Ionization Energies and Aqueous Redox Potentials of Organic Molecules: Comparison of DFT, Correlated ab initio Theory and Pair Natural Orbital Approaches

Supporting Information

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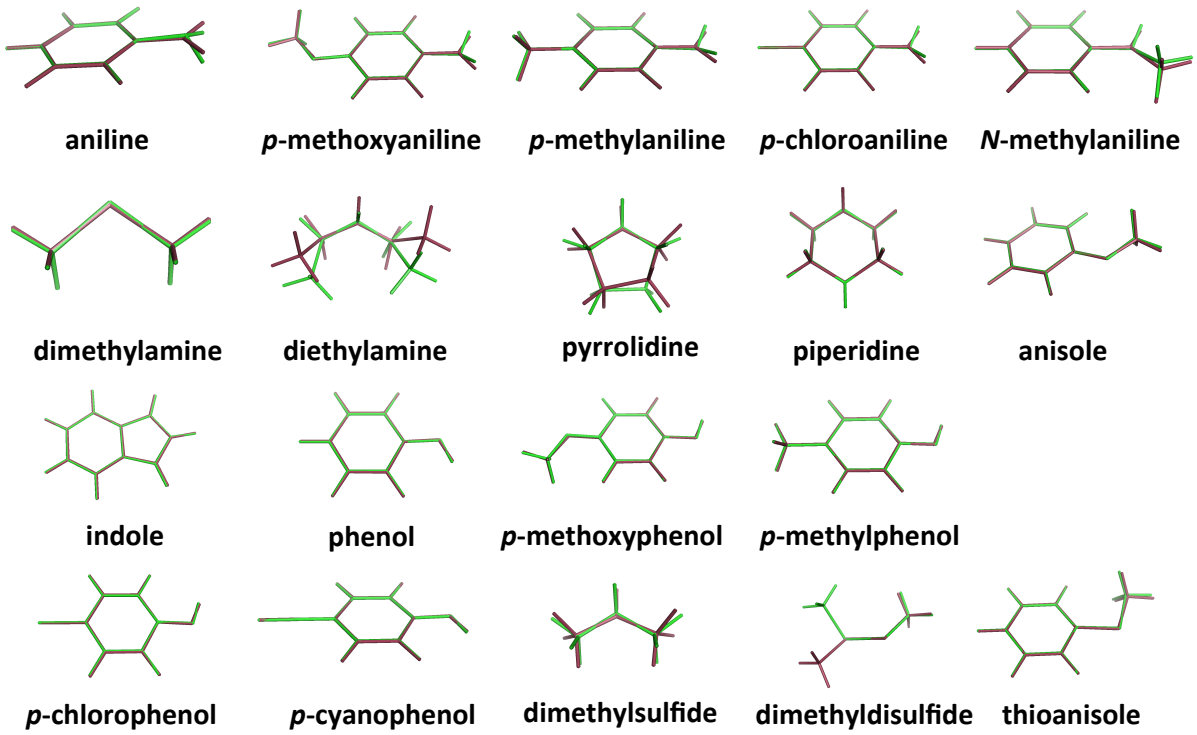

Figure S1. Overlays of gas-phase optimized reduced (green) and oxidized (red) forms.

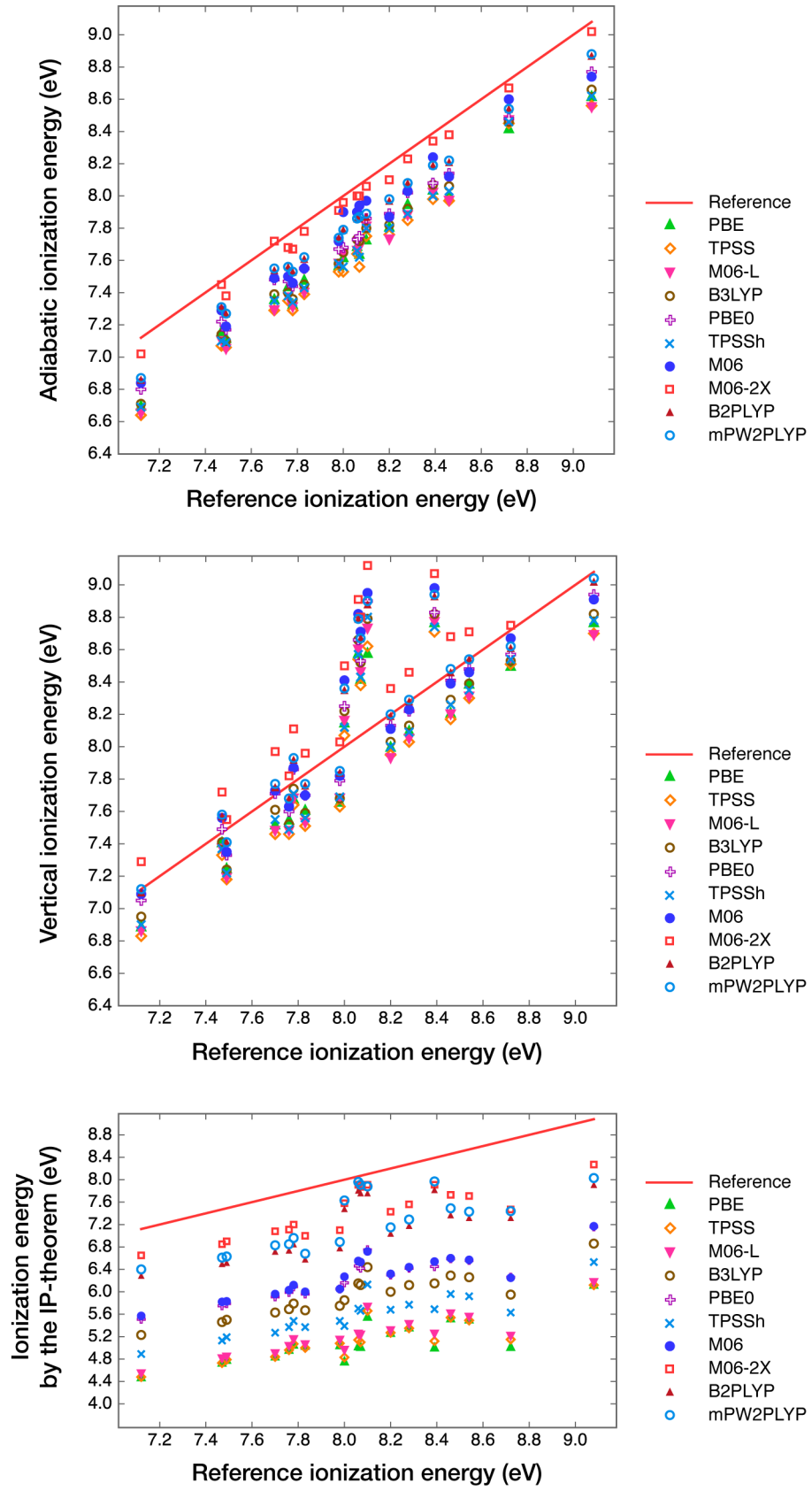

Figure S2. Plots of calculated ionization energies (eV) by ten density functionals compared with reference extrapolated CCSD(T)/cc-pVTZ energies, for adiabatic IEs, vertical IEs, and IEs estimated by HOMO energies ("IP-theorem" values).

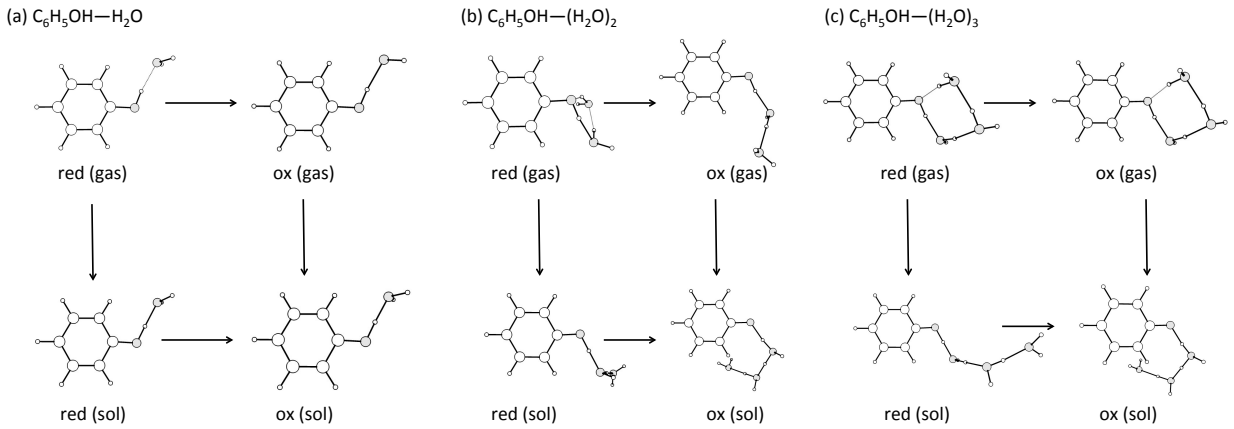

Figure S3. Optimized structures of three types of phenol-water clusters.

Table S1. RMSDs of internal coordinates from those of the gas-phase optimized reduced forms for bond lengths (Å), bond angles and dihedral angles (degrees).

	Oxidized			Reduced in solution			Oxidized in solution		
	Bonds	Bond angles	Dihedrals	Bonds	Bond angles	Dihedrals	Bonds	Bond angles	Dihedrals
aniline	0.02	3.13	65.91	0.01	2.74	65.93	0.02	3.02	65.91
p-methoxyaniline	0.14	5.17	51.44	0.14	4.44	51.45	0.14	4.92	51.44
p-methylaniline	0.05	4.03	54.39	0.04	3.62	54.16	0.05	3.92	54.33
N-methylaniline	0.02	2.04	12.23	0.17	6.02	120.19	0.17	6.65	120.09
dimethylamine	0.03	17.97	75.38	0.00	1.78	1.30	0.03	17.49	55.91
diethylamine	0.01	4.07	31.41	0.01	1.35	4.65	0.01	3.46	77.72
pyrrolidine	0.01	4.30	31.78	0.00	0.82	19.26	0.01	4.22	31.88
piperidine	0.02	2.83	21.47	0.00	0.69	1.74	0.02	2.84	36.68
anisole	0.02	1.65	0.01	0.00	0.22	0.08	0.02	1.45	0.00
indole	0.02	1.01	49.92	0.00	0.13	0.00	0.02	1.02	49.92
p-methoxyphenol	0.03	1.74	0.73	0.00	0.29	0.75	0.02	1.41	0.74
p-methylphenol	0.02	1.45	0.79	0.00	0.25	0.05	0.02	1.33	0.73
phenol	0.02	1.61	0.00	0.33	24.86	127.27	0.33	30.54	124.55
p-cyanophenol	0.02	1.33	48.20	0.00	0.34	8.09	0.02	1.32	44.44
dimethylsulfide	0.01	2.32	1.43	0.00	0.35	0.17	0.02	2.23	1.55
dimethyldisulfide	0.01	1.66	35.01	0.00	0.45	65.97	0.02	1.91	34.85
thioanisole	0.02	1.24	0.09	0.00	0.23	0.08	0.02	1.17	0.13
p-chloroaniline	0.03	2.99	66.03	0.01	2.64	66.04	0.03	2.90	66.03
p-chlorophenol	0.03	1.37	0.00	0.00	0.34	0.01	0.03	1.24	0.01

Table S2. Average and maximum errors in adiabatic ionization energies (eV) for selected wave function based methods and basis set combinations (reference values are obtained with CCSD(T)/cc-pVTZ combined with LPNO-CCSD[Q/5] extrapolation of the correlation energy).

Method	Basis set	MUE	MSE	UE_{max}	UE_{max} species
LPNO-CCSD	cc-pVDZ	0.43	-0.43	0.50	aniline
LPNO-CCSD	cc-pVTZ	0.21	-0.20	0.63	chlorophenol
LPNO-CCSD	cc-pVQZ	0.10	-0.10	0.14	methylaniline
LPNO-CCSD	cc-pV(D/T)Z	0.09	-0.06	0.49	chlorophenol
LPNO-CCSD	cc-pV[T/Q]Z	0.09	-0.06	0.51	chlorophenol
LPNO-CEPA	cc-pVDZ	0.47	-0.47	0.58	cyanophenol
LPNO-CEPA	cc-pVTZ	0.23	-0.23	0.68	chlorophenol
LPNO-CEPA	cc-pVQZ	0.10	-0.10	0.14	methylaniline
LPNO-CEPA	cc-pV(D/T)Z	0.11	-0.08	0.54	chlorophenol
LPNO-CEPA	cc-pV[T/Q]Z	0.12	-0.08	0.55	chlorophenol
LPNO-pCCSD	cc-pVDZ	0.41	-0.41	0.48	cyanophenol
LPNO-pCCSD	cc-pVTZ	0.17	-0.16	0.61	chlorophenol
LPNO-pCCSD	cc-pVQZ	0.06	-0.06	0.10	aniline
LPNO-pCCSD	cc-pV(D/T)Z	0.05	-0.02	0.46	chlorophenol
LPNO-pCCSD	cc-pV[T/Q]Z	0.05	-0.02	0.48	chlorophenol
F12-CCSD(T)	cc-pVDZ	0.13	-0.13	0.17	chloroaniline
CCSD	cc-pVDZ	0.45	-0.45	0.52	cyanophenol
CCSD	cc-pVTZ	0.22	-0.22	0.26	aniline
CCSD	cc-pV[D/T]Z	0.08	-0.08	0.12	aniline
CCSD(T)	cc-pVDZ	0.41	-0.41	0.47	cyanophenol
CCSD(T)	cc-pVTZ	0.14	-0.14	0.16	methoxyphenol
CCSD(T)	cc-pV[D/T]Z	0.02	0.02	0.05	thioanisole
MP2	cc-pVDZ	0.29	0.12	0.69	cyanophenol

MP2	cc-pVTZ	0.45	0.43	1.08	cyanophenol
MP2	cc-pVQZ	0.57	0.56	1.22	cyanophenol
MP2	cc-pV(D/T)Z	0.62	0.62	1.31	cyanophenol
MP2	cc-pV[T/Q]Z	0.65	0.65	1.39	aniline
RI-MP2	cc-pVTZ	0.45	0.43	1.08	cyanophenol
RI-MP2	cc-pV(D/T)Z	0.62	0.62	1.31	cyanophenol
RI-MP2	cc-pV(T/Q)Z	0.65	0.65	1.39	aniline
SCS-MP2	cc-pVDZ	0.23	0.03	0.56	cyanophenol
SCS-MP2	cc-pVTZ	0.35	0.34	0.95	cyanophenol
SCS-MP2	cc-pVQZ	0.46	0.46	1.09	cyanophenol
SCS-MP2	cc-pV(D/T)Z	0.52	0.52	1.17	cyanophenol
SCS-MP2	cc-pV[T/Q]Z	0.54	0.54	1.19	cyanophenol
OO-RI-MP2	cc-pVDZ	0.39	-0.39	0.47	cyanophenol
OO-RI-MP2	cc-pVTZ	0.11	-0.11	0.19	dimethyldisulfide
OO-RI-MP2	cc-pVQZ	0.04	-0.01	0.10	dimethyldisulfide
OO-RI-MP2	cc-pV(D/T)Z	0.06	0.06	0.13	phenol
OO-RI-MP2	cc-pV[T/Q]Z	0.07	0.06	0.13	pyrrolidine
F12-MP2	cc-pVTZ-F12	0.63	0.63	1.32	cyanophenol
HF	cc-pVTZ	1.42	-1.42	1.63	N_methylaniline

Table S3. Adiabatic ionization energies (eV) for the wave function methods listed in Table 3. Reference values are obtained with CCSD(T)/cc-pVTZ combined with LPNO-CCSD[Q/5] extrapolation of the correlation energy.

