 -1.376975 -1.070859 0.031037 1.140803 0.150731 2.115817 -2.512199	-0.067722 0.108603 0.038432 -0.008511 -0.034187 -0.040151 -0.070788 0.059651 0.357787 -0.142229 -0.064785 -0.182942 0.092542 -0.275734
(OH + phen. rad.) 19-20_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -613.5506484 ZPE (hartree): 0.1702240 <S^2>: 0 Rotational constants (GHz): 1.2039 0.5532 0.3869	-340.21 83.538 96.428 160.23 219.75 245.87 280.53 337.37 410.74 418.99 448.82 482.5 518.08 528.41 547.26 565.17 643.23 676.52 692.49 702.33 710.28 765.59 775.59 798.51 834.48 837.5 869.08 882.5 890.29 960.19 969.84 984.27 1003.5 1018.7 1058.8 1130.1 1151.6 1174.3 1185.7 1221.8 1240.1 1275.2 1306.9 1324.5 1372.2 1385.8 1437.8 1449.9 1482.7 1497.8 1542.3 1579.9 1632.6 1652.7 1763.2 3160.9 3164.8 3173.4 3177.3 3182.8 3188.9 3198.5 3248.5	C C C C C C H H H H C C C C H H C C C C H H O	-3.567081 -2.853552 -1.478742 -0.732232 -1.462025 -2.878366 -3.394854 -0.955494 -4.650638 -3.408800 0.706884 1.366228 0.600696 -0.761868 1.123401 -1.335923 1.510761 2.686623 3.489402 2.800163 4.556318 3.306811 1.024730	-0.210837 -1.421730 -1.443757 -0.244481 0.986356 0.967581 -2.353660 -2.384416 -0.213794 1.909840 -0.174607 1.067723 2.259877 2.217227 3.206515 3.132837 -1.519155 -1.135956 -0.033535 1.138724 -0.065716 2.095159 -2.505918	-0.121310 -0.232250 -0.185906 -0.041178 0.064648 0.024529 -0.350483 -0.244254 -0.148994 0.113408 -0.060018 0.014423 0.154740 0.182617 0.232323 0.277062 0.163368 -0.464782 -0.240466 -0.052124 -0.430573 -0.079424 0.674149
(OH + phen. rad.) 20	Theory: B3LYP/6-311G(d,p) Energy (hartree): -613.6551991	58.133 114.64 115.04 168.71 253.29 253.59 287.86 418.11 428.46 430.38 500.82 515.38 527.24 559.3 560.77	C C C	-3.385131 -2.375481 -1.048605	0.949135 1.935583 1.574103	-0.000297 -0.000598 -0.000595

		606.26 646.08 667.98 679.69 702.32	C	-0.659327	0.210599	-0.000303
	ZPE (hartree): 0.1734490	731.5 756.12 776.01 796.59 828.66	C	-1.685697	-0.793242	0.000066
		868.03 869.99 905.59 954.45 967.33	C	-3.042173	-0.381900	0.000036
	$<S^2>$: 0	975.37 990.22 1032.5 1054.3 1093	H	-2.648576	2.984804	-0.000790
		1143.4 1169.4 1183.1 1196.3 1235.1	H	-0.293380	2.351471	-0.000865
	Rotational constants (GHz):	1237.5 1289 1357 1368.8 1376.6 1403.9	H	-4.427938	1.245034	-0.000311
	0.9591	1449.2 1468.6 1484.4 1535.5 1561.3	H	-3.813743	-1.144944	0.000308
	0.5874	1597.2 1629.1 1659.7 2205.9 3158.8	C	0.687375	-0.241765	-0.000129
	0.3643	3162 3168.1 3179.5 3180.9 3190.7 3212	C	1.003156	-1.610578	0.000519
		3238.6	C	-0.024992	-2.581209	0.000896
			C	-1.333879	-2.174200	0.000749
			H	0.225858	-3.636315	0.001156
			H	-2.133375	-2.907381	0.000947
			C	2.205976	1.772113	0.002501
			C	1.972925	0.467326	-0.001539
			C	3.033231	-0.545967	-0.001512
			C	2.443925	-1.769015	-0.000520
			H	4.089160	-0.321589	-0.002542
			H	2.964999	-2.716348	-0.000583
