SUPPORTING INFORMATION

Theoretical study on the stability of formylphenol and formylaniline compounds and corresponding radicals: O-H or N-H vs C-H bond dissociation

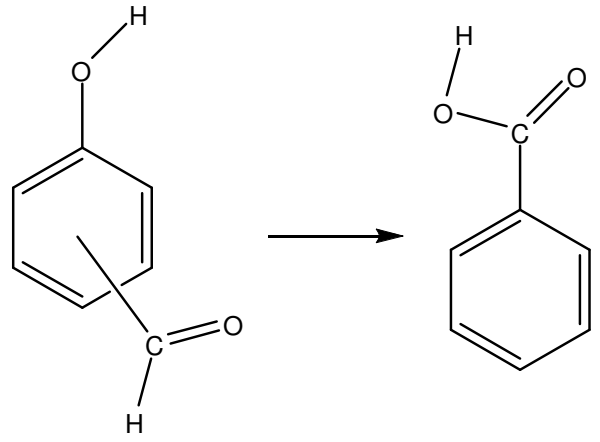
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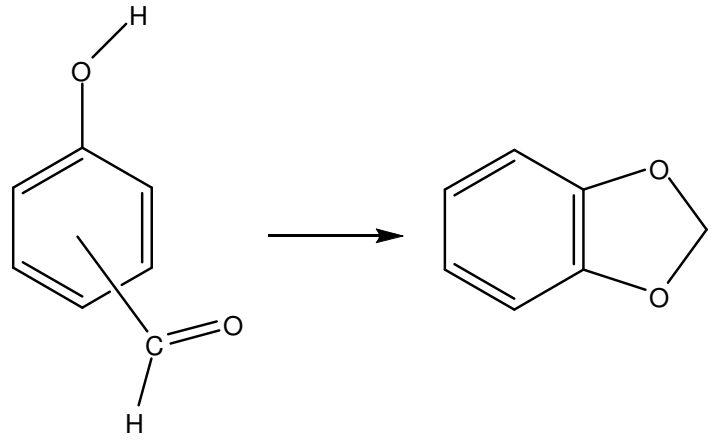
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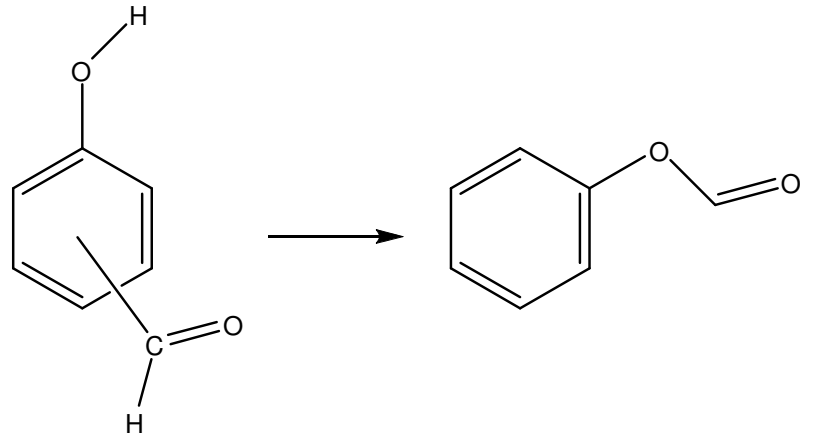
Reactions of isomerization of 2-, 3- and 4-formylphenol yielding benzoic acid (S1), 1,3-benzodioxole (S2), phenyl formate (S3), 2-furanacrolein (S4) and tropolone (S5) used for calculation of thermochemical data compiled in Table S1.



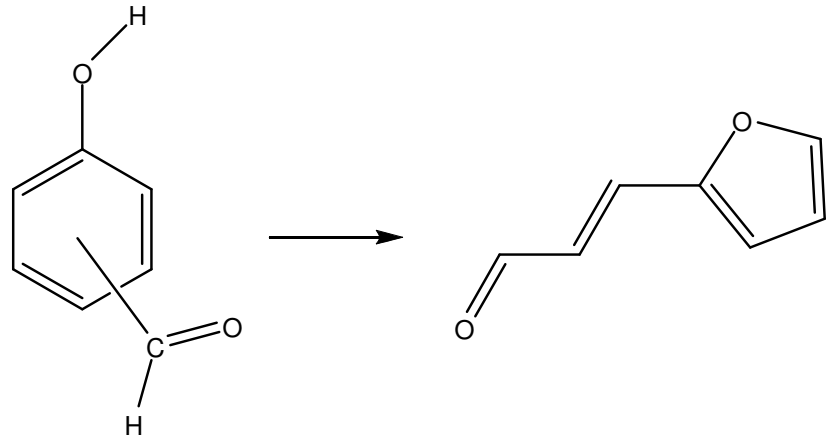
2- or 3- or 4-formylphenol benzoic acid (S1)



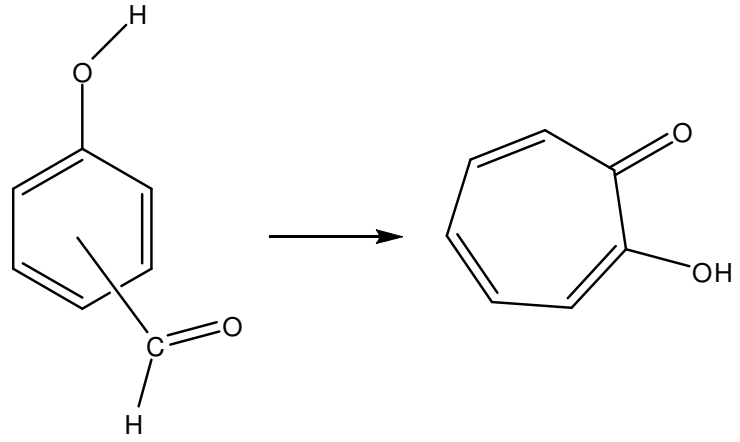
2- or 3- or 4-formylphenol 1,3-benzodioxole (S2)



2- or 3- or 4-formylphenol phenyl formate (S3)



2- or 3- or 4-formylphenol 2-furanacrolein (S4)



2- or 3- or 4-formylphenol tropolone (S5)

Table S1. Calculated gas-phase enthalpies of isomerization and of formation of 2-, 3-, and 4-formylphenol species (all values in kJ/mol).[a]

	Reaction	2-Formylphenol	3-Formylphenol	4-Formylphenol
Benzoic acid	Eq. S1	-56.5 (-55.7[b]; -48.4[c]) [-237.5]	-80.6 [-213.4]	-78.5 (-73.7[b]) [-215.5]
1,3-Benzodioxole	Eq. S2	79.4 (95.6[b]; 102.9[c]) [-222.1]	55.3 [-198.0]	57.4 (77.6[b]) [-200.1]
Phenylformate	Eq. S3	21.8 (22.5[b], 29.8[c]) [-237.6]	-2.3 [-213.5]	-0.2 (4.5[b]) [-215.6]
2-Furanacrolein	Eq. S4	134.3 (132.4[b], 139.7[c]) [-240.2]	110.2 [-216.1]	112.4 (114.4[b]) [-218.3]
Tropolone	Eq. S5	82.6 (82.9[b], 90.2[c]) [-238.0]	58.5 [-213.9]	60.6 (64.9[b]) [-216.0]

[a]Experimental enthalpies of isomerization (difference between experimental enthalpies of formation) are given in parenthesis; calculated enthalpies of formation for the three formylphenols appear in square brackets.