	CCSD(T)	LPNO-pCCSD	OO-MP2	CCSD	LPNO-CCSD	LPNO-CEPA	F12-CCSD(T)	SCS-MP2	F12-MP2	MP2	HF
	cc-pV[D/T]Z	cc-pV[T/Q]Z	cc-pV[T/Q]Z	cc-pV[D/T]Z	cc-pV[T/Q]Z	cc-pV[T/Q]Z	cc-pVDZ-F12	cc-pV[T/Q]Z	cc-pVTZ-F12	cc-pV[T/Q]Z	cc-pVTZ
aniline	7.77	7.72	7.65	7.64	7.68	7.64	7.64	8.59	8.64	9.15	6.14
p-methoxyaniline	7.13	7.13	7.15	7.04	7.06	7.01	6.98	7.75	7.75	7.85	5.79
p-methylaniline	7.51	7.46	7.58	7.38	7.40	7.36	7.36	8.18	8.32	8.31	5.95
N-methylaniline	7.49	7.44	7.56	7.36	7.40	7.36	7.34	8.34	8.48	8.47	5.84
dimethylamine	8.41	8.38	8.50	8.31	8.32	8.31	8.31	8.58	8.62	8.61	6.93
diethylamine	8.02	8.00	8.10	7.93	7.95	7.93	7.90	8.20	8.25	8.24	6.52
pyrrolidine	8.09	8.06	8.19	7.99	8.00	7.99	7.97	8.28	8.32	8.31	6.60
piperidine	8.09	8.10	8.11	8.02	8.07	8.03	7.96	8.32	8.35	8.34	6.75
anisole	8.30	8.28	8.38	8.18	8.22	8.18	8.16	8.88	9.04	9.03	6.76
indole	7.84	7.80	7.89	7.73	7.77	8.06	7.69	8.78	8.96	8.95	6.21
p-methoxyphenol	7.71	7.72	7.75	7.63	7.66	7.61	7.56	7.97	8.08	8.08	6.41
p-methylphenol	8.22	8.20	8.31	8.10	8.12	8.10	8.07	8.65	8.79	8.78	6.76
phenol	8.56	8.53	8.66	8.43	8.46	8.44	8.42	9.09	9.25	9.24	7.00
p-cyanophenol	9.11	9.07	9.14	9.00	9.04	8.97	8.93	10.27	10.40	10.40	7.53
dimethylsulfide	8.76	8.75	8.77	8.68	8.69	8.69	8.60	8.81	8.83	8.82	7.52
dimethyldisulfide	8.13	8.14	8.06	8.11	8.15	8.13	7.95	8.18	8.15	8.14	7.25
thioanisole	8.03	7.98	8.00	7.94	7.95	7.91	7.83	8.80	8.89	8.89	6.61
p-chloroaniline	7.79	7.98	7.81	7.67	7.95	7.91	7.61	8.56	8.68	8.68	6.31
p-chlorophenol	8.48	7.98	8.51	8.39	7.95	7.91	8.30	9.01	9.13	9.13	7.15
MUE	0.02	0.05	0.07	0.08	0.09	0.12	0.13	0.54	0.63	0.65	1.42
MSE	0.02	-0.02	0.06	-0.08	-0.06	-0.08	-0.13	0.54	0.63	0.65	-1.42

Table S4. Adiabatic ionization energies (eV) calculated by ten density functionals. MUE and MSE are calculated with respect to the reference values obtained with CCSD(T)/cc-pVTZ combined with LPNO-CCSD[Q/5] extrapolation.

	PBE	TPSS	M06-L	B3LYP	PBE0	TPSSh	M06	M06-	B2PLYP	mPW2PLYP	MUE	MSE	REF
aniline	7.44	7.35	7.37	7.40	7.47	7.38	7.50	7.68	7.56	7.56	0.29	-0.29	7.76
p-methoxyaniline	6.70	6.64	6.65	6.71	6.80	6.69	6.84	7.02	6.86	6.87	0.34	-0.34	7.12
p-methylaniline	7.12	7.06	7.05	7.10	7.17	7.09	7.19	7.38	7.27	7.27	0.32	-0.32	7.49
N-methylaniline	7.16	7.07	7.10	7.14	7.22	7.10	7.29	7.45	7.31	7.31	0.25	-0.25	7.47
dimethylamine	8.04	7.98	8.02	8.07	8.08	8.00	8.24	8.34	8.19	8.19	0.28	-0.28	8.39
diethylamine	7.62	7.53	7.64	7.65	7.68	7.56	7.90	7.96	7.79	7.79	0.29	-0.29	8.00
pyrrolidine	7.69	7.64	7.66	7.73	7.73	7.66	7.90	8.00	7.86	7.86	0.29	-0.29	8.06
piperidine	7.64	7.56	7.68	7.72	7.75	7.62	7.94	8.00	7.86	7.87	0.31	-0.31	8.07
anisole	7.95	7.85	7.88	7.92	8.02	7.89	8.03	8.23	8.08	8.08	0.29	-0.29	8.28
indole	7.48	7.39	7.40	7.45	7.55	7.43	7.55	7.78	7.61	7.62	0.30	-0.30	7.83
p-methoxyphenol	7.36	7.29	7.29	7.39	7.48	7.35	7.49	7.72	7.54	7.55	0.26	-0.25	7.70
p-methylphenol	7.81	7.76	7.73	7.82	7.89	7.80	7.87	8.10	7.97	7.98	0.33	-0.33	8.20
phenol	9.27	9.20	9.22	9.22	9.32	9.23	9.22	9.48	9.42	9.42	0.76	0.76	8.54
p-cyanophenol	8.62	8.56	8.55	8.66	8.77	8.62	8.74	9.02	8.87	8.88	0.35	-0.35	9.08
dimethylsulfide	8.42	8.45	8.47	8.46	8.48	8.46	8.60	8.67	8.54	8.54	0.21	-0.21	8.72
dimethyldisulfide	7.73	7.75	7.81	7.80	7.86	7.80	7.97	8.06	7.87	7.89	0.25	-0.25	8.10
thioanisole	7.57	7.53	7.58	7.58	7.67	7.58	7.72	7.91	7.74	7.74	0.32	-0.32	7.98
p-chloroaniline	7.33	7.29	7.31	7.36	7.44	7.34	7.46	7.67	7.53	7.53	0.35	-0.35	7.78
p-chlorophenol	8.00	7.97	7.97	8.06	8.14	8.03	8.12	8.38	8.21	8.22	0.35	-0.35	8.46
MUE	0.40	0.45	0.42	0.38	0.32	0.41	0.25	0.11	0.25	0.24			
MSE	-0.32	-0.38	-0.35	-0.30	-0.24	-0.34	-0.18	-0.01	-0.16	-0.15			

Table S5. Errors in ionization energies (eV) for Hartree–Fock, MP2, and OO-MP2, and singles amplitudes obtained from the latter.

	HF error	MP2 error	OO-MP2 error	singles amplitudes
aniline	-1.62	0.67	-0.08	0.08
p-methoxyaniline	-1.33	0.43	-0.17	0.12
p-methylaniline	-1.54	0.63	-0.09	0.09
N-methylaniline	-1.63	0.80	-0.09	0.09
dimethylamine	-1.46	0.04	-0.07	0.05
diethylamine	-1.48	0.07	-0.07	0.07
pyrrolidine	-1.46	0.08	-0.06	0.06
piperidine	-1.32	0.11	-0.11	0.09
anisole	-1.52	0.57	-0.07	0.12
indole	-1.62	0.92	-0.11	0.09
p-methoxyphenol	-1.29	0.18	-0.15	0.13
p-methylphenol	-1.44	0.41	-0.06	0.11
phenol	-1.54	0.51	-0.06	0.10
p-cyanophenol	-1.55	1.08	-0.13	0.14
dimethylsulfide	-1.20	-0.05	-0.10	0.03
dimethyldisulfide	-0.85	-0.11	-0.19	0.03
thioanisole	-1.37	0.72	-0.13	0.06
p-chloroaniline	-1.47	0.69	-0.15	0.10
p-chlorophenol	-1.31	0.47	-0.13	0.12

Table S6. Spin-squared expectation values for the oxidized form in the gas phase calculated by ten density functionals.

	PBE	TPSS	M06-L	B3LYP	PBE0	TPSSh	M06	M06-2X	B2PLYP	mPW2PLYP	MUE	MSE	REF
aniline	0.76	0.76	0.77	0.77	0.78	0.77	0.77	0.78	0.83	0.84	0.03	0.03	0.75
p-methoxyaniline	0.75	0.75	0.76	0.76	0.76	0.76	0.76	0.77	0.78	0.78	0.01	0.01	0.75
p-methylaniline	0.76	0.76	0.76	0.76	0.77	0.76	0.77	0.77	0.81	0.81	0.02	0.02	0.75
N-methylaniline	0.76	0.76	0.77	0.77	0.78	0.77	0.78	0.78	0.85	0.85	0.04	0.04	0.75
dimethylamine	0.75	0.75	0.76	0.75	0.76	0.76	0.76	0.76	0.76	0.76	0.01	0.01	0.75
diethylamine	0.75	0.75	0.76	0.75	0.76	0.76	0.76	0.76	0.76	0.76	0.01	0.01	0.75
pyrrolidine	0.75	0.75	0.76	0.75	0.76	0.76	0.76	0.76	0.76	0.76	0.01	0.01	0.75
piperidine	0.75	0.75	0.76	0.75	0.76	0.75	0.76	0.76	0.76	0.76	0.01	0.01	0.75
anisole	0.76	0.76	0.76	0.77	0.77	0.77	0.77	0.77	0.81	0.81	0.03	0.03	0.75
indole	0.76	0.76	0.76	0.76	0.77	0.76	0.77	0.77	0.81	0.81	0.02	0.02	0.75
p-methoxyphenol	0.75	0.75	0.75	0.76	0.76	0.76	0.76	0.77	0.78	0.78	0.01	0.01	0.75
p-methylphenol	0.75	0.76	0.76	0.76	0.76	0.76	0.76	0.77	0.78	0.78	0.01	0.01	0.75
phenol	0.76	0.76	0.76	0.76	0.77	0.77	0.77	0.77	0.80	0.81	0.02	0.02	0.75
p-cyanophenol	0.76	0.76	0.76	0.77	0.78	0.77	0.77	0.78	0.83	0.84	0.03	0.03	0.75
dimethylsulfide	0.75	0.76	0.76	0.75	0.76	0.76	0.75	0.75	0.76	0.76	0.01	0.01	0.75
dimethyldisulfide	0.75	0.75	0.75	0.76	0.76	0.76	0.75	0.75	0.76	0.76	0.01	0.01	0.75
thioanisole	0.76	0.76	0.76	0.76	0.77	0.76	0.77	0.77	0.81	0.82	0.02	0.02	0.75
p-chloroaniline	0.75	0.76	0.76	0.76	0.77	0.76	0.77	0.77	0.81	0.82	0.02	0.02	0.75
p-chlorophenol	0.75	0.75	0.76	0.76	0.76	0.76	0.76	0.77	0.78	0.78	0.01	0.01	0.75
MUE	0.00	0.01	0.01	0.01	0.02	0.01	0.01	0.02	0.04	0.04			
MSE	0.00	0.01	0.01	0.01	0.02	0.01	0.01	0.02	0.04	0.04			

Table S7. Spin-squared expectation values for the oxidized forms in aqueous solution calculated by ten density functionals.