			O	2.411146	2.909922	0.000879
(OH + phen. rad.) 21	Theory: B3LYP/6-311G(d,p)	108.4 140.99 198.84 242.64 280.57	C	3.280558	-0.137421	-0.050114
		390.18 413.75 436.89 470.52 493.9	C	2.697676	-1.428811	-0.005071
	Energy (hartree): -500.1783046	517.42 541.34 592.44 655.57 680.16	C	1.333475	-1.581274	0.017301
		703.3 730.66 761.04 789.15 826.52	C	0.482863	-0.447220	0.004299
	ZPE (hartree): 0.1608530	830.79 869.87 880.29 903.61 953.64	C	1.068572	0.867715	-0.009937
		969.97 974.08 1000.3 1034.5 1039.7	C	2.485323	0.980504	-0.046780
	$<S^2>$: 0	1100.6 1120 1159.7 1172 1181 1206.4	H	3.340100	-2.302049	0.017670
		1243.7 1285.1 1339.2 1354.8 1378.7	H	0.882398	-2.566010	0.059222
	Rotational constants (GHz):	1423.6 1427.9 1471.9 1474.4 1549.1	H	4.359728	-0.038193	-0.073988
	1.9177	1592.2 1598 1659.1 3159.8 3161.5	H	2.929272	1.970359	-0.067561
	0.6747	3168.7 3173.4 3177.8 3181.9 3190.5	C	-0.927870	-0.524956	-0.011391
	0.5007	3224.4	C	-1.725981	0.633250	-0.032901
			C	-1.152311	1.903765	0.069699
			C	0.230290	2.008963	0.041719
			H	-1.769219	2.791437	0.161705
			H	0.695583	2.988521	0.073858
			C	-1.868466	-1.587420	0.273415
			C	-3.169384	-1.185837	-0.162056
			C	-3.134499	0.186008	-0.093369
			H	-4.052318	-1.806759	-0.200828

			H	-3.987018	0.839102	0.061042
(OH + phen. rad.) 22	Theory: B3LYP/6-311G(d,p) Energy (hartree): -613.6734647 ZPE (hartree): 0.1762760 <S^2>: 0 Rotational constants (GHz): 1.2348 0.6349 0.4193	89.085 196.72 211.36 300.44 323.46 344.17 436.41 453.87 488.21 505.19 553.8 574.59 579.8 605 616.81 650.25 681.49 701.48 727.14 766.37 767.52 800.45 801.9 832.95 834.89 891.75 899.78 968.34 969.19 980.78 1012.1 1012.2 1033.7 1050.2 1062.9 1159.3 1186.4 1192.1 1234 1237.7 1242.9 1262.6 1338.8 1386.4 1389.3 1434.5 1449.9 1474.4 1499.5 1521.5 1531.1 1619.2 1660.6 1676.7 1706.8 3159.7 3166.8 3166.9 3176.8 3182.8 3183.1 3205.8 3206.2	C C C C C C H H H C C C C C C H H H O	3.313387 2.471238 1.115900 0.691464 1.472378 2.862681 2.889727 4.383920 3.586382 -0.691491 -1.472456 -0.690754 0.690632 -1.207720 1.207646 -1.115849 -2.471156 -3.313321 -2.862688 -2.889579 -4.383853 -3.586375 0.000007	-0.426707 -1.571723 -1.316744 0.008809 1.157863 0.896646 -2.569645 -0.599593 1.704063 0.008805 1.157840 2.379213 2.379238 3.333267 3.333274 -1.316864 -1.571786 -0.426764 0.896611 -2.569750 -0.599654 1.704040 -2.157828	0.000544 0.000192 -0.000464 -0.000606 -0.000126 0.000402 0.000515 0.000916 0.000660 -0.000552 -0.000211 -0.000178 -0.000094 0.000129 0.000027 -0.000314 0.000346 0.000527 0.000257 0.000714 0.000931 0.000560 -0.000351
