

Supporting information

A CCSD Estimation on O-H Bond Dissociation Enthalpies of

Pyrogallol

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Table S1. CCSD/6-31+G*-calculated total energy (TE, in hartree) and cartesian coordinates (Å) for the parent phenol, phenolic radical, pyrogallol and pyrogallic radicals.

Phenol: TE = -306.5466054

6	0	0.936327	-0.021414	-0.000161
8	0	2.312113	-0.111858	0.000042
6	0	0.263834	1.203617	0.000029
6	0	0.223972	-1.225229	-0.000011
6	0	-1.136023	1.220224	-0.000017
6	0	-1.171099	-1.194364	0.000046
1	0	2.695841	0.781482	0.000136
1	0	0.823910	2.140235	0.000052
1	0	0.772688	-2.165300	-0.000013
6	0	-1.860005	0.025733	0.000021
1	0	-1.657410	2.176915	0.000092
1	0	-1.725304	-2.132445	0.000120
1	0	-2.948665	0.042565	-0.000168

Phenolic radical: TE = -305.918101

6	0	1.047607	-0.000025	-0.000534
8	0	2.305154	-0.000034	0.000340
6	0	0.291590	-1.245707	-0.000140
6	0	0.291616	1.245730	-0.000142
6	0	-1.087331	-1.228795	0.000129
6	0	-1.087229	1.228843	0.000128
1	0	0.860443	-2.173642	0.000076
1	0	0.860547	2.173618	0.000141
6	0	-1.788479	-0.000012	-0.000041

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1	0	-1.645848	-2.163870	0.000254
1	0	-1.645818	2.163875	0.000202
1	0	-2.877197	0.000099	0.000212

Pyrogallol 1: TE = -456.6279455

8	0	-2.412934	-0.666360	-0.000016
6	0	-1.222314	0.012751	-0.000060
1	0	-2.219576	-1.623089	0.000067
6	0	-0.014221	-0.686402	0.000123
6	0	-1.222441	1.409162	0.000056
8	0	-0.078640	-2.065364	-0.000084
6	0	1.194394	0.009015	-0.000122
6	0	-0.005863	2.094208	-0.000006
1	0	-2.173636	1.936776	0.000016
8	0	2.320802	-0.796652	-0.000218
6	0	1.211959	1.403168	0.000043
1	0	0.830805	-2.417322	0.001112
1	0	-0.001884	3.182652	0.000047
1	0	3.122114	-0.246113	0.001191
1	0	2.159267	1.942690	-0.000096

Pyrogallolic radical 1a: TE = -456.0084882

8	0	-2.471046	-0.314017	0.000017
6	0	-1.182970	0.154712	0.000033
1	0	-2.446697	-1.289539	0.000202
6	0	-0.095861	-0.708645	-0.000078
6	0	-0.955205	1.532864	-0.000015
8	0	-0.307331	-2.048102	-0.000041
6	0	1.273333	-0.217340	-0.000001
6	0	0.372704	2.051475	0.000007
1	0	-1.812338	2.202947	0.000027
8	0	2.205204	-1.062148	0.000067
6	0	1.465889	1.223157	-0.000033
1	0	0.583002	-2.465440	-0.000037
1	0	0.506985	3.131600	-0.000004
1	0	2.487095	1.597238	-0.000003

Pyrogallolic radical 1b: TE = -456.017609

8	0	2.390192	-0.722355	-0.000058
6	0	1.244372	-0.007944	-0.000037

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1	0	2.133095	-1.670126	-0.000013
6	0	0.000000	-0.760080	0.000045
6	0	1.237878	1.373034	0.000031
8	0	0.000000	-2.022018	0.000081
6	0	-1.244371	-0.007943	-0.000036
6	0	0.000000	2.046087	0.000005
1	0	2.177187	1.921066	0.000012
8	0	-2.390192	-0.722354	-0.000062
6	0	-1.237878	1.373034	0.000036
1	0	0.000001	3.134808	0.000036
1	0	-2.133096	-1.670125	-0.000006
1	0	-2.177186	1.921067	0.000020