	PBE	TPSS	M06-L	B3LYP	PBE0	TPSSh	M06	M06-2X	B2PLYP	mPW2PLYP	MUE	MSE	REF
aniline	0.76	0.77	0.77	0.77	0.79	0.78	0.78	0.78	0.85	0.86	0.04	0.04	0.75
p-methoxyaniline	0.75	0.76	0.76	0.76	0.77	0.76	0.76	0.77	0.80	0.80	0.02	0.02	0.75
p-methylaniline	0.76	0.76	0.77	0.77	0.78	0.77	0.77	0.77	0.83	0.84	0.03	0.03	0.75
N-methylaniline	0.76	0.77	0.77	0.78	0.79	0.78	0.78	0.78	0.86	0.87	0.04	0.04	0.75
dimethylamine	0.75	0.75	0.76	0.75	0.76	0.76	0.76	0.76	0.76	0.76	0.01	0.01	0.75
diethylamine	0.75	0.75	0.76	0.75	0.76	0.76	0.76	0.76	0.76	0.76	0.01	0.01	0.75
pyrrolidine	0.75	0.75	0.76	0.75	0.76	0.76	0.76	0.76	0.76	0.76	0.01	0.01	0.75
piperidine	0.75	0.75	0.76	0.75	0.76	0.76	0.76	0.76	0.76	0.76	0.01	0.01	0.75
anisole	0.76	0.76	0.76	0.77	0.77	0.77	0.77	0.77	0.81	0.81	0.03	0.03	0.75
indole	0.76	0.76	0.76	0.76	0.77	0.76	0.77	0.77	0.82	0.82	0.03	0.03	0.75
p-methoxyphenol	0.75	0.75	0.75	0.76	0.76	0.76	0.76	0.77	0.77	0.77	0.01	0.01	0.75
p-methylphenol	0.75	0.76	0.76	0.76	0.76	0.76	0.76	0.77	0.78	0.78	0.01	0.01	0.75
phenol	0.76	0.76	0.76	0.77	0.77	0.77	0.77	0.77	0.81	0.81	0.03	0.03	0.75
p-cyanophenol	0.76	0.76	0.77	0.77	0.78	0.77	0.78	0.78	0.84	0.85	0.04	0.04	0.75
dimethylsulfide	0.75	0.76	0.76	0.75	0.76	0.76	0.75	0.75	0.76	0.76	0.01	0.01	0.75
dimethyldisulfide	0.75	0.75	0.75	0.76	0.76	0.76	0.75	0.75	0.76	0.76	0.01	0.01	0.75
thioanisole	0.76	0.76	0.76	0.77	0.77	0.77	0.77	0.77	0.82	0.82	0.03	0.03	0.75
p-chloroaniline	0.76	0.76	0.77	0.77	0.78	0.77	0.77	0.78	0.85	0.85	0.04	0.04	0.75
p-chlorophenol	0.75	0.76	0.76	0.76	0.76	0.76	0.76	0.77	0.79	0.79	0.02	0.02	0.75
MUE	0.00	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.05	0.05			
MSE	0.00	0.01	0.01	0.01	0.02	0.02	0.02	0.02	0.05	0.05			

Table S8. Contributions (in eV) of zero point vibrational energy, thermal energy, and entropy.

	ZPVE	Thermal	Entropy
aniline	0.02	0.00	-0.01
p-methoxyaniline	0.03	0.00	-0.01
p-methylaniline	-0.12	-0.05	0.09
N-methylaniline	0.01	0.01	-0.04
dimethylamine	-0.06	0.00	-0.03
diethylamine	-0.03	-0.01	0.01
pyrrolidine	-0.05	0.00	-0.01
piperidine	-0.02	0.01	-0.03
anisole	-0.01	0.01	-0.04
indole	0.02	-0.01	-0.01
p-methoxyphenol	0.03	0.00	-0.01
p-methylphenol	0.00	0.00	-0.02
phenol	0.01	0.00	-0.02
p-cyanophenol	-0.01	0.00	-0.03
dimethylsulfide	-0.04	0.01	-0.06
dimethyldisulfide	0.00	0.01	-0.04
thioanisole	0.00	0.00	-0.02
p-chloroaniline	0.02	0.00	-0.01
p-chlorophenol	0.02	0.00	-0.02

Table S9. Vertical ionization energies (eV) calculated by ten density functionals. The zero point vibrational energy correction is not considered.

	PBE	TPSS	M06-L	B3LYP	PBE0	TPSSh	M06	M06-2X	B2PLYP	mPW2PLYP	MUE	MSE	REF
aniline	7.55	7.46	7.48	7.52	7.60	7.49	7.63	7.82	7.68	7.68	0.18	-0.17	7.76
p-methoxyaniline	6.89	6.83	6.86	6.95	7.05	6.90	7.09	7.29	7.10	7.12	0.15	-0.11	7.12
p-methylaniline	7.25	7.18	7.19	7.24	7.33	7.22	7.35	7.55	7.41	7.41	0.19	-0.18	7.49
N-methylaniline	7.41	7.33	7.37	7.41	7.49	7.37	7.56	7.72	7.57	7.58	0.10	0.01	7.47
dimethylamine	8.77	8.71	8.77	8.82	8.83	8.74	8.98	9.07	8.93	8.94	0.47	0.47	8.39
diethylamine	8.15	8.07	8.16	8.22	8.25	8.12	8.41	8.50	8.35	8.36	0.26	0.26	8.00
pyrrolidine	8.58	8.54	8.60	8.66	8.66	8.57	8.82	8.91	8.79	8.79	0.63	0.63	8.06
piperidine	8.42	8.38	8.46	8.52	8.53	8.43	8.71	8.80	8.67	8.67	0.49	0.49	8.07
anisole	8.10	8.03	8.05	8.13	8.22	8.09	8.23	8.46	8.28	8.29	0.13	-0.09	8.28
indole	7.61	7.51	7.53	7.59	7.70	7.56	7.70	7.96	7.76	7.77	0.19	-0.16	7.83
p-methoxyphenol	7.52	7.46	7.48	7.61	7.71	7.55	7.73	7.97	7.75	7.77	0.13	-0.05	7.70
p-methylphenol	8.00	7.95	7.93	8.03	8.13	8.00	8.11	8.36	8.19	8.20	0.14	-0.11	8.20
phenol	8.39	8.30	8.31	8.39	8.48	8.35	8.46	8.71	8.54	8.54	0.13	-0.09	8.54
p-cyanophenol	8.77	8.70	8.69	8.82	8.94	8.78	8.91	9.21	9.02	9.04	0.22	-0.19	9.08
dimethylsulfide	8.50	8.51	8.55	8.53	8.57	8.54	8.67	8.75	8.61	8.62	0.14	-0.14	8.72
dimethyldisulfide	8.58	8.62	8.73	8.79	8.90	8.80	8.95	9.12	8.88	8.90	0.73	0.73	8.10
thioanisole	7.66	7.63	7.68	7.68	7.79	7.69	7.82	8.03	7.84	7.85	0.22	-0.21	7.98
p-chloroaniline	7.68	7.64	7.68	7.74	7.86	7.71	7.87	8.11	7.92	7.93	0.12	0.03	7.78
p-chlorophenol	8.21	8.17	8.20	8.29	8.41	8.26	8.39	8.68	8.46	8.48	0.15	-0.11	8.46
MUE	0.25	0.28	0.29	0.26	0.21	0.26	0.24	0.32	0.20	0.20			
MSE	-0.05	-0.11	-0.07	0.00	0.07	-0.05	0.12	0.32	0.14	0.15			

Table S10. Ionization energies (eV) estimated by Koopmans' theorem for ten density functionals.

	PBE	TPSS	M06-L	B3LYP	PBE0	TPSSh	M06	M06-2X	B2PLYP	mPW2PLYP	MUE	MSE	REF
aniline	4.97	4.96	5.03	5.69	5.99	5.37	6.03	7.11	6.74	6.85	1.89	-1.89	7.76
p-methoxyaniline	4.48	4.48	4.54	5.23	5.51	4.89	5.57	6.65	6.29	6.40	1.72	-1.72	7.12
p-methylaniline	4.79	4.79	4.84	5.50	5.79	5.19	5.83	6.90	6.52	6.63	1.81	-1.81	7.49
N-methylaniline	4.74	4.73	4.81	5.46	5.75	5.13	5.82	6.85	6.50	6.61	1.83	-1.83	7.47
dimethylamine	5.01	5.12	5.25	6.15	6.45	5.69	6.54	7.91	7.82	7.97	2.00	-2.00	8.39
diethylamine	4.76	4.83	4.96	5.85	6.16	5.39	6.27	7.58	7.48	7.63	1.91	-1.91	8.00
pyrrolidine	5.03	5.14	5.25	6.15	6.46	5.70	6.55	7.91	7.81	7.96	1.66	-1.66	8.06
piperidine	5.02	5.10	5.23	6.12	6.42	5.66	6.53	7.87	7.76	7.91	1.71	-1.71	8.07
anisole	5.37	5.35	5.42	6.12	6.42	5.77	6.44	7.56	7.18	7.29	1.99	-1.99	8.28
indole	5.04	5.00	5.06	5.67	5.96	5.37	6.00	7.00	6.58	6.68	1.99	-1.99	7.83
p-methoxyphenol	4.85	4.84	4.90	5.63	5.91	5.27	5.96	7.08	6.72	6.83	1.90	-1.90	7.70
p-methylphenol	5.27	5.27	5.31	6.00	6.30	5.68	6.32	7.43	7.04	7.15	2.02	-2.02	8.20
phenol	5.51	5.49	5.55	6.26	6.56	5.92	6.57	7.71	7.32	7.43	2.11	-2.11	8.54
p-cyanophenol	6.13	6.12	6.17	6.86	7.16	6.53	7.17	8.27	7.91	8.03	2.04	-2.04	9.08
dimethylsulfide	5.02	5.15	5.21	5.95	6.26	5.63	6.25	7.47	7.32	7.44	2.55	-2.55	8.72
dimethyldisulfide	5.56	5.66	5.73	6.44	6.75	6.13	6.72	7.91	7.76	7.88	1.45	-1.45	8.10
thioanisole	5.05	5.08	5.14	5.75	6.05	5.48	6.05	7.10	6.78	6.89	2.04	-2.04	7.98
p-chloroaniline	5.06	5.07	5.15	5.79	6.09	5.48	6.12	7.20	6.85	6.96	1.80	-1.80	7.78
p-chlorophenol	5.53	5.54	5.61	6.29	6.59	5.96	6.60	7.73	7.37	7.49	1.99	-1.99	8.46
MUE	2.94	2.91	2.84	2.11	1.81	2.46	1.77	0.62	0.91	0.79			
MSE	-2.94	-2.91	-2.84	-2.11	-1.81	-2.46	-1.77	-0.62	-0.91	-0.79			

Table S11. Adiabatic ionization energies (eV) at 298K calculated by ten density functionals. The zero point vibrational energy correction and thermal and entropic corrections are obtained with TPSS.

	PBE	TPSS	M06-L	B3LYP	PBE0	TPSSh	M06	M06-2X	B2PLYP	mPW2PLYP
aniline	7.45	7.36	7.38	7.41	7.48	7.39	7.51	7.69	7.57	7.57
p-methoxyaniline	6.72	6.66	6.67	6.73	6.82	6.71	6.86	7.04	6.88	6.89
p-methylaniline	7.04	6.98	6.97	7.02	7.09	7.01	7.11	7.30	7.19	7.19
N-methylaniline	7.14	7.05	7.08	7.12	7.20	7.08	7.27	7.43	7.29	7.29
dimethylamine	7.95	7.89	7.93	7.98	7.99	7.91	8.15	8.25	8.10	8.10
diethylamine	7.59	7.50	7.61	7.62	7.65	7.53	7.87	7.93	7.76	7.76
pyrrolidine	7.63	7.58	7.60	7.67	7.67	7.60	7.84	7.94	7.80	7.80
piperidine	7.60	7.52	7.64	7.68	7.71	7.58	7.90	7.96	7.82	7.83
anisole	7.91	7.81	7.84	7.88	7.98	7.85	7.99	8.19	8.04	8.04
indole	7.48	7.39	7.40	7.45	7.55	7.43	7.55	7.78	7.61	7.62
p-methoxyphenol	7.38	7.31	7.31	7.41	7.50	7.37	7.51	7.74	7.56	7.57
p-methylphenol	7.79	7.74	7.71	7.80	7.87	7.78	7.85	8.08	7.95	7.96
phenol	9.26	9.19	9.21	9.21	9.31	9.22	9.21	9.47	9.41	9.41
p-cyanophenol	8.58	8.52	8.51	8.62	8.73	8.58	8.70	8.98	8.83	8.84
dimethylsulfide	8.33	8.36	8.38	8.37	8.39	8.37	8.51	8.58	8.45	8.45
dimethyldisulfide	7.70	7.72	7.78	7.77	7.83	7.77	7.94	8.03	7.84	7.86
thioanisole	7.55	7.51	7.56	7.56	7.65	7.56	7.70	7.89	7.72	7.72
p-chloroaniline	7.34	7.30	7.32	7.37	7.45	7.35	7.47	7.68	7.54	7.54
p-chlorophenol	8.00	7.97	7.97	8.06	8.14	8.03	8.12	8.38	8.21	8.22

Table S12. Difference in solvation energies (eV) of reduced and oxidized forms calculated by ten density functionals combined with SMD.

	PBE	TPSS	M06-L	B3LYP	PBE0	TPSSh	M06	M06-2X	B2PLYP	mPW2PLYP	MUE	MSE	REF
aniline	-2.40	-2.42	-2.42	-2.43	-2.40	-2.42	-2.40	-2.40	-2.43	-2.44	0.07	0.07	-2.49
p-methoxyaniline	-2.13	-2.14	-2.15	-2.16	-2.14	-2.15	-2.14	-2.15	-2.16	-2.16	0.06	-0.06	-2.09
p-methylaniline	-2.27	-2.29	-2.29	-2.31	-2.27	-2.29	-2.28	-2.28	-2.31	-2.32	0.02	0.01	-2.30
N-methylaniline	-2.33	-2.33	-2.34	-2.37	-2.34	-2.34	-2.35	-2.36	-2.37	-2.38	0.06	-0.06	-2.29
dimethylamine	-2.77	-2.76	-2.78	-2.79	-2.78	-2.77	-2.78	-2.77	-2.79	-2.79	0.03	0.03	-2.81
diethylamine	-2.47	-2.44	-2.48	-2.50	-2.49	-2.46	-2.50	-2.46	-2.49	-2.50	0.11	-0.11	-2.37
pyrrolidine	-2.58	-2.58	-2.60	-2.61	-2.60	-2.59	-2.60	-2.59	-2.61	-2.62	0.07	-0.07	-2.53
piperidine	-2.41	-2.41	-2.43	-2.45	-2.44	-2.43	-2.44	-2.43	-2.45	-2.47	0.05	-0.05	-2.39
anisole	-2.22	-2.21	-2.23	-2.24	-2.21	-2.21	-2.24	-2.21	-2.23	-2.23	0.12	0.12	-2.34
indole	-2.19	-2.19	-2.20	-2.22	-2.19	-2.19	-2.21	-2.20	-2.21	-2.21	0.20	0.20	-2.40
p-methoxyphenol	-2.18	-2.17	-2.19	-2.20	-2.18	-2.17	-2.21	-2.20	-2.20	-2.21	0.05	-0.05	-2.14
p-methylphenol	-2.26	-2.26	-2.27	-2.29	-2.25	-2.26	-2.28	-2.26	-2.28	-2.29	0.24	0.24	-2.51
phenol	-2.32	-2.31	-2.33	-2.33	-2.31	-2.31	-2.33	-2.30	-2.32	-2.32	0.44	0.44	-2.76
p-cyanophenol	-2.47	-2.47	-2.49	-2.53	-2.51	-2.49	-2.54	-2.54	-2.55	-2.56	0.57	0.57	-3.08
dimethylsulfide	-2.81	-2.80	-2.80	-2.83	-2.81	-2.80	-2.83	-2.83	-2.84	-2.84	0.23	0.23	-3.05
dimethyldisulfide	-2.51	-2.49	-2.49	-2.52	-2.50	-2.49	-2.52	-2.52	-2.53	-2.53	0.39	-0.39	-2.12
thioanisole	-2.21	-2.19	-2.20	-2.23	-2.20	-2.19	-2.22	-2.21	-2.23	-2.23	0.01	0.00	-2.21
p-chloroaniline	-2.35	-2.37	-2.38	-2.40	-2.37	-2.38	-2.37	-2.39	-2.40	-2.41	0.39	0.39	-2.77
p-chlorophenol	-2.33	-2.33	-2.35	-2.37	-2.34	-2.34	-2.36	-2.35	-2.36	-2.37	1.11	1.11	-3.46
MUE	0.22	0.22	0.22	0.22	0.23	0.22	0.22	0.22	0.22	0.22			
MSE	0.15	0.16	0.14	0.12	0.15	0.15	0.13	0.14	0.12	0.12			

Table S13. Differences in solvation energies (eV) of reduced and oxidized form calculated by ten density functionals combined with COSMO.