(OH + phen. rad.) 23	Theory: B3LYP/6-311G(d,p) Energy (hartree): -538.3291898 ZPE (hartree): 0.1686020 <S^2>: 0 Rotational constants (GHz): 1.7335 0.5554 0.4206	98.06 128.08 224.81 238.53 243.77 379.92 411.63 434.74 451.22 462.99 472.49 519.62 559.77 579.08 593.46 666.02 677.87 727.1 754.62 775.23 779.58 804.9 846.72 884.54 885.41 939.47 965.01 979.17 980.3 998.13 1051.2 1080.6 1133.1 1144.9 1172.3 1177.1 1222.5 1229.6 1250.6 1299.4 1325.1 1363.6 1398.7 1435.4 1443.1 1474.1 1496.1 1542.1 1573 1639.4 1656.3 2038.3 3158.7 3160.8 3164 3166.9 3177.6 3179.1 3189.8 3202.3	C C C C C C H H C C C C H H C C	-3.652209 -2.780344 -1.543697 -0.712133 -1.510405 -2.934627 -4.733499 -3.482373 0.721801 1.352052 0.542975 -0.816267 1.042490 -1.400741 2.894379 3.522060	-0.521029 -1.609549 -1.593938 -0.469091 0.732539 0.674127 -0.554236 1.611391 -0.407118 0.868231 2.050723 1.988808 3.013780 2.902427 -1.482500 -0.221639	-0.000061 -0.000121 -0.000080 0.000037 0.000088 0.000042 -0.000111 0.000098 0.000028 -0.000058 -0.000005 0.000093 -0.000034 0.000196 0.000084 -0.000062

			C	2.764164	0.929635	-0.000129
			H	3.496442	-2.383946	0.000202
			H	4.604391	-0.159227	-0.000135
			H	3.245745	1.901861	-0.000250
			C	1.518997	-1.571494	0.000115
			H	1.027068	-2.538270	0.000213
(OH + phen. rad.) 24	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7827439 ZPE (hartree): 0.1933940 $<S^2>$: 0 Rotational constants (GHz): 1.0790 0.3361 0.2567	43.105 49.322 63.584 133.01 158.54 166.75 199.47 254.75 270.42 355.98 393.02 427.32 442.52 484.23 502.24 545.56 584.02 585.06 616.59 680.44 710.83 718.78 747.31 755.53 791.91 851.28 872.7 904.94 923.76 926.1 949.11 955.42 972.34 983.07 990.11 1001.3 1067.3 1147.1 1167.7 1192.8 1205.8 1211.8 1247.9 1275 1305 1355.6 1381.4 1406.9 1425.6 1437.4 1455.3 1482.9 1514.3 1571.2 1591.1 1637.5 1675.5 1701.6 2201 2991.8 3000.7 3053.8 3147.1 3159.7 3161.4 3169.3 3174.1 3178.3 3186	C	-1.839523	1.982776	0.000130
			C	-0.541242	2.370737	0.000142
			C	0.537904	1.411279	0.000118
			C	0.172844	0.021080	0.000391
			C	-1.126976	-0.388676	0.000521
			C	-2.200071	0.590199	0.000163
			C	1.850562	1.879277	-0.000110
			C	3.071080	1.154714	-0.000200
			C	3.260284	-0.189362	-0.000136
			C	4.090110	-1.164729	-0.000328
			C	-1.479072	-1.862905	0.001423
			C	-2.941871	-2.176561	-0.000413
			C	-3.881371	-1.211344	-0.001075
			C	-3.511856	0.178191	-0.000449
			O	4.718280	-2.161748	-0.000380
			H	-2.635631	2.719932	0.000028
			H	-0.287945	3.425511	0.000073
			H	1.962329	2.959899	-0.000249
			H	3.955543	1.797409	-0.000239
			H	0.976102	-0.706119	0.000547
			H	-1.009956	-2.352786	-0.863654
			H	-3.226525	-3.223362	-0.000962
			H	-4.934134	-1.470284	-0.002174
			H	-4.297848	0.926461	-0.000727
			H	-1.012988	-2.350742	0.869334
(OH + phen. rad.) 25	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7739696 ZPE (hartree): 0.1939700 $<S^2>$: 0 Rotational constants (GHz):	59.119 85.932 105.51 165.73 209.73 253.9 269.94 352.29 419.76 446.03 479.37 489.79 502.52 507.43 537.31 586.1 610.55 645.91 703.68 720.5 741.27 753.51 763.57 783.97 829.76 845.88 884.41 889.84 910 932.68 953.36 978.28 982.98 992.21 997.97 1023.7 1045.7 1063.9 1104.7 1165.3 1184.7 1198.9 1213.5 1223.7 1238.5 1256.2 1275.5	C	1.152462	2.152640	0.327886