[b]Taken from Bernardes, C. E. S; Minas da Piedade, M. E. *J. Phys. Chem. A* **2008**, *112*, 10029.

[c]Taken from Ribeiro da Silva, M. D. M. C.; Araújo, N. R. M. J. Chem. Thermodynamics **2007**, 39, 1372.

Table S2. G3(MP2)//B3LYP geometries (B3LYP/6-31G(d) approach).

Species	cartesian coordinates / Å			
benzene	C	0.000000	0.000000	1.396611
	H	0.000000	0.000000	2.483628
	C	1.209500	0.000000	0.698305
	C	1.209500	0.000000	-0.698305
	C	0.000000	0.000000	-1.396611
	C	-1.209500	0.000000	-0.698305
	C	-1.209500	0.000000	0.698305
	H	2.150885	0.000000	1.241814
	H	2.150885	0.000000	-1.241814
	H	0.000000	0.000000	-2.483628
	H	-2.150885	0.000000	-1.241814
	H	-2.150885	0.000000	1.241814
aniline	C	0.000000	0.015713	1.881647
	H	0.000000	0.021299	2.967625
	C	1.202609	0.011604	1.171766
	C	1.208246	0.002345	-0.221309
	C	0.000000	-0.001855	-0.938798
	C	-1.208246	0.002345	-0.221309
	C	-1.202609	0.011604	1.171766
	H	2.149755	0.013014	1.705651
	H	2.151751	0.003520	-0.763423
	N	0.000000	0.049034	-2.338204
	H	-2.151751	0.003520	-0.763423
	H	-2.149755	0.013014	1.705651
	H	-0.834901	-0.324075	-2.773614
	H	0.834901	-0.324075	-2.773614
phenylamino	C	-1.571617	-0.010710	-0.473326
	C	-1.551005	-0.010178	0.931668
	C	-0.325025	-0.001657	1.618190
	C	0.866937	0.006391	0.917208
	C	0.880171	0.005807	-0.516856
	C	-0.387679	-0.003104	-1.188816
	N	2.071807	0.013271	-1.131145
	H	-2.484753	-0.016352	1.486799
	H	-0.316198	-0.001256	2.704831
	H	1.827763	0.013177	1.422283
	H	-0.400138	-0.003469	-2.276812
	H	-2.523109	-0.017280	-0.998527
	H	1.923097	0.012987	-2.148964
phenylamide	C	-1.570905	-0.010884	-0.452334
	C	-1.589723	-0.010530	0.951689
	C	-0.341715	-0.001939	1.606848
	C	0.853791	0.005960	0.910901
	C	0.921675	0.006295	-0.538121
	C	-0.383900	-0.003074	-1.171549
	N	2.101974	0.014263	-1.152083
	H	-2.524953	-0.016578	1.508531
	H	-0.313374	-0.001530	2.700012
	H	1.804899	0.012441	1.442790
	H	-0.417219	-0.003890	-2.264117
	H	-2.517217	-0.017581	-1.000862
	H	1.918699	0.012338	-2.166374
aniline cation	C	0.000000	0.044023	1.858534
	H	0.000000	0.090306	2.943104
	C	1.230956	0.014233	1.160552
	C	1.245297	-0.044484	-0.212213
	C	0.000000	-0.074987	-0.927606
	C	-1.245297	-0.044484	-0.212213
	C	-1.230956	0.014233	1.160552
	H	2.164289	0.037734	1.713229
	H	2.179660	-0.068362	-0.765632

	N	0.000000	-0.131872	-2.262819
	H	-2.179660	-0.068362	-0.765632
	H	-2.164289	0.037734	1.713229
	H	-0.864010	-0.154352	-2.796336
	H	0.864010	-0.154352	-2.796336
phenol	C	0.003331	0.000000	0.941272
	O	0.059657	0.000000	2.309171
	C	1.219042	0.000000	0.248335
	C	1.216517	0.000000	-1.144434
	C	0.013951	0.000000	-1.857564
	C	-1.193496	0.000000	-1.159004
	C	-1.205089	0.000000	0.236871
	H	2.145211	0.000000	0.814544
	H	2.163812	0.000000	-1.677383
	H	0.019496	0.000000	-2.943524
	H	-2.137105	0.000000	-1.698364
	H	-2.149837	0.000000	0.778439
	H	-0.844372	0.000000	2.660066
phenoxyl	C	0.000000	0.000000	1.047854
	O	0.000000	0.000000	2.305865
	C	1.239566	0.000000	0.290248
	C	1.225597	0.000000	-1.088032
	C	0.000000	0.000000	-1.785504
	C	-1.225597	0.000000	-1.088032
	C	-1.239566	0.000000	0.290248
	H	2.164912	0.000000	0.858248
	H	2.158216	0.000000	-1.646095
	H	0.000000	0.000000	-2.871921
	H	-2.158216	0.000000	-1.646095
	H	-2.164912	0.000000	0.858248
phenoxide	C	-0.876787	0.000000	-0.885382
	C	-0.925332	0.000000	0.565545
	C	0.388037	0.000000	1.184096
	C	1.566603	0.000000	0.450029
	C	1.562400	0.000000	-0.954908
	C	0.314017	0.000000	-1.599427
	O	-2.005838	0.000000	1.225928
	H	0.414736	0.000000	2.274417
	H	2.523295	0.000000	0.980426
	H	2.491626	0.000000	-1.522832
	H	0.278337	0.000000	-2.692728
	H	-1.834923	0.000000	-1.40642
phenol cation	C	-0.831727	0.000000	-0.964727
	C	-0.816844	0.000000	0.467862
	C	0.416849	0.000000	1.206301
	C	1.602818	0.000000	0.514954
	C	1.591456	0.000000	-0.903052
	C	0.366404	0.000000	-1.632104
	O	-1.912285	0.000000	1.191497
	H	0.366216	0.000000	2.290248
	H	2.548569	0.000000	1.046468
	H	2.531575	0.000000	-1.446595
	H	0.389494	0.000000	-2.716953
	H	-1.779475	0.000000	-1.496869
	H	-2.731831	0.000000	0.656314
benzoic acid	C	0.013244	-0.221468	-0.000793
	C	0.013244	-1.707771	-0.000793
	C	1.250115	0.433727	-0.074894
	C	1.303114	1.824879	-0.078069
	C	0.121674	2.568255	-0.007289
	C	-1.112800	1.918366	0.066668
	C	-1.170849	0.525854	0.070145
	H	2.153217	-0.165297	-0.128999
	H	2.263029	2.330365	-0.135578
	H	0.162930	3.654304	-0.009761
	H	-2.030436	2.497418	0.121643
	H	-2.125361	0.014518	0.127330

