

Supporting Information

Performance of Edges on Carbon for the Catalytic Hydroxylation of Benzene to Phenol

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Catalysis Science & Technology

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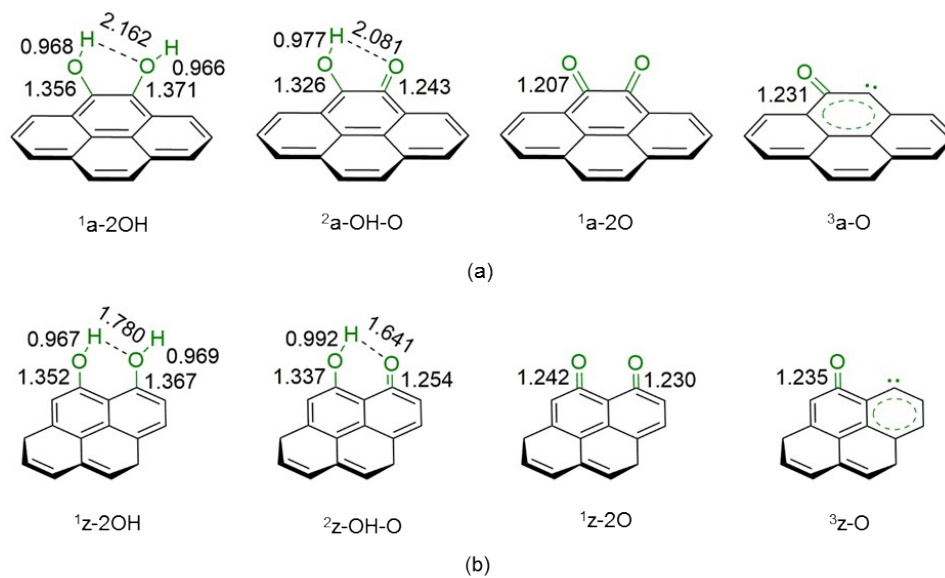


Figure S1. The geometric structures for the active sites of two models of carbon with (a) Armchair edges and (b) Zigzag edges in acetonitrile solution. For clarity, hydrogen atoms on carbon are not shown. Bond lengths are reported in Å.

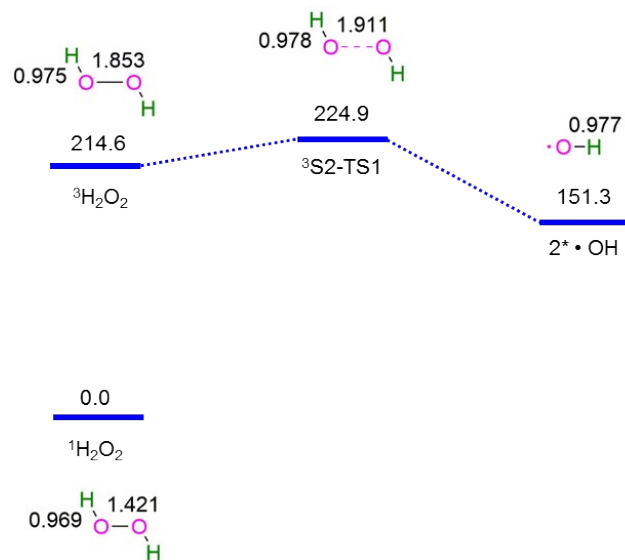


Figure S2. The geometric structures and the schematic energy diagrams with the relative Gibbs free energy (G_r , kJ mol^{-1}) relative to the singlet ground state H_2O_2 for the H_2O_2 decomposition in acetonitrile solution. Bond lengths are reported in Å.

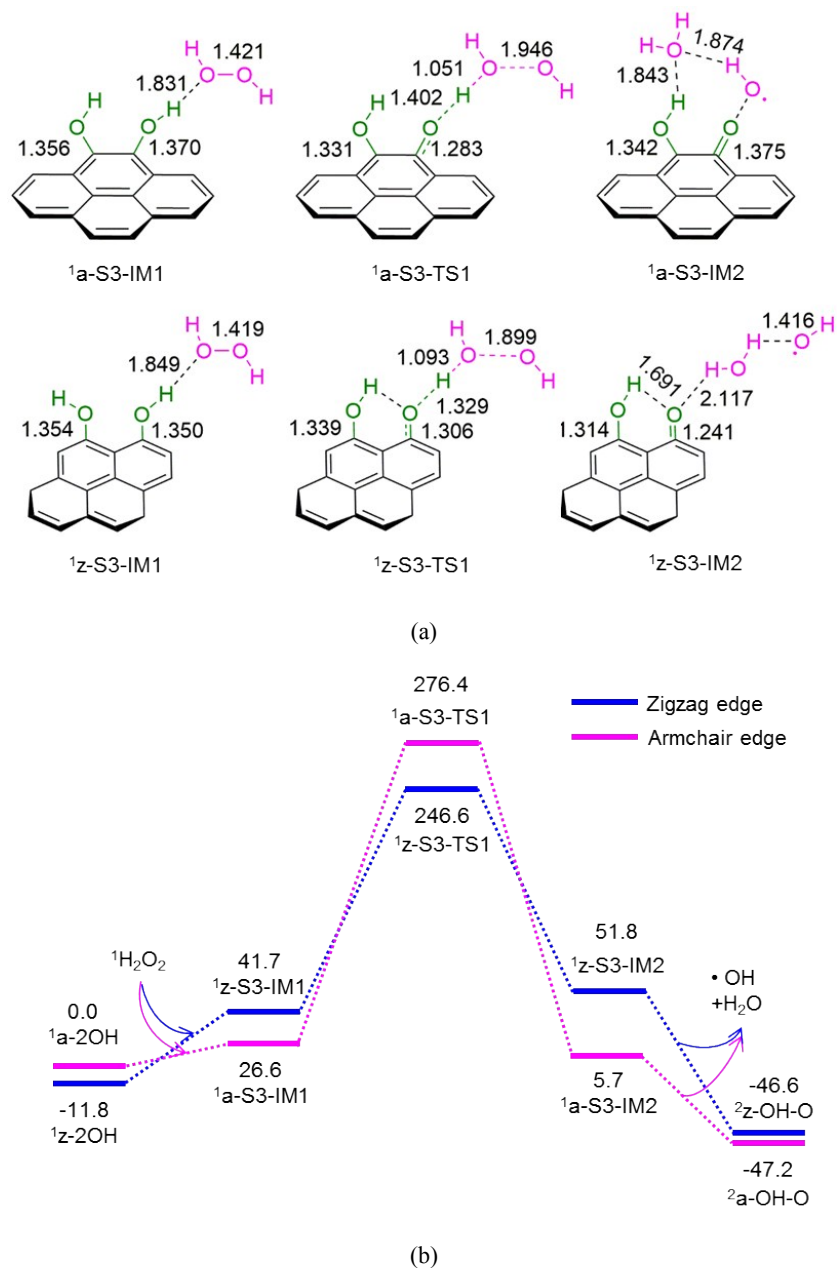


Figure S3. The geometric structures (a) and the schematic energy diagrams (b) with the relative Gibbs free energy (G_r , kJ mol⁻¹) relative to the ground state reactants ¹a-2OH/¹z-2OH + H₂O₂ for the H₂O₂ decomposition in acetonitrile solution. For clarity, hydrogen atoms on carbon are not shown. Bond lengths are reported in Å.

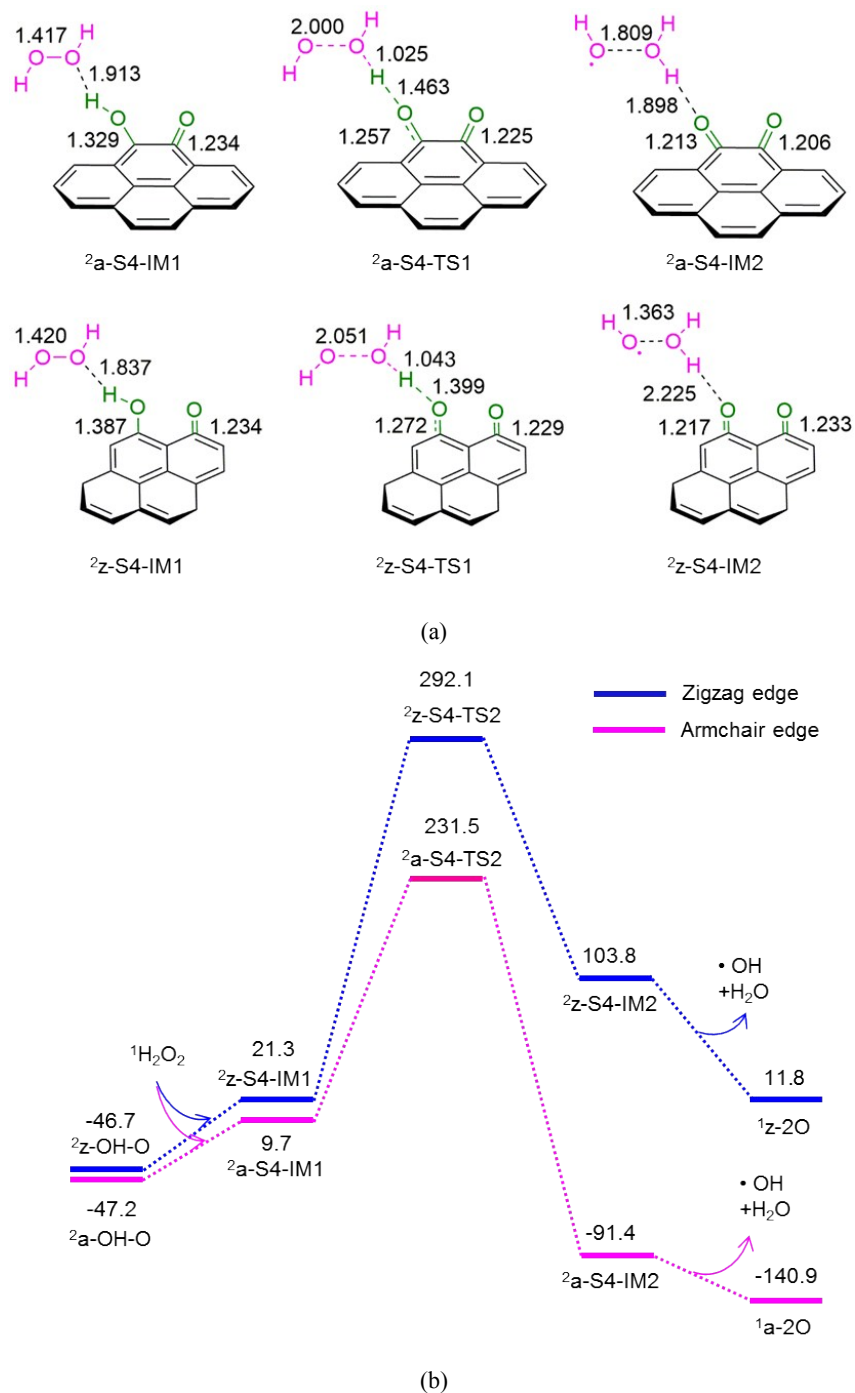
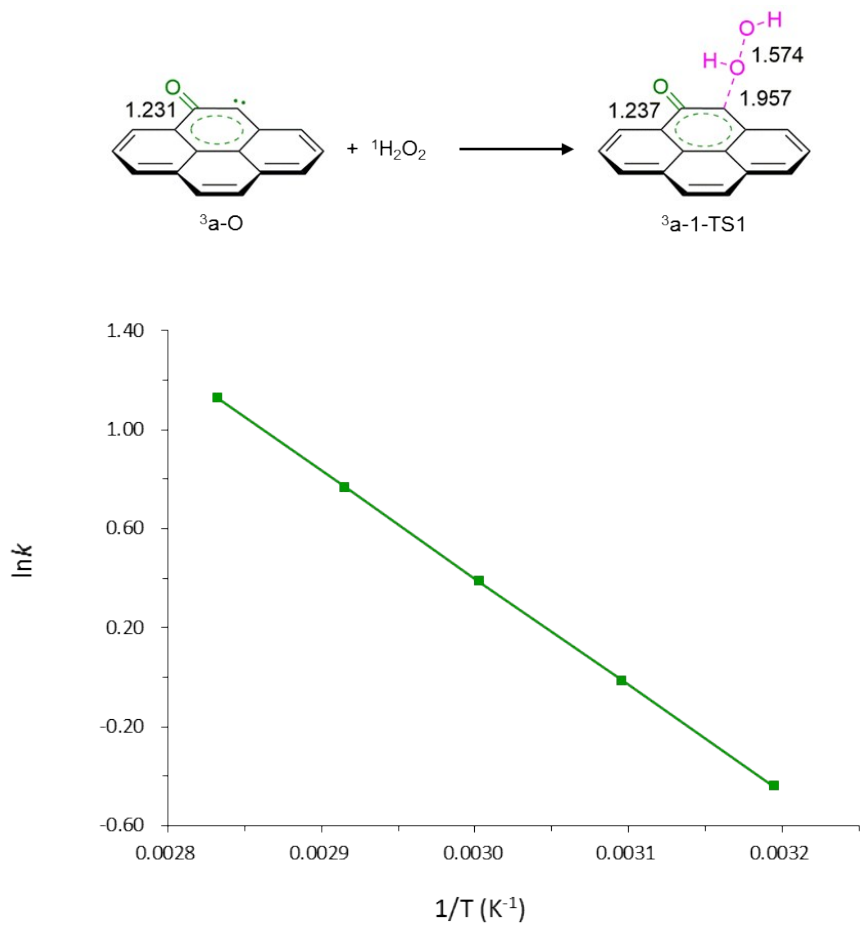
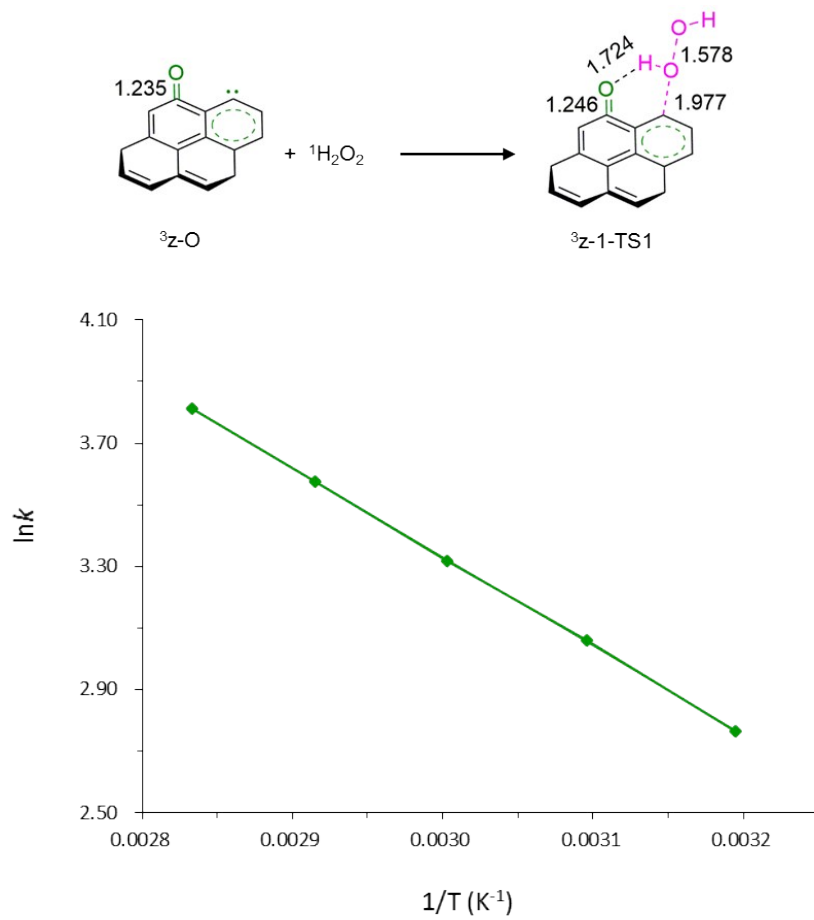


Figure S4. The geometric structures (a) and the schematic energy diagrams (b) with the relative Gibbs free energy (G_r , kJ mol⁻¹) relative to the ground state reactants ²a-OH-O/²z-OH-O + H₂O₂ for the H₂O₂ decomposition in acetonitrile solution. For clarity, hydrogen atoms on carbon are not shown. Bond lengths are reported in Å.



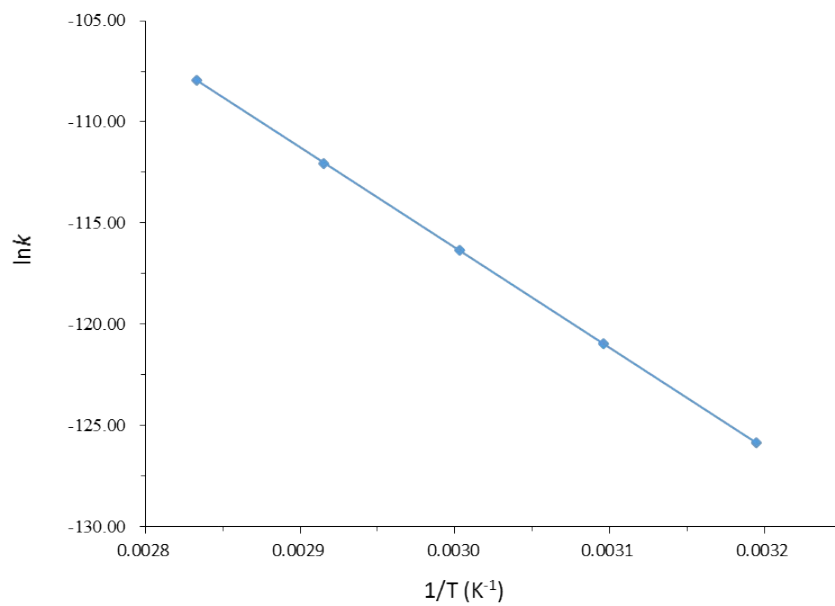
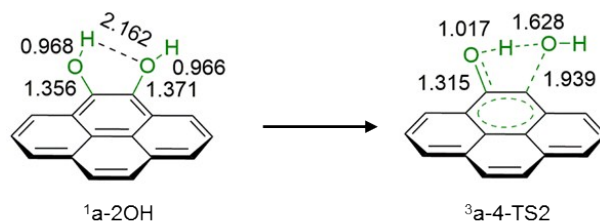
$$k_{CA-1} = 6.528 \times 10^5 \exp(-35,994/RT)$$

Figure S5. Arrhenius plots of rate constants for the crucial reaction step ${}^3\text{a-O} + {}^1\text{H}_2\text{O}_2 \rightarrow {}^3\text{a-1-TS1}$ for the gross reaction $\text{benzene} + \text{H}_2\text{O}_2 \rightarrow \text{phenol} + \text{H}_2\text{O}$ catalyzed by the defect armchair ${}^3\text{a-O}$, which is denoted as CA-1.