			C	-0.167602	2.408361	0.179129
			C	-1.061507	1.331714	-0.165936
			C	-0.505552	-0.010330	-0.303662
			C	0.811687	-0.283028	-0.138107
			C	1.714594	0.826142	0.164323
			C	-2.405442	1.336247	-0.383706
			C	-2.919968	-0.026764	-0.693296
			C	-1.626003	-0.950439	-0.600111

	1.1832 0.4775 0.3658	1354 1365.4 1411.8 1435.1 1444.2 1456.5 1549.9 1601.2 1628 1661.5 1688.9 1915.3 2966.9 2970.8 3125.7 3134.1 3154.2 3158.9 3167.4 3179.6 3181 3207.5	C C C C C O H H H H H H H H H H	-2.745736 1.365901 2.864205 3.634088 3.061842 -3.222933 1.838645 -0.559663 -3.056229 -3.695101 -1.479864 0.943261 3.310830 4.712400 3.723773 1.007588	-1.038286 -1.693068 -1.780595 -0.706308 0.605329 -1.625510 2.956189 3.411288 2.197489 -0.175973 -1.799071 -2.311480 -2.759494 -0.812379 1.439384 -2.171558	0.376750 -0.237051 -0.175299 0.067590 0.261797 1.296135 0.575498 0.306041 -0.312320 -1.440586 -1.263111 0.569514 -0.314501 0.121142 0.468664 -1.161263
(OH + phen. rad.) 25-26_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7372959 ZPE (hartree): 0.1914670 $<S^2>$: 0 Rotational constants (GHz): 1.2356 0.4462 0.3638	-399.15 57.034 86.398 101.52 166.77 207.55 241.96 265.01 326.4 408.15 422.9 456.54 472.2 498.88 502.45 538.11 580.51 607.18 624.28 654.41 704.99 727.57 747.03 749.61 799.36 810.18 854.6 860.1 868.12 924.86 959.31 963.2 968.5 983.2 990.48 1020 1054.9 1116.2 1160.7 1185.5 1199.4 1206.5 1208.8 1219.3 1242.7 1272.3 1323.4 1356.9 1378.7 1416.2 1434.2 1451.9 1465.9 1524.8 1575.8 1597.9 1628.4 1669.3 2051.7 2917.3 2930.6 3005 3148.5 3158 3165.7 3177.4 3179.6 3228.8 3242.8	C C C C C H H H C C C C H H C C C C H H H O	3.696918 3.009319 1.532980 0.889032 1.693179 3.047640 3.522151 1.353565 4.764311 3.635138 -0.463800 -1.082782 -0.264647 1.064335 -0.717416 1.700223 -3.225496 -1.484634 -2.785765 -2.424250 -1.396606 -3.520801 -3.159315 -3.303313	-0.569714 -1.686136 -1.676894 -0.312442 0.836513 0.710733 -2.640797 -2.083353 -0.626756 1.587569 -0.143001 1.183022 2.319561 2.138688 3.300736 2.981840 -0.829716 -1.058993 -0.335925 1.108829 -2.117930 -0.514924 1.898047 -1.186441	0.261297 -0.049920 -0.326098 -0.189864 0.136652 0.353391 -0.114722 -1.336981 0.448461 0.601766 -0.392511 -0.268564 0.057302 0.247762 0.147405 0.497879 0.510214 -0.763721 -0.805649 -0.510989 -0.946093 -1.597523 -0.457898 1.607639

			H	1.033079	-2.400047	0.340771
(OH + phen. rad.) 26	Theory: B3LYP/6-311G(d,p) Energy (hartree): -501.4662592 ZPE (hartree): 0.1851260 <S^2>: 0 Rotational constants (GHz): 1.7570 0.6768 0.4901	55.922 138.4 170.31 242.98 245.61 315.59 430.29 457.88 467.62 502.29 503.91 578.93 603.15 627.53 644.18 704.52 723.91 746.01 764.76 780.77 831.86 838.59 858.07 916.54 921.76 929.05 940.05 967.25 993.05 995.66 1015.1 1046.8 1105.3 1112.8 1167.6 1192.4 1195.2 1211.3 