Supporting Information

IEF-PCM Calculations of Absolute pKa for Substituted Phenols in Dimethylsulfoxide and Acetonitrile Solutions

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Table S1. B3LYP/6-311+G** and B3LYP/6-311++G(2df,2p) total energies (E_0, hartrees), enthalpies (H_{298}, hartrees) and free energies (G_{298}, hartrees) of phenols and corresponding phenoxide anions in gas phase

Phenols		B3LYP/6-311+G**			B3LYP/6-311++G(2df,2p)
		E_0	**H_{298}**	**G_{298}**	**E_0**
C_6H_5OH	anion	-306.9940	-306.8977	-306.9329	-307.0127
	phenol	-307.5586	-307.4480	-307.4835	-307.5791
4-$NH_2C_6H_4OH$	anion	-362.3609	-362.2465	-362.2857	-362.3825
	phenol	-362.9316	-362.8030	-362.8421	-362.9555
3-$NH_2C_6H_4OH$	anion	-362.3684	-362.2539	-362.2923	-362.3906
	phenol	-362.9358	-362.8071	-362.8458	-362.9598
2-$NH_2C_6H_4OH$	anion	-362.3732	-362.2585	-362.2963	-362.3953
	phenol	-362.9350	-362.8062	-362.8448	-362.9587

4-FC_6H_4OH	anion	-406.2662	-406.1772	-406.2145	-406.2888
	phenol	-406.8253	-406.7222	-406.7599	-406.8506
2-FC_6H_4OH	anion	-406.2670	-406.1779	-406.2152	-406.2900
	phenol	-406.8264	-406.7229	-406.7603	-406.8515
3-FC_6H_4OH	anion	-406.2730	-406.1839	-406.2212	-406.2959
	phenol	-406.8274	-406.7241	-406.7618	-406.8527
3-ClC_6H_4OH	anion	-766.6300	-766.5418	-766.5805	-766.6526
	phenol	-767.1812	-767.0789	-767.1179	-767.2059
2-$NO_2C_6H_4OH$	anion	-511.5820	-511.4803	-511.5229	-511.6124
	phenol	-512.1290	-512.0133	-512.0546	-512.1620
3-$NO_2C_6H_4OH$	anion	-511.5822	-511.4806	-511.5230	-511.6128
	phenol	-512.1218	-512.0062	-512.0488	-512.1548
4-CNC_6H_4OH	anion	-399.2921	-399.1947	-399.2342	-399.3161
	phenol	-399.8265	-399.7153	-399.7553	-399.8523
3,4,5-$Cl_3C_6H_2OH$	anion	-1685.8797	-1685.8078	-1685.8533	-1685.9107
	phenol	-1686.4139	-1686.3284	-1686.3740	-1686.4475
4-$NO_2C_6H_4OH$	anion	-511.5997	-511.4977	-511.5393	-511.6304
	phenol	-512.1240	-512.0084	-512.0508	-512.1572
2,4-$(NO_2)_2C_6H_3OH$	anion	-716.1732	-716.0662	-716.1147	-716.2160
	phenol	-716.6879	-716.5677	-716.6160	-716.7340
C_6F_5OH	anion	-803.3300	-803.2690	-803.3153	-803.3710
	phenol	-803.8569	-803.7822	-803.8284	-803.9029
2,4,6-$(NO_2)_3C_6H_2OH$	anion	-920.7396	-920.6276	-920.6830	-920.7945
	phenol	-921.2304	-921.1055	-921.1608	-921.2892
4-$CF_3C_6H_4OH$	anion	-644.1673	-644.0628	-644.1081	-644.2017
	phenol	-644.7092	-644.5905	-644.6364	-644.7466
3-$CF_3C_6H_4OH$	anion	-644.1610	-644.0565	-644.1015	-644.1958
	phenol	-644.7078	-644.5890	-644.6345	-644.7452
2-$CF_3C_6H_4OH$	anion	-644.1618	-644.0574	-644.1017	-644.1965
	phenol	-644.7075	-644.5885	-644.6330	-644.7448

3,5-$(CF_3)_2C_6H_3OH$	anion	-981.3241	-981.2113	-981.2665	-981.3753
	phenol	-981.8545	-981.7278	-981.7838	-981.9092
2,3,4,5,6-$(CF_3)_5C_6OH$	anion	-1992.7282	-1992.5925	-1992.6676	-1992.8326
	phenol	-1993.2143	-1993.0647	-1993.1401	-1993.3246
2,4,6-$Tf_3C_6H_2OH$	anion	-2964.3674	-2964.2063	-2964.2961	-2964.5829
	phenol	-2964.8409	-2964.6664	-2964.7580	-2965.0606
2,4,6-$(FSO_2)_3C_6H_2OH$	anion	-2250.8141	-2250.6975	-2250.7642	-2251.0118
	phenol	-2251.2848	-2251.1545	-2251.2208	-2251.4899

Tf denotes CF_3SO_2-

Table S2. IEF-PCM/B3LYP/6-31+G** free energies of solvation ($\Delta G_{solv.}$, kcal/mol) of phenols and corresponding phenoxide anions in DMSO