	O	−1.234440	−2.241347	0.073955
	O	1.006380	−2.405483	−0.060292
	H	−1.105353	−3.207713	0.066221
1,3-benzodioxole	C	−1.724279	0.005937	0.130048
	C	−1.692476	0.034691	1.537237
	C	−0.485048	0.034691	2.234346
	C	0.749515	0.005937	1.558294
	C	0.701360	−0.018858	0.178596
	C	−0.505349	−0.018858	−0.518098
	H	−2.657006	0.002281	−0.423649
	H	−2.629823	0.059349	2.085068
	H	−0.490810	0.059349	3.320028
	H	1.695394	0.002281	2.089210
	O	1.749306	−0.073488	−0.712135
	O	−0.257926	−0.073488	−1.871011
	C	1.159532	0.071671	−2.008369
	H	1.542427	−0.709426	−2.671562
	H	1.389244	1.070693	−2.406242
phenylformate	C	−0.193877	0.259352	0.218202
	O	−0.193877	1.659528	0.218202
	C	−1.046673	−0.290854	1.177992
	C	−1.149871	−1.674412	1.294137
	C	−0.404341	−2.506179	0.455071
	C	0.442148	−1.940421	−0.497621
	C	0.560517	−0.553785	−0.630841
	H	−1.615486	0.375886	1.818169
	H	−1.813560	−2.100892	2.041094
	H	−0.483528	−3.585835	0.544192
	H	1.025619	−2.579992	−1.154296
	H	1.216719	−0.118417	−1.369372
	C	0.537374	2.441654	−0.604795
	O	1.305129	2.104320	−1.468874
	H	0.308567	3.486336	−0.347280
tropolone	C	−2.044399	0.000000	−0.976989
	C	−2.032312	0.000000	0.401446
	C	−0.935581	0.000000	1.289832
	C	−0.929084	0.000000	−1.849306
	C	0.411302	0.000000	1.000631
	C	0.417517	0.000000	−1.573130
	C	1.107158	0.000000	−0.313320
	H	−3.020492	0.000000	−1.455398
	H	−3.006487	0.000000	0.886522
	H	−1.168270	0.000000	2.352110
	H	−1.178763	0.000000	−2.909281
	H	1.102008	0.000000	−2.417956
	O	2.356089	0.000000	−0.238402
	O	1.286404	0.000000	2.005955
	H	2.164452	0.000000	1.528595
2-furanacrolein	C	−2.723928	0.000086	0.207063
	C	−2.634110	0.000004	1.569573
	C	−1.241448	0.000101	1.868670
	C	−0.574264	0.000059	0.664453
	O	−1.490963	−0.000088	−0.358748
	H	−3.555279	0.000098	−0.481733
	H	−3.458114	−0.000019	2.268923
	H	−0.780738	0.000159	2.847055
	C	0.821674	0.000072	0.342583
	H	1.485349	0.000300	1.207129
	C	1.365781	−0.000173	−0.895975
	H	0.753173	−0.000406	−1.793042
	C	2.817486	−0.000163	−1.069827
	H	3.398122	−0.000286	−0.117689
	O	3.387255	0.000118	−2.147488
benzaldehyde	C	0.116729	0.000000	0.563309
	C	0.110534	0.000000	2.043603
	C	1.335244	0.000000	−0.127663
	C	1.349921	0.000000	−1.521784

	C	0.143867	0.000000	-2.226341
	C	-1.076703	0.000000	-1.540296
	C	-1.092149	0.000000	-0.149709
	H	2.268553	0.000000	0.431888
	H	2.294787	0.000000	-2.057942
	H	0.152878	0.000000	-3.313141
	H	-2.010775	0.000000	-2.095335
	H	-2.023379	0.000000	0.408656
	O	-0.890995	0.000000	2.733604
	H	1.121239	0.000000	2.510324
benzoyl	C	0.124264	0.000000	0.599595
	C	0.129611	0.000000	2.081463
	C	1.345453	0.000000	-0.086314
	C	1.359921	0.000000	-1.480124
	C	0.154720	0.000000	-2.186551
	C	-1.067899	0.000000	-1.504915
	C	-1.087367	0.000000	-0.113889
	H	2.270126	0.000000	0.483717
	H	2.305164	0.000000	-2.015328
	H	0.165798	0.000000	-3.273304
	H	-2.000724	0.000000	-2.062277
	H	-2.023078	0.000000	0.437255
	O	-0.808689	0.000000	2.821793
oxophenylmethanide	C	0.132898	-0.027685	0.619699
	C	0.165502	0.284622	2.192706
	C	1.335665	-0.086543	-0.097116
	C	1.357458	-0.125800	-1.491204
	C	0.155274	-0.027887	-2.211944
	C	-1.054408	0.072710	-1.515672
	C	-1.060907	0.045100	-0.118747
	H	2.264900	-0.085132	0.480582
	H	2.302840	-0.223862	-2.028914
	H	0.167645	-0.008712	-3.301844
	H	-1.990037	0.158035	-2.074992
	H	-1.993510	0.058840	0.450258
	O	-0.867591	-0.088282	2.776072
benzaldehyde cation	C	-1.280456	0.462114	-1.485895
	C	-1.366668	0.074878	-0.152317
	C	-0.180095	-0.068738	0.574650
	C	1.105445	0.098793	-0.055144
	C	1.176612	0.478201	-1.390656
	C	-0.005976	0.648134	-2.109064
	C	-0.214693	-0.515958	1.983432
	O	0.760018	-1.095227	2.431560
	H	2.001314	-0.049939	0.538990
	H	2.139565	0.624966	-1.867997
	H	0.027828	0.931998	-3.156967
	H	-2.183638	0.659085	-2.055650
	H	-2.332749	-0.065308	0.322931
	H	-1.137473	-0.403543	2.576175
2-formylphenol	C	-0.595796	0.000000	0.598775
	O	-0.644202	0.000000	1.938363
	C	0.637159	0.000000	-0.108968
	C	0.628214	0.000000	-1.518229
	C	-0.563568	0.000000	-2.222429
	C	-1.775975	0.000000	-1.509748
	C	-1.800719	0.000000	-0.121809
	C	1.895044	0.000000	0.618041
	H	1.581215	0.000000	-2.043579
	H	-0.566204	0.000000	-3.307709
	H	-2.716470	0.000000	-2.054671
	H	-2.734203	0.000000	0.431633
	H	0.291334	0.000000	2.265324
	O	1.992169	0.000000	1.848513
	H	2.814443	0.000000	0.000201
2-formylphenoxyl	C	-0.595796	0.000000	0.598775
	O	-0.644202	0.000000	1.938363