1239.2 1274.6 1347.4 1352.2 1386.5 1404.5 1418.4 1430.1 1434.6 1481.8 1553.3 1578.7 1618.8 1640.5 1681.7 2996.6 3008.1 3156.7 3158.4 3166.3 3177.7 3184.4 3194.4 3209.9 3223.3	C C C C C C H H H H C C C C C H H H H	-3.292770 -2.815887 -1.346538 -0.438162 -1.031538 -2.398750 -3.488623 -1.104934 -4.361373 -2.830668 0.924360 1.778135 1.178557 -0.174894 1.808345 -0.649972 1.812274 3.096765 3.087476 1.511662 3.965899 3.992295 -1.116802	-0.065498 -1.322488 -1.605371 -0.395967 0.940701 1.063913 -2.173514 -2.247518 0.118309 2.059841 -0.501765 0.694276 1.989343 2.106591 2.873214 3.081305 -1.650304 -1.177336 0.271718 -2.688187 0.902837 -1.784970 -2.228197	-0.005776 -0.002802 0.007755 0.002447 0.001988 -0.001560 -0.005741 -0.850300 -0.011692 -0.002885 -0.000017 -0.000333 0.001310 0.002319 0.001551 0.002819 -0.002046 -0.002915 -0.001761 -0.002643 -0.002174 -0.004235 0.883633
(OH + phen. rad.) 27	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7114382 ZPE (hartree): 0.1904790 <S^2>: 0 Rotational constants (GHz): 1.2099 0.3108 0.2483	39.128 61.092 66.936 119.13 146.07 190.78 240.84 246.22 277.34 384.54 394.83 419.26 434.8 460.28 500.39 538.01 549.62 596.66 625.36 673.84 689.08 724.33 746.85 763.91 786.01 806.72 815.67 868.29 883.57 908.17 934.8 967.17 971.22 979.03 997.81 1037.5 1042.5 1117.3 1141.1 1168.5 1180 1195.4 1235.9 1258.1 1276.6 1301.1 1342.1 1351.2 1369.4 1391.5 1411.8 1437.6 1481 1515.3 1560.1 1589.1 1647.5 1664.1 2187.6 2879.7 2964.2 2971.1 3124.1 3131.6 3150.5 3156 3167.9 3174.6 3181.1	C C C C C C H H H H C C C C C C H H H	3.991890 2.971352 1.575197 1.212352 2.270212 3.644050 3.216993 0.785683 5.025054 4.401040 -0.196664 -0.525446 0.500040 1.868215 0.225250 2.603466	-1.088923 -2.171081 -1.703661 -0.383187 0.624043 0.209731 -2.827862 -2.442092 -1.384570 0.982293 -0.074067 1.296519 2.261489 1.942358 3.311710 2.740193	0.175886 0.041377 -0.132486 -0.146104 -0.041761 0.126889 -0.810721 -0.232036 0.319117 0.226072 -0.200837 -0.022413 -0.100255 -0.079906 -0.179464 -0.064814

			C	-4.219066	-1.112556	0.010370
			C	-3.122618	-0.388313	-0.015771
			C	-3.044123	1.044345	0.139220
			C	-1.901678	1.771143	0.125554
			H	-2.159780	-0.902212	-0.180568
			H	-3.978531	1.581879	0.270479
			H	-2.012319	2.845174	0.251159
			O	-5.157977	-1.801536	0.027534
			H	3.014685	-2.859266	0.901928
(OH + phen. rad.) 27-29_TS	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.6881833 ZPE (hartree): 0.1896220 $<S^2>$: 0 Rotational constants (GHz): 0.9842 0.5121 0.3792	-234.97 41.519 47.681 93.959 139.56 169.78 225.61 262.54 283.87 387.87 407.49 438.78 442.9 451.95 469.47 500.13 565.18 594.59 618.96 639.97 678.97 703.37 723.35 747.69 773.02 798.02 803.67 829.32 889.24 894.92 920.22 948.87 956.16 969.6 979 992.67 1041.9 1110.8 1118.2 1159.4 1169.9 1186.6 1202.2 1243.5 1269.8 1302.4 1343.1 1363.1 1367.2 1396.2 1401.5 1432.1 1437 1518.3 1564.1 1586.4 1650.3 1675.8 2157.8 2930 2945.3 3142.4 3144.7 3152.5 3156.2 3163.8 3165.2 3168.8 3177.9	C	3.483968	-0.516972	0.273290