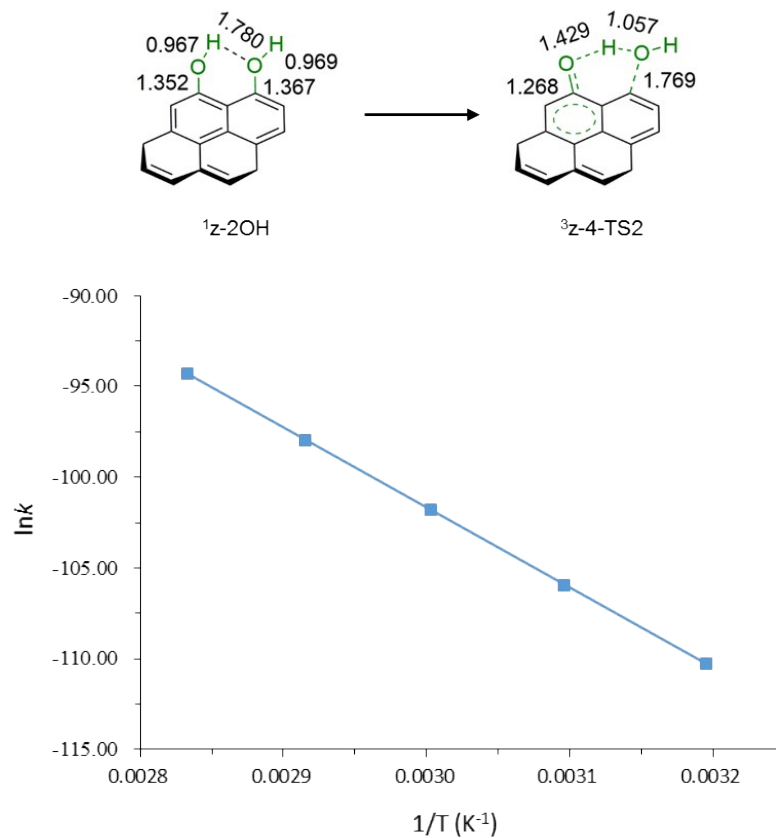
$$k_{\text{CZ-1}} = 1.603 \times 10^5 \exp(-23,984/RT)$$

Figure S6. Arrhenius plots of rate constants for the crucial reaction step $^3z\text{-O} + ^1\text{H}_2\text{O}_2 \rightarrow ^3z\text{-1-TS1}$ for the gross reaction benzene + $\text{H}_2\text{O}_2 \rightarrow$ phenol + H_2O catalyzed by the defect zigzag $^3z\text{-O}$, which is denoted as CZ-1.



$$k_{\text{CA-2}} = 6.927 \times 10^{13} \exp(-410,362/RT)$$

Figure S7: Arrhenius plots of rate constants for the crucial reaction step ${}^1\text{a-2OH} \rightarrow {}^3\text{a-4-TS2}$ for the whole reaction of benzene + $\text{H}_2\text{O}_2 \rightarrow$ phenol + H_2O catalyzed by the defect armchair ${}^3\text{a-O}$, which is denoted as CA-2.

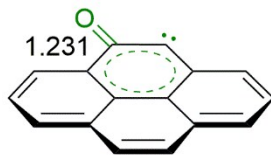


$$k_{u-2} = 2.594 \times 10^{13} \exp(-367,420/RT)$$

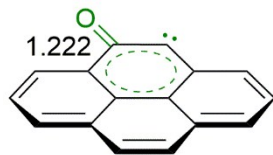
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Table S1: Snapshot and standard orientation of all the species in the solvent of acetonitrile under the temperature of 343.15 K calculated at the M06-2x level. For clarity, hydrogen atoms on ring are not shown.

³a-O

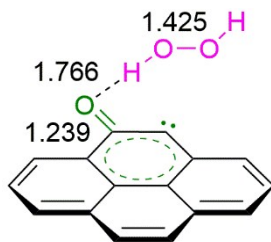


¹a-O

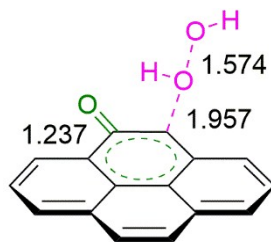


C	-3.582557	0.592086	0.000083
C	-3.160158	-0.728743	0.000255
C	-1.786874	-1.055104	0.000187
C	-0.835143	-0.018088	0.000088
C	-1.279821	1.345212	-0.000120
C	-2.655501	1.630706	-0.000096
C	-1.336161	-2.420196	0.000299
C	0.567500	-0.320247	-0.000086
C	0.979790	-1.674164	0.000000
C	-0.013127	-2.714419	0.000149
C	2.356331	-1.971466	-0.000095
H	2.666628	-3.011182	-0.000103
C	3.298718	-0.961355	-0.000165
C	2.894993	0.379420	-0.000153
C	1.548744	0.704812	-0.000050
C	1.133562	2.138352	0.000047
C	-0.286086	2.326353	-0.000207
H	-2.082193	-3.207841	0.000404
H	-4.642074	0.818856	0.000073
H	-3.885732	-1.535414	0.000446
H	-2.980961	2.664429	-0.000221
H	0.326217	-3.744853	0.000230
H	4.355047	-1.203631	-0.000207
H	3.629074	1.177027	-0.000196
O	1.943593	3.065458	-0.000156

C	3.588053	0.355010	-0.003114
C	3.063435	-0.918764	0.129141
C	1.668584	-1.158058	0.097209
C	0.798934	-0.061885	-0.008499
C	1.332705	1.265559	-0.170511
C	2.729802	1.434738	-0.205424
C	1.132905	-2.490065	0.157946
C	-0.616974	-0.288059	-0.062062
C	-1.121813	-1.602177	-0.016557
C	-0.206131	-2.702899	0.095836
C	-2.523402	-1.789297	-0.071215
H	-2.916556	-2.800323	-0.053207
C	-3.378146	-0.711120	-0.141118
C	-2.870486	0.602569	-0.144156
C	-1.508579	0.807843	-0.117702
C	-0.899263	2.159748	0.047456
C	0.482649	2.369316	-0.417178
H	1.826052	-3.320078	0.242747
H	4.660422	0.504645	0.011046
H	3.728967	-1.769670	0.239352
H	3.123956	2.432432	-0.364007
H	-0.611042	-3.708527	0.132565
H	-4.449003	-0.870407	-0.187898
H	-3.542517	1.453474	-0.173680
O	-1.481740	3.055463	0.641597

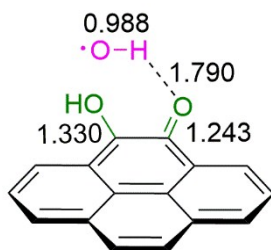
³a-1-IM1

C	-1.121539	3.554477	-0.002219
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C	0.166884	1.504474	-0.010752
C	0.111246	2.908660	-0.011024
C	-3.497576	0.641448	0.018641
C	-0.997900	-0.692999	-0.000847
C	-2.209726	-1.422694	0.009162
C	-3.460194	-0.714063	0.018927
C	-2.162244	-2.830313	0.008883
H	-3.095393	-3.383755	0.016407
C	-0.953509	-3.499397	-0.000853
C	0.248730	-2.782300	-0.010694
C	0.235146	-1.396837	-0.010223
C	1.512638	-0.642283	-0.020031
C	1.356448	0.777745	-0.018815
H	-4.443136	1.172768	0.026201
H	-1.160093	4.637070	-0.002937
H	-3.257465	3.331514	0.014466
H	1.035698	3.474229	-0.018280
H	-4.376507	-1.294498	0.026519
H	-0.932237	-4.582696	-0.000739
H	1.199954	-3.301829	-0.018624
O	2.619221	-1.200845	-0.027946
O	5.786922	0.105104	-0.011239
H	6.072461	0.271395	0.897693
O	4.526979	0.769647	-0.059876
H	3.899859	0.015185	-0.056848

³a-1-TS1

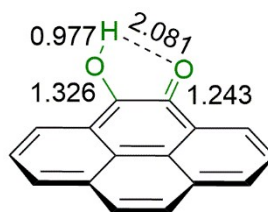
C	1.037663	3.287792	-0.019818
C	-0.349084	3.320440	-0.006602
C	-1.107802	2.130338	0.000204
C	-0.438871	0.891486	-0.005910
C	0.994777	0.868112	-0.018495
C	1.716415	2.072236	-0.025043
C	-2.545524	2.150796	0.013786
C	-1.183919	-0.334809	0.000039
C	-2.597896	-0.281660	0.014487
C	-3.256219	0.996500	0.021018
C	-3.329510	-1.484692	0.022652
H	-4.413387	-1.435534	0.034971
C	-2.685001	-2.706968	0.016308
C	-1.286363	-2.765430	-0.000141
C	-0.538379	-1.599291	-0.007758
C	0.944644	-1.664414	-0.025021
C	1.593714	-0.391481	-0.025096
H	-3.046393	3.112936	0.019516
H	1.598286	4.214871	-0.026387
H	-0.871820	4.271019	-0.001269
H	2.799550	2.038915	-0.035792
H	-4.340871	1.012897	0.032355
H	-3.261398	-3.624510	0.024314
H	-0.773815	-3.720525	-0.006516
O	1.583902	-2.723420	-0.038522
O	5.110086	-0.548666	0.004592
H	5.209082	-0.142118	0.878918
O	3.537730	-0.612757	-0.041041
H	3.435147	-1.582931	-0.047998

³a-1-IM2



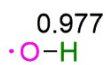
C	0.914781	-3.508709	-0.001219
C	2.096337	-2.787300	0.000624
C	2.078993	-1.379906	0.001254
C	0.841611	-0.700553	0.000039
C	-0.373053	-1.451020	-0.001288
C	-0.313162	-2.851513	-0.002171
C	3.301694	-0.622044	0.002862
C	0.819780	0.732027	0.000072
C	2.038391	1.452576	0.000926
C	3.282526	0.731956	0.002686
C	2.003399	2.858578	0.000018
H	2.940992	3.404503	0.000510
C	0.797928	3.537029	-0.001665
C	-0.407651	2.829328	-0.002185
C	-0.405244	1.441276	-0.001308
C	-1.679331	0.706835	-0.001392
C	-1.610491	-0.737011	-0.001877
H	4.240308	-1.165629	0.004188
H	0.939772	-4.591612	-0.001945
H	3.052654	-3.299014	0.001502
H	-1.213447	-3.456899	-0.003602
H	4.205996	1.301174	0.003756
H	0.784842	4.620522	-0.002557
H	-1.355946	3.353666	-0.003396
O	-2.779792	1.285098	-0.001077
O	-2.800786	-1.331304	-0.002409
H	-2.732191	-2.297884	-0.001390
O	-5.272733	0.069385	0.006751
H	-4.355527	0.436439	0.004564

²a-OH-O



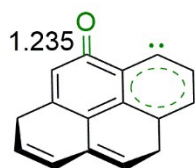
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C	2.696948	-1.849176	0.000068
C	1.291158	-1.767111	0.000036
C	0.673007	-0.498323	-0.000017
C	1.485665	0.673156	-0.000013
C	2.880334	0.556746	0.000029
C	0.470492	-2.949316	0.000066
C	-0.757753	-0.400935	-0.000025
C	-1.539238	-1.581357	0.000027
C	-0.881164	-2.860487	0.000062
C	-2.941667	-1.474941	0.000050
H	-3.534713	-2.383514	0.000096
C	-3.558708	-0.236629	0.000027
C	-2.791684	0.932226	-0.000033
C	-1.405789	0.859681	-0.000079
C	-0.600489	2.088572	-0.000200
C	0.835719	1.938879	-0.000071
H	0.964687	-3.914910	0.000105
H	4.556789	-0.783770	0.000095
H	3.163198	-2.828765	0.000108
H	3.491625	1.451220	0.000027
H	-1.496680	-3.753913	0.000097
H	-4.640354	-0.170356	0.000049
H	-3.268146	1.905830	-0.000068
O	-1.076749	3.236876	0.000024
O	1.556536	3.051834	-0.000060
H	0.926740	3.798379	-0.000158

• OH



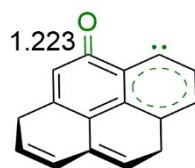
O	0.000000	0.000000	0.108523
H	0.000000	0.000000	-0.868186

$^3z\text{-O}$



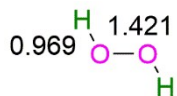
C	-3.702420	-0.508265	0.000048
C	-3.215289	0.797207	0.000054
C	-1.834132	1.048100	0.000032
C	-0.930457	-0.050271	-0.000005
C	-1.435161	-1.379108	-0.000007
C	-2.829811	-1.586007	0.000020
C	-1.308649	2.374855	0.000052
C	0.471177	0.190976	-0.000023
C	0.962651	1.528178	0.000004
C	0.045727	2.600929	0.000047
C	2.380605	1.745628	0.000059
H	2.734091	2.772089	0.000159
C	3.264418	0.717120	-0.000002
C	2.827308	-0.674362	-0.000231
C	1.375196	-0.899002	-0.000080
C	0.810848	-2.172996	-0.000060
C	-0.508392	-2.471765	-0.000024
H	-2.004738	3.206740	0.000089
H	-4.771930	-0.682568	0.000069
H	-3.901890	1.637103	0.000083
H	-3.208638	-2.602438	0.000020
H	0.430996	3.614997	0.000083
H	4.334166	0.893814	0.000072
H	-0.882087	-3.490972	-0.000023
O	3.628539	-1.614509	0.000019

$^1z\text{-O}$

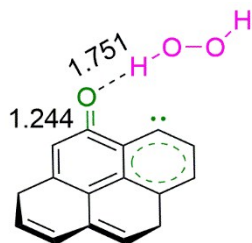


C	-3.675386	-0.499871	-0.296207
C	-3.199099	0.788137	-0.212207
C	-1.819333	1.042127	-0.015138
C	-0.927545	-0.052226	0.110318
C	-1.445373	-1.388529	0.012376
C	-2.796348	-1.594228	-0.192222
C	-1.301627	2.368696	0.030406
C	0.467473	0.203865	0.291997
C	0.953826	1.503985	0.222116
C	0.044967	2.590956	0.119938
C	2.388921	1.716021	0.091173
H	2.746698	2.740781	0.122816
C	3.248755	0.710428	-0.163158
C	2.809193	-0.692524	-0.218393
C	1.396550	-0.923458	0.162238
C	0.770776	-2.108287	0.260345
C	-0.501512	-2.439410	0.430430
H	-1.995561	3.199407	-0.039769
H	-4.732371	-0.679881	-0.452783
H	-3.874627	1.631722	-0.307566
H	-3.178619	-2.606537	-0.262465
H	0.440489	3.600598	0.091096
H	4.301794	0.898880	-0.339778
H	-0.842146	-3.259104	1.055816
O	3.581116	-1.609996	-0.458929

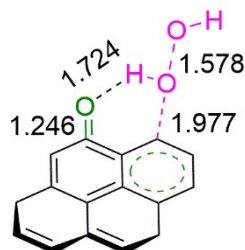
$^1\text{H}_2\text{O}_2$



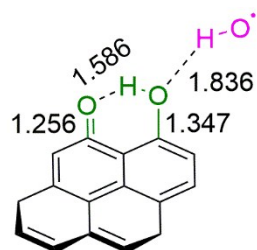
O	-0.702201	0.109817	-0.063628
H	-1.022664	-0.603226	0.509139
O	0.702199	-0.109820	-0.063649
H	1.022683	0.603248	0.509075

³_Z-1-IM1

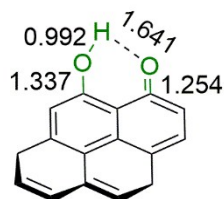
C	-3.521082	-2.309154	-0.004716
C	-3.867711	-0.959562	-0.009681
C	-2.878264	0.037039	-0.005542
C	-1.509667	-0.347081	0.002557
C	-1.163216	-1.725399	0.008613
C	-2.189001	-2.693421	0.004520
C	-3.205864	1.424999	-0.010973
C	-0.499016	0.652060	0.005550
C	-0.858411	2.029338	-0.000417
C	-2.223413	2.385997	-0.008117
C	0.183245	3.015947	0.002041
H	-0.109377	4.061247	-0.001409
C	1.496645	2.674278	0.006915
C	1.922029	1.286225	0.010093
C	0.865087	0.273770	0.011535
C	1.132046	-1.093618	0.018329
C	0.219780	-2.093266	0.016884
H	-4.252278	1.710489	-0.017303
H	-4.299211	-3.063319	-0.008381
H	-4.911189	-0.662805	-0.016423
H	-1.918134	-3.743702	0.008807
H	-2.486765	3.438333	-0.012572
H	2.276634	3.427252	0.007713
H	0.497140	-3.142893	0.021934
O	3.125582	0.971219	0.011124
O	4.127055	-1.571730	-0.019448
H	3.742566	-0.667377	-0.017837
O	5.523407	-1.303077	-0.120294
H	5.833122	-1.477449	0.778878

³_Z-1-TS1

C	-3.247678	-2.407908	0.002245
C	-3.666503	-1.079341	0.030556
C	-2.731739	-0.030463	0.025441
C	-1.344547	-0.340033	-0.009269
C	-0.923783	-1.697817	-0.038134
C	-1.897190	-2.719648	-0.031549
C	-3.134219	1.336736	0.054815
C	-0.388203	0.710629	-0.012822
C	-0.822997	2.065574	0.017838
C	-2.204783	2.348442	0.051019
C	0.160380	3.109450	0.017269
H	-0.190283	4.136296	0.040542
C	1.490222	2.842204	-0.009702
C	1.992003	1.481211	-0.041448
C	0.996178	0.405899	-0.042666
C	1.340628	-0.946669	-0.074404
C	0.473847	-1.988103	-0.071028
H	-4.194271	1.564527	0.081094
H	-3.983231	-3.203438	0.007264
H	-4.724208	-0.840298	0.057691
H	-1.570582	-3.753719	-0.052399
H	-2.523927	3.384926	0.073663
H	2.226894	3.637354	-0.008792
H	0.813410	-3.019175	-0.093197
O	3.214231	1.238002	-0.065941
O	3.259137	-1.422643	-0.061165
H	3.490267	-0.463437	-0.074135
O	4.713797	-2.012136	0.099961
H	4.608921	-2.409790	0.976461

³z-1-IM2

C	-2.784157	-2.744028	-0.051550
C	-3.395076	-1.495523	0.042722
C	-2.622805	-0.317777	0.058607
C	-1.209542	-0.419988	-0.023222
C	-0.586996	-1.695275	-0.118143
C	-1.404303	-2.851201	-0.131511
C	-3.215721	0.972615	0.153742
C	-0.411327	0.750213	-0.009453
C	-1.031502	2.024577	0.085059
C	-2.438091	2.106111	0.166998
C	-0.206486	3.198161	0.097765
H	-0.697451	4.163318	0.173120
C	1.146067	3.123768	0.020014
C	1.821765	1.847460	-0.080228
C	0.996754	0.648270	-0.091700
C	1.595180	-0.631804	-0.187160
C	0.820691	-1.780118	-0.200196
H	-4.296060	1.045957	0.216408
H	-3.393560	-3.639964	-0.062780
H	-4.475196	-1.416669	0.104718
H	-0.931662	-3.824504	-0.206755
H	-2.899074	3.085283	0.242121
H	1.766159	4.012774	0.029356
H	1.302031	-2.749164	-0.279023
O	3.073030	1.770898	-0.155366
O	2.935525	-0.735616	-0.268402
H	3.291978	0.202838	-0.245054
O	4.485158	-2.925425	0.592897
H	3.936437	-2.171488	0.284379

²z-OH-O

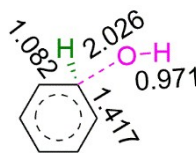
C	-2.875493	1.549625	-0.000003
C	-1.807974	2.386113	0.000031
C	-0.461034	1.892872	0.000011
C	-0.242957	0.489110	0.000006
C	-1.341783	-0.404262	-0.000005
C	-2.704756	0.110006	-0.000094
C	0.646535	2.767924	0.000021
C	1.082320	-0.011100	-0.000002
C	2.183792	0.884063	-0.000001
C	1.932797	2.284976	0.000011
C	3.491360	0.360199	-0.000007
H	4.332183	1.045405	-0.000004
C	3.704950	-1.016544	-0.000015
C	2.634639	-1.897422	-0.000019
C	1.302206	-1.417482	-0.000009
C	0.197498	-2.294105	-0.000014
C	-1.101717	-1.802136	0.000010
H	0.463227	3.837147	0.000039
H	-3.892218	1.925233	0.000010
H	-1.954960	3.461648	0.000064
H	2.776831	2.966079	0.000021
H	4.717613	-1.401996	-0.000021
H	2.803834	-2.968783	-0.000028
O	-2.119548	-2.669445	0.000092
H	0.354913	-3.367187	-0.000014
O	-3.692047	-0.663179	-0.000068
H	-2.950985	-2.127579	0.000211