Phenols		**$\Delta G_{solv,}$**
C_6H_5OH	anion	-51.86
	phenol	-2.75
4-$NH_2C_6H_4OH$	anion	-53.11
	phenol	-5.20
3-$NH_2C_6H_4OH$	anion	-54.34
	phenol	-5.08
2-$NH_2C_6H_4OH$	anion	-51.11
	phenol	-4.28
4-FC_6H_4OH	anion	-49.95
	phenol	-2.92
2-FC_6H_4OH	anion	-50.97
	phenol	-0.73
3-FC_6H_4OH	anion	-49.16
	phenol	-2.82
3-ClC_6H_4OH	anion	-47.76

	phenol	-2.87
2-$NO_2C_6H_4OH$	anion	-47.86
	phenol	-0.78
3-$NO_2C_6H_4OH$	anion	-45.15
	phenol	-4.35
4-CNC_6H_4OH	anion	-44.71
	phenol	-5.36
3,4,5-$Cl_3C_6H_2OH$	anion	-42.11
	phenol	-2.74
4-$NO_2C_6H_4OH$	anion	-43.69
	phenol	-5.41
2,4-$(NO_2)_2C_6H_3OH$	anion	-39.55
	phenol	-1.83
C_6F_5OH	anion	-42.12
	phenol	0.03
2,4,6-$(NO_2)_3C_6H_2OH$	anion	-35.23
	phenol	-2.77
4-$CF_3C_6H_4OH$	anion	-43.33
	phenol	-2.03
3-$CF_3C_6H_4OH$	anion	-44.62
	phenol	-1.90
2-$CF_3C_6H_4OH$	anion	-45.20
	phenol	1.51
3,5-$(CF_3)_2C_6H_3OH$	anion	-37.71
	phenol	-0.21
2,3,4,5,6-$(CF_3)_5C_6OH$	anion	-26.54
	phenol	4.95

Table S3. IEF-PCM/B3LYP/6-31+G** free energies of solvation ($\Delta G_{solv.}$, kcal/mol) of phenols and corresponding phenoxide anions in MeCN

Phenols		**$\Delta G_{solv,}$**
C_6H_5OH	anion	-56.20
	phenol	-2.64
2-$NO_2C_6H_4OH$	anion	-52.02
	phenol	-1.75
3-$NO_2C_6H_4OH$	anion	-49.45
	phenol	-4.95
4-CNC_6H_4OH	anion	-48.94
	phenol	-6.32
4-$NO_2C_6H_4OH$	anion	-47.64
	phenol	-6.07
2,4-$(NO_2)_2C_6H_3OH$	anion	-44.04
	phenol	-3.72
C_6F_5OH	anion	-45.68
	phenol	-0.70
2,4,6-$(NO_2)_3C_6H_2OH$	anion	-40.63
	phenol	-5.35
4-$CF_3C_6H_4OH$	anion	-47.01
	phenol	-1.98
3-$CF_3C_6H_4OH$	anion	-48.13
	phenol	-1.82
2-$CF_3C_6H_4OH$	anion	-48.39
	phenol	0.93
3,5-$(CF_3)_2C_6H_3OH$	anion	-40.63
	phenol	-0.20
2,3,4,5,6-$(CF_3)_5C_6OH$	anion	-27.33

	phenol	5.77
2,4,6-$Tf_3C_6H_2OH$	anion	-25.94
	phenol	6.49
2,4,6-$(FSO_2)_3C_6H_2OH$	anion	-36.13
	phenol	-3.59

Tf denotes CF_3SO_2-

Molecular Cartesian Coordinates
B3LYP/6-311+G** gas-phase geometries

$C_6H_5O^-$

C	-0.287463	-1.211848	-0.000039
C	-1.077741	0.000006	-0.000674
C	-0.287468	1.211849	-0.000045
C	1.100065	1.200020	0.000100
C	1.827775	0.000001	-0.000029
C	1.100061	-1.200024	0.000093
H	-0.831331	-2.153555	0.000215
H	-0.831317	2.153567	0.000205
H	1.636871	2.148624	0.000252
H	2.913257	-0.000004	0.000061
H	1.636875	-2.148625	0.000244
O	-2.346967	-0.000003	0.000324

C_6H_5OH

C	-0.262593	1.198048	-0.000003
C	-0.937862	-0.024011	0.000017
C	-0.221441	-1.221543	0.000005
C	1.169722	-1.188845	-0.000005
C	1.855041	0.026807	0.000005
C	1.131269	1.217261	-0.000004

H	-0.822778	2.128590	-0.000019
H	-0.764229	-2.158892	0.000009
H	1.721776	-2.122097	-0.000009
H	2.938186	0.045397	0.000006
H	1.649552	2.169612	-0.000008
O	-2.305027	-0.110294	-0.000024
H	-2.687108	0.773447	0.000124

4-$NH_2C_6H_4O^-$

C	-0.754229	-1.209991	-0.000017
C	-1.562193	-0.010040	-0.000305
C	-0.784892	1.207778	-0.000020
C	0.604191	1.213977	0.000026
C	1.350430	0.028678	-0.000022
C	0.633597	-1.178824	0.000025
H	-1.282102	-2.160473	0.000107
H	-1.336235	2.144771	0.000106
H	1.146307	2.157441	0.000093
H	1.188256	-2.118524	0.000088
O	-2.832045	-0.029493	0.000159
N	2.804687	0.093030	0.000019
H	3.192975	-0.373999	-0.814964
H	3.192929	-0.373950	0.815050

4-$NH_2C_6H_4OH$

C	-0.703137	1.214228	-0.000108
C	-1.417727	0.017509	0.002457
C	-0.723181	-1.190084	-0.000270
C	0.670677	-1.201811	-0.005622
C	1.399377	-0.007844	-0.006705
C	0.686636	1.199495	-0.006190
H	-1.246051	2.151832	0.002192
H	-1.265688	-2.131282	0.002177
H	1.194121	-2.152504	-0.014111