			C	2.778417	-1.575428	-0.522956
			C	1.382190	-1.211408	-0.909395
			C	0.790566	-0.027428	-0.563058
			C	1.563426	0.993251	0.156206
			C	2.910449	0.659367	0.573892
			H	3.357661	-1.805006	-1.434771
			H	0.793259	-1.951072	-1.442158
			H	4.492089	-0.735788	0.609996
			H	3.458617	1.397646	1.152649
			C	-0.598249	0.237250	-0.838888
			C	-1.219261	1.337611	-0.232978
			C	-0.424551	2.395476	0.217322
			C	0.956136	2.196113	0.440255
			H	-0.863420	3.372558	0.397829
			H	1.533362	2.988206	0.906776
			C	-2.050483	-1.832795	0.572581
			C	-2.436285	-1.088563	-0.464812
			C	-3.287470	0.123014	-0.248076
			C	-2.677674	1.311541	-0.156249
			H	-2.421256	-1.595210	-1.424698
			H	-4.363695	0.006855	-0.186889
			H	-3.239316	2.222991	0.025028
			O	-1.569437	-2.422011	1.448238
			H	2.781114	-2.531269	0.027533
(OH + phen. rad.) 28	Theory: B3LYP/6-311G(d,p) Energy (hartree): -614.7633035 ZPE (hartree): 0.1939070	64.278 92.146 141.92 154.43 209.66 256.97 268.16 344.34 383.72 427.09 447.41 474.79 502.17 512.93 581.24 612.84 619.78 664.01 700.33 708.03 757.47 770.26 795.92 803.59 832.48 839.66 859.53 891.78 915.05 918.15	C	3.516314	-0.164123	-0.100667
			C	2.850622	-1.431984	-0.546541
			C	1.352675	-1.353508	-0.532124
			C	0.672070	-0.245798	-0.180384
			C	1.375040	0.995587	0.178501
			C	2.826979	0.939066	0.222473

	$<S^2>$: 0	938.37 950.66 965.43 985.43 997.35	H	3.201025	-1.699027	-1.556970
		1015.6 1024.8 1073.3 1108.3 1115.7	H	0.815272	-2.255282	-0.810931
	Rotational constants (GHz):	1170 1196.3 1206 1224.4 1253.1 1282.6	H	4.600766	-0.160026	-0.055031
	1.1327	1312.2 1366.1 1372.2 1375.5 1423.3	H	3.351705	1.840657	0.524224
	0.5410	1431.6 1455.9 1559.3 1593 1648.2	C	-0.812014	-0.187422	-0.049841
	0.4233	1660.2 1710.7 1907.1 2952.6 2958.9	C	-1.463621	1.156396	-0.089003
		3118.3 3146.9 3149.1 3160.3 3168.7	C	-0.738350	2.262261	0.204891
		3176.8 3195.5 3215.5	C	0.684328	2.154786	0.399317
			H	-1.208222	3.238879	0.242522
			H	1.239991	3.052658	0.649159
			C	-1.481024	-1.259037	0.772097
			C	-1.900599	-1.193871	-0.638057
			C	-3.084032	-0.302685	-0.847697
			C	-2.832416	0.981959	-0.517913
			H	-1.673960	-2.004380	-1.327333
			H	-4.035096	-0.696566	-1.181379
			H	-3.553502	1.787518	-0.568886
			O	-1.465104	-1.867707	1.794103
			H	3.187023	-2.272544	0.081496
(OH + phen. rad.) 28-29_TS	Theory: B3LYP/6-311G(d,p)	-416.18 68.129 85.138 110.79 169.64	C	3.495006	-0.232471	0.025053
		217.5 224.45 273.31 313.73 406.64	C	2.825175	-1.499462	-0.427082
	Energy (hartree): -614.7406244	425.65 449.68 481.11 483.29 500.39	C	1.335963	-1.355598	-0.569671
		546.57 607.06 633.48 667.53 697.06	C	0.672733	-0.193688	-0.289242
	ZPE (hartree): 0.1916760	718.41 726.75 737.24 784.33 801.14	C	1.387696	1.014607	0.131541