	PBE	TPSS	M06-L	B3LYP	PBE0	TPSSh	M06	M06-2X	B2PLYP	mPW2PLYP	MUE	MSE	REF
aniline	-2.21	-2.23	-2.24	-2.23	-2.22	-2.23	-2.22	-2.22	-2.24	-2.24	0.26	0.26	-2.49
p-methoxyaniline	-1.99	-2.00	-2.02	-2.01	-2.00	-2.01	-2.00	-2.00	-2.01	-2.01	0.08	0.08	-2.09
p-methylaniline	-2.10	-2.12	-2.13	-2.13	-2.11	-2.12	-2.11	-2.11	-2.13	-2.14	0.18	0.18	-2.30
N-methylaniline	-2.14	-2.15	-2.16	-2.16	-2.15	-2.15	-2.15	-2.15	-2.17	-2.17	0.14	0.14	-2.29
dimethylamine	-2.67	-2.67	-2.69	-2.69	-2.69	-2.68	-2.69	-2.68	-2.69	-2.70	0.13	0.13	-2.81
diethylamine	-2.41	-2.38	-2.42	-2.43	-2.43	-2.39	-2.44	-2.40	-2.42	-2.43	0.04	-0.04	-2.37
pyrrolidine	-2.49	-2.49	-2.50	-2.51	-2.51	-2.50	-2.51	-2.50	-2.51	-2.52	0.03	0.03	-2.53
piperidine	-2.34	-2.35	-2.36	-2.38	-2.38	-2.36	-2.37	-2.37	-2.38	-2.39	0.02	0.02	-2.39
anisole	-2.04	-2.04	-2.06	-2.05	-2.04	-2.04	-2.06	-2.04	-2.05	-2.05	0.29	0.29	-2.34
indole	-2.00	-2.01	-2.02	-2.03	-2.01	-2.01	-2.03	-2.02	-2.02	-2.02	0.38	0.38	-2.40
p-methoxyphenol	-1.97	-1.96	-1.99	-1.98	-1.97	-1.97	-1.99	-1.97	-1.98	-1.98	0.16	0.16	-2.14
p-methylphenol	-2.09	-2.09	-2.11	-2.11	-2.09	-2.09	-2.11	-2.09	-2.10	-2.11	0.41	0.41	-2.51
phenol	-1.11	-1.08	-1.09	-1.13	-1.10	-1.09	-1.20	-1.13	-1.08	-1.08	1.65	1.65	-2.76
p-cyanophenol	-2.23	-2.24	-2.26	-2.28	-2.27	-2.25	-2.29	-2.30	-2.30	-2.30	0.81	0.81	-3.08
dimethylsulfide	-2.52	-2.51	-2.52	-2.52	-2.52	-2.51	-2.53	-2.53	-2.53	-2.53	0.53	0.53	-3.05
dimethyldisulfide	-2.23	-2.23	-2.24	-2.24	-2.24	-2.23	-2.25	-2.24	-2.25	-2.25	0.12	-0.12	-2.12
thioanisole	-1.98	-1.98	-1.99	-1.99	-1.98	-1.98	-2.00	-1.99	-2.00	-2.00	0.22	0.22	-2.21
p-chloroaniline	-2.13	-2.16	-2.17	-2.17	-2.16	-2.17	-2.15	-2.17	-2.17	-2.18	0.61	0.61	-2.77
p-chlorophenol	-2.11	-2.12	-2.14	-2.14	-2.13	-2.12	-2.14	-2.13	-2.13	-2.14	1.33	1.33	-3.46
MUE	0.40	0.40	0.39	0.38	0.39	0.39	0.38	0.39	0.38	0.38			
MSE	0.39	0.38	0.37	0.36	0.37	0.38	0.36	0.37	0.37	0.36			

Table S14. Solvation energies (eV) of reduced form and statistical errors calculated for ten density functionals combined with SMD.

	PBE	TPSS	M06-L	B3LYP	PBE0	TPSSh	M06	M06-[illegible]	B2PLY[illegible]	mPW2PLY[illegible]	MUE	MSE	REF
aniline	-0.17	-0.15	-0.13	-0.15	-0.19	-0.16	-0.16	-0.18	-0.15	-0.15	0.08	0.08	-0.24
p-methoxyaniline	-0.18	-0.17	-0.13	-0.18	-0.20	-0.18	-0.17	-0.20	-0.17	-0.18	0.15	0.15	-0.33
p-methylaniline	-0.14	-0.12	-0.09	-0.12	-0.16	-0.12	-0.13	-0.15	-0.12	-0.12	0.14	0.14	-0.27
N-methylaniline	-0.06	-0.05	-0.02	-0.04	-0.07	-0.05	-0.03	-0.04	-0.03	-0.03	0.16	0.16	-0.20
dimethylamine	-0.20	-0.20	-0.19	-0.20	-0.21	-0.21	-0.20	-0.22	-0.22	-0.22	0.04	-0.04	-0.17
diethylamine	-0.17	-0.18	-0.18	-0.17	-0.19	-0.18	-0.18	-0.21	-0.19	-0.19	0.01	0.00	-0.18
pyrrolidine	-0.23	-0.23	-0.22	-0.23	-0.24	-0.23	-0.23	-0.25	-0.24	-0.24	0.01	0.01	-0.24
piperidine	-0.20	-0.21	-0.20	-0.21	-0.22	-0.21	-0.21	-0.23	-0.22	-0.22	0.02	0.02	-0.23
anisole	-0.06	-0.06	-0.02	-0.06	-0.07	-0.06	-0.04	-0.09	-0.07	-0.07	0.05	0.05	-0.11
indole	-0.21	-0.19	-0.16	-0.19	-0.23	-0.20	-0.18	-0.23	-0.20	-0.21	0.05	0.05	-0.25
p-methoxyphenol	-0.24	-0.24	-0.20	-0.25	-0.26	-0.25	-0.23	-0.28	-0.26	-0.26	0.02	0.00	-0.25
p-methylphenol	-0.18	-0.17	-0.14	-0.18	-0.20	-0.18	-0.17	-0.21	-0.19	-0.19	0.08	0.08	-0.26
phenol	-0.20	-0.19	-0.16	-0.20	-0.22	-0.20	-0.19	-0.23	-0.21	-0.21	0.09	0.09	-0.29
p-cyanophenol	-0.36	-0.36	-0.35	-0.38	-0.38	-0.37	-0.36	-0.38	-0.36	-0.37	0.08	0.08	-0.45
dimethylsulfide	-0.05	-0.05	-0.04	-0.05	-0.06	-0.06	-0.03	-0.05	-0.05	-0.05	0.02	0.02	-0.07
dimethyldisulfide	-0.08	-0.08	-0.07	-0.08	-0.09	-0.09	-0.07	-0.09	-0.08	-0.09	0.01	-0.01	-0.07
thioanisole	-0.08	-0.07	-0.05	-0.07	-0.10	-0.08	-0.06	-0.10	-0.08	-0.08	0.04	0.04	-0.12
p-chloroaniline	-0.19	-0.18	-0.16	-0.18	-0.21	-0.18	-0.18	-0.20	-0.17	-0.17	0.08	0.08	-0.26
p-chlorophenol	-0.21	-0.21	-0.19	-0.22	-0.23	-0.22	-0.21	-0.24	-0.22	-0.23	0.17	0.17	-0.39
MUE	0.07	0.07	0.09	0.07	0.05	0.07	0.07	0.06	0.07	0.07			
MSE	0.06	0.07	0.09	0.06	0.04	0.06	0.07	0.04	0.06	0.06			

Table S15. Solvation energies (eV) of reduced forms and statistical errors calculated for ten density functionals combined with COSMO.

	PBE	TPSS	M06-L	B3LYP	PBE0	TPSSh	M06	M06-2X	B2PLYP	mPW2PLYP	MUE	MSE	REF
aniline	-0.25	-0.23	-0.21	-0.24	-0.26	-0.24	-0.24	-0.26	-0.23	-0.24	0.01	0.00	-0.24
p-methoxyaniline	-0.29	-0.27	-0.24	-0.28	-0.30	-0.28	-0.28	-0.30	-0.28	-0.28	0.05	0.05	-0.33
p-methylaniline	-0.24	-0.22	-0.20	-0.22	-0.25	-0.22	-0.23	-0.24	-0.22	-0.22	0.04	0.04	-0.27
N-methylaniline	-0.16	-0.14	-0.12	-0.14	-0.16	-0.14	-0.13	-0.13	-0.12	-0.12	0.06	0.06	-0.20
dimethylamine	-0.13	-0.13	-0.13	-0.13	-0.14	-0.14	-0.13	-0.15	-0.14	-0.14	0.03	0.03	-0.17
diethylamine	-0.13	-0.13	-0.13	-0.12	-0.14	-0.13	-0.13	-0.15	-0.14	-0.14	0.05	0.05	-0.18
pyrrolidine	-0.13	-0.13	-0.13	-0.13	-0.14	-0.13	-0.13	-0.15	-0.14	-0.14	0.10	0.10	-0.24
piperidine	-0.13	-0.13	-0.12	-0.13	-0.13	-0.13	-0.13	-0.14	-0.13	-0.13	0.10	0.10	-0.23
anisole	-0.19	-0.19	-0.15	-0.19	-0.20	-0.19	-0.17	-0.21	-0.20	-0.20	0.08	-0.08	-0.11
indole	-0.30	-0.29	-0.27	-0.29	-0.32	-0.30	-0.28	-0.32	-0.31	-0.31	0.05	-0.05	-0.25
p-methoxyphenol	-0.33	-0.34	-0.30	-0.34	-0.34	-0.34	-0.32	-0.36	-0.35	-0.35	0.09	-0.09	-0.25
p-methylphenol	-0.27	-0.26	-0.24	-0.27	-0.28	-0.27	-0.26	-0.29	-0.28	-0.28	0.01	-0.01	-0.26
phenol	-0.27	-0.27	-0.24	-0.27	-0.28	-0.27	-0.26	-0.29	-0.28	-0.28	0.02	0.02	-0.29
p-cyanophenol	-0.47	-0.47	-0.45	-0.48	-0.48	-0.47	-0.46	-0.48	-0.47	-0.47	0.02	-0.02	-0.45
dimethylsulfide	-0.14	-0.14	-0.13	-0.14	-0.15	-0.14	-0.13	-0.14	-0.14	-0.14	0.07	-0.07	-0.07
dimethyldisulfide	-0.16	-0.16	-0.15	-0.16	-0.17	-0.16	-0.15	-0.17	-0.16	-0.16	0.09	-0.09	-0.07
thioanisole	-0.20	-0.19	-0.17	-0.19	-0.21	-0.20	-0.18	-0.22	-0.20	-0.20	0.08	-0.08	-0.12
p-chloroaniline	-0.28	-0.26	-0.25	-0.27	-0.29	-0.27	-0.27	-0.28	-0.26	-0.26	0.01	-0.01	-0.26
p-chlorophenol	-0.28	-0.28	-0.26	-0.29	-0.30	-0.29	-0.28	-0.30	-0.29	-0.29	0.10	0.10	-0.39
MUE	0.06	0.06	0.06	0.06	0.06	0.06	0.05	0.06	0.06	0.06			
MSE	0.00	0.01	0.03	0.01	-0.01	0.00	0.01	-0.01	0.00	0.00			

Table S16. Solvation energies (eV) of the oxidized forms and statistical errors calculated for ten density functionals combined with SMD.