H	1.227647	2.140436	-0.015450
O	-2.792286	0.093416	0.009250
H	-3.163644	-0.794248	0.003783
N	2.803884	-0.015988	-0.075939
H	3.248913	0.813282	0.291002
H	3.239932	-0.851883	0.286618

3-$NH_2C_6H_4O^-$

C	-1.339072	1.007911	0.010859
C	-1.314699	-0.439848	-0.000485
C	0.012443	-1.009729	-0.014764
C	1.167115	-0.238107	-0.019982
C	1.097798	1.165356	-0.010367
C	-0.175280	1.757507	0.005619
H	-2.313121	1.488964	0.025326
H	0.082750	-2.096165	-0.022513
H	2.001746	1.767107	-0.036272
H	-0.244783	2.844829	0.013859
O	-2.366504	-1.149269	0.008556
N	2.450231	-0.872277	-0.083550
H	3.150661	-0.347632	0.427077
H	2.413333	-1.815556	0.283635

3-$NH_2C_6H_4OH$

C	-1.264627	1.058315	0.005658
C	-1.202569	-0.336751	0.000447
C	0.021944	-0.998348	-0.006217
C	1.215345	-0.267181	-0.007455
C	1.160316	1.136943	-0.003384
C	-0.071325	1.779158	0.003707
H	-2.222372	1.568494	0.011381
H	0.031843	-2.082463	-0.016238
H	2.078799	1.713593	-0.011172
H	-0.105959	2.862990	0.008022

O	-2.327549	-1.120179	0.002897
H	-3.109040	-0.558146	0.008433
N	2.443438	-0.927133	-0.070562
H	3.240255	-0.403514	0.259463
H	2.448299	-1.882409	0.254339

2-$NH_2C_6H_4O^-$

C	-0.790055	1.358818	0.005230
C	0.530399	0.816565	-0.009044
C	0.594551	-0.635467	-0.023655
C	-0.548573	-1.417868	-0.022558
C	-1.831946	-0.837885	0.006286
C	-1.932105	0.553921	0.015153
H	-0.878923	2.442170	0.025078
H	-0.445961	-2.502535	-0.051786
H	-2.718489	-1.464706	0.010015
H	-2.914390	1.023301	0.032120
O	1.609434	1.505438	0.003227
N	1.905689	-1.181384	-0.078718
H	2.545962	-0.398969	0.064877
H	2.062872	-1.901576	0.616426

2-$NH_2C_6H_4OH$

C	0.746190	1.364524	0.000705
C	-0.480046	0.713538	-0.005368
C	-0.553589	-0.691622	-0.008911
C	0.645476	-1.411012	-0.003653
C	1.877747	-0.759370	0.005019
C	1.934653	0.631095	0.005689
H	0.772937	2.450793	0.004738
H	0.604670	-2.495647	-0.012579
H	2.790776	-1.343248	0.009494
H	2.887356	1.146440	0.010687
O	-1.689651	1.375898	-0.000530

H	-1.541064	2.325863	0.034258
N	-1.799677	-1.313422	-0.073117
H	-2.579387	-0.733628	0.201347
H	-1.842933	-2.246719	0.307225

4-$FC_6H_4O^-$

C	-0.736340	-1.211193	-0.000052
C	-1.526291	0.000012	-0.000615
C	-0.736368	1.211194	-0.000059
C	0.655413	1.207879	0.000025
C	1.338315	0.000009	-0.000062
C	0.655419	-1.207880	0.000018
H	-1.276317	-2.153964	0.000217
H	1.217321	2.138283	0.000188
H	-1.276313	2.153986	0.000199
H	1.217369	-2.138261	0.000169
O	-2.796497	-0.000020	0.000358
F	2.732114	-0.000002	0.000094

4-FC_6H_4OH

C	0.672242	1.220336	-0.000010
C	1.380229	0.017031	-0.000022
C	0.692357	-1.197053	-0.000030
C	-0.702393	-1.212249	-0.000010
C	-1.383255	-0.007529	0.000026
C	-0.718678	1.209895	-0.000005
H	1.220978	2.153915	-0.000036
H	-1.253269	-2.144404	-0.000030
H	1.239380	-2.134814	-0.000057
H	-1.286200	2.132145	-0.000014
O	2.748705	0.094407	-0.000002
H	3.127268	-0.790593	0.000314
F	-2.742312	-0.017121	0.000015

2-$FC_6H_4O^-$

C	0.696644	1.387720	-0.000001
C	-0.624716	0.806343	-0.000230
C	-0.571960	-0.636881	-0.000046
C	0.581687	-1.388790	0.000003
C	1.839545	-0.761435	-0.000018
C	1.867653	0.637420	0.000053
H	0.738350	2.473850	0.000107
H	2.751386	-1.348717	0.000019
H	0.492948	-2.472210	0.000045
H	2.826411	1.153557	0.000137
O	-1.699203	1.472403	0.000085
F	-1.772065	-1.316885	0.000050

2-FC_6H_4OH

C	-0.641299	-1.413678	0.000143
C	0.552668	-0.695209	0.000042
C	0.482439	0.696965	0.000048
C	-0.714645	1.385459	0.000042
C	-1.903700	0.655349	-0.000184
C	-1.860043	-0.738650	0.000051
H	-0.593887	-2.495899	0.000339
H	-2.853542	1.175397	-0.000345
H	-0.704948	2.468410	-0.000049
H	-2.781542	-1.308644	0.000114
O	1.743811	-1.355158	-0.000216
H	2.462376	-0.710852	0.000077
F	1.669838	1.374604	0.000083