		809.6 841.01 892.05 914.83 925.1 935.69	C	2.829688	0.906466	0.270158
	$<S^2>$: 0	950.66 961.14 967.56 995.52 1024.2	H	3.277867	-1.824941	-1.379755
		1076 1108.9 1144.5 1166.3 1177.4	H	0.786949	-2.223370	-0.924041
	Rotational constants (GHz):	1200.2 1216 1236.9 1248.6 1300.9	H	4.573578	-0.261168	0.150789
	1.0975	1332.1 1363.6 1368.1 1418.9 1434.6	H	3.371456	1.792623	0.588720
	0.5478	1443 1468.7 1521.9 1569.2 1601.6	C	-0.753753	-0.023007	-0.346970
	0.4156	1630.4 1688.7 2083.8 2912.1 2927.3	C	-1.411024	1.222090	-0.123913
		2938.5 3137.8 3138.9 3152.4 3160.1	C	-0.690015	2.340266	0.229644
		3187.8 3200.2 3234.2	C	0.718315	2.198850	0.365213
			H	-1.169013	3.296344	0.401112
			H	1.302192	3.066058	0.658789
			C	-1.616058	-1.617098	0.618304
			C	-1.781303	-1.060720	-0.698506
			C	-3.087611	-0.268093	-0.667811
			C	-2.831444	1.017523	-0.341619
			H	-1.637145	-1.748674	-1.545174

			H	-4.045537	-0.733829	-0.845949
			H	-3.583544	1.790732	-0.247499
			O	-1.564657	-1.942360	1.727208
			H	3.080263	-2.312884	0.274748
(OH + phen. rad.) 29	Theory: B3LYP/6-311G(d,p) Energy (hartree): -501.4633775 ZPE (hartree): 0.1849290 <S^2>: 0 Rotational constants (GHz): 1.8571 0.6467 0.4811	81.93 126 193.14 248.38 269.46 305.23 423.66 448.91 449.86 452.31 509.98 570.66 614.17 647.93 669.9 706.8 738.62 746.57 783.98 819.74 834.77 841.67 866.44 867.05 903.59 914.67 950.97 958.85 969.2 997.86 1023.2 1042.5 1082.2 1097.1 1163.4 1184.7 1189.5 1245.2 1277.7 1285 1311.1 1363.3 1370.7 1408.5 1422.7 1426.8 1435.9 1471.2 1550.6 1589.2 1615.9 1649.3 1702.1 2956 2958.1 3151.9 3155.2 3159.8 3171.9 3175 3193.8 3207 3225.3	C	3.312116	0.004286	-0.000061
			C	2.793706	-1.395810	0.000122
			C	1.307222	-1.502660	0.000039
			C	0.466246	-0.436101	-0.000020
			C	1.041541	0.922972	-0.000011
			C	2.485361	1.060879	-0.000117
			H	3.200513	-1.945393	-0.865219
			H	4.387797	0.145075	-0.000166
			H	2.888126	2.069140	-0.000266
			C	-0.984577	-0.541609	-0.000069
			C	-1.799727	0.678191	-0.000023
			C	-1.204042	1.905626	0.000092
			C	0.221096	2.022087	0.000062
			H	-1.804127	2.810738	0.000190
			H	0.665346	3.011756	0.000073
			C	-1.855257	-1.605048	-0.000061
			C	-3.212223	-1.091992	-0.000021
			C	-3.187504	0.276249	0.000008
			H	-1.599896	-2.656447	-0.000041
			H	-4.035484	0.945937	0.000027
			H	-4.098892	-1.712129	-0.000001
			H	0.892513	-2.506010	0.000048
			H	3.200361	-1.945097	0.865726
(OH + phen. rad.) CO	Theory: B3LYP/6-311G(d,p) Energy (hartree): -113.3462354 ZPE (hartree): 0.0050570 <S^2>: 0 Rotational constants (GHz): 0.0000 58.0386 58.0386	2219.8	C	0.000000	0.000000	-0.643976
			O	0.000000	0.000000	0.482982

(OH + phen. rad.) H_2	Theory: B3LYP/6-311G(d,p) Energy (hartree): -1.1795710 ZPE (hartree): 0.0100680 $<S^2>$: 0 Rotational constants (GHz): 0.0000 1810.9604 1810.9604	4419.2	H H	0.000000 0.000000	0.000000 0.000000	0.372089 -0.372089