	PBE	TPSS	M06-L	B3LYP	PBE0	TPSSh	M06	M06-2X	B2PLYP	mPW2PLYP	MUE	MSE	REF
aniline	-2.57	-2.57	-2.55	-2.58	-2.59	-2.57	-2.56	-2.58	-2.58	-2.59	0.16	0.16	-2.73
p-methoxyaniline	-2.32	-2.31	-2.29	-2.34	-2.34	-2.32	-2.32	-2.35	-2.33	-2.34	0.09	0.09	-2.42
p-methylaniline	-2.41	-2.41	-2.39	-2.43	-2.43	-2.42	-2.41	-2.43	-2.43	-2.44	0.15	0.15	-2.57
N-methylaniline	-2.39	-2.38	-2.37	-2.40	-2.41	-2.39	-2.38	-2.40	-2.40	-2.41	0.10	0.10	-2.49
dimethylamine	-2.97	-2.97	-2.97	-2.99	-2.99	-2.98	-2.98	-2.99	-3.00	-3.01	0.01	-0.01	-2.98
diethylamine	-2.65	-2.62	-2.66	-2.67	-2.68	-2.64	-2.68	-2.67	-2.68	-2.69	0.11	-0.11	-2.55
pyrrolidine	-2.81	-2.81	-2.82	-2.84	-2.84	-2.82	-2.83	-2.84	-2.85	-2.86	0.06	-0.06	-2.77
piperidine	-2.61	-2.62	-2.63	-2.66	-2.66	-2.64	-2.65	-2.66	-2.67	-2.68	0.03	-0.03	-2.62
anisole	-2.28	-2.27	-2.25	-2.30	-2.28	-2.27	-2.28	-2.30	-2.30	-2.31	0.17	0.17	-2.45
indole	-2.39	-2.38	-2.36	-2.41	-2.42	-2.39	-2.39	-2.43	-2.41	-2.42	0.25	0.25	-2.65
p-methoxyphenol	-2.41	-2.41	-2.39	-2.45	-2.44	-2.42	-2.44	-2.48	-2.46	-2.47	0.05	-0.05	-2.39
p-methylphenol	-2.44	-2.43	-2.42	-2.46	-2.45	-2.44	-2.45	-2.47	-2.47	-2.47	0.32	0.32	-2.77
phenol	-2.52	-2.51	-2.50	-2.53	-2.52	-2.51	-2.52	-2.53	-2.53	-2.53	0.53	0.53	-3.05
p-cyanophenol	-2.83	-2.84	-2.84	-2.91	-2.89	-2.86	-2.90	-2.92	-2.92	-2.93	0.65	0.65	-3.53
dimethylsulfide	-2.85	-2.85	-2.84	-2.88	-2.87	-2.85	-2.87	-2.88	-2.89	-2.89	0.25	0.25	-3.12
dimethyldisulfide	-2.58	-2.57	-2.56	-2.60	-2.59	-2.58	-2.59	-2.61	-2.61	-2.61	0.40	-0.40	-2.19
thioanisole	-2.28	-2.27	-2.25	-2.30	-2.30	-2.27	-2.28	-2.31	-2.30	-2.31	0.04	0.04	-2.33
p-chloroaniline	-2.54	-2.55	-2.53	-2.58	-2.58	-2.56	-2.55	-2.58	-2.57	-2.58	0.46	0.46	-3.02
p-chlorophenol	-2.54	-2.55	-2.54	-2.59	-2.57	-2.56	-2.57	-2.59	-2.58	-2.59	1.27	1.27	-3.84
MUE	0.27	0.27	0.28	0.26	0.26	0.27	0.27	0.26	0.26	0.26			
MSE	0.21	0.22	0.23	0.19	0.19	0.21	0.20	0.18	0.18	0.18			

Table S17. Solvation energies (eV) of the oxidized forms and statistical errors calculated for ten density functionals combined with COSMO.

	PBE	TPSS	M06-L	B3LYP	PBE0	TPSSh	M06	M06-2X	B2PLYP	mPW2PLYP	MUE	MSE	REF
aniline	-2.47	-2.46	-2.45	-2.47	-2.49	-2.47	-2.46	-2.48	-2.47	-2.48	0.26	0.26	-2.73
p-methoxyaniline	-2.28	-2.27	-2.26	-2.29	-2.30	-2.28	-2.28	-2.30	-2.29	-2.29	0.14	0.14	-2.42
p-methylaniline	-2.34	-2.34	-2.33	-2.35	-2.36	-2.35	-2.34	-2.36	-2.35	-2.36	0.22	0.22	-2.57
N-methylaniline	-2.30	-2.29	-2.28	-2.30	-2.31	-2.30	-2.28	-2.28	-2.29	-2.30	0.20	0.20	-2.49
dimethylamine	-2.80	-2.80	-2.81	-2.82	-2.83	-2.81	-2.82	-2.83	-2.83	-2.84	0.16	0.16	-2.98
diethylamine	-2.53	-2.51	-2.56	-2.56	-2.57	-2.53	-2.57	-2.56	-2.56	-2.57	0.02	0.00	-2.55
pyrrolidine	-2.62	-2.62	-2.63	-2.64	-2.65	-2.63	-2.64	-2.64	-2.65	-2.66	0.13	0.13	-2.77
piperidine	-2.47	-2.47	-2.49	-2.50	-2.51	-2.49	-2.50	-2.51	-2.52	-2.53	0.12	0.12	-2.62
anisole	-2.23	-2.22	-2.21	-2.24	-2.24	-2.23	-2.23	-2.24	-2.24	-2.25	0.22	0.22	-2.45
indole	-2.31	-2.30	-2.29	-2.32	-2.34	-2.31	-2.31	-2.34	-2.32	-2.33	0.33	0.33	-2.65
p-methoxyphenol	-2.30	-2.30	-2.29	-2.32	-2.32	-2.31	-2.31	-2.33	-2.32	-2.33	0.08	0.08	-2.39
p-methylphenol	-2.36	-2.35	-2.34	-2.37	-2.37	-2.36	-2.37	-2.38	-2.38	-2.38	0.40	0.40	-2.77
phenol	-1.38	-1.35	-1.33	-1.40	-1.38	-1.36	-1.46	-1.42	-1.35	-1.36	1.67	1.67	-3.05
p-cyanophenol	-2.70	-2.71	-2.71	-2.75	-2.75	-2.73	-2.75	-2.77	-2.77	-2.78	0.79	0.79	-3.53
dimethylsulfide	-2.65	-2.65	-2.65	-2.66	-2.66	-2.65	-2.66	-2.67	-2.67	-2.67	0.46	0.46	-3.12
dimethyldisulfide	-2.39	-2.38	-2.38	-2.40	-2.40	-2.39	-2.39	-2.41	-2.40	-2.41	0.21	-0.21	-2.19
thioanisole	-2.18	-2.17	-2.16	-2.19	-2.20	-2.18	-2.18	-2.20	-2.20	-2.20	0.14	0.14	-2.33
p-chloroaniline	-2.41	-2.42	-2.41	-2.44	-2.45	-2.43	-2.42	-2.45	-2.43	-2.44	0.59	0.59	-3.02
p-chlorophenol	-2.40	-2.40	-2.40	-2.43	-2.42	-2.41	-2.42	-2.43	-2.42	-2.43	1.42	1.42	-3.84
MUE	0.41	0.41	0.42	0.39	0.39	0.40	0.40	0.39	0.39	0.39			
MSE	0.39	0.39	0.39	0.37	0.36	0.38	0.37	0.36	0.37	0.36			

Table S18. Redox potentials obtained for selected wave function methods.

	CCSD(T)	LPNO-pCCSD	OO-MP2	CCSD	LPNO-CCSD	LPNO-CEPA	F12-CCSD(T)	SCS-MP2	F12-MP2	MP2	HF
	cc-pV[D/T]Z	cc-pV[T/Q]Z	cc-pV[T/Q]Z	cc-pV[D/T]Z	cc-pV[T/Q]Z	cc-pV[T/Q]Z	cc-pVDZ-F12	cc-pV[T/Q]Z	cc-pVTZ-F12	cc-pV[T/Q]Z	cc-pVTZ
aniline	1.08	1.03	0.96	0.95	0.99	0.95	0.95	1.90	1.95	2.46	-0.55
p-methoxyaniline	0.73	0.73	0.75	0.64	0.66	0.61	0.58	1.35	1.35	1.45	-0.61
p-methylaniline	0.86	0.81	0.93	0.73	0.75	0.71	0.71	1.53	1.67	1.66	-0.70
N-methylaniline	0.86	0.81	0.93	0.73	0.77	0.73	0.71	1.71	1.85	1.84	-0.79
dimethylamine	1.28	1.25	1.37	1.18	1.19	1.18	1.18	1.45	1.49	1.48	-0.20
diethylamine	1.27	1.25	1.35	1.18	1.20	1.18	1.15	1.45	1.50	1.49	-0.23
pyrrolidine	1.17	1.14	1.27	1.07	1.08	1.07	1.05	1.36	1.40	1.39	-0.32
piperidine	1.36	1.37	1.38	1.29	1.34	1.30	1.23	1.59	1.62	1.61	0.02
anisole	1.77	1.75	1.85	1.65	1.69	1.65	1.63	2.35	2.51	2.50	0.23
indole	1.37	1.33	1.42	1.26	1.30	1.59	1.22	2.31	2.49	2.48	-0.26
p-methoxyphenol	1.28	1.29	1.32	1.20	1.23	1.18	1.13	1.54	1.65	1.65	-0.02
p-methylphenol	1.66	1.64	1.75	1.54	1.56	1.54	1.51	2.09	2.23	2.22	0.20
phenol	1.96	1.93	2.06	1.83	1.86	1.84	1.82	2.49	2.65	2.64	0.40
p-cyanophenol	2.32	2.28	2.35	2.21	2.25	2.18	2.14	3.48	3.61	3.61	0.74
dimethylsulfide	1.59	1.58	1.60	1.51	1.52	1.52	1.43	1.64	1.66	1.65	0.35
dimethyldisulfide	1.33	1.34	1.26	1.31	1.35	1.33	1.15	1.38	1.35	1.34	0.45
thioanisole	1.54	1.49	1.51	1.45	1.46	1.42	1.34	2.31	2.40	2.40	0.12
p-chloroaniline	1.15	1.34	1.17	1.03	1.31	1.27	0.97	1.92	2.04	2.04	-0.33
p-chlorophenol	1.87	1.37	1.90	1.78	1.34	1.30	1.69	2.40	2.52	2.52	0.54
MUE	0.28	0.28	0.30	0.29	0.28	0.30	0.30	0.69	0.78	0.80	1.29
MSE	0.16	0.12	0.19	0.06	0.07	0.06	0.01	0.67	0.76	0.79	-1.29

Table S19. Redox potentials calculated for ten density functionals combined with SMD.

	PBE	TPSS	M06-L	B3LYP	PBE0	TPSSh	M06	M06-2X	B2PLYP	mPW2PLYP	MUE	MSE	REF
aniline	0.76	0.66	0.68	0.70	0.80	0.69	0.83	1.01	0.86	0.85	0.24	-0.24	1.02
p-methoxyaniline	0.31	0.24	0.24	0.29	0.40	0.28	0.43	0.61	0.44	0.45	0.42	-0.42	0.79
p-methylaniline	0.48	0.40	0.40	0.43	0.54	0.43	0.55	0.74	0.60	0.59	0.40	-0.40	0.92
N-methylaniline	0.53	0.44	0.46	0.47	0.58	0.47	0.64	0.79	0.64	0.63	0.38	-0.38	0.95
dimethylamine	0.91	0.85	0.87	0.91	0.93	0.86	1.09	1.20	1.03	1.03	0.30	-0.30	1.27
diethylamine	0.84	0.78	0.85	0.84	0.87	0.79	1.09	1.19	0.99	0.98	0.44	-0.44	1.36
pyrrolidine	0.77	0.72	0.72	0.78	0.80	0.73	0.95	1.07	0.91	0.90	0.42	-0.42	1.26
piperidine	0.91	0.83	0.93	0.95	0.99	0.87	1.17	1.25	1.08	1.08	0.33	-0.33	1.34
anisole	1.41	1.32	1.33	1.36	1.49	1.37	1.47	1.70	1.53	1.53	0.19	-0.17	1.62
indole	1.02	0.92	0.92	0.95	1.09	0.96	1.06	1.30	1.13	1.12	0.10	-0.03	1.08
p-methoxyphenol	0.92	0.86	0.84	0.93	1.04	0.92	1.02	1.26	1.07	1.08	0.24	-0.24	1.23
p-methylphenol	1.25	1.20	1.15	1.23	1.34	1.24	1.29	1.54	1.39	1.39	0.11	-0.08	1.38
phenol	2.66	2.60	2.59	2.60	2.73	2.63	2.60	2.89	2.81	2.80	1.19	1.19	1.50
p-cyanophenol	1.83	1.76	1.74	1.81	1.94	1.81	1.88	2.16	2.00	2.00	0.18	0.18	1.71
dimethylsulfide	1.25	1.28	1.29	1.26	1.30	1.30	1.39	1.47	1.33	1.33	0.09	-0.07	1.39
dimethyldisulfide	0.91	0.95	1.01	0.97	1.04	1.00	1.14	1.23	1.03	1.05	0.65	-0.65	1.68
thioanisole	1.06	1.04	1.07	1.06	1.17	1.09	1.20	1.40	1.21	1.22	0.30	-0.30	1.45
p-chloroaniline	0.72	0.65	0.66	0.70	0.80	0.69	0.82	1.01	0.86	0.86	0.11	0.10	0.68
p-chlorophenol	1.39	1.36	1.34	1.41	1.52	1.41	1.48	1.75	1.57	1.58	0.83	0.83	0.65
MUE	0.39	0.43	0.41	0.40	0.36	0.41	0.30	0.28	0.33	0.33			
MSE	-0.18	-0.23	-0.22	-0.19	-0.10	-0.20	-0.06	0.12	-0.04	-0.04			

Table S20. Redox potentials calculated for ten density functionals combined with COSMO.

	PBE	TPSS	M06-L	B3LYP	PBE0	TPSSh	M06	M06-2X	B2PLYP	mPW2PLYP	MUE	MSE	REF
aniline	0.95	0.85	0.86	0.89	0.98	0.87	1.01	1.19	1.05	1.04	0.10	-0.05	1.02
p-methoxyaniline	0.46	0.38	0.38	0.45	0.54	0.42	0.58	0.75	0.59	0.60	0.28	-0.28	0.79
p-methylaniline	0.66	0.58	0.56	0.61	0.70	0.60	0.73	0.91	0.77	0.77	0.23	-0.23	0.92
N-methylaniline	0.71	0.61	0.63	0.65	0.75	0.64	0.81	0.96	0.82	0.81	0.21	-0.21	0.95
dimethylamine	1.00	0.94	0.96	1.01	1.02	0.95	1.18	1.29	1.13	1.12	0.21	-0.21	1.27
diethylamine	0.90	0.84	0.90	0.91	0.93	0.85	1.15	1.25	1.05	1.05	0.38	-0.38	1.36
pyrrolidine	0.86	0.81	0.81	0.88	0.89	0.82	1.05	1.16	1.01	1.00	0.33	-0.33	1.26
piperidine	0.98	0.90	1.00	1.02	1.05	0.94	1.24	1.32	1.16	1.16	0.26	-0.26	1.34
anisole	1.59	1.50	1.50	1.55	1.66	1.54	1.65	1.87	1.71	1.71	0.09	0.01	1.62
indole	1.20	1.10	1.10	1.14	1.26	1.14	1.24	1.48	1.32	1.31	0.15	0.15	1.08
p-methoxyphenol	1.06	1.00	0.97	1.08	1.17	1.06	1.17	1.40	1.22	1.23	0.13	-0.09	1.23
p-methylphenol	1.42	1.37	1.32	1.41	1.50	1.41	1.46	1.71	1.57	1.57	0.11	0.09	1.38
phenol	2.82	2.76	2.74	2.77	2.88	2.79	2.76	3.04	2.97	2.97	1.35	1.35	1.50
p-cyanophenol	2.07	2.00	1.97	2.07	2.17	2.05	2.13	2.40	2.25	2.25	0.43	0.43	1.71
dimethylsulfide	1.54	1.57	1.58	1.57	1.59	1.58	1.69	1.78	1.64	1.64	0.23	0.23	1.39
dimethyldisulfide	1.19	1.21	1.27	1.25	1.31	1.26	1.41	1.51	1.31	1.33	0.37	-0.37	1.68
thioanisole	1.29	1.25	1.28	1.29	1.39	1.30	1.42	1.62	1.44	1.45	0.11	-0.08	1.45
p-chloroaniline	0.93	0.87	0.87	0.92	1.01	0.90	1.04	1.23	1.09	1.08	0.31	0.31	0.68
p-chlorophenol	1.61	1.57	1.55	1.64	1.73	1.62	1.70	1.97	1.80	1.80	1.05	1.05	0.65
MUE	0.34	0.36	0.35	0.34	0.33	0.35	0.27	0.34	0.32	0.32			
MSE	0.00	-0.06	-0.05	-0.01	0.07	-0.03	0.11	0.29	0.14	0.14			

Table S21. Solvation energies (eV) for phenol-water clusters.