Ph

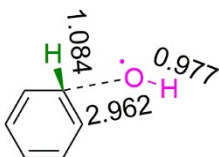
1.393



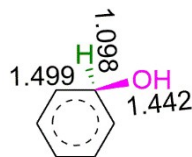
C	1.387928	-0.124454	0.000000
C	0.801630	1.139547	0.000000
C	-0.586041	1.264004	0.000000
C	-1.387929	0.124445	0.000000
C	-0.801637	-1.139542	0.000000
C	0.586049	-1.264001	0.000000
H	2.468073	-0.221511	0.000000
H	1.425838	2.026412	0.000000
H	-1.042136	2.247949	0.000000
H	-2.468072	0.221525	0.000000
H	-1.425826	-2.026420	0.000000
H	1.042123	-2.247955	0.000000

²2-HB-TS1

C	1.070923	1.214381	0.089963
C	1.698093	0.000000	0.388428
C	1.070923	-1.214380	0.089963
C	-0.183197	-1.219882	-0.493681
C	-0.861808	0.000000	-0.738377
C	-0.183198	1.219882	-0.493680
H	1.575071	2.149296	0.305765
H	2.682066	0.000000	0.843658
H	1.575071	-2.149296	0.305765
H	-0.674650	-2.154788	-0.736433
H	-1.742749	0.000000	-1.366474
H	-0.674650	2.154788	-0.736433
O	-2.121234	0.000000	0.848449
H	-1.440699	-0.000004	1.540868

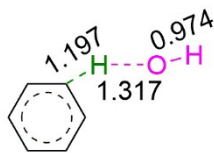
²2-IM1

C	0.920364	-1.208048	-0.262703
C	1.387933	-0.000002	-0.779334
C	0.920366	1.208046	-0.262706
C	-0.019159	1.207898	0.766320
C	-0.493102	0.000003	1.277598
C	-0.019162	-1.207896	0.766323
H	1.284661	-2.146735	-0.664861
H	2.117141	-0.000004	-1.581783
H	1.284666	2.146730	-0.664867
H	-0.387513	2.146484	1.165113
H	-1.229217	0.000004	2.073789
H	-0.387518	-2.146479	1.165118
O	-2.201244	0.000000	-1.142183
H	-1.255708	-0.000001	-1.388031

²Ph(H)OH

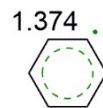
C	1.119966	1.225926	0.047261
C	1.814719	0.000066	0.203798
C	1.120126	-1.225852	0.047280
C	-0.206376	-1.249472	-0.255921
C	-1.018055	-0.000079	-0.422594
C	-0.206506	1.249422	-0.256016
H	1.658615	2.158635	0.177537
H	2.868529	0.000176	0.452432
H	1.658839	-2.158535	0.177485
H	-0.734545	-2.190572	-0.370089
H	-1.488545	-0.000155	-1.414900
H	-0.734764	2.190458	-0.370304
O	-2.146969	-0.000081	0.473961
H	-1.795626	0.000572	1.373308

²B-TS1



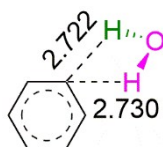
C	1.387903	1.201325	0.025692
C	-0.005552	1.225493	-0.051702
C	-0.677401	0.015523	-0.099993
C	-0.032948	-1.209436	-0.061108
C	1.360623	-1.217329	0.017267
C	2.064757	-0.015899	0.059389
H	1.940362	2.133691	0.060197
H	-0.544638	2.165539	-0.076863
H	-0.592972	-2.136972	-0.093615
H	1.891971	-2.162097	0.046008
H	3.147042	-0.028272	0.121721
O	-3.172615	0.020588	-0.015731
H	-1.869542	0.032513	-0.208748
H	-3.175593	-0.167168	0.939882

·Ph



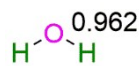
C	0.000000	1.320396	0.000006
C	-1.211299	0.630496	0.000002
C	-1.223425	-0.769288	-0.000004
C	0.000000	-1.395237	-0.000006
C	1.223425	-0.769289	-0.000004
C	1.211298	0.630497	0.000003
H	-0.000001	2.404355	0.000011
H	-2.149138	1.175360	0.000005
H	-2.157482	-1.320265	-0.000007
H	2.157483	-1.320263	-0.000006
H	2.149139	1.175359	0.000006

²B-IM2



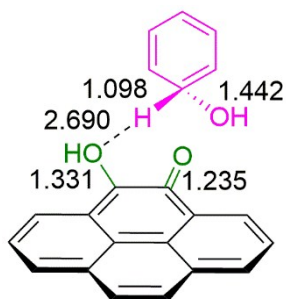
C	1.622500	1.139938	0.003022
C	0.230766	1.288816	-0.003583
C	-0.508912	0.130608	-0.007707
C	-0.006706	-1.148720	-0.006412
C	1.387302	-1.271897	0.000581
C	2.191159	-0.132783	0.004993
H	2.255883	2.020479	0.006703
H	-0.228106	2.271354	-0.006583
H	-0.647422	-2.023834	-0.010530
H	1.838820	-2.258139	0.003597
H	3.269999	-0.237882	0.010146
O	-3.716451	0.003233	0.004757
H	-3.127691	0.105162	-0.751290
H	-3.126530	0.061218	0.764529

H₂O



O	0.000000	0.000000	0.117827
H	0.000000	0.761172	-0.471306
H	0.000000	-0.761172	-0.471306

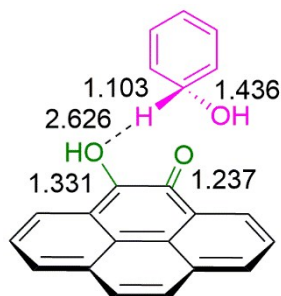
³a-3-IM1



C	-0.036169	3.419094	0.977162
C	1.109268	3.308601	0.207492
C	1.685911	2.048905	-0.043369
C	1.077341	0.888753	0.483105
C	-0.119209	1.007682	1.253122
C	-0.647911	2.281905	1.499924
C	2.883720	1.923993	-0.830912
C	1.661311	-0.394545	0.226884
C	2.843300	-0.487907	-0.547569
C	3.438252	0.711877	-1.070622
C	3.404689	-1.753477	-0.794364
H	4.312009	-1.817647	-1.386105
C	2.811966	-2.898890	-0.294382
C	1.639215	-2.810859	0.462138
C	1.063127	-1.576140	0.724480
C	-0.196615	-1.507619	1.494575
C	-0.755604	-0.186573	1.714041
H	3.331856	2.829685	-1.225808
H	-0.465699	4.393849	1.175207
H	1.581697	4.193988	-0.204561
H	-1.543403	2.418022	2.096728
H	4.343075	0.620310	-1.662285
H	3.253679	-3.868623	-0.491763
H	1.163942	-3.704707	0.849111
O	-1.911520	-0.182729	2.374088
C	-0.949061	0.038180	-2.090977
C	-1.490831	1.327726	-1.850579
C	-2.668150	1.460249	-1.071537
C	-3.293900	0.370285	-0.548413
C	-2.811144	-1.028998	-0.790488
C	-1.543969	-1.078727	-1.591755
H	-0.042332	-0.051726	-2.681528

H	-1.012748	2.206007	-2.266932
H	-3.070898	2.451604	-0.890190
H	-4.197808	0.477220	0.043168
H	-2.657267	-1.535456	0.172053
H	-1.127768	-2.063669	-1.780349
O	-3.840497	-1.824731	-1.412969
H	-4.026290	-1.428543	-2.273636
O	-0.769109	-2.517874	1.916115
H	-2.306267	0.701267	2.401274

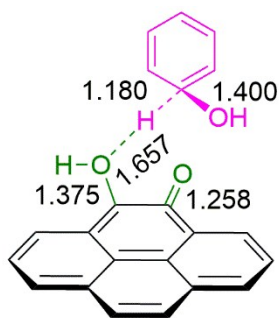
¹a-3-IM1



C	0.695323	3.527692	0.519397
C	1.896048	3.225047	-0.097173
C	2.316323	1.887256	-0.230431
C	1.495543	0.849073	0.260891
C	0.257198	1.168476	0.894132
C	-0.121982	2.511502	1.015364
C	3.566624	1.559301	-0.862657
C	1.915861	-0.514100	0.121735
C	3.149518	-0.807467	-0.509246
C	3.965661	0.271962	-0.994708
C	3.549653	-2.148743	-0.643808
H	4.496104	-2.366096	-1.128021
C	2.752176	-3.174553	-0.169641
C	1.534033	-2.888172	0.454279
C	1.111426	-1.574845	0.602166
C	-0.185518	-1.292910	1.255312
C	-0.579353	0.098277	1.340929
H	4.182660	2.372998	-1.230453
H	0.383933	4.560246	0.624835
H	2.533082	4.015243	-0.480054

H	-1.044490	2.796097	1.510208
H	4.909096	0.027254	-1.471435
H	3.070838	-4.204597	-0.280443
H	0.903658	-3.686412	0.828367
O	-1.776133	0.306734	1.885487
C	-1.853028	0.786759	-1.497371
C	-2.827781	1.700047	-1.045210
C	-4.015219	1.216753	-0.422937
C	-4.200387	-0.109983	-0.201622
C	-3.160335	-1.133809	-0.540480
C	-1.981979	-0.553168	-1.263184
H	-0.981787	1.159346	-2.026964
H	-2.705196	2.760734	-1.226904
H	-4.786918	1.925797	-0.142081
H	-5.112212	-0.478862	0.257168
H	-2.803876	-1.595599	0.395313
H	-1.237561	-1.257243	-1.622811
O	-3.724439	-2.237094	-1.266912
H	-4.052243	-1.891892	-2.106739
O	-0.916853	-2.190907	1.689945
H	-2.094495	1.206747	1.717439

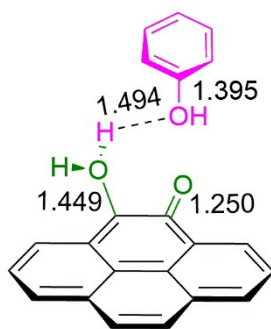
¹a-3-TS1



C	2.214302	-3.389858	-0.033898
C	3.226900	-2.539117	-0.452487
C	3.067663	-1.148458	-0.367854
C	1.859668	-0.614995	0.155514
C	0.835267	-1.495401	0.588633
C	1.026034	-2.870700	0.481552
C	4.093949	-0.242138	-0.813180

C	1.678230	0.801308	0.221061
C	2.694344	1.669685	-0.245980
C	3.915422	1.099175	-0.756128
C	2.490261	3.058728	-0.217208
H	3.271080	3.718979	-0.578788
C	1.293239	3.570284	0.260509
C	0.285944	2.728643	0.730876
C	0.455872	1.333834	0.732701
C	-0.544092	0.425217	1.202568
C	-0.438183	-0.978071	1.139400
H	5.014113	-0.663811	-1.205201
H	2.345903	-4.463605	-0.107714
H	4.151406	-2.939788	-0.855684
H	0.230214	-3.528944	0.810689
H	4.689646	1.776535	-1.102268
H	1.130653	4.642449	0.270065
C	-4.177472	-1.354691	-0.250504
C	-2.979615	-1.937508	-0.725921
C	-1.987667	-1.167633	-1.338226
C	-2.090689	0.200126	-1.337229
C	-3.226346	0.848309	-0.684109
C	-4.344827	-0.003116	-0.308819
H	-4.965668	-1.989397	0.134848
H	-2.865906	-3.014289	-0.690456
H	-1.118134	-1.648590	-1.770218
H	-1.328803	0.829009	-1.787878
H	-2.764237	0.924978	0.398660
H	-5.256364	0.481533	0.024038
O	-3.596979	2.127438	-1.115406
H	-2.836830	2.717362	-1.034223
O	-1.732088	0.911172	1.695342
H	-1.614705	1.793865	2.075981
H	-0.633044	3.183227	1.086710
O	-1.363254	-1.761265	1.475542

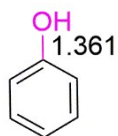
1a-3-IM2



C	-2.856266	-2.477905	-0.617205
C	-3.431906	-1.360997	-0.031016
C	-2.743563	-0.139458	0.006367
C	-1.445481	-0.051177	-0.564248
C	-0.868486	-1.203134	-1.158568
C	-1.579304	-2.398231	-1.174750
C	-3.315762	1.030266	0.620920
C	-0.730286	1.186730	-0.503689
C	-1.305862	2.315077	0.125443
C	-2.632651	2.198553	0.675492
C	-0.571179	3.508517	0.225806
H	-1.017669	4.370385	0.709064
C	0.716474	3.567761	-0.284446
C	1.302682	2.462512	-0.902075
C	0.595913	1.255383	-1.028169
C	1.130676	0.072492	-1.602271
C	0.520831	-1.184112	-1.69617
H	-4.311898	0.950862	1.044464
H	-3.398232	-3.416731	-0.639758
H	-4.423289	-1.418818	0.406638
H	-1.113292	-3.267823	-1.623555
H	-3.069107	3.073661	1.146181
H	1.285941	4.487297	-0.203497
C	1.214333	-2.486471	1.736826
C	0.297109	-1.798408	2.529216
C	0.413387	-0.419020	2.683493
C	1.429418	0.280132	2.03658
C	2.320808	-0.427080	1.241445
C	2.239195	-1.803774	1.089688
H	1.133250	-3.560745	1.616719
H	-0.502600	-2.335233	3.025845
H	-0.295259	0.123699	3.298908

H	1.513588	1.359091	2.129139
H	3.046943	0.177262	-0.95221
H	2.955427	-2.320816	0.461434
O	3.313503	0.233059	0.516859
H	3.397642	1.150818	0.826146
O	2.556681	0.063553	1.859838
H	2.854152	0.699204	-2.539619
H	2.311601	2.560319	-1.289992
O	1.058859	-2.221408	-2.140511

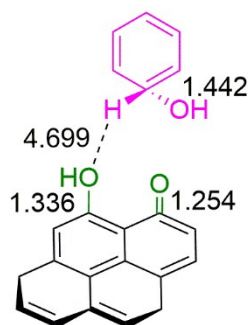
PhOH



C	1.121951	1.219221	0.000083
C	-0.270042	1.195919	-0.000043
C	-0.936706	-0.028407	-0.000088
C	-0.216755	-1.222472	-0.000006
C	1.172815	-1.184870	0.000132
C	1.850975	0.033052	0.000173
H	1.635951	2.173938	0.000113
H	-0.840270	2.119714	-0.000108
H	-0.754108	-2.163934	-0.000048
H	1.728750	-2.115833	0.000199
H	2.934109	0.056261	0.000273
O	-2.295022	-0.114584	-0.000185
H	-2.677692	0.771859	-0.000454

¹a-3-IM3

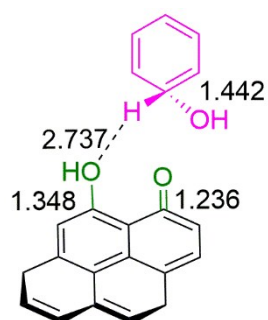
C	-3.579253	0.122973	0.000643
C	-3.101083	-1.178156	0.000360
C	-1.721774	-1.432852	-0.000153
C	-0.810526	-0.342855	-0.000224
C	-1.315258	0.982957	-0.000100
C	-2.688935	1.197457	0.000327
C	-1.203456	-2.775950	-0.000495
C	0.597786	-0.602190	-0.000251
C	1.081259	-1.931252	-0.000328
C	0.129840	-3.013283	-0.000639
C	2.465866	-2.168385	-0.000024
H	2.831227	-3.189188	-0.000103
C	3.347802	-1.099096	0.000494
C	2.890441	0.218769	0.000541
C	1.514350	0.492583	0.000062
C	0.947923	1.792519	-0.000164
C	-0.401465	2.160303	-0.000271
H	-1.912289	-3.597791	-0.000632
H	-4.647529	0.307196	0.001114
H	-3.789200	-2.017272	0.000581
H	-3.050712	2.218909	0.000473
H	0.510990	-4.029263	-0.000896
H	4.416476	-1.283355	0.000887
H	3.617443	1.024095	0.001018
O	1.870499	2.919576	0.000006
H	2.420840	3.011548	0.807342
O	-0.838014	3.330784	-0.000218
H	2.421773	3.010993	-0.806754

³_z-3-IM1

C	4.055006	-1.257266	0.295646
C	3.914891	0.069097	0.698739
C	2.755073	0.799747	0.372631
C	1.727229	0.166334	-0.372349
C	1.870603	-1.188922	-0.781310
C	3.055188	-1.882755	-0.433478
C	2.580739	2.154078	0.774951
C	0.541036	0.871435	-0.693541
C	0.400574	2.226083	-0.287367
C	1.436462	2.841648	0.449073
C	-0.799498	2.932775	-0.630404
H	-0.885642	3.970011	-0.321749
C	-1.810433	2.335519	-1.310754
C	-1.724785	0.947906	-1.723474
C	-0.499413	0.227259	-1.405381
C	-0.342048	-1.128440	-1.793252
C	0.829984	-1.813535	-1.498304
H	3.368117	2.634340	1.345775
H	4.953269	-1.805140	0.555410
H	4.698157	0.554009	1.271464
H	1.312336	3.874612	0.756961
H	-2.719429	2.869898	-1.562930
C	-0.273139	-1.624887	1.954401
C	-1.137917	-2.500070	1.248790
C	-2.417163	-2.045687	0.837956
C	-2.829130	-0.774952	1.099606
C	-1.981990	0.208422	1.848867
C	-0.646387	-0.347155	2.239931
H	0.702644	-1.983518	2.267555
H	-0.825081	-3.513723	1.030968
H	-3.074023	-2.726478	0.306427
H	-3.809252	-0.430555	0.785111

H	-1.834398	1.104337	1.230733
H	0.017559	0.320281	2.781363
O	-2.683605	0.720900	2.999616
H	-2.846568	-0.025178	3.590477
O	-1.313692	-1.769756	-2.449625
H	-2.060137	-1.124095	-2.547527
H	0.925862	-2.849344	-1.805848
H	3.166403	-2.915804	-0.745085
O	-2.667592	0.392173	-2.335611

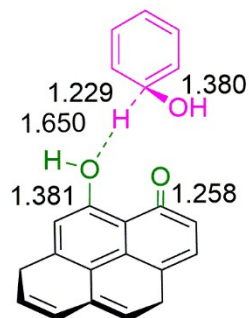
¹_z-3-IM1



H	4.441165	0.665121	-1.132512
H	3.239756	-2.470185	1.545303
H	0.463070	2.081146	-3.295723
H	-3.687306	0.039933	-2.259689
C	-1.943454	2.291611	0.818189
C	-0.850698	3.068400	0.354049
C	0.460581	2.781062	0.808769
C	0.695054	1.755359	1.674332
C	-0.403472	0.896577	2.220526
C	-1.754659	1.261471	1.687407
H	-2.943762	2.526963	0.469242
H	-1.020600	3.886598	-0.334973
H	1.288075	3.388117	0.455889
H	1.700208	1.538483	2.023814
H	-0.191134	-0.155989	1.979774
H	-2.593197	0.670316	2.043102
O	-0.396005	0.901474	3.661296
H	-0.578873	1.806131	3.945385
O	-1.571634	-3.079328	1.010436
O	-3.396715	-1.822212	-0.474806
H	-4.223111	-1.535904	-0.890090
H	0.889163	-3.164045	1.645285

C	3.989114	-0.914551	0.255811
C	3.669541	0.029524	-0.710924
C	2.341925	0.190092	-1.162952
C	1.323752	-0.626087	-0.623656
C	1.659873	-1.604912	0.364746
C	2.999100	-1.727501	0.792339
C	2.010104	1.178740	-2.146537
C	-0.035492	-0.475160	-1.053429
C	-0.323328	0.514510	-2.023489
C	0.725518	1.332199	-2.555464
C	-1.657269	0.684484	-2.446157
H	-1.882634	1.444496	-3.187097
C	-2.660681	-0.095602	-1.932987
C	-2.383259	-1.084479	-0.965581
C	-1.074038	-1.297647	-0.519222
C	-0.738448	-2.323920	0.497975
C	0.649450	-2.417576	0.895245
H	2.804512	1.798264	-2.548522
H	5.014220	-1.018478	0.591484