	C	0.637159	0.000000	-0.108968
	C	0.628214	0.000000	-1.518229
	C	-0.563568	0.000000	-2.222429
	C	-1.775975	0.000000	-1.509748
	C	-1.800719	0.000000	-0.121809
	C	1.895044	0.000000	0.618041
	H	1.581215	0.000000	-2.043579
	H	-0.566204	0.000000	-3.307709
	H	-2.716470	0.000000	-2.054671
	H	-2.734203	0.000000	0.431633
	H	0.291334	0.000000	2.265324
	O	1.992169	0.000000	1.848513
	H	2.814443	0.000000	0.000201
2-hydroxybenzoyl	C	-0.615753	1.572103	0.516723
	C	-0.615753	0.169645	0.516723
	C	0.335877	-0.522505	-0.281859
	C	1.259368	0.204812	-1.056828
	C	1.251599	1.590024	-1.050308
	C	0.307362	2.263622	-0.257930
	O	-1.523189	-0.466703	1.278220
	C	0.352304	-1.977824	-0.295644
	O	-0.368820	-2.733685	0.309504
	H	1.974105	-0.351303	-1.656616
	H	1.963994	2.149267	-1.648132
	H	0.294481	3.350385	-0.247121
	H	-1.346097	2.090459	1.129609
	H	-1.400447	-1.434963	1.175218
2-formylphenoxyde	C	-1.923052	0.000000	-1.238399
	C	-1.920504	0.000000	0.137088
	C	-0.690688	0.000000	0.922659
	C	0.534141	0.000000	0.116663
	C	0.481131	0.000000	-1.293209
	C	-0.715678	0.000000	-1.985714
	O	-0.708704	0.000000	2.181016
	C	1.817060	0.000000	0.784109
	O	2.933697	0.000000	0.245645
	H	1.435140	0.000000	-1.819686
	H	-0.739091	0.000000	-3.073970
	H	-2.876443	0.000000	-1.771939
	H	-2.851853	0.000000	0.701966
	H	1.737846	0.000000	1.891162
2-hydroxyphenyloxomethanide	C	-1.768871	0.000000	-1.496120
	C	-1.766236	0.000000	-0.100524
	C	-0.542276	0.000000	0.598356
	C	0.686883	0.000000	-0.117262
	C	0.638954	0.000000	-1.510931
	C	-0.568293	0.000000	-2.217301
	O	-0.522350	0.000000	1.939397
	C	2.080043	0.000000	0.577296
	O	1.935872	0.000000	1.855121
	H	1.601884	0.000000	-2.026079
	H	-0.581655	0.000000	-3.306775
	H	-2.721411	0.000000	-2.027093
	H	-2.695850	0.000000	0.467282
	H	0.527626	0.000000	2.135440
2-formylphenol cation	C	-0.607122	1.652071	0.516654
	C	-0.607122	0.214154	0.516654
	C	0.342449	-0.528401	-0.291420
	C	1.242339	0.178066	-1.057216
	C	1.235087	1.602375	-1.051045
	C	0.309172	2.323575	-0.263102
	O	-1.479029	-0.393709	1.258637
	C	0.304661	-2.006725	-0.259263
	O	-0.508938	-2.608350	0.433101
	H	1.966169	-0.349406	-1.673187
	H	1.954169	2.138360	-1.662975
	H	0.323868	3.408484	-0.275608

	H	−1.337100	2.161422	1.137857
	H	−1.353466	−1.401396	1.151784
	H	1.033317	−2.551684	−0.879341
3-formylphenol	C	−1.370335	0.560886	0.000000
	O	−2.305141	1.555470	0.000000
	C	0.000000	0.807893	0.000000
	C	0.899177	−0.267084	0.000000
	C	0.429872	−1.585549	0.000000
	C	−0.945562	−1.823815	0.000000
	C	−1.844907	−0.760484	0.000000
	H	0.397861	1.820343	0.000000
	C	2.355635	−0.002498	0.000000
	H	1.136569	−2.411589	0.000000
	H	−1.323489	−2.842300	0.000000
	H	−2.917247	−0.928977	0.000000
	H	−1.853683	2.414301	0.000000
	O	2.858250	1.105420	0.000000
	H	2.991837	−0.914996	0.000000
3-formylphenoxyl	C	−1.647043	0.000000	−1.150827
	C	−1.685833	0.000000	0.300667
	C	−0.409018	0.000000	0.991219
	C	0.780077	0.000000	0.286953
	C	0.768914	0.000000	−1.129436
	C	−0.445545	0.000000	−1.833724
	O	−2.773240	0.000000	0.932187
	C	2.077751	0.000000	1.011421
	O	3.162616	0.000000	0.465514
	H	−0.428571	0.000000	2.078314
	H	1.722048	0.000000	−1.648974
	H	−0.434028	0.000000	−2.920203
	H	−2.601857	0.000000	−1.667631
	H	1.991586	0.000000	2.119250
3-hydroxybenzoyl	C	−1.357518	0.493962	0.000000
	O	−2.340551	1.441131	0.000000
	C	0.000000	0.807177	0.000000
	C	0.949311	−0.229145	0.000000
	C	0.546379	−1.567959	0.000000
	C	−0.817217	−1.868680	0.000000
	C	−1.765571	−0.849519	0.000000
	H	0.342961	1.839464	0.000000
	C	2.396118	0.091836	0.000000
	H	1.298040	−2.350766	0.000000
	H	−1.146436	−2.903749	0.000000
	H	−2.828847	−1.068447	0.000000
	H	−1.934597	2.322237	0.000000
	O	2.910533	1.170772	0.000000
3-formylphenoxide	C	−1.636649	0.000000	−1.127225
	C	−1.713433	0.000000	0.321810
	C	−0.408345	0.000000	0.952189
	C	0.791510	0.000000	0.232826
	C	0.801666	0.000000	−1.178746
	C	−0.434039	0.000000	−1.829921
	O	−2.798979	0.000000	0.967223
	C	2.046804	0.000000	0.987947
	O	3.186118	0.000000	0.533464
	H	−0.384464	0.000000	2.042772
	H	1.746706	0.000000	−1.712464
	H	−0.460533	0.000000	−2.922008
	H	−2.585221	0.000000	−1.664018
	H	1.901308	0.000000	2.096939
3-hydroxyphenyloxomethanide	C	1.870915	0.674302	−0.012668
	C	1.302443	−0.602832	0.005428
	C	−0.082234	−0.761288	−0.024488
	C	−0.940813	0.344589	−0.030337
	C	−0.366588	1.622810	−0.015460
	C	1.017738	1.789306	−0.039118
	O	2.167755	−1.693495	0.040667