	$\Delta\Delta G_{solv}$			ΔG_{solv}(Red)			ΔG_{solv}(Ox)		
	C_6H_5OH–H_2O	C_6H_5OH–$(H_2O)_2$	C_6H_5OH–$(H_2O)_3$	C_6H_5OH–H_2O	C_6H_5OH–$(H_2O)_2$	C_6H_5OH–$(H_2O)_3$	C_6H_5OH–H_2O	C_6H_5OH–$(H_2O)_2$	C_6H_5OH–$(H_2O)_3$
PBE	-1.92	-1.86	-1.75	-0.56	-0.51	-0.61	-2.49	-2.37	-2.36
TPSS	-1.93	-1.87	-1.75	-0.55	-0.50	-0.60	-2.48	-2.36	-2.35
M06-L	-1.94	-1.87	-1.77	-0.52	-0.47	-0.56	-2.46	-2.34	-2.33
B3LYP	-1.95	-1.88	-1.77	-0.55	-0.50	-0.60	-2.50	-2.38	-2.37
PBE0	-1.91	-1.85	-1.74	-0.58	-0.52	-0.62	-2.49	-2.37	-2.36
TPSSh	-1.92	-1.86	-1.75	-0.56	-0.50	-0.60	-2.48	-2.36	-2.35
M06	-1.95	-1.87	-1.77	-0.54	-0.49	-0.58	-2.48	-2.36	-2.35
M06-2X	-1.93	-1.86	-1.75	-0.58	-0.52	-0.62	-2.50	-2.38	-2.37
B2PLYP	-1.95	-1.86	-1.78	-0.55	-0.52	-0.61	-2.50	-2.38	-2.38
mPW2PLYP	-1.95	-1.86	-1.78	-0.56	-0.52	-0.61	-2.50	-2.38	-2.38

Cartesian coordinates of optimized structures

	X	Y	Z
	AnilinelRed.lgas-phase		
C	-0.07998	-0.05882	-0.25175
N	-0.05754	-0.08642	-1.65493
C	-0.08327	1.16346	0.44021
H	-0.12309	2.09590	-0.11931
C	-0.03218	1.18694	1.83166
H	-0.03811	2.14451	2.34611
C	0.02417	0.00003	2.56465
H	0.06306	0.02261	3.64945
C	0.02731	-1.21657	1.87966
H	0.06820	-2.15189	2.43207
C	-0.02355	-1.25121	0.48848
H	-0.01684	-2.20598	-0.03352
H	-0.42801	-0.93970	-2.05922
H	-0.46951	0.73045	-2.09287
	p-MethoxyanilinelRed.lgas-phase		
C	0.07727	-0.04344	-0.33671
N	0.02632	-0.02957	-1.74787
C	0.07115	1.14529	0.39979
H	0.08709	2.10093	-0.12020
C	0.04048	1.13336	1.79728
H	0.03914	2.07814	2.33013
C	0.01447	-0.08203	2.48567
O	-0.01553	-0.20961	3.85940
C	0.02142	-1.27819	1.75767
H	0.00380	-2.22041	2.29743
C	0.05055	-1.25809	0.36980
H	0.04935	-2.19831	-0.17771
C	-0.03361	1.00213	4.61587
H	-0.06358	0.69441	5.66219
H	-0.92249	1.60319	4.38246
H	0.86988	1.59899	4.43295
H	0.43498	0.80625	-2.15431
H	0.44061	-0.85473	-2.17017
	p-MethylanilinelRed.lgas-phase		
C	0.21797	-0.04476	-0.28300
N	0.24190	-0.06584	-1.68880
C	0.18538	1.16779	0.41965
H	0.23532	2.10778	-0.12639
C	0.08585	1.17814	1.80984
H	0.06500	2.13481	2.32813
C	0.01404	-0.00527	2.55217
C	-0.09498	0.01266	4.05949
C	0.04824	-1.21203	1.83965
H	-0.00233	-2.15541	2.38023
C	0.14710	-1.23909	0.45232
H	0.16694	-2.19331	-0.07063
H	-0.10216	1.03916	4.43872
H	0.74570	-0.51256	4.52934
H	-1.01539	-0.47694	4.40079
H	0.66629	0.75666	-2.10443
H	0.64399	-0.91129	-2.07977
	N-MethylanilinelRed.lgas-phase		
C	0.01648	-0.03275	0.02730
N	-1.42012	0.13578	-0.15371
C	-2.09986	-0.56223	-1.15257
C	-1.43134	-1.14549	-2.24388
C	-2.15428	-1.78382	-3.25235
C	-3.54444	-1.86728	-3.19897
C	-4.21207	-1.29627	-2.11073
C	-3.50550	-0.65270	-1.10258
H	0.31882	-1.08616	0.13915
H	0.55730	0.39214	-0.82501
H	0.31758	0.51796	0.92157
H	-1.93936	0.19911	0.71355
H	-0.34877	-1.10058	-2.30831
H	-1.61544	-2.22556	-4.08692
H	-4.09939	-2.36873	-3.98599
H	-5.29575	-1.35339	-2.04593
H	-4.03738	-0.20603	-0.26433
	DimethylaminelRed.lgas-phase		
N	-0.20243	1.25823	-0.64778
H	0.97754	1.85704	-2.36192

C	-0.03471	1.50930	-2.08208
C	0.17195	2.42107	0.16221
H	-0.25595	0.59417	-2.63983
H	-0.53370	3.23585	-0.03612
H	-0.75032	2.27791	-2.39556
H	0.38678	0.47023	-0.38187
H	0.10072	2.16329	1.22333
H	1.19099	2.80074	-0.04098

DiethylaminelRed.lgas-phase

N	-0.22575	1.96877	-0.25638
C	0.29066	1.49565	-1.54633
C	0.35542	1.36841	0.95581
C	-0.37227	0.13882	1.52285
C	0.06306	0.01968	-1.92286
H	0.38384	2.14106	1.73685
H	-0.15979	2.13222	-2.31813
H	0.10209	-0.19323	2.45481
H	-0.37331	-0.70013	0.82081
H	0.43630	-0.17379	-2.93648
H	0.58671	-0.65851	-1.24115
H	-1.24150	1.88787	-0.23355
H	-1.41545	0.38656	1.75540
H	-1.00412	-0.23136	-1.90287
H	1.39919	1.11805	0.73012
H	1.36716	1.70921	-1.55980

PyrrolidinelRed.lgas-phase

C	-0.41455	-2.33585	-0.82659
C	-0.72361	-2.60654	-2.31246
C	-0.98204	-1.19410	-2.91763
C	-0.79962	-0.22906	-1.72930
N	0.13161	-0.96742	-0.85786
H	0.17458	-0.55961	0.07561
H	0.31733	-3.03221	-0.40513
H	-1.34330	-2.40795	-0.23040
H	-1.58185	-3.27452	-2.42856
H	0.13440	-3.07825	-2.79912
H	-1.97906	-1.10402	-3.35815
H	-0.25054	-0.97547	-3.70035
H	-1.77579	-0.04184	-1.24422
H	-0.37142	0.73559	-2.01961

PiperidinelRed.lgas-phase

C	-4.80934	1.28730	0.15769
C	-4.77998	-0.19584	-0.22258
C	-3.49390	-0.85933	0.29412
C	-2.25457	-0.07698	-0.16759
C	-2.38110	1.40158	0.21057
N	-3.61154	1.95235	-0.38068
H	-4.87542	1.37465	1.26114
H	-5.69328	1.77573	-0.26732
H	-1.52930	1.97169	-0.17667
H	-2.37153	1.49253	1.31565
H	-4.82563	-0.27872	-1.31585
H	-5.66374	-0.70066	0.18674
H	-3.43751	-1.90158	-0.04243
H	-3.51684	-0.88032	1.39352
H	-2.15385	-0.15299	-1.25766
H	-1.34594	-0.49743	0.28081
H	-3.66282	2.95117	-0.18500

AnisolelRed.lgas-phase

C	-0.00001	-0.05451	-0.43590
C	-0.00001	1.14233	0.27525
H	-0.00001	2.09103	-0.25522
C	-0.00001	1.14822	1.67373
H	-0.00001	2.09313	2.20599
C	-0.00001	-0.06838	2.36549
C	-0.00001	-1.27764	1.65559
H	-0.00001	-2.20972	2.21277
C	-0.00001	-1.26479	0.26591
H	-0.00001	-2.20761	-0.27471
H	-0.00001	-0.04877	-1.52172
O	0.00000	-0.18305	3.73433
C	0.00000	1.03219	4.49149
H	0.00000	0.72291	5.53745
H	-0.89692	1.62858	4.28200
H	0.89692	1.62857	4.28200

Indole|Red.|gas-phase

C	2.15315	-0.68489	0.00001
C	2.15363	0.72506	0.00000
C	0.96642	1.44511	0.00000
C	-0.25523	0.74838	0.00001
C	-0.22890	-0.67635	0.00001
C	0.96407	-1.40503	0.00001
H	0.98003	2.53197	0.00000
H	3.09936	-1.21870	0.00001
H	3.10300	1.25347	0.00000
C	-1.63531	1.14188	0.00001
H	-2.02611	2.14977	0.00002
C	-2.38444	-0.00741	0.00000
N	-1.54239	-1.10618	0.00000
H	-3.45681	-0.14319	0.00000
H	-1.84321	-2.06896	0.00000
H	0.96650	-2.49211	0.00002

p-Methoxyphenol|Red.|gas-phase

C	0.04253	0.23653	-0.17820
C	0.09863	1.35655	0.65976
H	0.17371	2.34431	0.21463
C	0.06178	1.20126	2.04164
H	0.10748	2.07828	2.68620
C	-0.03359	-0.07658	2.60438
O	-0.09417	-0.28935	3.96852
H	-0.08705	0.57342	4.41375
C	-0.07133	-1.19365	1.77368
H	-0.13577	-2.18277	2.21611
C	-0.03364	-1.04123	0.38621
H	-0.06609	-1.92586	-0.23963
O	0.07154	0.49431	-1.53193
C	0.00622	-0.63756	-2.40341
H	0.03315	-0.22983	-3.41453
H	0.86366	-1.30630	-2.25210
H	-0.92575	-1.19853	-2.25567

p-Methylphenol|Red.|gas-phase

C	-0.00002	0.06307	-0.20146
C	-0.00002	1.28060	0.48219
C	-0.00001	1.29199	1.87772
O	0.00001	2.45700	2.61529
C	-0.00002	0.08391	2.58112
C	-0.00002	-1.11854	1.88193
H	-0.00001	-2.05106	2.44274
C	-0.00002	-1.15753	0.47924
C	0.00000	-2.47362	-0.26402
H	-0.00002	0.06979	-1.28932
H	0.00001	3.20904	2.00064
H	-0.00001	0.10311	3.66680
H	-0.00002	2.21808	-0.07192
H	0.00000	-2.31264	-1.34625
H	-0.88305	-3.07373	-0.01331
H	0.88306	-3.07371	-0.01331

Phenol|Red.|gas-phase

C	-0.14442	-0.49232	0.00006
H	-2.06519	-0.49038	0.00014
O	-1.35372	-1.15173	0.00013
C	1.01301	-1.27614	0.00004
C	2.25999	-0.65588	-0.00002
C	2.36644	0.73728	-0.00007
C	1.20571	1.51049	-0.00005
C	-0.05020	0.90271	0.00002
H	0.91921	-2.35777	0.00008
H	3.15722	-1.26904	-0.00003
H	3.34224	1.21333	-0.00012
H	1.27159	2.59519	-0.00008
H	-0.95448	1.50933	0.00003

p-Cyanophenol|Red.|gas-phase

C	0.01268	-0.00947	-0.23662
C	0.00155	1.20396	0.43899
C	-0.00469	1.22397	1.83930
O	-0.01538	2.38710	2.56018
C	0.00004	0.02466	2.56215
C	0.01132	-1.18562	1.88599
H	0.01517	-2.11761	2.44179
C	0.01762	-1.21873	0.47868
C	0.02936	-2.46765	-0.21534

H	0.01772	-0.02758	-1.32159
H	-0.01760	3.14133	1.94709
H	-0.00505	0.06062	3.64670
H	-0.00216	2.13739	-0.12010
N	0.03363	-3.48604	-0.77826

DimethylsulfidelRed.lgas-phase

S	-0.22551	0.17907	0.56222
C	0.21796	1.41051	-0.70711
C	0.22183	1.11786	2.05970
H	-0.00750	0.95715	-1.67530
H	-0.37630	2.32141	-0.59089
H	-0.37190	2.03313	2.13820
H	-0.00186	0.47204	2.91216
H	1.28854	1.35983	2.06377
H	1.28459	1.64875	-0.66279