3-$FC_6H_4O^-$

C	-1.260784	1.048964	0.000000
C	-1.310977	-0.399364	-0.000191
C	-0.009247	-1.036408	-0.000017

C	1.141926	-0.284916	0.000055
C	1.182218	1.106015	-0.000013
C	-0.067552	1.750852	0.000017
H	-2.211794	1.573799	0.000086
H	2.123610	1.640094	-0.000001
H	0.042233	-2.119466	0.000054
H	-0.092154	2.839145	0.000054
O	-2.392942	-1.055015	0.000085
F	2.358683	-0.956035	0.000002

3-FC_6H_4OH

C	1.178058	1.095782	0.000041
C	1.194209	-0.301169	0.000088
C	-0.000553	-1.022746	0.000104
C	-1.188890	-0.314354	0.000045
C	-1.247699	1.072147	-0.000015
C	-0.042011	1.769155	-0.000031
H	2.110287	1.651512	-0.000009
H	-2.205276	1.575620	-0.000066
H	0.005015	-2.104607	0.000187
H	-0.051514	2.852804	-0.000052
O	2.352325	-1.026273	-0.000165
H	3.109841	-0.431859	0.000356
F	-2.349516	-1.014020	-0.000054

3-$ClC_6H_4O^-$

C	-1.880446	0.820188	-0.000001
C	-1.606612	-0.600308	-0.000020
C	-0.193040	-0.932977	-0.000007
C	0.766069	0.055391	-0.000002
C	0.488470	1.422397	-0.000001
C	-0.873046	1.769559	0.000003
H	-2.924160	1.120913	0.000011
H	1.276528	2.162894	-0.000001

H	0.080353	-1.981135	0.000004
H	-1.138057	2.825408	0.000011
O	-2.509820	-1.484362	0.000012
Cl	2.504443	-0.438746	0.000002

3-ClC_6H_4OH

C	-1.813188	0.898278	-0.000021
C	-1.511851	-0.464935	0.000171
C	-0.183681	-0.895471	0.000250
C	0.830483	0.057476	0.000418
C	0.557994	1.419777	0.000058
C	-0.777564	1.824898	-0.000011
H	-2.850613	1.207972	-0.000302
H	1.364554	2.140375	-0.000226
H	0.060294	-1.951794	0.000329
H	-1.009884	2.883652	-0.000268
O	-2.561057	-1.340497	-0.000297
H	-2.236720	-2.247222	0.000371
Cl	2.502804	-0.491126	-0.000160

2-$NO_2C_6H_4O^-$

C	-1.906194	0.926669	-0.018914
C	-0.452485	1.095151	-0.029781
C	0.265675	-0.185400	0.010004
C	-0.414521	-1.419540	0.032332
C	-1.789958	-1.494865	0.043381
C	-2.534570	-0.288412	0.017849
H	-2.473080	1.852306	-0.042786
H	-2.289643	-2.456673	0.075860
H	0.190753	-2.316434	0.048526
H	-3.622133	-0.330663	0.027079
O	0.050291	2.233393	-0.086401
N	1.699229	-0.248711	0.009876
O	2.360360	0.777917	0.187244

O	2.250827	-1.362456	-0.164222

2-$NO_2C_6H_4OH$

C	1.831909	1.009896	0.000100
C	0.427870	0.994416	-0.000055
C	-0.215182	-0.266336	-0.000207
C	0.523844	-1.457978	-0.000101
C	1.903192	-1.414361	-0.000053
C	2.552561	-0.169765	0.000019
H	2.322255	1.975355	0.000073
H	2.475901	-2.332870	0.000066
H	-0.015710	-2.395020	-0.000026
H	3.635855	-0.128236	-0.000035
O	-0.207025	2.170586	0.000131
H	-1.170757	1.984310	0.000395
N	-1.664688	-0.362242	0.000039
O	-2.320218	0.699052	-0.000286
O	-2.190242	-1.462523	0.000284

3-$NO_2C_6H_4O^-$

C	-2.131396	0.816380	-0.000162
C	-1.833843	-0.600044	-0.000133
C	-0.418847	-0.900042	-0.000329
C	0.531607	0.110500	0.000057
C	0.214968	1.476262	0.000448
C	-1.146113	1.793592	0.000274
H	-3.181281	1.095079	-0.000355
H	-0.111705	-1.936667	-0.000665
H	0.990699	2.226255	0.000766
H	-1.438380	2.841335	0.000492
O	-2.723991	-1.494929	-0.000046
N	1.957741	-0.264669	0.000007
O	2.805284	0.633904	-0.000848
O	2.260985	-1.458125	0.000742

3-$NO_2C_6H_4OH$

C	-2.071617	0.891597	0.000077
C	-1.739112	-0.467138	-0.000157
C	-0.402804	-0.859761	-0.000242
C	0.576749	0.128754	0.000041
C	0.277632	1.484590	0.000304
C	-1.067075	1.852397	0.000222
H	-3.117715	1.172252	0.000168
H	-0.110113	-1.902239	-0.000334
H	1.073624	2.214913	0.000640
H	-1.333674	2.902450	0.000384
O	-2.768290	-1.361252	-0.000275
H	-2.428819	-2.262803	0.000400
N	1.996041	-0.295403	0.000017
O	2.851243	0.579607	-0.000824
O	2.229770	-1.498278	0.000743

4-$CNC_6H_4O^-$

C	1.061857	1.218874	-0.000040
C	1.850972	-0.000017	-0.000674
C	1.061828	-1.218877	-0.000044
C	-0.313384	-1.212391	0.000033
C	-1.048822	0.000026	-0.000083
C	-0.313349	1.212427	0.000028
H	1.608063	2.157593	0.000248
H	1.607995	-2.157620	0.000240
H	-0.859286	-2.152188	0.000139
H	-0.859229	2.152238	0.000135
O	3.108974	-0.000026	0.000393
C	-2.462223	0.000031	0.000012
N	-3.627230	-0.000036	0.000100