	C	−2.522083	0.157179	0.251196
	O	−2.929479	−0.952245	−0.134863
	H	−0.552344	−1.751129	−0.084014
	H	−1.039977	2.482502	0.028089
	H	1.456269	2.788652	−0.074664
	H	2.952910	0.781640	0.018654
	H	1.600660	−2.480149	0.058179
3-formylphenol cation	C	−0.029761	0.000000	−0.001667
	O	0.041436	0.000000	1.308949
	C	1.226221	0.000000	−0.696145
	C	1.225871	0.000000	−2.069565
	C	−0.012869	0.000000	−2.776916
	C	−1.253156	0.000000	−2.087528
	C	−1.274913	0.000000	−0.713509
	H	2.141009	0.000000	−0.109496
	C	2.504963	0.000000	−2.862900
	H	0.023237	0.000000	−3.863129
	H	−2.180927	0.000000	−2.650540
	H	−2.211127	0.000000	−0.161008
	H	−0.833508	0.000000	1.747974
	O	2.492263	0.000000	−4.070631
	H	3.440502	0.000000	−2.273222
4-formylphenol	C	0.122690	0.000000	1.768768
	O	0.188165	0.000000	3.127706
	C	1.336865	0.000000	1.069063
	C	1.320584	0.000000	−0.319397
	C	0.108887	0.000000	−1.027357
	C	−1.100120	0.000000	−0.313356
	C	−1.098091	0.000000	1.073587
	H	2.266224	0.000000	1.628966
	H	2.260053	0.000000	−0.868403
	C	0.105882	0.000000	−2.500486
	H	−2.031404	0.000000	−0.871588
	H	−2.035681	0.000000	1.626776
	H	−0.711470	0.000000	3.492161
	O	−0.893966	0.000000	−3.196325
	H	1.118512	0.000000	−2.963890
4-formylphenoxyl	C	−0.645802	−0.386772	−1.399584
	C	−0.645802	1.072109	−1.399584
	C	−0.102828	1.739918	−0.222848
	C	0.385074	1.010026	0.834532
	C	0.367991	−0.405277	0.797511
	C	−0.153105	−1.090733	−0.331810
	O	−1.093054	1.726402	−2.368868
	C	0.896299	−1.173746	1.942460
	O	0.920090	−2.390752	1.994021
	H	−0.104539	2.825378	−0.226557
	H	0.790106	1.509654	1.712319
	H	−0.145336	−2.176373	−0.314973
	H	−1.051442	−0.877958	−2.278687
	H	1.283962	−0.559048	2.782603
4-hydroxybenzoyl	C	0.905526	0.636849	1.262495
	C	0.905526	−0.764903	1.262495
	C	0.199759	−1.477506	0.278507
	C	−0.499336	−0.785566	−0.696180
	C	−0.507186	0.624159	−0.707125
	C	0.200739	1.322522	0.279873
	O	1.573339	−1.496425	2.193567
	C	−1.245458	1.375025	−1.736431
	O	−1.897175	0.947315	−2.645064
	H	0.218838	−2.562459	0.305107
	H	−1.050707	−1.318754	−1.464907
	H	0.191306	2.408591	0.266720
	H	1.454863	1.180815	2.028386
	H	2.018966	−0.898786	2.814866
4-formylphenoxide	C	−1.532421	0.000000	−0.404602
	C	−1.600512	0.000000	1.054660

	C	−0.299360	0.000000	1.713494
	C	0.878868	0.000000	1.007753
	C	0.908795	0.000000	−0.413087
	C	−0.344074	0.000000	−1.089167
	O	−2.686019	0.000000	1.685563
	C	2.157322	0.000000	−1.120908
	O	2.338351	0.000000	−2.345611
	H	−0.304803	0.000000	2.802559
	H	1.832708	0.000000	1.541541
	H	−0.324115	0.000000	−2.178209
	H	−2.485060	0.000000	−0.933038
	H	3.050910	0.000000	−0.441339
4-hydroxyphenyloxomethanide	C	−0.544439	−0.403535	−1.323496
	C	−0.544439	0.997580	−1.323496
	C	−0.085239	1.700121	−0.207209
	C	0.371262	0.980064	0.902513
	C	0.383340	−0.414507	0.931875
	C	−0.081893	−1.087958	−0.199077
	O	−0.995331	1.726072	−2.419587
	C	0.942179	−1.205985	2.290378
	O	0.864817	−2.432109	2.102315
	H	−0.095242	2.789725	−0.231526
	H	0.737103	1.502981	1.791851
	H	−0.063009	−2.181894	−0.153170
	H	−0.909730	−0.934445	−2.211496
	H	−1.269636	1.077241	−3.086405
4-formylphenol cation	C	−0.021765	0.001697	−0.003691
	O	0.047330	−0.002033	1.305627
	C	1.235029	−0.001790	−0.698023
	C	1.233165	0.000562	−2.066230
	C	−0.002890	−0.005617	−2.779214
	C	−1.247647	0.007686	−2.082752
	C	−1.270656	0.005997	−0.712457
	H	2.147345	−0.009000	−0.110473
	H	2.155449	−0.000712	−2.638341
	C	0.027119	−0.000282	−4.271972
	H	−2.176342	0.012202	−2.646815
	H	−2.206591	0.005853	−0.159629
	H	−0.827817	−0.000912	1.744124
	O	1.078767	0.065944	−4.874996
	H	−0.948947	−0.038541	−4.787991
N-formylaniline	C	0.028164	0.004787	−0.998316
	C	−0.041464	0.000450	0.403139
	C	1.137621	−0.098166	1.157269
	C	2.372891	−0.191467	0.522102
	C	2.449197	−0.187712	−0.871834
	C	1.274130	−0.089468	−1.618262
	N	−1.261788	0.092067	1.109526
	H	3.412247	−0.260440	−1.368783
	H	1.084905	−0.101633	2.244505
	H	3.276441	−0.267185	1.120966
	H	1.320088	−0.085476	−2.704064
	H	−0.882578	0.080926	−1.575916
	C	−2.539693	0.196616	0.623763
	H	−1.182661	0.078716	2.118590
	O	−2.876266	0.231468	−0.545446
	H	−3.270873	0.248647	1.454417
N-phenyl-*N*-formylamino	C	−0.919955	0.209889	−1.789314
	C	−0.903685	0.169059	−0.407155
	C	0.345231	0.101646	0.295444
	C	1.552444	0.091145	−0.473962
	C	1.514635	0.131264	−1.855034
	C	0.279535	0.191030	−2.521388
	N	0.485625	0.090188	1.633897
	C	−0.577297	−0.087402	2.498643
	O	−1.523624	−0.846436	2.344927
	H	0.250614	0.225468	−3.606834