DimethyldisulfidelRed.lgas-phase

S	1.22686	0.00501	-1.03040
S	1.02619	-0.08580	1.01887
C	0.00940	1.38692	1.42564
C	-0.24634	-0.89334	-1.65566
H	-0.99532	1.29543	1.00909
H	-0.04995	1.40902	2.51880
H	-0.26759	-1.90686	-1.25276
H	-0.12735	-0.92972	-2.74355
H	0.49841	2.29266	1.06437
H	-1.16470	-0.35776	-1.40843

ThioanisolelRed.lgas-phase

C	-0.00022	-0.04344	-0.52124
C	0.00041	1.11094	0.25908
H	0.00057	2.08930	-0.21460
C	0.00085	1.03103	1.65335
H	0.00133	1.94510	2.23726
C	0.00068	-0.21991	2.28308
C	0.00005	-1.38369	1.49544
H	-0.00009	-2.35844	1.97669
C	-0.00041	-1.29169	0.10761
H	-0.00090	-2.20200	-0.48612
H	-0.00057	0.02577	-1.60503
S	0.00113	-0.45737	4.04233
C	-0.00051	1.23916	4.69731
H	0.00023	1.12562	5.78384
H	-0.90011	1.77999	4.39323
H	0.89745	1.78213	4.39222

p-ChloroanilinelRed.lgas-phase

C	0.00128	-0.09563	-0.23869
C	0.11718	1.10464	0.45681
C	0.17386	1.12311	1.85998
C	0.10894	-0.09994	2.54714
C	-0.00740	-1.30314	1.85667
H	-0.05417	-2.24208	2.39806
C	-0.06127	-1.29607	0.46493
H	-0.03898	-0.09790	-1.32279
H	0.14689	-0.11048	3.63409
H	0.16113	2.03976	-0.09690
Cl	-0.20546	-2.81635	-0.41173
N	0.21613	2.33739	2.55948
H	0.61448	2.27146	3.48974
H	0.62819	3.10569	2.04147

p-ChlorophenollRed.lgas-phase

C	-0.00001	0.02144	-0.17985
C	0.00000	1.23268	0.51169
C	0.00001	1.24289	1.90956
O	0.00000	2.40545	2.64490
C	0.00001	0.03706	2.61693
C	0.00000	-1.17244	1.92828
H	0.00000	-2.11135	2.47136
C	-0.00001	-1.17331	0.53388
H	-0.00002	0.00928	-1.26440
H	-0.00001	3.16102	2.03450
H	0.00001	0.05747	3.70215
H	0.00000	2.16899	-0.04315
Cl	-0.00002	-2.70376	-0.33371

AnilinelOx.lgas-phase

C	-0.00001	0.00000	-0.22905

N	0.00001	0.00000	-1.56902
C	-0.00002	1.24411	0.48347
H	-0.00002	2.17829	-0.07129
C	0.00000	1.23016	1.85687
H	0.00001	2.16345	2.41035
C	0.00001	0.00000	2.55454
H	0.00002	0.00000	3.64038
C	-0.00001	-1.23016	1.85687
H	0.00000	-2.16345	2.41035
C	-0.00002	-1.24411	0.48347
H	-0.00001	-2.17829	-0.07129
H	0.00002	0.86644	-2.09961
H	0.00002	-0.86644	-2.09960

p-Methoxyaniline|Ox.lgas-phase

C	0.00000	-0.02809	-0.33711
N	-0.00003	-0.00977	-1.68265
C	0.00003	1.19677	0.39724
H	0.00002	2.14077	-0.14049
C	0.00005	1.18670	1.76963
H	0.00006	2.12306	2.31522
C	0.00006	-0.05446	2.46104
O	0.00004	-0.18470	3.78343
C	0.00002	-1.28103	1.73388
H	0.00001	-2.21051	2.29366
C	0.00000	-1.27110	0.36756
H	-0.00003	-2.20368	-0.18929
H	-0.00003	0.86148	-2.20029
H	-0.00005	-0.86787	-2.22198
C	-0.00003	0.99927	4.63775
H	-0.00004	0.60341	5.65083
H	-0.90325	1.58608	4.45318
H	0.90316	1.58615	4.45322

p-Methylaniline|Ox.lgas-phase

C	0.00000	0.00087	-0.30039
N	-0.00001	-0.00427	-1.64185
C	0.00001	1.24143	0.41232
H	0.00000	2.17649	-0.14110
C	0.00001	1.23337	1.78437
H	0.00000	2.17385	2.32702
C	0.00000	0.01456	2.51581
C	-0.00001	0.00705	4.00728
C	0.00001	-1.21409	1.79220
H	0.00000	-2.15052	2.34265
C	0.00001	-1.23438	0.42280
H	0.00001	-2.17383	-0.12307
H	-0.00001	0.85949	-2.17488
H	-0.00001	-0.87211	-2.16820
H	-0.00001	1.01469	4.42519
H	0.87735	-0.53629	4.38466
H	-0.87736	-0.53629	4.38465

N-Methylaniline|Ox.lgas-phase

C	0.03947	0.00911	0.03206
N	-1.41635	-0.09948	-0.10588
C	-2.08805	-0.66721	-1.12734
C	-1.40343	-1.25107	-2.23689
C	-2.13756	-1.81809	-3.25407
C	-3.54863	-1.82333	-3.20278
C	-4.23076	-1.24889	-2.11091
C	-3.52016	-0.67606	-1.08201
H	0.48956	-0.98820	0.04907
H	0.45290	0.58488	-0.80164
H	0.25394	0.52088	0.96904
H	-1.97860	0.29391	0.64559
H	-0.31970	-1.24564	-2.27371
H	-1.62918	-2.26480	-4.10236
H	-4.11309	-2.27466	-4.01300
H	-5.31534	-1.25910	-2.08305
H	-4.02856	-0.22826	-0.23180

Dimethylamine|Ox.lgas-phase

N	-0.01818	1.37967	-0.71064
H	-0.02165	2.55235	-2.43644
C	-0.20237	1.52327	-2.13138
C	0.35135	2.42880	0.20359
H	0.47917	0.82851	-2.64845
H	0.47831	3.36986	-0.32839
H	-1.22526	1.20440	-2.38944

H	-0.16327	0.44582	-0.31413
H	-0.42624	2.51139	0.98021
H	1.27832	2.13553	0.72249

DiethylaminelOx.lgas-phase

N	-0.30711	1.45143	-0.26665
C	0.29543	1.49067	-1.57734
C	0.39363	1.24634	0.98281
C	-0.35670	0.29912	1.93152
C	0.04591	0.14986	-2.33707
H	0.47225	2.24547	1.45430
H	-0.17691	2.30652	-2.13777
H	0.20398	0.24532	2.86791
H	-0.42728	-0.70367	1.50373
H	0.50335	0.26168	-3.32387
H	0.51581	-0.68343	-1.81120
H	-1.32701	1.53468	-0.21580
H	-1.36005	0.67196	2.15846
H	-1.02272	-0.03990	-2.46004
H	1.40933	0.91614	0.74897
H	1.36448	1.67651	-1.45929

PyrrolidinelOx.lgas-phase

C	-0.25138	-2.38508	-0.90049
C	-0.95674	-2.58968	-2.25145
C	-0.80171	-1.21985	-2.94775
C	-0.89216	-0.21662	-1.78595
N	-0.40345	-0.96782	-0.64929
H	-0.18559	-0.53505	0.25239
H	0.83699	-2.58585	-0.96022
H	-0.62350	-2.96082	-0.04326
H	-2.01118	-2.82734	-2.08070
H	-0.50760	-3.40546	-2.81858
H	-1.57312	-1.03671	-3.69627
H	0.17613	-1.13226	-3.43110
H	-1.93825	0.06881	-1.55681
H	-0.33230	0.72247	-1.88426

PiperidinelOx.lgas-phase

C	-4.83521	1.32556	0.28817
C	-4.78387	-0.17410	-0.22380
C	-3.49591	-0.83558	0.25951
C	-2.25395	-0.05790	-0.16781
C	-2.36269	1.43888	0.34320
N	-3.61537	1.95519	-0.12916
H	-4.87261	1.31445	1.38234
H	-5.69327	1.85631	-0.12571
H	-1.53933	2.04693	-0.03313
H	-2.37308	1.42892	1.43798
H	-4.85046	-0.16992	-1.31646
H	-5.68177	-0.65803	0.17300
H	-3.44003	-1.84572	-0.17030
H	-3.51454	-0.95497	1.34927
H	-2.13997	-0.04535	-1.25649
H	-1.33384	-0.45855	0.26898
H	-3.62040	2.49704	-0.99513

AnisolelOx.lgas-phase

C	-0.00002	-0.07133	-0.42645
C	-0.00001	1.17063	0.26593
H	-0.00001	2.09627	-0.30088
C	0.00000	1.20498	1.63914
H	0.00000	2.14767	2.17412
C	0.00000	-0.03534	2.34740
C	0.00000	-1.29192	1.64898
H	0.00000	-2.20334	2.23840
C	-0.00001	-1.29691	0.27559
H	-0.00001	-2.23463	-0.27009
H	-0.00002	-0.07283	-1.51260
O	0.00000	-0.14562	3.66068
C	0.00000	1.03786	4.53123
H	-0.00001	0.62730	5.53791
H	-0.90462	1.61986	4.34254
H	0.90462	1.61985	4.34255

IndolelOx.lgas-phase

C	2.15482	-0.66518	0.00000
C	2.16835	0.73019	0.00002
C	0.97371	1.45600	0.00000
C	-0.25110	0.74452	0.00000

C	-0.22770	-0.67814	-0.00001
C	0.93957	-1.40533	-0.00002
H	0.98099	2.54176	0.00001
H	3.09304	-1.21119	0.00002
H	3.11716	1.25577	0.00003
C	-1.60374	1.14306	-0.00002
H	-2.00422	2.14804	-0.00003
C	-2.38583	-0.04397	0.00003
N	-1.56993	-1.10630	0.00001
H	-3.46209	-0.15494	0.00004
H	-1.87740	-2.07388	0.00003
H	0.95526	-2.49096	-0.00001

p-MethoxyphenolOx.lgas-phase

C	0.03117	0.20556	-0.16130
C	0.08578	1.36957	0.66926
H	0.15198	2.34018	0.18850
C	0.05409	1.24111	2.03098
H	0.09490	2.11771	2.67219
C	-0.03323	-0.05750	2.60256
O	-0.06923	-0.27380	3.91650
H	-0.02867	0.55978	4.42592
C	-0.08783	-1.21970	1.77973
H	-0.15399	-2.19067	2.25990
C	-0.05630	-1.09403	0.41523
H	-0.09758	-1.97600	-0.21321
O	0.06886	0.45253	-1.46100
C	0.02023	-0.64273	-2.43210
H	0.06498	-0.14697	-3.39888
H	0.88540	-1.29390	-2.28780
H	-0.91926	-1.18813	-2.31708

p-MethylphenolOx.lgas-phase

C	0.00001	0.09462	-0.23517
C	0.00000	1.29029	0.43496
C	-0.00001	1.27912	1.86185
O	-0.00003	2.38779	2.58881
C	0.00001	0.05129	2.59292
C	0.00001	-1.12942	1.90216
H	0.00000	-2.07234	2.44123
C	0.00000	-1.14839	0.47134
C	-0.00002	-2.44350	-0.25716
H	0.00000	0.08161	-1.32091
H	-0.00004	3.19566	2.03507
H	-0.00001	0.09290	3.67742
H	-0.00001	2.23698	-0.09978
H	-0.00002	-2.31637	-1.34013
H	-0.87482	-3.04222	0.03775
H	0.87478	-3.04224	0.03773

PhenolOx.lgas-phase

C	-0.14195	-0.47841	0.00006
H	-2.06649	-0.52579	0.00015
O	-1.29294	-1.12863	0.00013
C	1.03345	-1.30084	0.00004
C	2.26291	-0.69184	-0.00002
C	2.34834	0.72300	-0.00006
C	1.17824	1.53418	-0.00005
C	-0.06213	0.94985	0.00002
H	0.91022	-2.37923	0.00008
H	3.17055	-1.28636	-0.00003
H	3.32407	1.20053	-0.00011
H	1.27598	2.61501	-0.00009
H	-0.97286	1.54357	0.00003

p-CyanophenolOx.lgas-phase

C	0.01257	0.01274	-0.26049
C	0.00164	1.21288	0.39708
C	-0.00455	1.21845	1.82581
O	-0.01487	2.33231	2.53611
C	0.00015	0.00313	2.58114
C	0.01121	-1.19384	1.91770
H	0.01509	-2.13328	2.46017
C	0.01753	-1.20878	0.48869
C	0.02910	-2.44013	-0.19790
H	0.01759	-0.02986	-1.34464
H	-0.01768	3.13877	1.97859
H	-0.00510	0.06477	3.66472
H	-0.00222	2.15185	-0.15057
N	0.03379	-3.46267	-0.76744