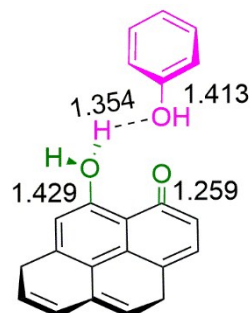
¹_z-3-TS1



C	-3.978085	-2.367766	0.258676
C	-4.325563	-1.061527	0.574259
C	-3.418247	-0.008138	0.367581
C	-2.130225	-0.295465	-0.173047
C	-1.790927	-1.641027	-0.489439
C	-2.723304	-2.662998	-0.267197
C	-3.752561	1.348966	0.690547
C	-1.180726	0.756442	-0.399997
C	-1.555108	2.082918	-0.059263
C	-2.848942	2.343842	0.483039
C	-0.617398	3.119668	-0.268825
H	-0.900583	4.134182	0.000189
C	0.620631	2.870426	-0.794001
C	1.067789	1.550746	-1.177602
C	0.109208	0.478688	-0.951638
C	0.398182	-0.897554	-1.234043
C	-0.484704	-1.908885	-1.010404
H	-4.733882	1.559273	1.102069
H	-4.691366	-3.168144	0.424438
H	-5.304081	-0.836680	0.985628
H	-2.454365	-3.685582	-0.509851
H	-3.098560	3.372002	0.729323
H	1.330409	3.677831	-0.945438
C	1.495407	-0.697416	2.016083
C	1.789662	0.673723	2.039009
C	2.888647	1.197148	1.360158
C	3.712085	0.361391	0.634336
C	3.384231	-1.030035	0.520729
C	2.305649	-1.556327	1.313503
H	0.639318	-1.080802	2.557385
H	1.144286	1.343397	2.597448

H	3.096359	2.259149	1.393996
H	4.562700	0.744683	0.080645
H	2.608660	-0.802433	-0.404720
H	2.111097	-2.622765	1.264602
O	4.299451	-1.956949	0.064187
H	4.911340	-1.531298	-0.551644
O	1.662724	-1.203463	-1.696205
H	1.711851	-2.161414	-1.848502
H	-0.200558	-2.936115	-1.221761
O	2.221971	1.384637	-1.649055

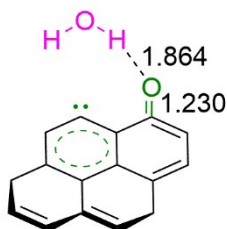
¹_z-3-IM2



C	-4.496559	-1.190501	1.000561
C	-4.415321	0.187024	0.847655
C	-3.264656	0.783165	0.305504
C	-2.176730	-0.048070	-0.092391
C	-2.276265	-1.458493	0.075421
C	-3.439779	-2.013504	0.620928
C	-3.152074	2.204862	0.139801
C	-0.993269	0.532276	-0.654958
C	-0.919983	1.941291	-0.796810
C	-2.022733	2.749860	-0.386890
C	0.256151	2.498991	-1.348965
H	0.314780	3.579806	-1.449069
C	1.306015	1.718889	-1.757007
C	1.296623	0.281183	-1.653697
C	0.096694	-0.288324	-1.068246
C	-0.065184	-1.684569	-0.841095

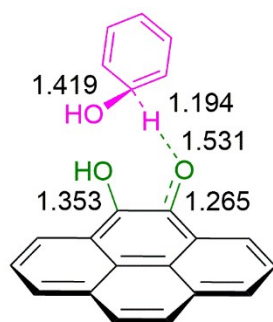
C	-1.158721	-2.273454	-0.309009	C	-1.282527	-0.056616	0.127998
H	-3.985242	2.829416	0.443430	C	-2.475692	0.731635	-0.230970
H	-5.393809	-1.632045	1.420686	C	1.378855	2.604503	0.139237
H	-5.242592	0.822291	1.146258	C	1.193811	-0.205791	0.102886
H	-3.505654	-3.089051	0.744755	C	2.454934	0.433131	0.004720
H	-1.938531	3.825890	-0.509320	C	2.520317	1.855276	0.062895
H	2.199420	2.168954	-2.178373	C	3.614537	-0.358208	-0.182300
C	1.805948	0.678775	2.389518	H	4.575512	0.139349	-0.260467
C	2.719945	1.675165	2.059353	C	3.528120	-1.728112	-0.281396
C	3.733123	1.417209	1.136876	C	2.279490	-2.371547	-0.203967
C	3.835968	0.165831	0.536700	C	1.125872	-1.635081	-0.010209
C	2.908488	-0.803669	0.874731	C	-0.168676	-2.217114	0.377586
C	1.894299	-0.576445	1.790527	C	-1.197085	-1.398136	0.200203
H	1.015884	0.873568	3.105375	H	1.426203	3.687945	0.118539
H	2.642527	2.653700	2.519021	H	-3.197904	2.785163	-0.358219
H	4.445369	2.192867	0.880192	H	-1.027312	3.836723	0.113805
H	4.600896	-0.055495	-0.196533	H	3.493070	2.332326	0.011525
H	1.963308	-2.257537	-0.669428	H	4.423835	-2.319237	-0.430986
H	1.178646	-1.360646	2.017551	H	2.217451	-3.451067	-0.287212
O	2.975531	-2.045553	0.204642	O	-4.227203	-2.493949	0.104475
H	3.033413	-2.765633	0.856685	H	-3.416996	-3.000770	-0.006940
O	1.031422	-2.531058	-1.193643	H	-0.201499	-3.118564	0.982050
H	0.801770	-3.467509	-1.027209	O	-3.565959	0.205481	-0.450429
O	2.273049	-0.417857	-2.030569	H	-3.970049	-1.582183	-0.112790
H	-1.202086	-3.347782	-0.158516				

¹z-3-IM4



C	-2.312071	2.186270	-0.180271
C	-1.116665	2.754933	0.079673
C	0.105663	1.978885	0.217656
C	0.021613	0.592317	0.275981

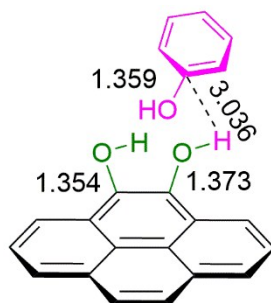
¹a-4-TS1



C	1.259761	3.595233	0.266070
C	2.414693	3.057282	-0.273578
C	2.593682	1.664174	-0.322976
C	1.574541	0.815461	0.170163
C	0.383441	1.378324	0.702288
C	0.246932	2.764640	0.753195
C	3.794253	1.077421	-0.859997
C	1.760316	-0.605936	0.155140
C	2.955443	-1.153866	-0.375013
C	3.966103	-0.265649	-0.886263
C	3.125657	-2.547565	-0.383821
H	4.041470	-2.962885	-0.791513
C	2.140506	-3.381305	0.119424
C	0.963164	-2.845815	0.647029
C	0.762401	-1.470304	0.667770
C	-0.482375	-0.913635	1.222098
C	-0.677464	0.484608	1.129940
H	4.562020	1.742569	-1.241175
H	1.134472	4.670781	0.313343
H	3.197947	3.703534	-0.655297
H	-0.641191	3.219813	1.177599
H	4.873335	-0.701612	-1.291596
H	2.282743	-4.455763	0.105678
H	0.190507	-3.493463	1.044335
O	-1.767323	0.977723	1.763069
C	-2.146397	1.276628	-1.142453
C	-3.441256	1.638166	-0.880969
C	-4.437476	0.658470	-0.552295
C	-4.108578	-0.652913	-0.501706
C	-2.709347	-1.090283	-0.590304
C	-1.724391	-0.060409	-0.952316
H	-1.433424	2.012799	-1.495398

H	-3.744726	2.672414	-1.003837
H	-5.462832	0.977495	-0.406635
H	-4.854542	-1.420483	-0.322021
H	-2.433562	-1.347695	0.542024
H	-0.793013	-0.391736	-1.400476
O	-2.498010	-2.351849	-1.204004
H	-2.687918	-2.256930	-2.145259
O	-1.413217	-1.661180	1.639547
H	-2.084532	1.777262	1.312778

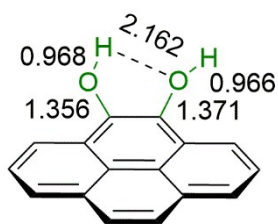
¹a-4-IM2



C	0.474307	3.562008	0.500070
C	1.722039	3.327287	-0.064717
C	2.212682	2.020527	-0.178937
C	1.419384	0.937660	0.280451
C	0.143933	1.189719	0.854481
C	-0.311978	2.508149	0.958883
C	3.505598	1.739197	-0.750241
C	1.904833	-0.400364	0.172735
C	3.182683	-0.648431	-0.393243
C	3.967761	0.470398	-0.850168
C	3.642156	-1.967095	-0.495754
H	4.619356	-2.152628	-0.929045
C	2.856573	-3.024647	-0.053171
C	1.599562	-2.794905	0.500025
C	1.113104	-1.490378	0.620299
C	-0.191458	-1.209796	1.161810
C	-0.645683	0.066042	1.279873
H	4.103291	2.575381	-1.098184
H	0.106559	4.578083	0.589055

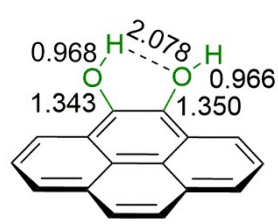
H	2.330411	4.152884	-0.418469	C	-0.698581	-0.502526	0.006209
H	-1.278989	2.714601	1.403639	C	-1.376401	-1.749198	0.009772
H	4.943011	0.268528	-1.281069	C	-0.598917	-2.962640	0.019901
H	3.224243	-4.040797	-0.140871	C	-2.776208	-1.770764	-0.000328
H	0.990522	-3.624383	0.838278	H	-3.291317	-2.725373	0.004686
O	-1.881493	0.239813	1.851644	C	-3.495431	-0.583017	-0.024102
C	-3.391162	1.360474	-0.921969	C	-2.843616	0.647130	-0.031691
C	-4.452162	0.702813	-0.299660	C	-1.445756	0.708407	-0.008645
C	-4.438033	-0.689713	-0.218788	C	-0.721261	1.951788	0.005004
C	-3.378127	-1.420120	-0.744535	C	0.638021	1.984740	0.000694
C	-2.320289	-0.752918	-1.362800	H	1.331958	-3.848020	0.022313
C	-2.326768	0.639118	-1.457576	H	4.611243	-0.376414	-0.019549
H	-3.387207	2.442816	-0.993686	H	3.431044	-2.552718	-0.000180
H	-5.278074	1.268552	0.114338	H	3.335003	1.740973	-0.023842
H	-5.256629	-1.213169	0.262384	H	-1.130757	-3.908305	0.027411
H	-3.354186	-2.502235	-0.680869	H	-4.578972	-0.609380	-0.041015
H	-1.830339	-1.929628	1.771797	H	-3.437626	1.553606	-0.064613
H	-1.497926	1.150881	-1.938161	O	-1.357894	3.165358	-0.031513
O	-1.305459	-1.507796	-1.859017	H	-2.174415	3.140371	0.483864
H	-0.598376	-0.932895	-2.179800	O	1.318548	3.157635	0.010208
O	-0.953223	-2.265826	1.531615	H	0.679970	3.883549	0.054196
H	-2.448007	0.764316	1.264321				

¹a-2OH



C	3.527546	-0.402487	-0.013577
C	2.867861	-1.625505	-0.002981
C	1.469138	-1.678482	0.004741
C	0.727439	-0.467758	-0.000888
C	1.415245	0.773938	-0.009339
C	2.812918	0.792062	-0.016674
C	0.754444	-2.929395	0.016432

³a-2OH

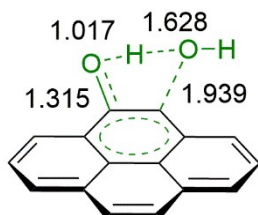


C	3.558412	-0.436477	-0.000899
C	2.890656	-1.646228	-0.000061
C	1.445391	-1.695088	0.000408
C	0.718331	-0.473130	-0.000860
C	1.430371	0.771918	-0.000987
C	2.866020	0.772204	-0.001379
C	0.745654	-2.906118	0.001503

C	-0.698730	-0.493709	-0.000297
C	-1.384784	-1.738150	0.000314
C	-0.647311	-2.926721	0.001497
C	-2.831158	-1.739309	0.000114
H	-3.347871	-2.692285	0.000128
C	-3.537785	-0.552419	-0.000973
C	-2.886785	0.678020	-0.001486
C	-1.448615	0.733619	-0.001104
C	-0.740775	1.925230	-0.000283
C	0.697160	1.947547	-0.000291
H	1.304046	-3.836247	0.002193
H	4.642871	-0.424981	-0.001151
H	3.438195	-2.581898	0.000277
H	3.396428	1.715377	-0.001488
H	-1.178033	-3.872837	0.001773
H	-4.621863	-0.573799	-0.001555
H	-3.481568	1.583722	-0.002854
O	-1.282300	3.161309	0.000866
H	-2.248529	3.141419	0.008210
O	1.327627	3.133979	0.001404
H	0.677408	3.852096	0.004999

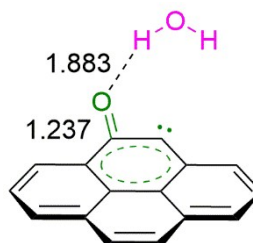
C	-1.413592	-1.749591	0.027270
C	-0.668711	-2.972870	0.142044
C	-2.823440	-1.743504	-0.002426
H	-3.348314	-2.690777	0.065516
C	-3.533501	-0.559164	-0.115259
C	-2.857441	0.657867	-0.198951
C	-1.458317	0.697504	-0.174341
C	-0.743989	1.922883	-0.254958
C	0.673223	1.921443	-0.221950
H	1.249381	-3.886494	0.238335
H	4.601717	-0.500275	0.020603
H	3.366833	-2.638292	0.158882
H	3.367715	1.646653	-0.126048
H	-1.218064	-3.905527	0.212375
H	-4.616386	-0.577958	-0.135768
H	-3.406183	1.589406	-0.284741
O	-0.984060	3.563823	0.757970
H	-1.788376	3.899031	0.345601
O	1.246287	3.104403	-0.239636
H	0.463336	3.695040	0.032879

³a-4-TS2



C	3.518402	-0.501770	0.004525
C	2.827535	-1.700240	0.080590
C	1.417885	-1.727719	0.065126
C	0.708294	-0.511878	-0.039677
C	1.430872	0.715442	-0.105266
C	2.828153	0.707808	-0.080903
C	0.687630	-2.962238	0.155694
C	-0.721249	-0.523409	-0.060568

³a-4-IM3

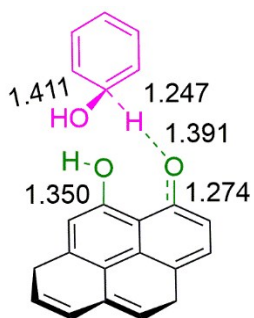


C	-0.717160	-3.480897	0.004670
C	-1.895208	-2.759562	-0.005078
C	-1.880444	-1.351196	-0.006054
C	-0.637053	-0.675276	0.002544
C	0.563317	-1.432182	0.010156
C	0.515502	-2.816808	0.011745
C	-3.098299	-0.587834	-0.015099
C	-0.621863	0.758411	0.002344

C	-1.828415	1.482785	-0.005386
C	-3.075397	0.767615	-0.014617
C	-1.782572	2.893845	-0.003361
H	-2.717351	3.444544	-0.007221
C	-0.572896	3.572970	0.004320
C	0.630301	2.873159	0.011412
C	0.625006	1.468041	0.010623
C	1.783110	0.690140	0.017500
C	1.876671	-0.737189	0.014111
H	-4.039864	-1.126578	-0.022040
H	-0.743860	-4.564213	0.005996
H	-2.851977	-3.271183	-0.012529
H	1.443471	-3.376903	0.016719
H	-3.996416	1.340540	-0.019923
H	-0.562705	4.656396	0.005559
H	1.578652	3.397886	0.018177
O	5.001035	0.629717	-0.086503
H	4.573741	1.341875	0.400151
O	2.953581	-1.345945	0.013603
H	4.371775	-0.108671	-0.040679

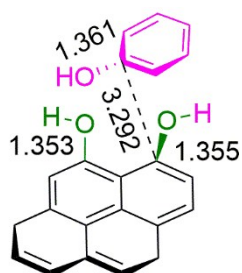
C	-1.280263	0.798145	-0.273192
C	-2.148385	1.783213	0.258387
C	-3.441136	1.408714	0.762479
C	-1.725251	3.121415	0.279951
H	-2.385103	3.878731	0.690106
C	-0.490155	3.479094	-0.209621
C	0.373954	2.514611	-0.752344
C	-0.003765	1.163466	-0.799272
C	0.855004	0.111728	-1.358651
C	0.462357	-1.233633	-1.198221
H	-4.836258	-0.156971	1.118078
H	-2.907569	-4.276728	-0.304877
H	-4.401274	-2.510593	0.579770
H	-0.649816	-3.690173	-1.151517
H	-4.077766	2.193103	1.158601
H	-0.168096	4.516017	-0.185523
C	1.034341	-0.913456	1.633966
C	1.616125	0.111529	2.310184
C	2.955102	0.546676	2.005772
C	3.665247	-0.076073	1.037250
C	3.034017	-1.058411	0.154786
C	1.703278	-1.537706	0.521692
H	0.074504	-1.307393	1.950513
H	1.096492	0.569065	3.145515
H	3.403107	1.338362	2.594886
H	4.691830	0.197144	0.813910
H	2.766541	-0.296647	-0.795132
H	1.497329	-2.589164	0.349076
O	3.881448	-2.002357	-0.463026
H	4.167467	-2.635693	0.206177
O	2.031629	0.333123	-1.793676
H	1.024284	-1.964572	-1.769765
O	1.577485	2.897954	-1.229642
H	1.665899	3.854245	-1.120352

¹_z-4-TS1



C	-2.579106	-3.243512	-0.292688
C	-3.416471	-2.258148	0.201059
C	-3.005474	-0.913645	0.220985
C	-1.719749	-0.573157	-0.271823
C	-0.871938	-1.593999	-0.765980
C	-1.308037	-2.915755	-0.771290
C	-3.857373	0.120822	0.741783

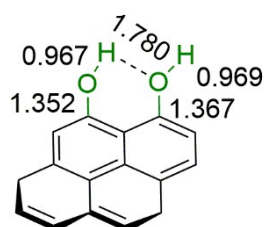
¹z-4-IM2



C	3.896341	-1.693157	-0.111034
C	3.983645	-0.391081	0.369476
C	2.907608	0.493277	0.222895
C	1.722360	0.048618	-0.426070
C	1.643701	-1.284460	-0.907284
C	2.741382	-2.139813	-0.743242
C	2.969031	1.844284	0.716439
C	0.604212	0.928129	-0.580744
C	0.708034	2.256253	-0.086441
C	1.917820	2.682756	0.564264
C	-0.380223	3.120734	-0.230301
H	-0.306456	4.136481	0.143807
C	-1.544393	2.692148	-0.838027
C	-1.670603	1.384475	-1.314626
C	-0.599915	0.474399	-1.202191
C	-0.646935	-0.905906	-1.649470
C	0.430942	-1.724359	-1.525627
H	3.877395	2.172560	1.210685
H	4.735859	-2.368922	0.010140
H	4.885399	-0.046908	0.864761
H	2.676169	-3.157845	-1.112451
H	1.962190	3.702015	0.934715
H	-2.387681	3.368195	-0.944272
O	-1.807872	-1.352864	-2.186558
O	-2.832102	0.996255	-1.889593
H	-3.454321	1.734846	-1.860435
H	0.361406	-2.753463	-1.867321
H	-1.701238	-2.287305	-2.408878
C	-2.736562	0.333482	1.736029
C	-1.594368	0.721926	2.431755
C	-0.535448	-0.176781	2.560818
C	-0.614170	-1.450453	2.007197
C	-1.761410	-1.825905	1.308289