	H	2.489688	0.047705	0.071314
	H	2.438504	0.118680	-2.426200
	H	-1.869625	0.257685	-2.314886
	H	-1.826132	0.168771	0.159919
	H	-0.438882	0.482089	3.436587
phenylaminobenzoyl	C	-0.885033	0.000000	-1.807310
	C	-0.879172	0.000000	-0.412338
	C	0.345620	0.000000	0.265366
	C	1.546974	0.000000	-0.455161
	C	1.524334	0.000000	-1.847862
	C	0.307635	0.000000	-2.532225
	N	0.424149	0.000000	1.687046
	C	-0.581779	0.000000	2.590701
	O	-1.775219	0.000000	2.428281
	H	0.289850	0.000000	-3.618111
	H	2.497158	0.000000	0.075206
	H	2.462147	0.000000	-2.396595
	H	-1.838135	0.000000	-2.329057
	H	-1.805967	0.000000	0.147521
	H	1.356187	0.000000	2.078441
N-phenylformamidate ion	C	-0.869910	0.000000	-1.815954
	C	-0.865886	0.000000	-0.422342
	C	0.357981	0.000000	0.312832
	C	1.548283	0.000000	-0.467834
	C	1.530853	0.000000	-1.857675
	C	0.317136	0.000000	-2.557129
	N	0.525384	0.000000	1.682353
	C	-0.526009	0.000000	2.513650
	O	-1.763019	0.000000	2.322871
	H	0.298378	0.000000	-3.645973
	H	2.490499	0.000000	0.076647
	H	2.474179	0.000000	-2.405898
	H	-1.827876	0.000000	-2.338918
	H	-1.788724	0.000000	0.143368
	H	-0.174678	0.000000	3.578036
N-formylaniline acyl carbanion	C	-0.134117	-2.053374	0.144049
	C	-0.567862	-0.790972	0.515852
	C	-0.457063	0.349395	-0.357264
	C	0.145235	0.062738	-1.634667
	C	0.566433	-1.211934	-1.991701
	C	0.439941	-2.299866	-1.115979
	N	-0.901233	1.549116	0.051856
	C	0.339641	2.581729	1.764091
	O	0.528322	1.795230	2.592671
	H	0.771814	-3.296380	-1.400898
	H	0.263966	0.887583	-2.340103
	H	1.009579	-1.364059	-2.978689
	H	-0.244534	-2.877902	0.851758
	H	-1.012252	-0.623927	1.494560
	H	-0.699758	2.242734	-0.677275
N-formylaniline cation	C	-0.909805	0.000000	-1.837649
	C	-0.910362	0.000000	-0.462130
	C	0.349654	0.000000	0.230471
	C	1.581801	0.000000	-0.512430
	C	1.552012	0.000000	-1.883944
	C	0.306776	0.000000	-2.560760
	N	0.443050	0.000000	1.584554
	C	-0.598410	0.000000	2.569371
	O	-1.768331	0.000000	2.304440
	H	0.286655	0.000000	-3.646430
	H	2.527223	0.000000	0.023509
	H	2.476644	0.000000	-2.451430
	H	-1.852587	0.000000	-2.374777
	H	-1.829849	0.000000	0.106401
	H	1.385580	0.000000	1.971965
	H	-0.178376	0.000000	3.585792

2-formylaniline	C	0.599604	−0.037544	0.613346
	N	0.604023	−0.069702	1.972374
	C	1.805716	−0.056260	−0.124784
	C	1.790966	0.003310	−1.508461
	C	0.584107	0.082956	−2.225609
	C	−0.604781	0.096317	−1.517573
	C	−0.630886	0.034841	−0.110158
	H	2.749930	−0.113962	0.411876
	H	2.735917	−0.011827	−2.046032
	H	0.588539	0.130626	−3.309738
	H	−1.555522	0.151786	−2.044487
	C	−1.921169	0.029090	0.564419
	H	−0.289619	−0.133602	2.448444
	H	1.461349	−0.243306	2.473036
	O	−2.107994	−0.036683	1.778885
	H	−2.796144	0.085401	−0.117867
N-(2-formyl)phenylamino	C	0.254987	−0.569544	0.066931
	C	0.254998	0.884949	0.066935
	C	−0.982911	1.536897	−0.257971
	C	−2.125773	0.820269	−0.557955
	C	−2.102393	−0.585961	−0.551836
	C	−0.916340	−1.259192	−0.240519
	N	1.299533	1.665112	0.341075
	C	1.450032	−1.369070	0.380624
	O	2.554797	−0.934695	0.670543
	H	−0.972736	2.622236	−0.255288
	H	−3.047312	1.342507	−0.799830
	H	−3.000502	−1.148924	−0.787583
	H	−0.901518	−2.347649	−0.236628
	H	2.109817	1.070753	0.553741
	H	1.281539	−2.467243	0.336475
2-aminobenzoyl	C	−0.252771	0.626532	−0.032323
	C	−0.228881	−0.802686	−0.027391
	C	1.013369	−1.441932	0.181787
	C	2.166289	−0.700053	0.387057
	C	2.143785	0.704856	0.393486
	C	0.936810	1.349224	0.182638
	N	−1.373957	−1.527516	−0.188645
	C	−1.480449	1.366629	−0.282206
	O	−2.592289	0.960542	−0.512055
	H	1.053080	−2.528900	0.186919
	H	3.105196	−1.224555	0.546498
	H	3.055800	1.269527	0.557328
	H	0.875250	2.433877	0.171449
	H	−2.214771	−1.043049	−0.476100
	H	−1.307457	−2.514043	−0.387433
2-formylphenylamide	C	−0.276174	0.557884	−0.066748
	C	−0.276202	−0.920346	−0.066745
	C	1.021025	−1.519532	0.246781
	C	2.138935	−0.782212	0.516927
	C	2.112743	0.647945	0.510562
	C	0.918315	1.268137	0.221903
	N	−1.290250	−1.712531	−0.311819
	C	−1.446639	1.329799	−0.349607
	O	−2.594169	0.937609	−0.626919
	H	1.046555	−2.607865	0.252982
	H	3.076707	−1.293510	0.743577
	H	3.011857	1.220831	0.727821
	H	0.864810	2.359972	0.208953
	H	−2.102833	−1.120227	−0.508207
	H	−1.264009	2.437592	−0.305478
2-aminophenyloxomethanide	C	−0.254788	0.079910	−0.632607
	C	−0.214045	0.092156	0.790482
	C	1.022763	−0.009492	1.459157
	C	2.217452	−0.021929	0.737345
	C	2.199956	0.034304	−0.661266
	C	0.962208	0.053210	−1.313334