Pyrogallolic radical 1c: TE = -456.0066869

8	0	-2.427850	-0.586796	0.000039
6	0	-1.242763	0.055572	0.000045
1	0	-2.215751	-1.547609	0.000082
6	0	-0.051130	-0.790128	-0.000005
6	0	-1.163740	1.437247	-0.000039
8	0	-0.185516	-2.038358	-0.000085
6	0	1.236635	-0.106482	0.000056
6	0	0.105429	2.033820	0.000008
1	0	-2.072076	2.035197	-0.000025
8	0	2.317250	-0.927795	0.000009
6	0	1.296399	1.274164	-0.000051
1	0	0.179875	3.119880	-0.000039
1	0	3.131017	-0.391761	0.000245
1	0	2.260875	1.782722	-0.000059

Pyrogallolic radical 1d: TE = -456.0027865

6	0	-0.548678	2.007801	0.000369
6	0	0.816163	1.593668	-0.000427
6	0	-1.561794	1.087385	0.000061
1	0	-0.770967	3.073358	0.000488
6	0	1.131382	0.239527	-0.000074
6	0	-1.279415	-0.345783	-0.000088
1	0	1.610261	2.340536	-0.001293
1	0	-2.610278	1.377256	0.000254
8	0	-2.189090	-1.205337	-0.000077
8	0	2.420014	-0.267166	-0.001700
6	0	0.127925	-0.733470	0.000036

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8	0	0.418713	-2.051487	0.000266
1	0	3.069222	0.456268	0.011232
1	0	1.391164	-2.150274	0.002152

Table S2. B3LYP/6-31+G*-calculated thermal correction to enthalpy (TCE, in hartree) and cartesian coordinates (Å) for the parent phenol, phenolic radical, pyrogallol and pyrogallic radicals.

Phenol: TCE = 0.110983

C,0,0.0379233173,0.0004409267,0.9390064352
O,0,0.0389474521,0.0008191873,2.3124391647
C,0,1.2162298511,0.0003467468,0.1849772261
C,0,-1.2076067112,-0.0001404852,0.3015645411
C,0,1.1439676887,-0.0001983029,-1.2114113342
C,0,-1.2661996243,-0.0007361924,-1.0920242559
H,0,0.9518044419,0.001046258,2.6406802397
H,0,2.1844010098,0.0007403657,0.6836835991
H,0,-2.1093298685,-0.0001556745,0.9068189752
C,0,-0.0941575431,-0.0006708969,-1.8576198884
H,0,2.0636141393,-0.0001895224,-1.791398693
H,0,-2.2360491446,-0.001185476,-1.5834626827
H,0,-0.1469620662,-0.0010602265,-2.9427911

Phenolic radical: TCE = 0.097837

C,0,0.0000448122,0.0002382401,1.0471392428
O,0,0.0001020865,0.0001857418,2.3074213852
C,0,1.2414058941,0.0006493517,0.2911795515
C,0,-1.2413738153,-0.0005798526,0.291289574
C,0,1.226794958,0.0004787463,-1.0886939199
C,0,-1.2268913877,-0.0007254272,-1.088590928
H,0,2.1677924359,0.0011153828,0.8582294298
H,0,-2.1677058503,-0.0010034746,0.8584296886
C,0,-0.000086713,-0.0002038993,-1.7872299947
H,0,2.1599804247,0.0008555727,-1.6464080403
H,0,-2.1601301865,-0.0012860476,-1.6462183833
H,0,-0.0001160057,-0.0003103213,-2.8739649302

Pyrogallol 1: TCE = 0.121679

O,0,-0.619308471,0.0085293549,-2.4228004594
C,0,-0.6200355123,0.003996698,-1.0570001788

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H,0,0.3032042087,0.0088231925,-2.7323358385
C,0,0.5897547961,0.000741015,-0.3552955459
C,0,-1.8307686529,0.0025577425,-0.3598709119
O,0,1.7518946279,0.0024038189,-1.0928757943
C,0,0.5879520397,-0.0038695904,1.0402354498
C,0,-1.8201011923,-0.0020973645,1.0360548666
H,0,-2.7596331406,0.0050984641,-0.9211092059
O,0,1.8420494596,-0.0066622305,1.6191268039
C,0,-0.6149240524,-0.0053466555,1.7474213095
H,0,2.5095914554,-0.0010186151,-0.4838723123
H,0,-2.7602829424,-0.0032269266,1.5799399502
H,0,1.7680450896,-0.0108545881,2.5852483723
H,0,-0.6092741576,-0.0088801435,2.8352546962