4-CNC_6H_4OH

C	-1.007216	1.222947	0.000036
C	-1.710344	0.014608	-0.000062
C	-1.018740	-1.200489	0.000009
C	0.369291	-1.207880	0.000044
C	1.082682	-0.001253	-0.000058
C	0.377893	1.213971	0.000023
H	-1.560957	2.153410	0.000089
H	-1.565121	-2.138452	0.000057
H	0.905854	-2.148510	0.000153
H	0.925112	2.148506	-0.000002
O	-3.069485	0.086399	0.000032
H	-3.450934	-0.798249	-0.000253
C	2.511317	-0.008493	-0.000111
N	3.667517	-0.015481	0.000059

3,4,5-$Cl_3C_6H_2O^-$

C	-1.213893	1.535606	0.000095
C	-0.000042	2.322501	0.000648
C	1.213838	1.535649	0.000092
C	1.190024	0.158384	0.000059
C	0.000010	-0.589056	0.000209
C	-1.190030	0.158342	0.000060
H	-2.159393	2.062667	-0.000190
H	2.159319	2.062745	-0.000204
Cl	2.754149	-0.694039	-0.000133
Cl	0.000045	-2.347439	0.000051
Cl	-2.754126	-0.694133	-0.000134
O	-0.000064	3.581428	-0.000364

3,4,5-$Cl_3C_6H_2OH$

C	-0.864913	1.714754	-0.000121
C	0.463360	2.134808	-0.000305
C	1.493939	1.198083	-0.000069

C	1.189267	-0.159982	-0.000043
C	-0.135850	-0.610125	0.000232
C	-1.153305	0.357243	0.000044
H	-1.660989	2.446414	-0.000282
H	2.531878	1.508709	-0.000001
Cl	2.519394	-1.292150	-0.000155
Cl	-0.508684	-2.307902	0.000214
Cl	-2.832577	-0.120750	-0.000148
O	0.688864	3.478819	0.000386
H	1.634951	3.659277	0.000269

4-$NO_2C_6H_4O^-$

C	1.421524	-1.225037	-0.000133
C	2.208238	-0.000017	-0.000422
C	1.421552	1.225025	0.000196
C	0.051573	1.220660	0.000060
C	-0.664181	0.000063	-0.000180
C	0.051545	-1.220550	-0.000022
H	1.972437	-2.160331	0.000135
H	1.972514	2.160292	0.000533
H	-0.512789	2.144920	0.000308
H	-0.512885	-2.144792	-0.000173
O	3.461600	-0.000017	0.000188
N	-2.076681	0.000018	-0.000065
O	-2.688443	-1.091317	0.000353
O	-2.688659	1.091200	-0.000210

4-$NO_2C_6H_4OH$

C	-1.373672	1.226196	-0.000086
C	-2.075322	0.015080	0.000000
C	-1.384174	-1.202186	0.000082
C	0.003345	-1.210764	0.000108
C	0.688624	0.000660	0.000018
C	0.011144	1.219823	-0.000045

H	-1.929125	2.155417	-0.000218
H	-1.931176	-2.139548	0.000219
H	0.558687	-2.138470	0.000115
H	0.575546	2.142075	-0.000053
O	-3.431837	0.086216	-0.000027
H	-3.814978	-0.797943	0.000002
N	2.157808	-0.006790	0.000017
O	2.734696	1.075460	0.000184
O	2.724230	-1.095033	-0.000237

2,4-$(NO_2)_2C_6H_3O^-$

C	0.016095	2.106076	-0.049642
C	1.259990	1.335554	-0.065460
C	1.029934	-0.118117	-0.005734
C	-0.232362	-0.679982	-0.003469
C	-1.365746	0.131418	0.004625
C	-1.224348	1.543922	-0.014266
H	0.138761	3.183283	-0.074580
H	-0.340097	-1.755176	0.006317
H	-2.119472	2.152299	-0.002909
O	2.364102	1.886202	-0.160855
N	2.149507	-1.043640	0.027780
O	1.994027	-2.169162	-0.471511
O	3.194520	-0.685232	0.562219
N	-2.664367	-0.458737	0.043352
O	-3.656666	0.292131	0.048859
O	-2.768052	-1.696063	0.068404

2,4-$(NO_2)_2C_6H_3OH$

C	-0.055278	2.068193	0.000342
C	-1.188626	1.233617	-0.000055
C	-0.978337	-0.168863	-0.000110
C	0.306171	-0.710643	-0.000125
C	1.385771	0.147644	0.000140

C	1.216681	1.538561	0.000412
H	-0.219282	3.138104	0.000670
H	0.445054	-1.782311	-0.000394
H	2.089347	2.177412	0.000797
O	-2.383079	1.815444	-0.000405
H	-3.062748	1.104811	-0.000526
N	-2.106111	-1.095046	-0.000039
O	-1.889809	-2.290923	0.000982
O	-3.251354	-0.606268	-0.000456
N	2.747852	-0.415628	-0.000072
O	3.682009	0.376461	0.000104
O	2.859377	-1.634008	-0.000648

$C_6F_5O^-$

C	-1.192757	-0.727687	0.000052
C	0.000038	-1.538678	0.000233
C	1.192783	-0.727642	0.000049
C	1.192021	0.654705	0.000032
C	-0.000027	1.372705	0.000099
C	-1.192053	0.654651	0.000024
F	-2.397157	-1.359659	-0.000047
F	2.397227	-1.359550	-0.000050
F	2.368651	1.337123	-0.000056
F	-0.000064	2.737061	-0.000024
F	-2.368706	1.337032	-0.000057
O	0.000051	-2.794549	-0.000104