	N	−1.415867	0.235209	1.490318
	C	−1.553058	−0.193170	−1.534759
	O	−2.620390	−0.189284	−0.863037
	H	1.041995	−0.049176	2.551636
	H	3.165588	−0.081835	1.272985
	H	3.133967	0.035606	−1.223742
	H	0.890985	0.002833	−2.403206
	H	−2.196827	0.029102	0.837890
	H	−1.444448	−0.278657	2.366399
2-formylaniline cation	C	−0.228919	0.000071	−0.634395
	C	−0.212687	−0.007369	0.817552
	C	1.041740	0.006914	1.517315
	C	2.223483	0.027593	0.809269
	C	2.205438	0.034790	−0.601613
	C	0.977936	0.020909	−1.304369
	N	−1.359557	−0.027351	1.488371
	C	−1.502452	−0.014142	−1.399204
	O	−2.603534	−0.032697	−0.874383
	H	1.038692	0.001129	2.603717
	H	3.171370	0.038390	1.337158
	H	3.139390	0.051098	−1.154354
	H	0.984960	0.026753	−2.391180
	H	−2.235878	−0.037052	0.947224
	H	−1.384445	−0.033077	2.504495
	H	−1.396160	−0.006813	−2.497926
3-formylaniline	C	−0.689768	−0.027323	1.310943
	N	−0.708496	−0.004070	2.705434
	C	0.519227	−0.012146	0.605302
	C	0.523283	0.025273	−0.793351
	C	−0.678224	0.046311	−1.512317
	C	−1.885195	0.029252	−0.813466
	C	−1.894612	−0.006576	0.578430
	H	1.473123	−0.026217	1.126026
	C	1.811288	0.035744	−1.523200
	H	−0.662675	0.073448	−2.598902
	H	−2.828873	0.042895	−1.351968
	H	−2.841602	−0.013278	1.113982
	H	−1.539798	−0.389272	3.135653
	H	0.135578	−0.339066	3.152610
	O	2.909392	0.008230	−0.999774
	H	1.712597	0.070919	−2.631288
N-(3-formyl)phenylamino	C	−1.637700	0.006273	−1.127559
	C	−1.658138	0.012760	0.306777
	C	−0.392737	0.007027	0.977845
	C	0.796295	−0.004303	0.265060
	C	0.779274	−0.010433	−1.146649
	C	−0.441366	−0.005062	−1.829788
	N	−2.765148	0.023717	1.062442
	C	2.091333	−0.010002	0.989786
	O	3.179331	−0.019878	0.448663
	H	−0.400246	0.011888	2.064776
	H	1.726394	−0.019291	−1.676425
	H	−0.451892	−0.009797	−2.916247
	H	−2.586618	0.010445	−1.659485
	H	−3.591191	0.026691	0.450118
	H	2.003182	−0.004492	2.098025
3-aminobenzoyl	C	1.782708	0.758638	−0.000976
	C	1.315980	−0.571751	−0.007682
	C	−0.067509	−0.791191	−0.008267
	C	−0.955070	0.294560	−0.004720
	C	−0.482564	1.611975	0.001534
	C	0.894738	1.831293	0.004122
	N	2.213118	−1.637588	−0.071782
	C	−2.417880	0.055467	−0.003073
	O	−2.996016	−0.991112	0.005784
	H	−0.470263	−1.800717	−0.014852
	H	−1.189445	2.435320	0.005686

	H	1.285519	2.844998	0.010932
	H	2.854760	0.943537	-0.005295
	H	3.135857	-1.452364	0.300714
	H	1.850866	-2.527064	0.247875
3-formylphenylamide	C	-1.630237	0.006231	-1.119230
	C	-1.692283	0.013121	0.330532
	C	-0.383176	0.006856	0.946482
	C	0.805713	-0.004573	0.218186
	C	0.810595	-0.010914	-1.196841
	C	-0.434602	-0.005170	-1.830745
	N	-2.780831	0.023999	1.090086
	C	2.059494	-0.009827	0.975288
	O	3.198935	-0.019692	0.521449
	H	-0.351339	0.011493	2.035936
	H	1.750048	-0.019797	-1.739020
	H	-0.477543	-0.009741	-2.922362
	H	-2.576162	0.010308	-1.664990
	H	-3.596888	0.026817	0.462069
	H	1.913197	-0.003878	2.084138
3-aminophenyloxomethanide	C	-1.301410	-1.393410	-0.518262
	C	-1.363844	0.006883	-0.477243
	C	-0.255465	0.732645	-0.026065
	C	0.948772	0.103618	0.339432
	C	1.000698	-1.301382	0.258755
	C	-0.112246	-2.038296	-0.127859
	N	-2.548682	0.678968	-0.910679
	C	2.268466	0.941672	0.463372
	O	2.162354	2.027185	1.059059
	H	-0.310237	1.818820	0.092773
	H	1.945221	-1.794459	0.500370
	H	-0.076023	-3.129547	-0.135878
	H	-2.151249	-1.967275	-0.888703
	H	-3.385866	0.176898	-0.623509
	H	-2.589741	1.614932	-0.515553
3-formylaniline cation	C	-1.471960	-0.021154	-1.390741
	C	-1.469866	-0.068914	0.046077
	C	-0.230971	-0.036040	0.764175
	C	0.958121	0.041682	0.067192
	C	0.943856	0.088067	-1.345081
	C	-0.276193	0.056056	-2.063144
	N	-2.623505	-0.144140	0.716893
	C	2.249991	0.075172	0.839696
	O	2.268196	0.035792	2.047144
	H	-0.208970	-0.071223	1.850781
	H	1.883866	0.149239	-1.888017
	H	-0.263519	0.092751	-3.147426
	H	-2.416892	-0.046651	-1.925725
	H	-3.520413	-0.169367	0.239896
	H	-2.646682	-0.179027	1.732424
	H	3.173713	0.137701	0.233621
4-formylaniline	C	0.122883	0.037376	1.771295
	N	0.129489	0.019551	3.155333
	C	1.331322	0.021748	1.046567
	C	1.311767	-0.011447	-0.340061
	C	0.099917	-0.027919	-1.046657
	C	-1.104850	-0.011813	-0.321292
	C	-1.098540	0.020318	1.061527
	H	2.277246	0.031290	1.583086
	H	2.250907	-0.021904	-0.889975
	C	0.092643	-0.058736	-2.515261
	H	-2.039551	-0.022888	-0.874061
	H	-2.035113	0.028770	1.614687
	H	-0.712181	0.336052	3.617670
	H	0.975669	0.334456	3.610457
	O	-0.907448	-0.071159	-3.213227
	H	1.105328	-0.070520	-2.980092

N-(4-formyl)phenylamino	C	−1.516193	−0.006479	−0.403902
	C	−1.538412	−0.010298	1.037205
	C	−0.274332	−0.006117	1.722575
	C	0.910349	0.001641	1.017103
	C	0.903442	0.005461	−0.393627
	C	−0.326652	0.001227	−1.093217
	N	−2.645419	−0.017160	1.780805
	C	2.176069	0.013716	−1.139426
	O	2.261157	0.017230	−2.355098
	H	−0.297524	−0.009259	2.807527
	H	1.862379	0.004836	1.543540
	H	−0.297862	0.004237	−2.178544
	H	−2.464575	−0.009888	−0.936796
	H	−3.468377	−0.019199	1.164163
	H	3.089020	0.016646	−0.505007
4-aminobenzoyl	C	−0.010829	0.001605	−0.000221
	C	−0.003155	0.002647	1.412604
	C	1.234449	0.001606	2.088141
	C	2.421225	−0.000966	1.371894
	C	2.415860	−0.001011	−0.031713
	C	1.178587	−0.000381	−0.706786
	N	−1.190747	−0.045030	2.118524
	C	3.686300	0.000679	−0.766136
	O	3.866228	0.002748	−1.951561
	H	1.249839	−0.001591	3.175427
	H	3.374793	−0.000045	1.892643
	H	1.174934	0.001028	−1.792975
	H	−0.962211	−0.001762	−0.527783
	H	−2.025907	0.252539	1.632762
	H	−1.162173	0.248859	3.085384
4-formylphenylamide	C	−1.517629	−0.006315	−0.390769
	C	−1.575552	−0.010472	1.067382
	C	−0.271884	−0.005876	1.715243
	C	0.897364	0.001682	1.003179
	C	0.925081	0.005607	−0.422671
	C	−0.336896	0.001251	−1.084330
	N	−2.672456	−0.017730	1.797426
	C	2.161248	0.013509	−1.142304
	O	2.331021	0.017600	−2.371945
	H	−0.270353	−0.008762	2.803560
	H	1.851768	0.004894	1.534943
	H	−0.330409	0.004177	−2.173327
	H	−2.467333	−0.009484	−0.929715
	H	−3.477494	−0.019926	1.155820
	H	3.062453	0.016094	−0.472089
4-aminophenyloxomethanide	C	−1.426156	−0.040600	−0.409435
	C	−1.431147	−0.033478	0.995133
	C	−0.205074	−0.007336	1.675677
	C	0.992795	−0.004712	0.953764
	C	1.016277	0.012257	−0.440069
	C	−0.215396	−0.004575	−1.101064
	N	−2.663302	−0.110156	1.716507
	C	2.467035	−0.061211	−1.232313
	O	2.282758	0.121545	−2.449242
	H	−0.205066	0.006487	2.769314
	H	1.957198	−0.016089	1.472025
	H	−0.178657	0.028872	−2.194482
	H	−2.383804	−0.071182	−0.939687
	H	−3.414952	0.340210	1.200287
	H	−2.583676	0.348368	2.620773
4-formylaniline cation	C	−1.468968	0.022727	−0.449221
	C	−1.461406	0.036778	0.988808
	C	−0.214370	0.020807	1.706818
	C	0.964655	−0.007929	1.003949
	C	0.952749	−0.021697	−0.413589
	C	−0.279320	−0.005945	−1.125714
	N	−2.612927	0.064701	1.661119