C	-2.826471	-0.936399	1.173183
H	-3.564246	1.024971	1.618789
H	-1.526233	1.714157	2.862956
H	0.363462	0.116581	3.093030
H	0.206368	-2.154110	2.097356
H	-3.712622	-1.238828	0.623795
O	-1.795018	-3.077789	0.774741
H	-2.622986	-3.200255	0.292886

¹z-2OH

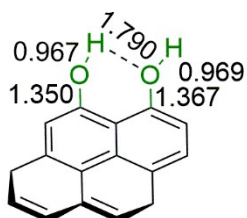


C	2.783715	1.621947	-0.000036
C	1.680742	2.452116	0.000089
C	0.382930	1.925585	0.000045
C	0.214793	0.517400	-0.000016
C	1.351324	-0.344919	-0.000129
C	2.637133	0.232101	-0.000207
C	-0.776049	2.776327	0.000161
C	-1.108313	-0.026867	-0.000037
C	-2.237900	0.836564	0.000000
C	-2.027807	2.260562	0.000107
C	-3.524335	0.281621	-0.000052
H	-4.383687	0.943611	-0.000018
C	-3.697620	-1.096823	-0.000118
C	-2.599100	-1.950882	-0.000124
C	-1.298830	-1.434539	-0.000059
C	-0.145991	-2.289799	0.000012
C	1.103792	-1.771329	0.000049
H	-0.617532	3.849888	0.000330
H	3.789218	2.026292	0.000019
H	1.814385	3.528761	0.000233
H	-2.897430	2.909111	0.000237
H	-4.699086	-1.512306	-0.000169
H	-2.740149	-3.026368	-0.000183

O	2.216994	-2.564851	0.000303
H	1.973156	-3.500782	0.001554
H	-0.286640	-3.366519	0.000089
O	3.786826	-0.479954	-0.000384
H	3.586307	-1.427633	0.000440

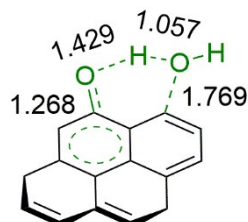
O	-3.789955	-0.572157	0.022684
H	-3.548180	-1.510513	0.034703

³_z-2OH



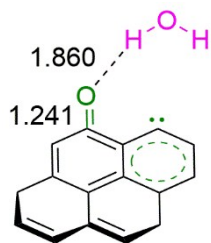
C	-2.852326	1.575220	0.001031
C	-1.778695	2.437057	-0.006712
C	-0.424831	1.925639	-0.005068
C	-0.219409	0.511097	-0.002747
C	-1.340512	-0.385583	-0.002699
C	-2.677558	0.193029	0.006221
C	0.679310	2.772902	-0.004141
C	1.102255	0.003370	-0.000600
C	2.216673	0.893523	0.000618
C	1.986555	2.265140	-0.001424
C	3.552844	0.341060	0.004816
H	4.394212	1.024454	0.006294
C	3.752523	-1.031043	0.007465
C	2.679755	-1.909785	0.005294
C	1.323074	-1.410198	0.001300
C	0.234130	-2.262395	-0.005681
C	-1.081144	-1.751333	-0.008455
H	0.516849	3.845357	-0.005085
H	-3.868990	1.953071	0.005378
H	-1.929718	3.509686	-0.009749
H	2.831425	2.945650	-0.000202
H	4.763330	-1.423386	0.010789
H	2.836246	-2.982083	0.006332
O	-2.141018	-2.615024	-0.025214
H	-1.845332	-3.532597	0.045987
H	0.382079	-3.338396	-0.009517

³_z-4-TS2



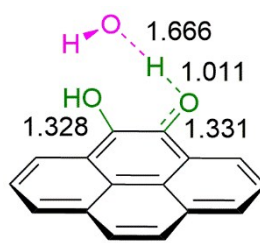
C	-2.773353	1.692512	-0.048256
C	-1.673360	2.488265	-0.034784
C	-0.346473	1.938355	-0.028492
C	-0.186477	0.531869	-0.093853
C	-1.322343	-0.316193	-0.178225
C	-2.650456	0.254895	-0.069522
C	0.797346	2.761409	0.061049
C	1.115714	-0.034582	-0.042174
C	2.247738	0.807110	0.059683
C	2.058382	2.216107	0.102253
C	3.540151	0.229504	0.112629
H	4.404385	0.879913	0.190461
C	3.693336	-1.151151	0.065193
C	2.587736	-1.986594	-0.030232
C	1.270958	-1.457526	-0.087233
C	0.142000	-2.280066	-0.258428
C	-1.136278	-1.701203	-0.379231
H	0.663996	3.837377	0.099342
H	-3.774301	2.107003	-0.014669
H	-1.778383	3.568024	-0.002376
H	2.930797	2.857217	0.170417
H	4.686845	-1.582723	0.104078
H	2.717711	-3.062946	-0.067459
O	-2.402722	-2.520643	0.544940
H	-2.622046	-3.314932	0.033730
H	0.282569	-3.348624	-0.391141
O	-3.668445	-0.493686	0.034464
H	-3.129959	-1.781926	0.340121

³_z-4-IM3



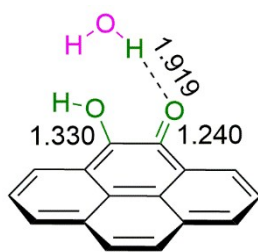
C	2.304798	2.213563	0.006964
C	1.076017	2.788533	0.002615
C	-0.127653	2.007761	0.000678
C	-0.025293	0.588093	0.005773
C	1.247083	-0.033416	0.013025
C	2.473132	0.769626	0.010660
C	-1.404539	2.608226	-0.009150
C	-1.202509	-0.209232	0.003018
C	-2.478169	0.419184	-0.006756
C	-2.546182	1.843769	-0.012894
C	-3.633283	-0.379444	-0.010980
H	-4.605061	0.102575	-0.018997
C	-3.539550	-1.769404	-0.005336
C	-2.300390	-2.391432	0.003533
C	-1.114869	-1.627473	0.008137
C	0.177880	-2.242143	0.017525
C	1.257816	-1.426576	0.019338
H	-1.470290	3.690846	-0.013927
H	3.208720	2.811914	0.006455
H	0.978798	3.869545	-0.000282
H	-3.522551	2.315902	-0.021672
H	-4.442554	-2.368098	-0.008080
H	-2.226977	-3.473457	0.007166
O	4.307138	-2.497085	-0.077770
H	3.573337	-2.980570	0.314067
H	0.257441	-3.324741	0.021733
O	3.596945	0.242548	0.012724
H	4.030747	-1.565429	-0.042995

²_a-5-TS1



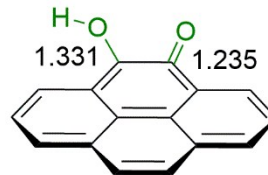
C	2.304798	2.213563	0.006964
C	1.076017	2.788533	0.002615
C	-0.127653	2.007761	0.000678
C	-0.025293	0.588093	0.005773
C	1.247083	-0.033416	0.013025
C	2.473132	0.769626	0.010660
C	-1.404539	2.608226	-0.009150
C	-1.202509	-0.209232	0.003018
C	-2.478169	0.419184	-0.006756
C	-2.546182	1.843769	-0.012894
C	-3.633283	-0.379444	-0.010980
H	-4.605061	0.102575	-0.018997
C	-3.539550	-1.769404	-0.005336
C	-2.300390	-2.391432	0.003533
C	-1.114869	-1.627473	0.008137
C	0.177880	-2.242143	0.017525
C	1.257816	-1.426576	0.019338
H	-1.470290	3.690846	-0.013927
H	3.208720	2.811914	0.006455
H	0.978798	3.869545	-0.000282
H	-3.522551	2.315902	-0.021672
H	-4.442554	-2.368098	-0.008080
H	-2.226977	-3.473457	0.007166
O	4.307138	-2.497085	-0.077770
H	3.573337	-2.980570	0.314067
H	0.257441	-3.324741	0.021733
O	3.596945	0.242548	0.012724
H	4.030747	-1.565429	-0.042995

²a-5-IM2

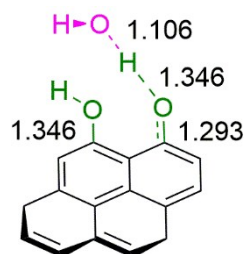


C	-0.583806	3.567958	-0.019781
C	-1.837017	2.983546	0.014946
C	-1.978713	1.584449	0.022367
C	-0.819368	0.772331	-0.006235
C	0.455407	1.386253	-0.039929
C	0.563363	2.769761	-0.046205
C	-3.273757	0.961422	0.059786
C	-0.949927	-0.655158	-0.003924
C	-2.235853	-1.237241	0.030845
C	-3.396133	-0.387297	0.063797
C	-2.362555	-2.638838	0.031382
H	-3.354931	-3.075955	0.059456
C	-1.240440	-3.448631	-0.001960
C	0.034528	-2.888503	-0.035070
C	0.203877	-1.496792	-0.034153
C	1.492621	-0.878738	-0.064280
C	1.672236	0.557120	-0.063958
H	-4.150278	1.600188	0.084153
H	-0.488506	4.647400	-0.026542
H	-2.730013	3.599459	0.036232
H	1.548479	3.220421	-0.073551
H	-4.373142	-0.857846	0.093276
H	-1.348185	-4.526566	-0.001995
H	0.881859	-3.565622	-0.060451
O	2.634891	-1.558838	-0.089993
O	5.401351	-0.121205	0.195561
H	5.816827	0.743993	0.257005
O	2.811029	1.048345	-0.082821
H	4.456858	0.075307	0.085534
H	2.496077	-2.517037	-0.080864

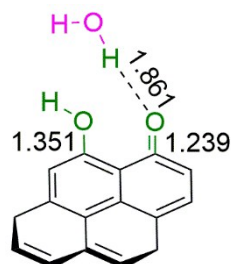
trans-²a-OH-O



C	3.451209	-0.784362	0.000056
C	2.647109	-1.911080	0.000074
C	1.245212	-1.788925	0.000046
C	0.657388	-0.504880	-0.000019
C	1.492450	0.654115	-0.000027
C	2.884381	0.488065	0.000011
C	0.399963	-2.953495	0.000088
C	-0.770584	-0.380806	-0.000017
C	-1.578015	-1.544736	0.000039
C	-0.948997	-2.837504	0.000086
C	-2.977366	-1.409454	0.000055
H	-3.589302	-2.305411	0.000106
C	-3.565958	-0.157886	0.000017
C	-2.771753	0.992847	-0.000048
C	-1.387893	0.892041	-0.000081
C	-0.566643	2.121590	-0.000208
C	0.872963	1.945034	-0.000080
H	0.875436	-3.928419	0.000136
H	4.529806	-0.886067	0.000084
H	3.087977	-2.902138	0.000123
H	3.556956	1.338782	0.000002
H	-1.583215	-3.717760	0.000128
H	-4.645850	-0.066501	0.000030
H	-3.226362	1.976574	-0.000096
O	-1.069171	3.249785	-0.000019
O	1.565895	3.081015	-0.000043
H	2.519977	2.921158	0.000039

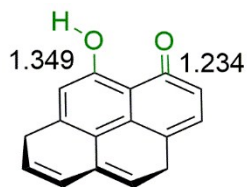
²_z-5-TS1

C	-2.555970	1.669761	0.027341
C	-1.464046	2.456391	-0.110652
C	-0.126332	1.930241	-0.054918
C	0.039991	0.523899	0.049125
C	-1.077881	-0.332045	0.144870
C	-2.404928	0.246754	0.294761
C	1.009884	2.759767	-0.130638
C	1.344731	-0.028228	0.034861
C	2.476979	0.823862	-0.018614
C	2.280312	2.230541	-0.098352
C	3.766420	0.247278	0.000934
H	4.634400	0.896970	-0.029973
C	3.923487	-1.135551	0.057168
C	2.820045	-1.975390	0.084780
C	1.501949	-1.446975	0.069255
C	0.369066	-2.278323	0.027190
C	-0.941269	-1.745491	-0.012213
H	0.868004	3.832392	-0.213926
H	-3.560663	2.080323	0.033259
H	-1.587936	3.526906	-0.240732
H	3.148818	2.878336	-0.144184
H	4.920124	-1.561503	0.071086
H	2.950134	-3.052050	0.109578
O	-3.341498	-0.639264	-1.070730
H	-2.990553	-0.373625	-1.933333
O	-1.981192	-2.473580	-0.257189
H	-2.851309	-1.585443	-0.773039
H	0.492211	-3.354826	-0.032898
O	-3.152685	-0.282497	1.280600
H	-3.994849	0.196311	1.343338

²_z-5-IM2

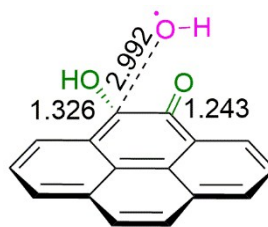
C	3.657109	-1.964468	0.044117
C	3.858950	-0.586545	0.078224
C	2.767488	0.301009	0.057097
C	1.446605	-0.222291	0.002001
C	1.249639	-1.626927	-0.033549
C	2.374289	-2.484707	-0.011020
C	2.950779	1.711148	0.088728
C	0.321838	0.646047	-0.020607
C	0.550226	2.051879	0.010590
C	1.867606	2.553693	0.064396
C	-0.569565	2.945092	-0.017203
H	-0.372166	4.012278	0.004086
C	-1.836666	2.479015	-0.068044
C	-2.142708	1.052799	-0.092148
C	-1.001160	0.123557	-0.073334
C	-1.162339	-1.286223	-0.110170
C	-0.066464	-2.131190	-0.088718
H	3.959648	2.106994	0.130613
H	4.509436	-2.633494	0.060736
H	4.863745	-0.180043	0.121364
H	2.214450	-3.557162	-0.036392
H	2.009097	3.629156	0.084638
H	-2.689006	3.148701	-0.087366
H	-0.221363	-3.206222	-0.114949
O	-3.327007	0.690143	-0.123826
O	-2.410700	-1.799641	-0.167919
H	-2.353424	-2.765763	-0.209883
O	-5.274652	-1.270209	0.335521
H	-4.938714	-2.140600	0.565465
H	-4.476583	-0.747524	0.149309

trans-²z-OH-O

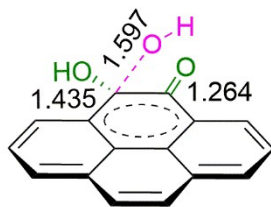


C	-2.887970	1.557313	0.000056
C	-1.825914	2.391675	0.000092
C	-0.484357	1.887191	0.000043
C	-0.267221	0.478002	-0.000012
C	-1.364742	-0.428448	-0.000064
C	-2.743307	0.101799	-0.000106
C	0.614004	2.772375	0.000088
C	1.072759	0.002979	-0.000007
C	2.168005	0.910090	0.000037
C	1.905347	2.308520	0.000080
C	3.480535	0.404957	0.000042
H	4.310868	1.102841	0.000076
C	3.714769	-0.968413	0.000007
C	2.655639	-1.861422	-0.000030
C	1.320705	-1.394515	-0.000038
C	0.224014	-2.280948	-0.000071
C	-1.081582	-1.820390	-0.000083
H	0.415116	3.838840	0.000135
H	-3.905261	1.932531	0.000122
H	-1.965407	3.468244	0.000173
H	2.741933	2.998662	0.000118
H	4.732723	-1.339948	0.000013
H	2.835375	-2.931054	-0.000054
O	-2.104181	-2.699763	-0.000122
H	-1.743188	-3.596579	-0.000137
H	0.408777	-3.351523	-0.000091
O	-3.750198	-0.611062	0.000053

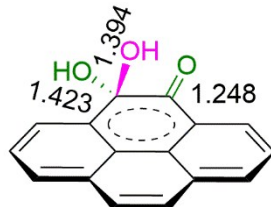
³a-6-IM1



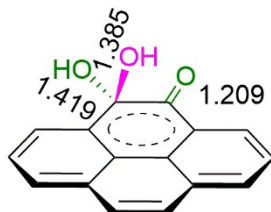
C	3.228791	-1.177176	-0.381598
C	2.315336	-2.216061	-0.284921
C	0.932614	-1.959516	-0.199338
C	0.475423	-0.624872	-0.212982
C	1.424536	0.436383	-0.308090
C	2.793608	0.146267	-0.396127
C	-0.023858	-3.029376	-0.094610
C	-0.927132	-0.347922	-0.110994
C	-1.844779	-1.420704	-0.006244
C	-1.350533	-2.771528	-0.002626
C	-3.219164	-1.139310	0.094954
H	-3.917429	-1.965886	0.175310
C	-3.677338	0.166170	0.092835
C	-2.775192	1.229164	-0.010942
C	-1.413269	0.983726	-0.113049
C	-0.465490	2.102169	-0.221373
C	0.937233	1.773807	-0.319017
H	0.346247	-4.049053	-0.089458
H	4.288601	-1.393046	-0.446109
H	2.656649	-3.245760	-0.272320
H	3.507166	0.958453	-0.467912
H	-2.069254	-3.580250	0.076871
H	-4.739087	0.367733	0.172561
H	-3.126489	2.254556	-0.013089
O	-0.795663	3.299998	-0.236678
O	1.641286	0.689301	2.379100
H	2.263987	-0.054451	2.262436
O	1.787844	2.785122	-0.412286
H	1.257166	3.605015	-0.394641

³a-6-TS1

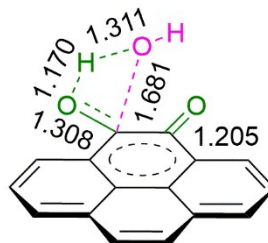
C	-2.124832	2.781241	-0.068819
C	-0.808034	3.211886	-0.060199
C	0.250251	2.290306	-0.022563
C	-0.031680	0.902412	0.007151
C	-1.386708	0.480626	0.019424
C	-2.416361	1.418176	-0.024912
C	1.622985	2.724227	-0.014344
C	1.041573	-0.045091	0.023071
C	2.381277	0.410610	0.024632
C	2.637567	1.828035	0.013847
C	3.430414	-0.524158	0.023968
H	4.454759	-0.167482	0.028495
C	3.155315	-1.884958	0.007376
C	1.840432	-2.344881	-0.007640
C	0.770414	-1.442852	0.006563
C	-0.589206	-1.927520	-0.012136
C	-1.674245	-0.950980	0.100547
H	1.821451	3.790596	-0.031244
H	-2.934028	3.500280	-0.109159
H	-0.578888	4.271966	-0.086222
H	-3.455315	1.100673	-0.041502
H	3.670276	2.161033	0.020099
H	3.971722	-2.598473	0.002059
H	1.627587	-3.407234	-0.026615
O	-0.931879	-3.136462	-0.151495
O	-2.660421	-1.363592	1.058019
H	-3.282912	-0.627422	1.232890
O	-2.814947	-1.401167	-0.923097
H	-2.631651	-2.376648	-0.952018

³a-6-IM2

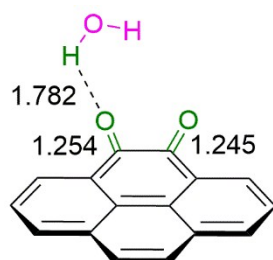
C	-2.996066	1.863707	-0.236929
C	-1.934105	2.722508	-0.144224
C	-0.610804	2.214848	-0.034415
C	-0.395662	0.802487	-0.008595
C	-1.515814	-0.060777	-0.065646
C	-2.782249	0.465786	-0.191727
C	0.499422	3.069735	0.040292
C	0.936899	0.289749	0.030013
C	2.031675	1.181974	0.085070
C	1.795499	2.559831	0.109040
C	3.384672	0.668016	0.071684
H	4.208981	1.366355	0.140083
C	3.609655	-0.721084	-0.065825
C	2.565632	-1.591338	-0.157704
C	1.176288	-1.110686	-0.079742
C	0.101593	-2.033456	-0.167041
C	-1.317788	-1.546159	0.142205
H	0.339405	4.142650	0.034546
H	-4.005470	2.244517	-0.334101
H	-2.078694	3.797355	-0.160669
H	-3.633593	-0.204364	-0.247064
H	2.638652	3.240248	0.156810
H	4.628099	-1.090382	-0.101051
H	2.723343	-2.656137	-0.270691
O	0.245888	-3.244825	-0.428626
O	-1.485048	-1.855625	1.521326
H	-2.358751	-1.536195	1.789616
O	-2.242241	-2.249341	-0.627894
H	-1.903845	-3.156565	-0.684667