C_6F_5OH

C	0.245942	1.365724	0.000103
C	1.321013	0.475581	-0.000074
C	1.034529	-0.888495	-0.000222
C	-0.267740	-1.366944	-0.000051
C	-1.326170	-0.466392	-0.000089
C	-1.063478	0.899854	-0.000070

F	0.475381	2.682403	0.000302
F	2.073545	-1.750711	0.000175
F	-0.501659	-2.681573	0.000123
F	-2.587006	-0.909493	-0.000060
F	-2.076881	1.769142	0.000003
O	2.584158	0.958896	-0.000627
H	3.211742	0.224954	0.002548

2,4,6-$(NO_2)_3C_6H_2O^-$

C	-0.550764	1.217942	-0.024800
C	-1.384175	0.001580	-0.114014
C	-0.553496	-1.216673	-0.024797
C	0.817484	-1.215811	0.003491
C	1.516394	-0.001734	0.023256
C	0.820257	1.213880	0.003475
H	1.359977	-2.150516	0.021910
H	1.364839	2.147369	0.021871
O	-2.591639	0.002850	-0.321480
N	2.950414	-0.003358	0.089075
O	3.541909	1.083919	0.114644
O	3.539414	-1.091984	0.115282
N	-1.207628	-2.521715	0.005505
O	-2.267509	-2.625552	0.608482
O	-0.640973	-3.464638	-0.559242
N	-1.201808	2.524483	0.005530
O	-2.261941	2.630609	0.607690
O	-0.632493	3.466318	-0.558403

2,4,6-$(NO_2)_3C_6H_2OH$

C	0.487938	1.211625	-0.013362
C	1.266677	0.022510	-0.021643
C	0.540197	-1.190750	-0.003540
C	-0.837507	-1.231440	-0.003203
C	-1.546776	-0.032686	0.022545

C	-0.901854	1.188585	0.018159
H	-1.358730	-2.179156	-0.021082
H	-1.461463	2.113432	0.031317
O	2.582076	-0.004797	-0.080738
H	2.899371	0.928621	-0.109274
N	-3.023172	-0.069036	0.048151
O	-3.610042	1.002847	0.058414
O	-3.553386	-1.170334	0.057645
N	1.259633	-2.484896	0.015407
O	0.812482	-3.365979	-0.704557
O	2.212903	-2.583818	0.766372
N	1.140641	2.522868	-0.040140
O	0.451996	3.520815	-0.002655
O	2.382602	2.544700	-0.101810

4-$CF_3C_6H_4O^-$

C	0.000000	0.003611	-2.188300
C	0.000000	-0.051108	-0.722186
C	0.000000	0.015517	2.172826
C	1.208563	-0.026733	0.004867
C	-1.208563	-0.026733	0.004867
C	-1.216489	0.000044	1.382715
C	1.216489	0.000044	1.382715
H	2.150529	-0.039492	-0.536314
H	-2.150529	-0.039492	-0.536314
H	-2.156223	0.006775	1.927303
H	2.156223	0.006775	1.927303
O	0.000000	0.038188	3.432603
F	0.000000	1.286135	-2.729431
F	-1.094193	-0.588312	-2.763024
F	1.094193	-0.588312	-2.763024

4-$CF_3C_6H_4OH$

C	-0.058730	-0.002813	-2.443242

C	-0.046741	0.030342	-0.944034
C	-0.040351	-0.010135	1.843289
C	-1.252719	-0.003795	-0.237245
C	1.160913	0.040433	-0.248286
C	1.167044	0.022758	1.142387
C	-1.253326	-0.022322	1.149297
H	-2.193637	-0.008260	-0.773628
H	2.098223	0.070356	-0.789111
H	2.109883	0.036974	1.680259
H	-2.179716	-0.043794	1.709456
O	-0.101173	-0.027408	3.204844
F	-0.176720	-1.268435	-2.928231
F	1.074639	0.505820	-2.979570
F	-1.094796	0.697558	-2.963194
H	0.787207	-0.017279	3.577010

3-$CF_3C_6H_4O^-$

H	-0.575635	-0.141802	-2.176037
C	-0.598300	-0.080139	-1.095936
C	-0.647570	0.065270	1.806985
C	0.587691	-0.047539	-0.344063
C	-1.806369	-0.042258	-0.388227
C	-1.843627	0.027436	0.995179
C	0.580447	0.024865	1.043253
C	1.894526	-0.009140	-1.068951
H	-2.741886	-0.071951	-0.943878
H	-2.794253	0.054080	1.520761
H	1.510607	0.047562	1.599549
O	-0.666558	0.127037	3.069855
F	2.936418	-0.517812	-0.357257
F	2.284308	1.262716	-1.412096
F	1.880203	-0.698327	-2.249138

3-$CF_3C_6H_4OH$

H	-0.479929	-0.156003	-2.374373
C	-0.505679	-0.091392	-1.294870
C	-0.555995	0.060335	1.497321
C	0.681731	-0.046217	-0.561656
C	-1.718326	-0.062287	-0.613628
C	-1.750791	0.014207	0.776705
C	0.667157	0.031151	0.827708
C	2.003315	-0.018399	-1.283159
H	-2.648990	-0.101583	-1.167270
H	-2.701939	0.034716	1.300194
H	1.585176	0.061239	1.399715
O	-0.515406	0.132286	2.860263
H	-1.409463	0.140461	3.217924
F	2.394728	1.251618	-1.563268
F	1.956085	-0.674654	-2.464247
F	2.998327	-0.575478	-0.557358