	C	2.230814	−0.052945	−1.185567
	O	2.237966	−0.065045	−2.398567
	H	−0.222967	0.031684	2.792957
	H	1.913560	−0.020251	1.533049
	H	−0.243430	−0.017313	−2.210422
	H	−2.417824	0.035053	−0.977916
	H	−3.509363	0.076559	1.182930
	H	−2.640161	0.075229	2.676655
	H	3.162025	−0.064280	−0.589464

Table S3. G3(MP2)//B3LYP enthalpies.

Species	Enthalpy / a.u.	Species	Enthalpy / a.u.
C	-37.788425	3-hydroxyphenyloxomethanide	-419.565581
N	-54.524582	3-formylphenol cation	-419.850732
O	-74.989704	4-formylphenol	-420.180399
H	-0.499780	4-formylphenoxyl	-419.534616
benzene	-231.835152	4-hydroxybenzoyl	-419.535586
aniline	-287.120095	4-formylphenoxide	-419.651321
phenylamino	-286.471298	4-hydroxyphenyloxomethanide	-419.561792
phenylamide	-286.537216	4-formylphenol cation	-419.851049
aniline cation	-286.831357	*N*-formylaniline	-400.323366
phenol	-306.986455	*N*-phenyl-*N*-formylamino	-399.663447
phenoxyl	-306.343007	phenylaminobenzoyl	-399.673780
phenoxide	-306.431902	*N*-phenylformamidate ion	-399.771993
phenol cation	-306.669544	*N*-formylaniline acyl carbanion	-399.731428
benzoic acid	-420.210283	*N*-formylaniline cation	-400.012255
1,3-benzodioxole	-420.158545	2-formylaniline	-400.319644
phenylformate	-420.180480	*N*-(2-formyl)phenylamino	-399.662950
tropolone	-420.157304	2-aminobenzoyl	-399.672309
2-furanacrolein	-420.137604	2-formylphenylamide	-399.756148
benzaldehyde	-345.027560	2-aminophenyloxomethanide	-399.702541
benzoyl	-344.382757	2-formylaniline cation	-400.022869
oxophenylmethanide	-344.410809	3-formylaniline	-400.313452
benzaldehyde cation	-344.670898	*N*-(3-formyl)phenylamino	-399.662395
2-formylphenol	-420.188770	3-aminobenzoyl	-399.668357
2-formylphenoxyl	-419.532903	3-formylphenylamide	-399.745476
2-hydroxybenzoyl	-419.540266	3-aminophenyloxomethanide	-399.694543
2-formylphenoxyde	-419.646069	3-formylaniline cation	-400.012643
2-hydroxyphenyloxomethanide	-419.587058	4-formylaniline	-400.315144
2-formylphenol cation	-419.864788	*N*-(4-formyl)phenylamino	-399.663967
3-formylphenol	-420.179593	4-aminobenzoyl	-399.670271
3-formylphenoxyl	-419.533181	4-formylphenylamide	-399.760831
3-hydroxybenzoyl	-419.534164	4-aminophenyloxomethanide	-399.692384
3-formylphenoxide	-419.639542	4-formylaniline cation	-400.013791

Table S4. (RO)B3LYP/6-311+G(2d,2p)//(U)B3LYP/6-311+G(2d,2p) enthalpies.

Species	Enthalpy / a.u.
H[a]	-0.497640
H[b]	-0.499796
aniline	-287.575481
phenylamino	-286.931318
phenol	-307.459732
phenoxyl	-306.920567
benzaldehyde	-345.681197
benzoyl	-345.026593
2-formylphenol	-420.820289
2-formylphenoxyl	-420.169705
2-hydroxybenzoyl	-420.173985
3-formylphenol	-420.809745
3-formylphenoxyl	-420.169767
3-hydroxybenzoyl	-420.166719
4-formylphenol	-420.811439
4-formylphenoxyl	-420.170930
4-hydroxybenzoyl	-420.169208
N-formylaniline	-400.936001
N-phenyl-*N*-formylamino	-400.282790
phenylaminobenzoyl	-400.288873
2-formylaniline	-400.933905
N-(2-formyl)phenylamino	-400.279809
2-aminobenzoyl	-400.289774
3-formylaniline	-400.925870
N-(3-formyl)phenylamino	-400.279141
3-aminobenzoyl	-400.283166
4-formylaniline	-400.929182
N-(4-formyl)phenylamino	-400.280870
4-aminobenzoyl	-400.287326

[a]From the exact energy (-0.500000 Hartree).
[b]From the UB3LYP/6-311+G(2d,2p) energy.

Table S5. Experimental $\Delta_f H^o_m(g)$ in kJ/mol at T=298.15 K.

Species	$\Delta_f H^o_m(g)$	Reference
H	218.00	1
C	716.67	1
N	472.68	1
O	249.17	1
benzene	82.6 ± 0.7	2
aniline	87.1 ± 1.1	2
phenol	-96.4 ± 0.9	2
benzaldehyde	-36.7 ± 2.8	2
benzoic acid	-294 ± 2.2	2
1,3-benzodioxole	-142.7 ± 2.9	2
phenylformate	-215.8 ± 3.0	2
2-furanacrolein	-105.9 ± 2.3	2
tropolone	-155.4 ± 1.5	2
2-formylphenol	-238.3 ± 2.5	3
	-245.6 ± 2.2	4
4-formylphenol	-220.3 ± 2.0	3

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