Pyrogallolic radical 1a: TCE = 0.109037

O,0,-0.6337145398,0.0026584905,-2.4127598055
C,0,-0.5922963099,-0.0000612744,-1.0480206827
H,0,0.2752550598,0.0066650341,-2.7586561906
C,0,0.6174261819,0.0031682737,-0.3543604606
C,0,-1.7778142551,-0.0062575388,-0.3153518545
O,0,1.7818431536,0.0090549751,-1.0283055896
C,0,0.6752036641,0.0004068448,1.1034983108
C,0,-1.7591655026,-0.009198083,1.1085911877
H,0,-2.7207264894,-0.0088666555,-0.8536846836
O,0,1.8184609135,0.0035845117,1.6344947018
C,0,-0.5817267414,-0.0061092266,1.816710749
H,0,2.4843829026,0.0104975138,-0.3373223402
H,0,-2.7099047254,-0.014065737,1.6344192517
H,0,-0.5514851877,-0.0083079478,2.9014060118

Pyrogallolic radical 1b: TCE = 0.110087

O,0,-0.5859872428,0.0129261511,-2.4195178479
C,0,-0.6264049421,0.0224512628,-1.0764410443
H,0,0.3615277651,-0.0316241978,-2.6711347334
C,0,0.6516317271,-0.0320713914,-0.3853188544
C,0,-1.8122470773,0.0809150493,-0.3657805394
O,0,1.7385998754,-0.0850076212,-1.0282402203
C,0,0.6398335018,-0.0234146179,1.0685433647
C,0,-1.7598489951,0.086441905,1.0407198741
H,0,-2.7601477853,0.1213677307,-0.8923099889
O,0,1.8347902422,-0.074501903,1.6810174395

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C,0,-0.5542297308,0.0353331714,1.7652679946
H,0,-2.6942679644,0.1325280143,1.5933473892
H,0,2.5120871931,-0.1089512678,0.9717591863
H,0,-0.5508291093,0.0414144318,2.8503184044

Pyrogallolic radical 1c: TCE = 0.109233

O,0,-0.5643892193,0.0059748395,-2.4222736621
C,0,-0.6150445075,0.002328006,-1.0834478024
H,0,0.3944960645,0.0077172842,-2.6492210366
C,0,0.6819376932,0.0017921847,-0.4037439643
C,0,-1.8120816173,-0.0005849066,-0.3855783034
O,0,1.727091033,0.0045826669,-1.1015714945
C,0,0.6587235723,-0.0022588678,1.0523185669
C,0,-1.7650255783,-0.0042582633,1.0148102746
H,0,-2.7561368946,0.0000028013,-0.9205755209
O,0,1.870882616,-0.0028959902,1.6507142046
C,0,-0.5501374103,-0.0051094198,1.7300694696
H,0,-2.6965533529,-0.0065632898,1.5740067597
H,0,1.7643544599,-0.0058402653,2.6161170078
H,0,-0.5650686272,-0.0080610582,2.8181509606

Pyrogallolic radical 1d: TCE = 0.108663

C,0,-1.7325341925,0.0026107322,-1.1466302993
C,0,-1.7674043815,-0.0016629939,0.2753406009
C,0,-0.5389105067,0.0055011043,-1.8223110081
H,0,-2.673457983,0.0037439665,-1.6897907509
C,0,-0.5837706115,-0.0034623002,1.0021887523
C,0,0.7306489267,0.0040356012,-1.1126362763
H,0,-2.7232152064,-0.0033747421,0.7951245754
H,0,-0.4890312733,0.008947724,-2.9064975042
O,0,1.8352057812,0.0063729,-1.7031246921
O,0,-0.5059120381,-0.0069776559,2.3801354202
C,0,0.6571058768,-0.0007602381,0.3495649767
O,0,1.8065041719,-0.0024546469,1.0423437063
H,0,-1.3893708331,-0.0162221688,2.7784082619
H,0,1.5978813083,-0.0061909899,1.994819465