¹a-6-IM2

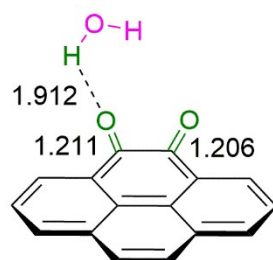
C	-2.922262	1.961052	-0.209082
C	-1.811279	2.772256	-0.157128
C	-0.518236	2.213777	-0.068832
C	-0.373721	0.809695	-0.037348
C	-1.528174	-0.004166	-0.054239
C	-2.781803	0.563211	-0.147633
C	0.650960	3.049282	-0.003569
C	0.954500	0.236021	-0.004529
C	2.079425	1.085936	0.064348
C	1.890990	2.511809	0.077105
C	3.370442	0.518068	0.087521
H	4.226863	1.181105	0.155192
C	3.551124	-0.847946	0.012403
C	2.439687	-1.691967	-0.103715
C	1.162192	-1.160287	-0.104019
C	-0.005718	-2.048485	-0.265384
C	-1.376324	-1.493090	0.173267
H	0.511545	4.125032	-0.016647
H	-3.911869	2.395934	-0.287193
H	-1.913195	3.851962	-0.184780
H	-3.659956	-0.071616	-0.167129
H	2.769930	3.145252	0.131782
H	4.549461	-1.268045	0.030732
H	2.566957	-2.765251	-0.188214
O	0.056346	-3.188330	-0.664238
O	-1.352508	-1.768593	1.564988
H	-2.098914	-1.307426	1.974752
O	-2.402419	-2.172210	-0.462233
H	-2.142986	-3.104870	-0.511620

¹a-6-TS2

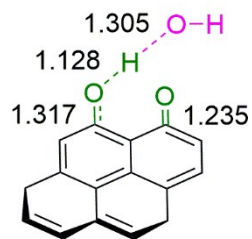
C	-2.892146	2.010724	-0.253714
C	-1.769751	2.802832	-0.152217
C	-0.483547	2.227742	-0.058007
C	-0.355861	0.822935	-0.072315
C	-1.522830	0.027675	-0.140846
C	-2.769277	0.611954	-0.237485
C	0.693546	3.045886	0.058642
C	0.960297	0.227377	-0.027851
C	2.093771	1.060296	0.092008
C	1.924202	2.487381	0.145613
C	3.376555	0.474261	0.128817
H	4.240478	1.122498	0.233380
C	3.537948	-0.891472	0.022870
C	2.417298	-1.716618	-0.137493
C	1.146616	-1.169685	-0.156507
C	-0.025193	-2.055018	-0.365586
C	-1.416082	-1.463030	-0.039720
H	0.568344	4.123171	0.078799
H	-3.873396	2.462973	-0.336518
H	-1.858189	3.884224	-0.145983
H	-3.646121	-0.021990	-0.296696
H	2.810829	3.105254	0.239468
H	4.529442	-1.327049	0.053046
H	2.533496	-2.789140	-0.244557
O	0.062498	-3.197134	-0.739651
O	-1.442094	-1.863299	1.593146
H	-1.733951	-1.114548	2.143581
O	-2.463742	-2.202952	-0.298150
H	-2.317502	-2.357758	0.995476

³a-6-IM3

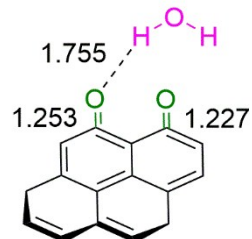
C	2.051250	2.624358	-0.080067
C	0.763515	3.130992	-0.034255
C	-0.341645	2.243971	-0.006637
C	-0.122217	0.833025	-0.026911
C	1.183959	0.329174	-0.073162
C	2.260655	1.248655	-0.098785
C	-1.656848	2.729242	0.039851
C	-1.245395	-0.060146	0.002961
C	-2.571469	0.466337	0.048415
C	-2.752450	1.856931	0.066932
C	-3.679761	-0.416126	0.075351
H	-4.680224	0.000445	0.108733
C	-3.473473	-1.786428	0.057624
C	-2.179329	-2.292764	0.014054
C	-1.047816	-1.443208	-0.014904
C	0.303212	-2.031992	-0.060556
C	1.447545	-1.115832	-0.096317
H	-1.824379	3.800836	0.055593
H	2.899963	3.297040	-0.099060
H	0.578459	4.199218	-0.017664
H	3.272108	0.860212	-0.131227
H	-3.758335	2.260801	0.102225
H	-4.317852	-2.464409	0.076203
H	-2.009598	-3.363051	0.000247
O	0.449908	-3.268499	-0.068157
O	5.227182	-0.726194	0.197615
H	5.508297	-1.056905	1.055608
O	2.620873	-1.554574	-0.145133
H	4.309458	-1.037177	0.093175

¹a-6-IM3

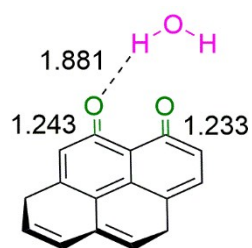
C	2.063742	2.606245	-0.015363
C	0.774561	3.094768	-0.005770
C	-0.335892	2.223896	-0.000401
C	-0.120135	0.828882	-0.004756
C	1.211622	0.345079	-0.014833
C	2.283479	1.223884	-0.019596
C	-1.676835	2.741596	0.009327
C	-1.258444	-0.061506	0.000941
C	-2.561242	0.481526	0.010331
C	-2.742278	1.907419	0.014405
C	-3.672012	-0.389444	0.015742
H	-4.668152	0.040677	0.022946
C	-3.503752	-1.757949	0.011996
C	-2.212592	-2.300240	0.002935
C	-1.105435	-1.468809	-0.002381
C	0.246609	-2.067858	-0.012120
C	1.466085	-1.107540	-0.019352
H	-1.810315	3.817910	0.012411
H	2.906674	3.286490	-0.019293
H	0.592585	4.164458	-0.002331
H	3.295786	0.835927	-0.026229
H	-3.754940	2.295439	0.021727
H	-4.365516	-2.414314	0.015971
H	-2.065929	-3.374077	-0.000092
O	0.454219	-3.255966	-0.014563
O	5.294208	-0.684238	-0.029175
H	5.756238	-1.053828	0.729280
O	2.571681	-1.600902	-0.029283
H	4.407814	-1.069524	0.003159

¹z-6-TS1

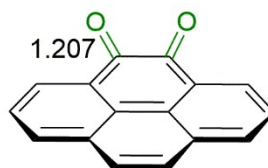
C	-2.621337	1.653723	-0.011854
C	-1.548980	2.444662	-0.169096
C	-0.196239	1.910518	-0.066752
C	0.003422	0.503624	0.054656
C	-1.098709	-0.361384	0.122701
C	-2.454548	0.232044	0.420074
C	0.921753	2.755602	-0.132118
C	1.312185	-0.025201	0.034016
C	2.428211	0.840048	-0.013097
C	2.202966	2.237738	-0.088796
C	3.723729	0.290377	-0.002822
H	4.580364	0.955831	-0.028966
C	3.904482	-1.089243	0.037692
C	2.805757	-1.938469	0.061283
C	1.487354	-1.428701	0.060855
C	0.357663	-2.276559	0.015023
C	-0.941051	-1.760933	-0.015796
H	0.768505	3.824488	-0.225655
H	-3.634175	2.040107	-0.036158
H	-1.653900	3.507397	-0.359349
H	3.059440	2.902862	-0.130158
H	4.905340	-1.502152	0.041136
H	2.950994	-3.013852	0.072559
O	-3.363958	-0.713832	-1.038963
H	-3.066940	-0.480451	-1.927309
O	-1.999839	-2.518772	-0.213069
H	-2.756446	-1.793049	-0.628695
H	0.500128	-3.351818	-0.031621
O	-3.057859	-0.144451	1.429331

¹z-6-IM2

C	-0.659331	3.341407	0.009020
C	0.676015	3.210027	0.024282
C	1.291169	1.899876	0.018320
C	0.463509	0.742364	-0.002375
C	-0.957455	0.843427	-0.021086
C	-1.574335	2.177003	-0.014348
C	2.694710	1.789175	0.034565
C	1.110581	-0.514038	-0.006391
C	2.518506	-0.616346	0.010605
C	3.310103	0.558833	0.030396
C	3.115263	-1.891837	0.007020
H	4.198966	-1.956300	0.019540
C	2.351090	-3.062978	-0.011185
C	0.975923	-2.973814	-0.026430
C	0.325877	-1.702554	-0.024364
C	-1.051646	-1.610189	-0.041078
C	-1.772639	-0.342858	-0.042878
H	3.285040	2.698399	0.049899
H	-1.135272	4.316149	0.013323
H	1.326938	4.078076	0.040989
H	4.390713	0.471421	0.042667
H	2.840155	-4.028466	-0.012995
H	0.362659	-3.869008	-0.039948
O	-4.393087	-2.731881	0.028362
H	-4.979581	-2.673016	0.787599
O	-3.024721	-0.366627	-0.066097
H	-3.927360	-1.870775	-0.002882
H	-1.652199	-2.516245	-0.053335
O	-2.783953	2.381606	-0.025926

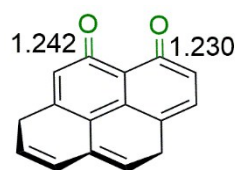
³z-6-IM2

C	-0.569501	3.385478	-0.014324
C	0.768108	3.205593	-0.058694
C	1.340255	1.892843	-0.041688
C	0.480343	0.748196	-0.007089
C	-0.911764	0.904538	0.013483
C	-1.496104	2.259090	0.071486
C	2.739091	1.721982	-0.065759
C	1.080858	-0.561774	0.005687
C	2.486836	-0.700417	-0.008316
C	3.301474	0.472210	-0.048822
C	3.058604	-1.990867	0.018674
H	4.139255	-2.081126	0.007691
C	2.258709	-3.125439	0.060400
C	0.876714	-3.006434	0.072520
C	0.265017	-1.733208	0.044992
C	-1.127510	-1.589370	0.038751
C	-1.767939	-0.302010	-0.021153
H	3.366801	2.605726	-0.097226
H	-1.014519	4.374053	-0.011218
H	1.443537	4.054019	-0.102157
H	4.379214	0.352570	-0.065089
H	2.715998	-4.107438	0.083406
H	0.244261	-3.886701	0.102035
O	-4.433727	-2.699178	-0.171443
H	-5.041335	-2.723123	0.573783
O	-3.004901	-0.238985	-0.131165
H	-4.022552	-1.820963	-0.135893
H	-1.770026	-2.463592	0.039973
O	-2.703845	2.464926	0.208084

¹a-2O

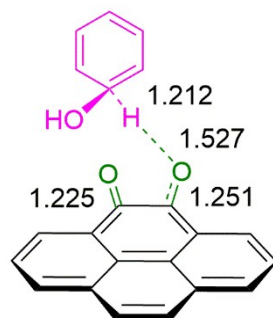
C	3.536759	-0.457579	-0.005963
C	2.825298	-1.638797	-0.005417
C	1.414124	-1.639226	-0.003035
C	0.722984	-0.408268	-0.000182
C	1.470615	0.794603	0.000547
C	2.854838	0.765213	-0.001699
C	0.676639	-2.873509	-0.001313
C	-0.722984	-0.408269	0.000146
C	-1.414122	-1.639228	0.003033
C	-0.676636	-2.873510	0.001330
C	-2.825296	-1.638800	0.005436
H	-3.343977	-2.591951	0.007271
C	-3.536759	-0.457583	0.005982
C	-2.854839	0.765209	0.001690
C	-1.470616	0.794601	-0.000593
C	-0.776231	2.101698	-0.008865
C	0.776229	2.101700	0.008769
H	1.235308	-3.803179	-0.002950
H	4.619959	-0.472153	-0.008866
H	3.343980	-2.591947	-0.007228
H	3.402669	1.700371	-0.000697
H	-1.235302	-3.803182	0.002989
H	-4.619958	-0.472159	0.008907
H	-3.402670	1.700368	0.000684
O	-1.350329	3.162768	-0.028172
O	1.350324	3.162769	0.028258

¹z-20



C	3.733084	-0.882343	0.000232
C	3.429532	0.483207	0.000075
C	2.101848	0.951086	-0.000096
C	1.042335	0.018152	-0.000201
C	1.344439	-1.375808	-0.000013
C	2.707338	-1.802011	0.000186
C	1.819924	2.341353	-0.000089
C	-0.309601	0.434815	-0.000244
C	-0.551770	1.837168	-0.000100
C	0.512676	2.762026	-0.000055
C	-1.914677	2.316120	0.000207
H	-2.077556	3.389142	0.000489
C	-2.944660	1.453855	0.000238
C	-2.756966	-0.014608	-0.000378
C	-1.379076	-0.506883	-0.000419
C	-1.103769	-1.928502	-0.000714
C	0.315866	-2.294277	-0.000003
H	2.640233	3.050251	0.000013
H	4.765383	-1.207627	0.000408
H	4.234279	1.212542	0.000157
H	2.915971	-2.867112	0.000317
H	0.275800	3.820279	0.000075
H	-3.973189	1.798753	0.000568
O	-1.944384	-2.842253	0.000378
H	0.541184	-3.357446	0.000237
O	-3.755772	-0.732606	0.000370

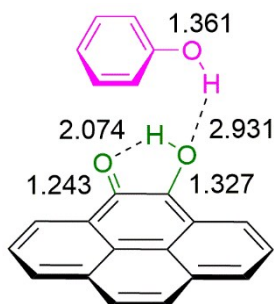
²a-7-TS1



C	1.807919	-3.500826	0.138186
C	2.890203	-2.785419	-0.337467
C	2.886682	-1.376946	-0.321494
C	1.757993	-0.694258	0.188467
C	0.661402	-1.441654	0.683489
C	0.693109	-2.828103	0.651091
C	4.006378	-0.620504	-0.815878
C	1.737472	0.745160	0.186295
C	2.850191	1.458564	-0.312955
C	3.990230	0.733466	-0.808573
C	2.817786	2.866921	-0.326890
H	3.677959	3.406045	-0.709984
C	1.708914	3.552270	0.134767
C	0.604077	2.851997	0.626743
C	0.607043	1.460944	0.661016
C	-0.557707	0.739488	1.177339
C	-0.533008	-0.753458	1.223785
H	4.864383	-1.163656	-1.197778
H	1.821806	-4.584410	0.117899
H	3.759775	-3.300781	-0.732085
H	-0.158050	-3.381313	1.031401
H	4.835319	1.301315	-1.183211
H	1.694161	4.635818	0.115774
H	-0.268394	3.382329	0.990039
O	-1.493344	-1.367732	1.671750
C	-4.117318	-1.381357	-0.320099
C	-2.953111	-1.882750	-0.934814
C	-1.987849	-1.017474	-1.469826
C	-2.128626	0.341919	-1.325460
C	-3.226582	0.890437	-0.540332
C	-4.298591	-0.030964	-0.188608
H	-4.881155	-2.069690	0.021665

H	-2.827811	-2.953930	-1.045157
H	-1.137615	-1.420792	-2.008104
H	-1.411641	1.035604	-1.753312
H	-2.658032	0.990192	0.524940
H	-5.197121	0.384531	0.255224
O	-3.589231	2.224905	-0.805031
H	-4.037536	2.248951	-1.659429
O	-1.589386	1.333459	1.560709

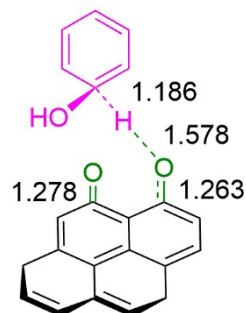
²a-7-IM2



C	3.860611	0.499248	0.414020
C	3.542885	-0.807189	0.087731
C	2.279229	-1.132122	-0.438523
C	1.328613	-0.102371	-0.635806
C	1.670908	1.230472	-0.298228
C	2.924439	1.520085	0.221543
C	1.923462	-2.488994	-0.756861
C	0.024781	-0.428452	-1.135911
C	-0.298698	-1.769598	-1.434111
C	0.691422	-2.793969	-1.230889
C	-1.591055	-2.080235	-1.899190
H	-1.831881	-3.115177	-2.118898
C	-2.543691	-1.087267	-2.069915
C	-2.238572	0.241299	-1.781148
C	-0.963714	0.582283	-1.316983
C	-0.622086	1.919795	-0.975239
C	0.678321	2.299674	-0.473376
H	2.665698	-3.264322	-0.598078
H	4.836639	0.734238	0.822430
H	4.266133	-1.601664	0.240136

H	3.163454	2.545503	0.479351
H	0.422170	-3.819084	-1.462784
H	-3.534318	-1.344818	-2.425806
H	-2.985453	1.015942	-1.907130
O	0.883305	3.496439	-0.206996
C	0.284758	-0.411020	2.507512
C	-0.096586	-1.746389	2.404667
C	-1.398692	-2.056152	2.011357
C	-2.310195	-1.047419	1.718577
C	-1.913786	0.286635	1.817426
C	-0.617577	0.608933	2.217218
H	1.296311	-0.154060	2.805018
H	0.612102	-2.536196	2.625618
H	-1.708611	-3.092273	1.926427
H	-3.322880	-1.276784	1.406084
H	-1.080009	3.717989	-0.837305
H	-0.319180	1.651280	2.290619
O	-2.833277	1.239375	1.504121
H	-2.429742	2.114847	1.562370
O	-1.517414	2.889324	-1.113534

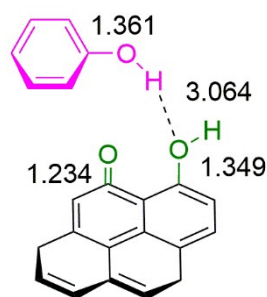
²z-7-TS1



C	-0.378945	2.871916	-0.421101
C	0.893916	3.113197	-0.012797
C	1.837109	2.052459	0.101085
C	1.431037	0.733474	-0.216787
C	0.087159	0.459085	-0.644197
C	-0.840338	1.546604	-0.760286
C	3.167983	2.314027	0.528269
C	2.394024	-0.310848	-0.082278

C	3.713649	-0.032467	0.345106
C	4.083788	1.310291	0.648543
C	4.642365	-1.093293	0.467246
H	5.650952	-0.865269	0.795237
C	4.278483	-2.401454	0.174797
C	2.987627	-2.690398	-0.245076
C	2.025483	-1.660490	-0.383326
C	0.722756	-1.930273	-0.806305
C	-0.281101	-0.914006	-0.970108
H	3.439405	3.339128	0.759465
H	-1.103093	3.674900	-0.510300
H	1.215086	4.120199	0.235458
H	5.098381	1.513060	0.973845
H	5.005584	-3.198805	0.275718
H	2.696923	-3.709494	-0.476176
O	-1.417177	-1.265523	-1.394658
H	0.429794	-2.947774	-1.043972
O	-2.058478	1.405333	-1.118303
C	-3.384339	-1.398006	0.538754
C	-2.647259	-0.622679	1.536678
C	-2.637121	0.730226	1.467048
C	-3.399979	1.381439	0.450219
C	-4.432131	0.664614	-0.230467
C	-4.453541	-0.686738	-0.161346
H	-2.569238	-1.367697	-0.321668
H	-2.047542	-1.165588	2.260972
H	-2.021496	1.322637	2.133283
H	-3.439590	2.463079	0.453766
H	-5.152343	1.210922	-0.826308
H	-5.188555	-1.278813	-0.697335
O	-3.603298	-2.754200	0.825895
H	-4.246395	-2.815452	1.542525