2-$CF_3C_6H_4O^-$

O	-2.242077	-0.086346	0.513942
C	-1.139268	-0.046348	-0.088625
C	1.388644	0.044191	-1.516334
C	0.154051	-0.001827	0.584584
C	-1.040739	-0.040626	-1.535560
C	0.162409	0.002473	-2.207419
C	1.356846	0.041269	-0.125217
C	0.176842	-0.001242	2.069922
H	-1.981689	-0.072710	-2.077190
H	0.163717	0.004315	-3.296449
H	2.289166	0.073443	0.428550
H	2.332662	0.078077	-2.048876
F	-0.459377	1.062590	2.643637
F	1.456710	0.043591	2.582867
F	-0.383115	-1.107293	2.643951

2-$CF_3C_6H_4OH$

H	2.314707	0.020422	-2.050315
C	1.375571	0.011536	-1.511553
C	-1.056682	-0.001660	-0.111020
C	1.369360	0.032221	-0.124188
C	0.161018	-0.022019	-2.199347
C	-1.041980	-0.025661	-1.508222
C	0.164595	0.024207	0.587762
H	2.301562	0.055454	0.425222
H	0.151142	-0.039313	-3.283204
H	-1.992410	-0.042869	-2.027111
C	0.198621	-0.031103	2.085174
O	-2.281912	-0.017383	0.478631
F	-0.082793	-1.269589	2.565100
F	-0.739855	0.797113	2.650474
F	1.385895	0.327595	2.600881
H	-2.221620	0.174484	1.421541

3,5-$(CF_3)_2C_6H_3O^-$

H	-0.494289	0.018801	-2.770272
C	-0.497121	0.021004	-1.686497
C	-0.500731	0.044075	1.092225
C	-1.785611	0.017169	-1.030275
C	0.694615	0.037257	-0.976418
C	0.732322	0.046781	0.424315
C	-1.710251	0.027501	0.414725
O	-2.877140	0.007816	-1.659220
C	1.990582	-0.026118	-1.725414
H	1.667506	0.074980	0.963506
H	-2.647563	0.030020	0.958178
C	-0.493750	-0.008669	2.589308
F	0.522298	0.711953	3.145227
F	2.402948	-1.310065	-1.966135
F	3.024676	0.561677	-1.060131
F	1.943335	0.570293	-2.945718

F	-0.335685	-1.279923	3.074871
F	-1.636140	0.455448	3.157726

3,5-$(CF_3)_2C_6H_3OH$

H	-0.332303	0.003172	-2.699872
C	-0.310149	0.004521	-1.617939
C	-0.293169	0.032531	1.163812
C	-1.514624	-0.013399	-0.912039
C	0.890311	0.037517	-0.918839
C	0.915323	0.049119	0.476199
C	-1.509178	0.000116	0.481726
O	-2.660354	-0.037387	-1.646492
C	2.190369	0.006022	-1.683147
H	1.853749	0.086485	1.010859
H	-2.442316	-0.003506	1.034331
C	-0.300884	-0.004055	2.670820
H	-3.431885	-0.045030	-1.069604
F	2.594544	-1.266339	-1.919827
F	3.189749	0.613387	-1.009237
F	2.089260	0.611600	-2.885701
F	-0.406994	-1.273413	3.135988
F	-1.345401	0.683709	3.187474
F	0.823953	0.514948	3.201489

2,3,4,5,6-$(CF_3)_5C_6O^-$

C	0.349773	-0.136196	-2.996868
C	0.195981	0.006940	-1.497157
C	0.190266	0.037376	1.331985
C	-1.011443	0.005597	-0.807491
C	1.462477	0.198131	-0.792572
C	1.407365	0.037911	0.659578
C	-1.040723	-0.056348	0.617191
C	-2.317574	0.259826	-1.579571
O	2.498277	0.529602	-1.379112

C	2.768928	-0.073948	1.312666
C	-2.300563	-0.502577	1.331539
C	0.165782	0.327735	2.842659
F	-0.715181	-0.742344	-3.589090
F	1.401698	-0.927580	-3.304704
F	0.536065	1.036031	-3.652238
F	-2.898419	-0.841193	-2.097865
F	-2.110345	1.122421	-2.602881
F	-3.248511	0.868596	-0.809078
F	-3.062266	-1.303710	0.538674
F	-3.131016	0.471320	1.782220
F	-2.010359	-1.273767	2.413833
F	0.318068	-0.752496	3.635119
F	-0.984201	0.932406	3.220734
F	1.137019	1.210150	3.177684
F	2.724787	-0.659140	2.540652
F	3.408279	1.110599	1.475468
F	3.592781	-0.866293	0.591270

2,3,4,5,6-$(CF_3)_5C_6OH$

C	0.305688	-0.011191	-3.022474
C	0.209633	0.009395	-1.495051
C	0.183639	0.040674	1.326643
C	-1.013986	-0.009373	-0.798287
C	1.416358	0.041842	-0.765287
C	1.404500	0.013192	0.645835
C	-1.027476	-0.098077	0.607647
C	-2.332258	0.238756	-1.567093
O	2.625845	0.183017	-1.322945
C	2.780744	-0.116696	1.319897
C	-2.301200	-0.562561	1.345225
C	0.150355	0.414183	2.828244
F	-0.701162	-0.643496	-3.619406
F	1.432081	-0.698366	-3.418328
F	0.425415	1.218617	-3.547771

F	-2.851999	-0.864699	-2.118651
F	-2.118861	1.141547	-2.548650
F	-3.265051	0.788537	-0.776451
F	-3.007024	-1.392869	0.547860
F	-3.125475	0.403078	1.762302
F	-1.956092	-1.301253	2.420385
F	0.338987	-0.612396	3.662378
F	-1.018894	0.996570	3.146535
F	1.093058	1.347326	3.073563
F	2.700026	-0.508462	2.599581
F	3.474036	1.033561	1.278469
F	3.510539	-1.067383	0.701583
H	2.627581	-0.016780	-2.267045

2,4,6-$Tf_3C_6H_2O^-$

O	-0.419322	-2.443814	0.000000
C	-0.588840	-1.223259	0.000000
C	-0.722625	1.655961	0.000000
C	-0.672667	-0.413745	1.214908
C	-0.672667	-0.413745	-1.214908
C	-0.707499	0.960445	-1.221120
C	-0.707499	0.960445	1.221120
S	-0.775630	-1.237799	2.793790
S	-0.775630	-1.237799	-2.793790
H	-0.737054	1.497740	-2.161693
H	-0.737054	1.497740	2.161693
S	-0.728016	3.406507	0.000000
C	1.117036	3.878631	0.000000
O	-0.630451	-0.218776	3.838407
O	-1.872903	-2.196609	2.850813
C	0.836685	-2.276271	2.927494
O	-1.872903	-2.196609	-2.850813
O	-0.630451	-0.218776	-3.838407
C	0.836685	-2.276271	-2.927494
O	-1.222042	3.914714	-1.278974

O	-1.222042	3.914714	1.278974
F	1.188778	-2.307771	4.222475
F	1.825368	-1.695654	2.236191
F	0.670975	-3.520681	2.508537
F	1.730200	3.393840	-1.086582
F	1.730200	3.393840	1.086582
F	1.235111	5.211429	0.000000
F	1.188778	-2.307771	-4.222475
F	0.670975	-3.520681	-2.508537
F	1.825368	-1.695654	-2.236191

2,4,6-$Tf_3C_6H_2OH$

O	2.393664	0.977154	0.371731
C	1.227034	0.424537	0.085027
C	-1.344385	-0.573467	-0.463065
C	0.894325	-0.935771	0.311803
C	0.220629	1.246001	-0.469404
C	-1.047805	0.762181	-0.739575
C	-0.382019	-1.428955	0.054173
S	2.112505	-2.085832	0.939978
S	0.559193	2.966152	-0.954552
H	-1.791974	1.422014	-1.171107
H	-0.616260	-2.468746	0.251978
S	-2.984837	-1.211159	-0.815126
H	2.981967	0.342699	0.835357
O	3.202005	-1.289156	1.525768
O	1.466543	-3.168036	1.658775
C	2.843697	-2.848065	-0.648738
O	1.780117	3.037803	-1.737439
O	-0.707762	3.505066	-1.432682
C	0.882526	3.860350	0.714123
O	-3.602637	-0.369834	-1.829200
O	-2.900849	-2.661797	-0.914039
C	-3.916579	-0.848992	0.807709
F	3.327056	-1.872590	-1.417781

F	1.890986	-3.501706	-1.307688
F	3.815050	-3.680171	-0.307097
F	-3.900736	0.462970	1.052206
F	-3.324684	-1.487466	1.819274
F	-5.168122	-1.267636	0.683825
F	2.159255	3.790105	1.057184
F	0.132176	3.293662	1.666566
F	0.527166	5.129601	0.564992

2,4,6-$(FSO_2)_3C_6H_2O^-$

C	1.483043	-0.002341	-0.127702
C	0.790935	1.218565	-0.107020
C	-0.583279	1.217558	-0.080404
C	-1.411982	0.002159	-0.016994
C	-0.587019	-1.215777	-0.080327
C	0.787172	-1.221106	-0.106896
H	1.333853	2.155522	-0.127032
H	1.327173	-2.159734	-0.126767
S	-1.382577	2.794793	-0.136958
O	-0.387132	3.850059	-0.067162
O	-2.453941	2.858367	-1.103062
S	-1.391272	-2.790510	-0.136970
O	-2.463070	-2.850554	-1.102826
O	-0.399117	-3.848891	-0.067611
S	3.222756	-0.005028	-0.135911
O	3.745303	-1.274152	-0.600857
O	3.749312	1.261773	-0.602666
O	-2.631269	0.003985	0.096274
F	-2.114822	2.815696	1.337122
F	-2.123240	-2.809439	1.337232
F	3.571681	-0.004358	1.493485

2,4,6-$(FSO_2)_3C_6H_2OH$

C	-1.490530	-0.157664	0.046510

C	-0.947865	1.115987	-0.022232
C	0.435012	1.255530	-0.089109
C	1.304140	0.136419	-0.104142
C	0.694741	-1.137765	-0.034180
C	-0.677876	-1.291317	0.052297
H	-1.586069	1.991967	-0.017297
H	-1.106586	-2.283893	0.124559
S	1.093971	2.904775	-0.115615
O	2.456694	2.844581	-0.617720
O	0.125146	3.851068	-0.592668
S	1.687803	-2.634296	-0.102424
O	0.816836	-3.760710	0.123678
O	2.638466	-2.583530	-1.180079
S	-3.260510	-0.345234	0.138551
O	-3.584451	-1.618028	0.730197
O	-3.857852	0.903740	0.539028
O	2.622176	0.195406	-0.165854
H	2.937165	1.108285	-0.325238
F	1.245675	3.169849	1.483634
F	2.530293	-2.424528	1.275372
F	-3.578923	-0.501724	-1.458756