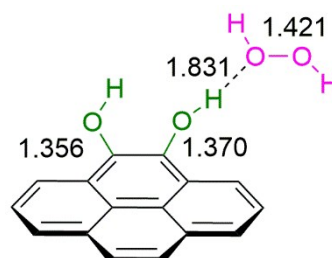
²_z-7-IM2



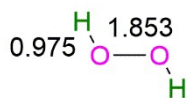
C	3.033214	0.206555	-2.045292
C	2.613392	1.460275	-1.606102
C	1.302109	1.654687	-1.134620
C	0.402702	0.554140	-1.105996
C	0.837835	-0.718503	-1.557742
C	2.163302	-0.872184	-2.025455
C	0.860330	2.921262	-0.659876
C	-0.920708	0.708467	-0.608881
C	-1.319628	1.993123	-0.137201
C	-0.415656	3.075211	-0.178214
C	-2.638893	2.167464	0.395915
H	-2.920807	3.155018	0.748269
C	-3.507994	1.135692	0.463623
C	-3.167500	-0.209735	0.000364
C	-1.812782	-0.397729	-0.555373
C	-1.344640	-1.658458	-1.012129
C	-0.057817	-1.805871	-1.501389
H	1.550767	3.757517	-0.680621
H	4.048269	0.073752	-2.401225
H	3.296113	2.303260	-1.618704
H	2.489385	-1.850995	-2.360513
H	-0.749576	4.039513	0.190341
H	-4.506517	1.259888	0.867899
C	0.062252	-0.035244	2.514915
C	1.064815	0.925994	2.618441
C	2.353890	0.618121	2.183630
C	2.639548	-0.630352	1.641711
C	1.624718	-1.581810	1.534919
C	0.335812	-1.290221	1.978128
H	-0.945580	0.190493	2.848156
H	0.845350	1.902060	3.035341
H	3.143977	1.357347	2.260499

H	3.635623	-0.878239	1.292093
H	-1.698857	-3.499810	-1.293498
H	-0.446068	-2.039543	1.893627
O	1.946251	-2.786344	0.988071
H	1.144773	-3.314284	0.879012
O	-2.169849	-2.724761	-0.958421
O	-4.002540	-1.113622	0.090631
H	0.272466	-2.783473	-1.843172

¹a-S3-IM1

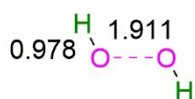


³H₂O₂



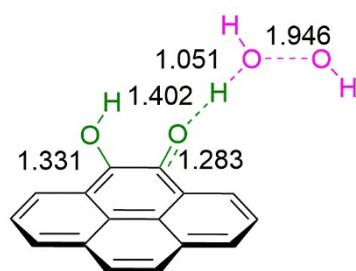
O	0.918427	0.121344	-0.000010
H	1.056110	-0.844262	0.000030
O	-0.918445	-0.121346	-0.000010
H	-1.055965	0.844281	0.000133

³S2-TS1

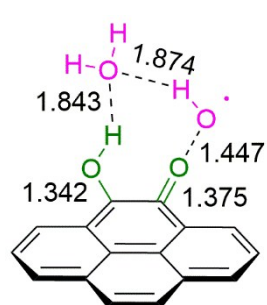


O	-0.955398	-0.106684	-0.014657
H	-1.107134	0.852739	0.101265
O	0.955587	-0.106540	0.014655
H	1.105623	0.853057	-0.101249

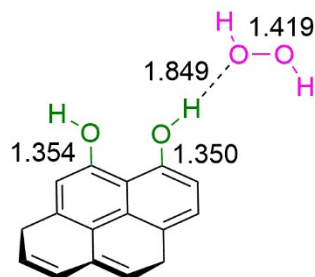
O	-4.068666	-0.525620	0.945231
O	-3.086732	-0.269047	1.940151
H	-3.052671	-1.348823	-0.336568
C	3.570686	-1.689116	0.371597
C	3.736787	-0.312708	0.470658
C	2.652808	0.550362	0.270487
C	1.378546	0.005696	-0.037112
C	1.223059	-1.402441	-0.131291
C	2.325971	-2.236396	0.073500
C	2.790036	1.981977	0.364431
C	0.262891	0.870018	-0.245755
C	0.428844	2.277008	-0.157256
C	1.732357	2.802658	0.162121
C	-0.670942	3.113995	-0.380755
H	-0.541230	4.188610	-0.308392
C	-1.910074	2.573392	-0.701837
C	-2.085542	1.195144	-0.796652
C	-1.012597	0.327189	-0.562006
C	-1.152525	-1.104652	-0.612815
C	-0.085632	-1.926433	-0.421499
H	3.767766	2.387305	0.603353
H	4.418264	-2.346273	0.528818
H	4.709391	0.106755	0.705418
H	2.203559	-3.310187	0.000808
H	1.845743	3.879576	0.232878
H	-2.752060	3.230919	-0.886179
H	-3.057895	0.797205	-1.061773
O	-2.350075	-1.699503	-0.911515
O	-0.215102	-3.274584	-0.482149
H	-1.145910	-3.477065	-0.659031
H	-2.892168	0.670383	1.785942
H	-4.846233	-0.782515	1.466089

¹a-S3-TS1

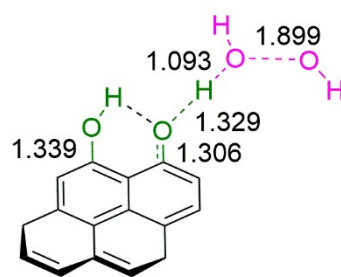
O	-5.000199	0.193370	-0.080054
O	-4.034067	-0.937506	1.175417
H	-3.290666	-1.182386	0.473679
C	3.714512	-1.784503	0.152457
C	3.920253	-0.412053	0.230059
C	2.841327	0.485057	0.152778
C	1.530836	-0.022277	-0.005348
C	1.330829	-1.431206	-0.082367
C	2.432210	-2.297827	-0.002507
C	3.035287	1.907541	0.227689
C	0.424175	0.872237	-0.089496
C	0.643284	2.268124	-0.022598
C	1.983792	2.759669	0.143097
C	-0.455626	3.142807	-0.126226
H	-0.279903	4.212103	-0.075072
C	-1.736899	2.649177	-0.301509
C	-1.965349	1.272081	-0.365265
C	-0.899744	0.376266	-0.250449
C	-1.121365	-1.052045	-0.297653
C	0.003819	-1.914543	-0.225174
H	4.045718	2.282736	0.349843
H	4.558854	-2.460791	0.212308
H	4.923142	-0.015820	0.349935
H	2.273430	-3.367972	-0.061286
H	2.134311	3.832721	0.195593
H	-2.571496	3.334627	-0.392504
H	-2.969451	0.893448	-0.520082
O	-2.277593	-1.598199	-0.401521
O	-0.217702	-3.225460	-0.277601
H	-1.181898	-3.346231	-0.366053
H	-3.718090	-0.168725	1.674822
H	-5.775501	-0.382381	0.003962

¹a-S3-IM2

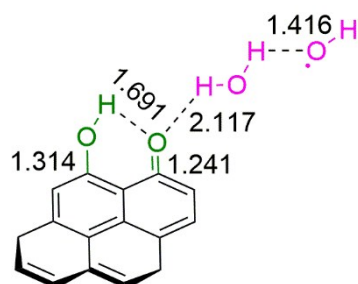
O	-4.862303	-0.781350	0.185604
O	-3.205894	1.334031	0.832175
H	-5.359235	-1.386756	0.751011
C	1.503175	-3.452443	0.039226
C	2.618801	-2.628802	0.119497
C	2.481254	-1.235795	0.091472
C	1.184567	-0.668909	-0.020089
C	0.054270	-1.522884	-0.102339
C	0.226151	-2.908174	-0.069529
C	3.619855	-0.356240	0.173315
C	1.029421	0.749951	-0.050232
C	2.166864	1.593252	0.032171
C	3.470587	0.989182	0.144695
C	1.991119	2.982292	0.001299
H	2.860904	3.627550	0.062929
C	0.717090	3.526503	-0.108903
C	-0.406773	2.708018	-0.192943
C	-0.265849	1.318195	-0.164640
C	-1.394196	0.429445	-0.257127
C	-1.259852	-0.926698	-0.210461
H	4.604974	-0.803025	0.259118
H	1.626160	-4.529014	0.062465
H	3.611690	-3.057816	0.205655
H	-0.640677	-3.554517	-0.128247
H	4.333834	1.643767	0.205782
H	0.593354	4.603344	-0.130972
H	-1.395829	3.141776	-0.280086
O	-2.648032	0.959805	-0.449054
O	-2.297311	-1.775196	-0.273616
H	-3.150678	-1.301752	-0.255671
H	-3.942429	0.695435	0.880698
H	-5.452644	-0.558675	-0.546026

¹z-S3-IM1

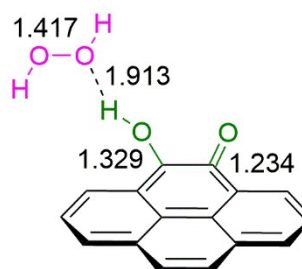
O	4.764802	-1.348713	-0.439321
O	4.801637	-0.192464	0.382857
H	3.238979	0.763284	0.128538
C	-0.873746	-3.742481	0.021078
C	-2.122119	-3.130433	0.017887
C	-2.227347	-1.733831	0.011714
C	-1.044306	-0.944580	0.008977
C	0.224273	-1.581001	0.016104
C	0.289236	-2.980793	0.020659
C	-3.506948	-1.074902	0.006192
C	-1.122419	0.484532	-0.001231
C	-2.404987	1.095578	-0.009397
C	-3.586919	0.275656	-0.003752
C	-2.491489	2.490380	-0.022401
H	-3.467833	2.963473	-0.028023
C	-1.349447	3.266562	-0.032031
C	-0.079219	2.683229	-0.025883
C	0.064644	1.280717	-0.005622
C	1.342908	0.588728	0.015167
C	1.403745	-0.770822	0.018825
H	-4.402422	-1.687499	0.009628
H	-0.805613	-4.824888	0.024118
H	-3.028241	-3.726829	0.020057
H	1.261112	-3.463144	0.025585
H	-4.550121	0.775977	-0.009348
H	-1.424711	4.349864	-0.044535
O	2.463071	1.341342	0.033063
H	5.080264	-0.542901	1.244716
H	5.537995	-1.216703	-1.010663
H	2.371963	-1.262192	0.020896
O	1.016094	3.478769	-0.044927
H	0.728638	4.400863	-0.052070

¹z-S3-TS1

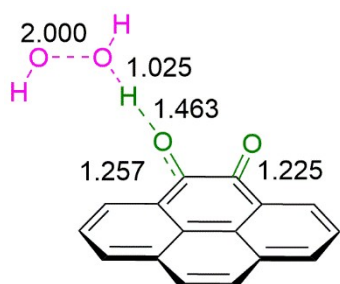
O	3.750683	-2.046051	0.720104
O	2.038371	-2.316776	1.494099
H	3.384509	-1.336793	-0.026069
C	-2.751192	-2.749772	-0.288417
C	-3.409327	-1.563208	0.004045
C	-2.701874	-0.349415	0.082041
C	-1.302658	-0.353134	-0.136453
C	-0.631923	-1.574351	-0.436436
C	-1.376434	-2.762127	-0.507886
C	-3.360445	0.892506	0.375745
C	-0.564638	0.866550	-0.069529
C	-1.240327	2.073537	0.222868
C	-2.656933	2.052055	0.442363
C	-0.494372	3.268585	0.289667
H	-1.010930	4.195947	0.514678
C	0.865134	3.276661	0.076949
C	1.545875	2.081781	-0.213012
C	0.841192	0.865462	-0.290314
C	1.518837	-0.382955	-0.582764
C	0.773521	-1.564433	-0.652259
H	-4.432403	0.881142	0.541183
H	-3.311419	-3.675919	-0.346227
H	-4.480857	-1.558351	0.173504
H	-0.865389	-3.690695	-0.738604
H	-3.155476	2.989929	0.664730
H	1.437096	4.195751	0.128119
O	2.812938	-0.384719	-0.756720
H	2.124933	-1.511010	2.037215
H	3.771385	-2.929033	0.318810
H	1.276532	-2.480781	-0.936628
O	2.867715	2.150406	-0.412206
H	3.177760	1.230479	-0.592571

¹_z-S3-IM2

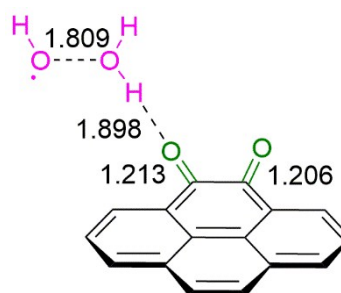
O	-6.837210	-0.550455	-0.011868
O	-4.689748	-1.554294	0.732520
H	-7.158274	-0.939358	-0.828784
C	2.252321	-3.447208	-0.074365
C	3.215598	-2.434790	0.034509
C	2.877990	-1.061620	0.058620
C	1.522940	-0.700972	-0.031883
C	0.519188	-1.727623	-0.140871
C	0.924944	-3.108555	-0.161717
C	3.876069	-0.056682	0.168521
C	1.150924	0.656129	-0.011731
C	2.154024	1.644075	0.096929
C	3.514129	1.267419	0.186617
C	1.752825	3.024007	0.117447
H	2.523440	3.782286	0.203681
C	0.446336	3.383094	0.033580
C	-0.566266	2.378893	-0.078249
C	-0.217709	1.022297	-0.102519
C	-1.242837	0.011301	-0.213556
C	-0.803569	-1.396848	-0.226864
H	4.916193	-0.353573	0.237679
H	2.560734	-4.484077	-0.090534
H	4.265577	-2.704957	0.104101
H	0.155492	-3.868698	-0.247789
H	4.265664	2.044211	0.271306
H	0.136964	4.421215	0.050517
O	-2.450159	0.287307	-0.295625
H	-4.005267	-0.984225	0.371692
H	-5.614523	-1.137131	0.395824
H	-1.571639	-2.160391	-0.310369
O	-1.815927	2.778831	-0.157008
H	-2.391450	1.976076	-0.228273

²_a-S4-IM1

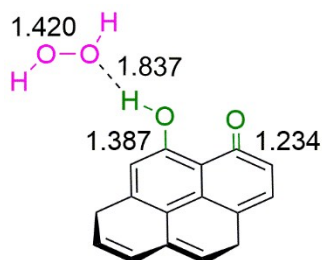
O	-4.474542	0.271607	1.272511
O	-3.997159	-1.031869	0.988790
H	-2.808692	-1.617506	-0.391009
C	3.898508	-1.225683	0.433452
C	3.843793	0.154292	0.509656
C	2.633238	0.837116	0.297622
C	1.462165	0.094380	0.011528
C	1.533610	-1.317206	-0.063387
C	2.744588	-1.961266	0.145614
C	2.559412	2.272194	0.356632
C	0.225711	0.780854	-0.221379
C	0.189862	2.191872	-0.182474
C	1.392854	2.919416	0.124178
C	-1.017252	2.862384	-0.456250
H	-1.034406	3.946465	-0.423780
C	-2.159132	2.151495	-0.785733
C	-2.139004	0.757901	-0.819663
C	-0.966084	0.052787	-0.511852
C	-0.921717	-1.377242	-0.495994
C	0.318011	-2.115462	-0.341563
H	3.465629	2.824107	0.582973
H	4.838096	-1.740143	0.598039
H	4.736836	0.729769	0.729972
H	2.780650	-3.042672	0.085285
H	1.340226	4.002320	0.159346
H	-3.075906	2.676603	-1.027870
H	-3.040390	0.234259	-1.119530
O	-2.014571	-2.119572	-0.642800
O	0.340294	-3.347851	-0.410256
H	-3.967970	-1.457123	1.861187
H	-3.657641	0.798404	1.277102

²a-S4-TS1

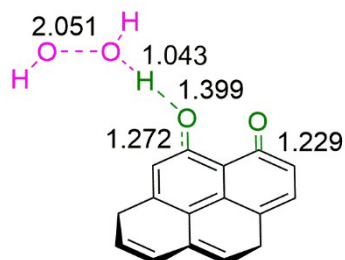
O	-5.033429	0.358365	0.370485
O	-4.023258	-1.264356	0.958056
H	-3.266943	-1.433122	0.287117
C	3.920249	-1.421308	0.239984
C	3.958822	-0.044183	0.310341
C	2.770506	0.712340	0.193907
C	1.532139	0.042838	0.000861
C	1.509345	-1.364644	-0.066905
C	2.698381	-2.078852	0.053320
C	2.789457	2.130172	0.261241
C	0.326250	0.808257	-0.127592
C	0.382883	2.221982	-0.063108
C	1.630888	2.862846	0.137223
C	-0.811408	2.979151	-0.200896
H	-0.750893	4.060638	-0.145192
C	-2.022868	2.345491	-0.414670
C	-2.082315	0.957045	-0.487548
C	-0.916530	0.168758	-0.327724
C	-1.005005	-1.278146	-0.369715
C	0.234306	-2.089398	-0.251851
H	3.739747	2.631889	0.410421
H	4.833558	-1.997185	0.328211
H	4.897850	0.479366	0.454857
H	2.661956	-3.161028	0.000157
H	1.659603	3.945789	0.189096
H	-2.929160	2.927738	-0.530948
H	-3.033913	0.475449	-0.673389
O	-2.107861	-1.869245	-0.492499
O	0.185436	-3.313053	-0.294707
H	-3.641803	-0.742341	1.677212
H	-5.827685	-0.194975	0.350552

²a-S4-IM2

O	-3.317322	1.164489	1.781019
O	-4.090367	-1.395344	0.966973
H	-3.430528	-1.858213	0.427911
C	3.948688	-0.893342	0.522507
C	3.740926	0.469729	0.524698
C	2.468175	1.013907	0.247771
C	1.391333	0.143789	-0.025078
C	1.625108	-1.252981	-0.030176
C	2.885033	-1.759494	0.238713
C	2.258544	2.436476	0.233637
C	0.088867	0.698919	-0.314149
C	-0.077028	2.100462	-0.337697
C	1.041932	2.956824	-0.050939
C	-1.342120	2.640528	-0.650471
H	-1.454186	3.719655	-0.669423
C	-2.416576	1.823829	-0.936439
C	-2.261659	0.432636	-0.894525
C	-1.032908	-0.125120	-0.576134
C	-0.901622	-1.589351	-0.480478
C	0.519392	-2.187307	-0.328779
H	3.104007	3.080998	0.449122
H	4.930711	-1.297198	0.737289
H	4.559577	1.149208	0.738095
H	3.036244	-2.832853	0.229843
H	0.884182	4.029846	-0.069537
H	-3.378350	2.253064	-1.189446
H	-3.101672	-0.213998	-1.122389
O	-1.844661	-2.351707	-0.490141
O	0.656302	-3.380308	-0.443122
H	-4.417469	-2.042800	1.601186
H	-3.580639	0.258239	1.494744

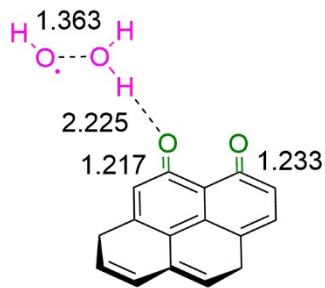
²_z-S4-IM1

O	4.595990	-1.206789	-0.334099
O	5.527851	-0.652483	0.582783
H	3.246296	0.036026	-0.241595
C	-1.616217	-3.596227	-0.002185
C	-2.725449	-2.754148	0.037871
C	-2.566769	-1.356535	0.036367
C	-1.256988	-0.804264	-0.000795
C	-0.132307	-1.669128	-0.048785
C	-0.335519	-3.069029	-0.044416
C	-3.685382	-0.478406	0.079393
C	-1.058780	0.603440	-0.002572
C	-2.207704	1.446536	0.048133
C	-3.499948	0.881177	0.084472
C	-2.035652	2.869378	0.052986
H	-2.925118	3.490632	0.092020
C	-0.805491	3.425361	0.014735
C	0.418497	2.624587	-0.036922
C	0.252362	1.157161	-0.044472
C	1.358568	0.265599	-0.102761
C	1.159773	-1.107594	-0.095693
H	-4.683537	-0.901801	0.106325
H	-1.757038	-4.670760	-0.000563
H	-3.727633	-3.167828	0.067847
H	0.529614	-3.722490	-0.078461
H	-4.353792	1.549593	0.118668
H	-0.667509	4.500915	0.020376
O	2.604019	0.763042	-0.164011
H	5.681323	-1.394177	1.189966
H	5.128228	-1.344779	-1.135019
H	2.020650	-1.768319	-0.131910
O	1.513459	3.191921	-0.067148

²_z-S4-TS1

O	-4.102755	-0.585780	0.841325
O	-4.703996	1.232548	0.107159
H	-3.414360	-1.026323	0.193049
C	0.292911	3.774799	-0.143515
C	1.596201	3.314594	0.019577
C	1.884339	1.934538	0.062357
C	0.829713	1.002254	-0.063655
C	-0.502644	1.475400	-0.232993
C	-0.749373	2.871259	-0.265389
C	3.215739	1.462328	0.231404
C	1.087743	-0.400729	-0.030409
C	2.438501	-0.830649	0.144010
C	3.474755	0.114111	0.270160
C	2.733569	-2.237513	0.192861
H	3.768212	-2.535642	0.328204
C	1.756069	-3.156180	0.075047
C	0.348292	-2.781967	-0.116760
C	0.037200	-1.337717	-0.153672
C	-1.320020	-0.859002	-0.322563
C	-1.542945	0.554961	-0.363420
H	4.018775	2.184563	0.328299
H	0.095349	4.839276	-0.170656
H	2.415390	4.019220	0.118532
H	-1.770810	3.216087	-0.385742
H	4.489192	-0.245872	0.401144
H	1.964003	-4.219723	0.108195
O	-2.321511	-1.635160	-0.433418
H	-4.490909	1.582994	0.983317
H	-4.980054	-0.901970	0.585708
H	-2.562889	0.904344	-0.502029
O	-0.498262	-3.664092	-0.240851

²z-S4-IM2



O	7.445905	-0.162669	0.515416
O	5.219453	0.592060	-0.197682
H	7.972679	-0.451143	-0.233560
C	-4.805048	-0.584341	0.066786
C	-4.373836	0.745039	0.075948
C	-3.004587	1.086311	0.052736
C	-2.037468	0.060886	0.018018
C	-2.471982	-1.298376	0.015859
C	-3.872463	-1.595168	0.038645
C	-2.588543	2.437580	0.062146
C	-0.651856	0.381673	-0.021448
C	-0.268993	1.763852	-0.011352
C	-1.243641	2.762187	0.034675
C	1.135988	2.121848	-0.039496
H	1.383829	3.177417	-0.010060
C	2.091790	1.183750	-0.107186
C	1.752893	-0.252818	-0.179352
C	0.314427	-0.628487	-0.061975
C	-0.097669	-2.030773	0.007790
C	-1.537305	-2.306198	0.005026
H	-3.342108	3.217753	0.092639
H	-5.863061	-0.809944	0.084142
H	-5.103083	1.549345	0.101117
H	-4.176653	-2.636446	0.035343
H	-0.932759	3.800033	0.046421
H	3.153740	1.415738	-0.141483
O	0.685673	-2.978817	0.091893
H	4.661406	-0.188303	-0.258708
H	6.214053	0.247605	0.099730
H	-1.836573	-3.349656	0.017654
O	2.626255	-1.082349	-0.356397

Table S2: Thermal correction to Gibbs free energy (G_0 , hartree), sum of electronic and thermal free energies (G_c , hartree) with ZPE and thermal corrections, and the relative Gibbs free energies (G_r) (kJ mol⁻¹) of various species with respect to the triplet state reactants ³a-O/³z-O + H₂O₂ for the H₂O₂ decomposition at M06-2x/6-311++G(d, p) level in acetonitrile solution under the temperature of 343.15 K and the pressure of 1.0 atm.

Species	G_0	G_c	G_r
¹ H ₂ O ₂	0.00073	-151.54665	
³ a-O	0.14090	-689.44648	
³ a-O + ¹ H ₂ O ₂	0.14163	-840.99313	0.0
¹ a-O	0.14217	-689.42735	
¹ a-O + ¹ H ₂ O ₂	0.14290	-840.97400	50.2
³ a-1-IM1	0.16201	-840.98307	26.4
³ a-1-TS1	0.16115	-840.96061	85.4
³ a-1-IM2	0.16327	-841.08497	-241.1
² a-OH-O	0.15776	-765.35436	
·OH	-0.01159	-75.74451	
² a-OH-O + ·OH	0.14617	-841.09888	-277.6
³ z-O	0.14031	-689.44508	
³ z-O + ¹ H ₂ O ₂	0.14104	-840.99173	3.7
¹ z-O	0.14172	-689.42522	
¹ z-O + ¹ H ₂ O ₂	0.14245	-840.97187	55.8
³ z-1-IM1	0.16158	-840.98379	24.5
³ z-1-TS2	0.16060	-840.96326	78.4
³ z-1-IM2	0.16065	-841.09043	-255.5
² z-OH-O	0.15669	-765.35416	
² z-OH-O + ·OH	0.14511	-841.09867	-277.1

Table S3: Thermal correction to Gibbs free energy (G_0 , hartree), sum of electronic and thermal free energies (G_c , hartree) with ZPE and thermal corrections, and the relative Gibbs free energies (G_r) (kJ mol⁻¹) of various species with respect to the reaction of hydroxyl radical with benzene at M06-2x/6-311++G(d, p) level in acetonitrile solution under the temperature of 343.15 K and the pressure of 1.0 atm.

Species	G_0	G_c	G_r
Ph	0.06810	-232.14002	
·OH	-0.01159	-75.74451	
Ph + ·OH	0.05652	-307.88453	0.0
² 2-IM1	0.07080	-307.87583	22.9
² 2-HB-TS1	0.07503	-307.86364	54.8
² Ph(H)OH	0.07803	-307.89059	-15.9
² 2-B-TS1	0.06808	-307.86150	60.5
² 2-B-IM2	0.06954	-307.88558	-2.7
·Ph	0.05463	-231.46731	
H ₂ O	0.00058	-76.42928	
·Ph + H ₂ O	0.05521	-307.89659	-31.7

Table S4: Thermal correction to Gibbs free energy (G_0 , hartree), sum of electronic and thermal free energies (G_c , hartree) with ZPE and thermal corrections, and the relative Gibbs free energies (G_r) (kJ mol⁻¹) of various species with respect to hydroxybenzene radical attacking the oxygen atom of hydroxyl group on the armchair and zigzag semiquinones of carbon at M06-2x/6-311++G(d, p) level in acetonitrile solution under the temperature of 343.15 K and the pressure of 1.0 atm.

Species	G_0	G_c	G_r
² a-OH-O	0.15776	-765.35436	
² Ph(H)OH	0.07803	-307.89059	
² a-OH-O + ² Ph(H)OH	0.23578	-1073.24495	0.0
¹ a-3-IM1	0.25873	-1073.22478	53.0
³ a-3-IM1	0.25829	-1073.22544	51.2
¹ a-3-TS1	0.25939	-1073.20981	92.3
¹ a-3-IM2	0.26387	-1073.25639	-30.0
¹ a-3-IM3	0.16870	-765.89117	
PhOH	0.07081	-307.36649	
¹ a-3-IM3 + PhOH	0.23951	-1073.25765	-33.3
H ₂ O	0.00058	-76.42928	
¹ a-O	0.14217	-689.42735	
¹ a-O + PhOH + H ₂ O	0.21356	-1073.22311	57.3
³ a-O	0.14090	-689.44648	
³ a-O + PhOH + H ₂ O	0.21229	-1073.24225	7.1
² z-OH-O	0.15669	-765.35416	
² z-OH-O + ² Ph(H)OH	0.23472	-1073.24475	0.5
¹ z-3-IM1	0.25795	-1073.21877	68.7
³ z-3-IM1	0.25874	-1073.23309	31.1
¹ z-3-TS1	0.25772	-1073.20766	97.9
¹ z-3-IM2	0.26338	-1073.24984	-12.8
¹ z-3-IM4	0.15923	-765.84643	
¹ z-3-IM4 + PhOH	0.23004	-1073.21292	
¹ z-O	0.14172	-689.42522	84.1
¹ z-O + PhOH + H ₂ O	0.21311	-1073.22099	
³ z-O	0.14031	-689.44508	62.9
³ z-O + PhOH + H ₂ O	0.21170	-1073.24084	

Table S5: Thermal correction to Gibbs free energy (G_0 , hartree), sum of electronic and thermal free energies (G_c , hartree) with ZPE and thermal corrections, and the relative Gibbs free energies (G_r) (kJ mol⁻¹) of various species with respect hydroxybenzene radical attacking the oxygen atom of carbonyl group on the armchair and zigzag semiquinones of carbon at M06-2x/6-311++G(d, p) level in acetonitrile solution under the temperature of 343.15 K and the pressure of 1.0 atm.

Species	G_0	G_c	G_r
² a-OH-O	0.15776	-765.35436	
² Ph(H)OH	0.07803	-307.89059	
² a-OH-O + ² Ph(H)OH	0.23578	-1073.24495	0.0
¹ a-3-IM1	0.25873	-1073.22478	53.0
³ a-3-IM1	0.25829	-1073.22544	51.2
¹ a-4-TS1	0.26414	-1073.21959	66.6
¹ a-4-IM2	0.26166	-1073.32053	-198.4
PhOH	0.07081	-307.36649	
¹ a-2OH	0.17005	-765.96354	
¹ a-2OH + PhOH	0.24086	-1073.33002	-223.4
³ a-2OH	0.16344	-765.88724	
³ a-2OH + PhOH	0.23425	-1073.25373	-23.0
³ a-4-TS2	0.16316	-765.80938	
³ a-4-TS2 + PhOH	0.23397	-1073.17586	181.4
³ a-4-IM3	0.16017	-765.86587	
³ a-4-IM3 + PhOH	0.23098	-1073.23236	33.1
H ₂ O	0.00058	-76.42928	
³ a-O	0.14090	-689.44648	
³ a-O + H ₂ O + PhOH	0.21229	-1073.24225	7.1
² z-OH-O	0.15669	-765.35416	
² z-OH-O + ² Ph(H)OH	0.23472	-1073.24475	0.5
¹ z-3-IM1	0.25795	-1073.21877	68.7
³ z-3-IM1	0.25874	-1073.23309	31.1
¹ z-4-TS1	0.26163	-1073.21886	68.5
¹ z-4-IM2	0.26424	-1073.31521	-184.5
¹ z-2OH	0.16975	-765.96804	
¹ z-2OH + PhOH	0.24056	-1073.33453	-235.2
³ z-2OH	0.16355	-765.88845	
³ z-2OH + PhOH	0.23436	-1073.25494	-26.2
³ z-4-TS2	0.16276	-765.82880	
³ z-4-TS2 + PhOH	0.23357	-1073.19529	130.4
³ z-4-IM3	0.15919	-765.86606	
³ z-4-IM3 + PhOH	0.22999	-1073.23254	32.6
³ z-O	0.14031	-689.44508	

${}^3\text{z-O} + \text{H}_2\text{O} + \text{PhOH}$	0.21170	-1073.24084	10.8
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Table S6: Thermal correction to Gibbs free energy (G_0 , hartree), sum of electronic and thermal free energies (G_c , hartree) with ZPE and thermal corrections, and the relative Gibbs free energies (G_r) (kJ mol⁻¹) of various species with respect to the conversion of hydroquinone to semiquinone with the armchair and zigzag carbon oxidized by hydroxyl at M06-2x/6-311++G(d, p) level in acetonitrile solution under the temperature of 343.15 K and the pressure of 1.0 atm.

Species	G_0	G_c	G_r
¹ a-2OH	0.17005	-765.96354	
•OH	-0.01159	-75.74451	
¹ a-2OH + •OH	0.15846	-841.70805	0.0
² a-5-TS1	0.17588	-841.69529	33.5
² a-5-IM2	0.17427	-841.76743	-155.9
² a-OH-O	0.15776	-765.35436	
H ₂ O	0.00058	-76.42928	
² a-OH-O + H ₂ O	0.15834	-841.78364	-198.5
trans- ² a-OH-O	0.15716	-765.34576	
trans- ² a-OH-O + H ₂ O	0.15775	-841.77504	-175.9
¹ z-2OH	0.16975	-765.96804	
¹ z-2OH + •OH	0.15816	-841.71256	-11.8
² z-5-TS1	0.17792	-841.70520	7.5
² z-5-IM2	0.17498	-841.76180	-141.1
² z-OH-O	0.16930	-765.35416	
² z-OH-O + H ₂ O	0.16988	-841.78344	-197.9
trans- ² z-OH-O	0.15598	-765.33994	
trans- ² z-OH-O + H ₂ O	0.15656	-841.76922	-160.6

Table S7: Thermal correction to Gibbs free energy (G_0 , hartree), sum of electronic and thermal free energies (G_c , hartree) with ZPE and thermal corrections, and the relative Gibbs free energies (G_r) (kJ mol⁻¹) of various species with respect to the reaction from semiquinone to quinone with the armchair and zigzag carbon oxidized by hydroxyl at M06-2x/6-311++G(d, p) level in acetonitrile solution under the temperature of 343.15 K and the pressure of 1.0 atm.

Species	G_0	G_c	G_r
·OH	-0.01159	-75.74451	
² a-OH-O	0.15776	-765.35436	
² a-OH-O + ·OH	0.14617	-841.09888	0.0
trans- ² a-OH-O	0.15716	-765.34576	
trans- ² a-OH-O + ·OH	0.14558	-841.09028	22.6
³ a-6-IM1	0.16138	-841.08961	24.3
³ a-6-TS1	0.16822	-841.01531	219.4
³ a-6-IM2	0.16617	-841.08621	33.3
¹ a-6-IM2	0.17299	-841.17980	-212.4
¹ a-6-TS2	0.16673	-841.11351	-38.4
¹ a-6-IM3	0.16535	-841.17967	-212.1
³ a-6-IM3	0.15979	-841.10864	-25.6
¹ a-2O	0.14708	-764.76292	
H ₂ O	0.00058	-76.42928	
¹ a-2O + H ₂ O	0.14766	-841.19220	-245.0
	0.16930	-765.35416	
² z-OH-O	0.15771	-841.09867	
² z-OH-O + ·OH	0.15598	-765.33994	0.5
trans- ² a-OH-O	0.14439	-841.08445	
trans- ² a-OH-O + ·OH	0.16065	-841.09043	37.9
³ z-1-IM2	0.16689	-841.08890	22.2
¹ z-6-TS1	0.16320	-841.12678	26.2
¹ z-6-IM2	0.15863	-841.12302	-73.3
³ z-6-IM2	0.14491	-764.70473	-63.4
¹ z-2O	0.14549	-841.13401	
¹ z-2O + H ₂ O	-0.01159	-75.74451	-92.2

Table S8: Thermal correction to Gibbs free energy (G_0 , hartree), sum of electronic and thermal free energies (G_c , hartree) with ZPE and thermal corrections, and the relative Gibbs free energies (G_r) (kJ mol⁻¹) of various species with respect to the phenol formation from hydroxybenzene radical on the armchair and zigzag quinones of carbon at M06-2x/6-311++G(d, p) level in acetonitrile solution under the temperature of 343.15 K and the pressure of 1.0 atm.

Species	G_0	G_c	G_r
¹ a-2O	0.14708	-764.76292	
² Ph(H)OH	0.07803	-307.89059	
¹ a-2O + ² Ph(H)OH	0.22511	-1072.65351	0.0
² a-7-TS1	0.24394	-1072.62592	72.4
² a-7-IM2	0.25061	-1072.71215	-153.9
² a-OH-O	0.15776	-765.35436	
PhOH	0.07081	-307.36649	
² a-OH-O + PhOH	0.22857	-1072.72085	-176.8
¹ z-2O	0.14491	-764.70473	
² z-7-TS1	0.24634	-1072.58933	168.5
² z-7-IM2	0.24691	-1072.59171	162.2
² z-OH-O	0.24956	-1072.69699	-114.2
² z-7-IM1	0.16930	-765.35416	
² z-OH-O + PhOH	0.24011	-1072.72065	-176.3

Table S9: Thermal correction to Gibbs free energy (G_0 , hartree), sum of electronic and thermal free energies (G_c , hartree) with ZPE and thermal corrections, and the relative Gibbs free energies (G_r) (kJ mol⁻¹) of various species with respect to the singlet ground state H₂O₂ for the H₂O₂ decomposition at M06-2x/6-311++G(d, p) level in acetonitrile solution under the temperature of 343.15 K and the pressure of 1.0 atm.

Species	G_0	G_c	G_r
¹ H ₂ O ₂	0.00073	-151.54665	0.0
³ H ₂ O ₂	-0.00480	-151.46492	214.6
³ S2-TS1	-0.00668	-151.46097	224.9
·OH	-0.01159	-75.74451	
2* ·OH	-0.02317	-151.48903	151.3

Table S10: Thermal correction to Gibbs free energy (G_0 , hartree), sum of electronic and thermal free energies (G_c , hartree) with ZPE and thermal corrections, and the relative Gibbs free energies (G_r) (kJ mol⁻¹) of various species with respect to the ground state reactants ¹a-2OH/¹z-2OH + H₂O₂ for the H₂O₂ decomposition at M06-2x/6-311++G(d, p) level in acetonitrile solution under the temperature of 343.15 K and the pressure of 1.0 atm.

Species	G_0	G_c	G_r
¹ a-2OH	0.17005	-765.96354	
¹ H ₂ O ₂	0.00073	-151.54665	
¹ a-2OH + ¹ H ₂ O ₂	0.17078	-917.51019	0.0
¹ a-S3-IM1	0.19032	-917.50008	26.6
¹ a-S3-TS1	0.18531	-917.40490	276.4
¹ a-S3-IM2	0.19236	-917.50801	5.7
² a-OH-O	0.15776	-765.35436	
·OH	-0.01159	-75.74451	
H ₂ O	0.00058	-76.42928	
² a-OH-O + ·OH + H ₂ O	0.14675	-917.52815	-47.2
¹ z-2OH	0.16975	-765.96804	
¹ z-2OH + ¹ H ₂ O ₂	0.17048	-917.51469	-11.8
¹ z-S3-IM1	0.19090	-917.49431	41.7
¹ z-S3-TS1	0.18585	-917.41628	246.6
¹ z-S3-IM2	0.18109	-917.49047	51.8
² z-OH-O	0.16930	-765.35416	
² z-OH-O + ·OH + H ₂ O	0.15829	-917.52795	-46.6

Table S11: Thermal correction to Gibbs free energy (G_0 , hartree), sum of electronic and thermal free energies (G_c , hartree) with ZPE and thermal corrections, and the relative Gibbs free energies (G_r) (kJ mol⁻¹) of various species with respect to the reactants ²a-OH-O/²z-OH-O + H₂O₂ for the H₂O₂ decomposition at M06-2x/6-311++G(d, p) level in acetonitrile solution under the temperature of 343.15 K and the pressure of 1.0 atm.

Species	G_0	G_c	G_r
² a-OH-O	0.15776	-765.35436	
¹ H ₂ O ₂	0.00073	-151.54665	
² a-OH-O + ¹ H ₂ O ₂	0.15849	-916.90101	-47.2
² a-S4-IM1	0.17764	-916.87935	9.7
² a-S4-TS2	0.17847	-916.79486	231.5
² a-S4-IM2	0.17281	-916.91784	-91.4
·OH	-0.01159	-75.74451	
H ₂ O	0.00058	-76.42928	
¹ a-2O	0.14708	-764.76292	
¹ a-2O + ·OH + H ₂ O	0.13608	-916.93672	-140.9
² z-OH-O	0.16930	-765.35416	
² z-OH-O + ¹ H ₂ O ₂	0.17003	-916.90081	-46.7
² z-S4-IM1	0.17611	-916.87493	21.3
² z-S4-TS2	0.17015	-916.77177	292.1
² z-S4-IM2	0.16579	-916.84351	103.8
¹ z-2O	0.14491	-764.70473	
¹ z-2O + ·OH + H ₂ O	0.13391	-916.87852	11.8