	DimethylsulfidelOx.lgas-phase		
S	-0.21522	0.23227	0.56818
C	0.21303	1.39260	-0.73163
C	0.21419	1.09774	2.08011
H	-0.02555	0.91267	-1.68214
H	-0.37109	2.31117	-0.59196
H	-0.36580	2.02794	2.13208
H	-0.02826	0.43295	2.91077
H	1.28521	1.33600	2.05974
H	1.28290	1.62591	-0.66003
	DimethyldisulfidelOx.lgas-phase		
S	0.16688	0.43509	-1.07670
S	-0.18771	0.00896	0.86498
C	0.14827	1.62054	1.65380
C	-0.16892	-1.17649	-1.86557
H	-0.54808	2.36801	1.26962
H	-0.03273	1.43562	2.71606
H	0.52717	-1.92400	-1.48097
H	0.01281	-0.99174	-2.92773
H	1.18951	1.90054	1.48452
H	-1.21025	-1.45643	-1.69679
	ThioanisolelOx.lgas-phase		
C	0.00000	-0.06034	-0.51264
C	-0.00001	1.13250	0.24247
H	-0.00001	2.09168	-0.26537
C	-0.00001	1.08468	1.62140
H	-0.00001	2.00093	2.20033
C	0.00000	-0.18037	2.26499
C	-0.00001	-1.38667	1.49906
H	-0.00001	-2.34598	2.00890
C	-0.00001	-1.31533	0.12103
H	-0.00002	-2.22503	-0.47032
H	-0.00001	-0.00529	-1.59726
S	0.00000	-0.41978	3.96704
C	0.00000	1.22626	4.72743
H	0.00000	1.03623	5.80255
H	-0.90383	1.76951	4.44242
H	0.90384	1.76951	4.44242
	p-ChloroanilinelOx.lgas-phase		
C	-0.00001	-0.02293	-0.23096
C	0.00000	1.16877	0.44668
C	0.00000	1.17588	1.87777
C	0.00001	-0.06110	2.59746
C	0.00000	-1.24952	1.91406
H	0.00000	-2.19651	2.44245
C	-0.00001	-1.23921	0.49675
H	-0.00002	-0.04783	-1.31510
H	0.00002	-0.05047	3.68374
H	0.00000	2.11037	-0.09508
Cl	-0.00003	-2.72050	-0.35026
N	-0.00001	2.34040	2.54363
H	-0.00001	3.23025	2.05551
H	-0.00001	2.37113	3.55809
	p-ChlorophenollOx.lgas-phase		
C	-0.00001	0.04562	-0.20190
C	-0.00001	1.24061	0.46956
C	0.00000	1.23614	1.89569
O	0.00000	2.34787	2.61827
C	0.00000	0.01450	2.63511
C	0.00000	-1.17783	1.96067
H	0.00000	-2.12394	2.49083
C	-0.00001	-1.17015	0.53938
H	-0.00001	0.01009	-1.28596
H	0.00000	3.15500	2.06378
H	0.00001	0.06180	3.71937
H	-0.00001	2.18291	-0.07239
Cl	-0.00001	-2.64719	-0.30028
	AnilinelRed.lSMD		
C	-0.00008	0.00004	-0.24285
N	-0.00036	-0.00002	-1.61655
C	-0.00004	1.21166	0.48157
H	0.00001	2.15512	-0.05963
C	0.00010	1.20298	1.87430
H	0.00021	2.15077	2.40701

C	0.00001	-0.00001	2.58862
H	0.00000	-0.00002	3.67444
C	-0.00008	-1.20298	1.87428
H	-0.00012	-2.15082	2.40691
C	0.00001	-1.21159	0.48156
H	-0.00002	-2.15502	-0.05969
H	-0.00038	0.86565	-2.13397
H	0.00083	-0.86580	-2.13380

p-Methoxyaniline|Red.|SMD

C	0.00006	-0.02356	-0.34747
N	0.00006	0.00168	-1.72770
C	-0.00002	1.16295	0.40604
H	0.00009	2.12262	-0.10540
C	-0.00018	1.13686	1.80420
H	-0.00024	2.07771	2.34383
C	-0.00027	-0.08452	2.48239
O	-0.00053	-0.21833	3.86952
C	-0.00007	-1.27493	1.74534
H	-0.00005	-2.22593	2.27117
C	0.00009	-1.24720	0.35541
H	0.00018	-2.18290	-0.19858
H	-0.00093	0.87641	-2.22876
H	0.00089	-0.85460	-2.25958
C	0.00011	1.00641	4.62720
H	-0.00006	0.70208	5.67442
H	-0.89726	1.59935	4.41637
H	0.89812	1.59839	4.41643

p-Methylaniline|Red.|SMD

C	0.00019	0.00239	-0.32328
N	0.00025	-0.00101	-1.69973
C	0.00021	1.20851	0.40421
H	0.00032	2.15563	-0.13087
C	0.00012	1.19672	1.79898
H	0.00011	2.14759	2.32860
C	0.00003	0.00259	2.53220
C	-0.00009	-0.00094	4.04320
C	0.00004	-1.19464	1.79821
H	-0.00009	-2.14649	2.32644
C	0.00014	-1.20539	0.40633
H	0.00007	-2.15195	-0.12984
H	-0.00114	0.86329	-2.21916
H	0.00021	-0.86805	-2.21454
H	-0.00012	1.02049	4.43633
H	0.88178	-0.51438	4.44627
H	-0.88203	-0.51436	4.44614

N-Methylaniline|Red.|SMD

C	0.00003	-0.04521	-0.36634
C	-0.00012	1.15536	0.34760
H	-0.00018	2.10297	-0.18577
C	-0.00024	1.17462	1.74278
H	-0.00040	2.13115	2.25489
C	-0.00016	-0.03351	2.47669
N	-0.00022	-0.08910	3.85033
C	0.00020	1.03628	4.77247
H	-0.00055	-1.01252	4.26208
C	0.00001	-1.24696	1.74400
H	0.00015	-2.18910	2.28859
C	0.00012	-1.24652	0.35455
H	0.00027	-2.19755	-0.17254
H	0.00053	1.97700	4.22397
H	0.88933	1.01756	5.41316
H	-0.88892	1.01825	5.41318
H	0.00016	-0.04760	-1.45210

Dimethylamine|Red.|SMD

N	-0.23154	1.23910	-0.63667
H	0.97841	1.86069	-2.31297
C	-0.03872	1.51073	-2.07458
C	0.16533	2.41945	0.15569
H	-0.23745	0.60369	-2.65144
H	-0.53056	3.24096	-0.04127
H	-0.74563	2.28137	-2.39754
H	0.42566	0.49589	-0.39399
H	0.11771	2.18150	1.22158
H	1.18262	2.77182	-0.07859

Diethylamine|Red.|SMD

N	-0.27093	1.97790	-0.24942
C	0.26731	1.52789	-1.55496
C	0.37348	1.32149	0.92338
C	-0.42820	0.17016	1.52903
C	0.12861	0.03943	-1.88813
H	0.53237	2.07922	1.70079
H	-0.23869	2.11514	-2.32916
H	0.08006	-0.22342	2.41769
H	-0.56458	-0.65323	0.82072
H	0.52437	-0.15539	-2.89270
H	0.68521	-0.59099	-1.18636
H	-1.26092	1.72546	-0.23041
H	-1.42056	0.51757	1.84207
H	-0.92284	-0.27114	-1.87454
H	1.36777	0.97710	0.61957
H	1.32488	1.81325	-1.58783

PyrrolidinelRed.lSMD

C	-0.40599	-2.33379	-0.83484
C	-0.72198	-2.60620	-2.31371
C	-0.98058	-1.19468	-2.91825
C	-0.78803	-0.23337	-1.73489
N	0.16229	-0.96104	-0.85443
H	0.10832	-0.56774	0.08641
H	0.30896	-3.04156	-0.40695
H	-1.32912	-2.37606	-0.23618
H	-1.58268	-3.27172	-2.42103
H	0.13049	-3.08301	-2.80659
H	-1.98115	-1.10060	-3.34864
H	-0.25666	-0.97899	-3.70970
H	-1.74975	-0.05949	-1.22776
H	-0.37798	0.73698	-2.02720

PiperidinelRed.lSMD

C	-4.80610	1.28624	0.14309
C	-4.77854	-0.19646	-0.22394
C	-3.49370	-0.86030	0.29270
C	-2.25587	-0.07754	-0.16933
C	-2.38371	1.40046	0.19542
N	-3.61217	1.97299	-0.40585
H	-4.85095	1.38601	1.24218
H	-5.69929	1.76822	-0.26624
H	-1.52299	1.96507	-0.17606
H	-2.39582	1.50184	1.29521
H	-4.83710	-0.29936	-1.31578
H	-5.66238	-0.69080	0.19696
H	-3.43728	-1.90266	-0.04287
H	-3.51664	-0.87840	1.39170
H	-2.14066	-0.17239	-1.25737
H	-1.34849	-0.48732	0.29052
H	-3.66461	2.94756	-0.10589

AnisolelRed.lSMD

C	-0.00003	-0.05461	-0.43755
C	-0.00003	1.14220	0.27744
H	-0.00003	2.09218	-0.25001
C	-0.00004	1.14562	1.67671
H	-0.00002	2.08881	2.21116
C	-0.00005	-0.07415	2.36306
C	-0.00004	-1.28346	1.65257
H	-0.00001	-2.22021	2.20250
C	0.00001	-1.26779	0.26105
H	0.00007	-2.20934	-0.28109
H	0.00002	-0.04617	-1.52332
O	-0.00006	-0.18697	3.73974
C	0.00002	1.04382	4.49591
H	0.00002	0.73883	5.54237
H	-0.89844	1.63192	4.28193
H	0.89853	1.63184	4.28197

IndolelRed.lSMD

C	2.15314	-0.68642	0.00000
C	2.15608	0.72582	0.00001
C	0.96852	1.44911	0.00000
C	-0.25544	0.75235	-0.00002
C	-0.23158	-0.67535	0.00000
C	0.96170	-1.40568	-0.00002
H	0.98466	2.53607	0.00002
H	3.09874	-1.22140	0.00000
H	3.10631	1.25300	0.00007

C	-1.63659	1.14421	-0.00003
H	-2.03075	2.15152	-0.00002
C	-2.38138	-0.01230	-0.00001
N	-1.54148	-1.10695	0.00001
H	-3.45287	-0.15266	0.00011
H	-1.84469	-2.07109	0.00006
H	0.95845	-2.49207	-0.00003

p-Methoxyphenol|Red.|SMD

C	0.03086	0.24167	-0.17968
C	0.09256	1.36022	0.66059
H	0.16541	2.35199	0.22410
C	0.06095	1.20214	2.04322
H	0.10915	2.07399	2.69100
C	-0.03273	-0.07910	2.59663
O	-0.06793	-0.29141	3.97224
H	-0.01577	0.57267	4.41763
C	-0.09441	-1.19459	1.76436
H	-0.16718	-2.18763	2.19780
C	-0.06294	-1.03854	0.37536
H	-0.11224	-1.92050	-0.25289
O	0.06932	0.50056	-1.54177
C	0.00509	-0.64479	-2.41649
H	0.04716	-0.23985	-3.42780
H	0.85815	-1.31165	-2.25025
H	-0.93401	-1.19113	-2.27640

p-Methylphenol|Red.|SMD

C	0.00005	0.06411	-0.20246
C	0.00003	1.28313	0.48092
C	0.00005	1.28825	1.87624
O	-0.00001	2.46554	2.61444
C	0.00006	0.08185	2.58230
C	0.00002	-1.12252	1.88230
H	-0.00002	-2.05458	2.44317
C	0.00002	-1.15905	0.47862
C	-0.00004	-2.47422	-0.26426
H	0.00008	0.07219	-1.28999
H	-0.00025	3.21730	1.99536
H	0.00008	0.09507	3.66848
H	-0.00003	2.22247	-0.06726
H	0.00002	-2.31408	-1.34639
H	-0.88213	-3.07476	-0.01172
H	0.88193	-3.07490	-0.01165

Phenol|Red.|SMD

C	0.00946	-0.01666	-0.25930
H	0.01551	-0.03879	-1.34480
C	-0.00688	1.20432	0.42159
H	-0.01356	2.13792	-0.13398
C	-0.01478	1.24202	1.81572
H	-0.02741	2.18681	2.35120
C	-0.00611	0.04229	2.53316
O	-0.01438	0.12641	3.91791
H	-0.00645	-0.77661	4.28287
C	0.01038	-1.18631	1.86641
H	0.01713	-2.11267	2.43590
C	0.01801	-1.20782	0.47043
H	0.03078	-2.16398	-0.04524

p-Cyanophenol|Red.|SMD

C	0.01246	-0.00575	-0.24086
C	0.00160	1.20512	0.43503
C	-0.00446	1.21633	1.83630
O	-0.01504	2.38641	2.55402
C	0.00011	0.01882	2.56414
C	0.01107	-1.19142	1.89029
H	0.01482	-2.12321	2.44502
C	0.01720	-1.21381	0.48161
C	0.02855	-2.45600	-0.20831
H	0.01729	-0.02376	-1.32514
H	-0.01737	3.13995	1.93562
H	-0.00488	0.05050	3.64863
H	-0.00214	2.14150	-0.11563
N	0.03500	-3.47835	-0.77176

Dimethylsulfide|Red.|SMD

S	-0.22511	0.18148	0.56245
C	0.21782	1.40853	-0.71287
C	0.22069	1.11518	2.06502

H	-0.00899	0.95552	-1.68064
H	-0.37544	2.31822	-0.59128
H	-0.37384	2.02921	2.13836
H	-0.00223	0.46927	2.91727
H	1.28645	1.35691	2.06334
H	1.28399	1.64349	-0.66425

Dimethyldisulfide|Red.|SMD

S	-1.04094	0.52758	-1.24745
S	-1.25851	0.46872	0.81116
C	0.23108	1.32718	1.44168
C	-0.01582	-0.94101	-1.62934
H	0.26813	2.35012	1.06509
H	0.11788	1.33732	2.53014
H	0.97216	-0.85042	-1.17568
H	0.08259	-0.94748	-2.71926
H	1.13495	0.77739	1.17545
H	-0.51796	-1.85113	-1.29894

Thioanisole|Red.|SMD

C	-0.00061	-0.04417	-0.52331
C	0.00086	1.11109	0.25845
H	0.00116	2.08970	-0.21373
C	0.00202	1.03025	1.65375
H	0.00325	1.94355	2.23848
C	0.00169	-0.22322	2.27953
C	0.00015	-1.38824	1.49308
H	-0.00034	-2.36431	1.97112
C	-0.00092	-1.29450	0.10374
H	-0.00218	-2.20392	-0.49067
H	-0.00152	0.02611	-1.60690
S	0.00340	-0.45049	4.04406
C	-0.00114	1.24547	4.70126
H	-0.00038	1.12606	5.78684
H	-0.90285	1.78198	4.39960
H	0.89732	1.78716	4.39914

p-Chloroaniline|Red.|SMD

C	-0.00004	-0.04863	-0.21830
C	-0.00006	1.15899	0.47346
C	-0.00005	1.18779	1.88458
C	-0.00006	-0.04297	2.57544
C	0.00001	-1.25162	1.88546
H	0.00009	-2.18799	2.43353
C	0.00001	-1.24729	0.49211
H	-0.00008	-0.05116	-1.30327
H	-0.00002	-0.04808	3.66233
H	-0.00010	2.09316	-0.08215
Cl	0.00008	-2.78680	-0.38818
N	0.00003	2.37834	2.56535
H	0.00037	3.25721	2.07070
H	-0.00021	2.39776	3.57367

p-Chlorophenol|Red.|SMD

C	0.00002	0.02320	-0.18128
C	0.00008	1.23465	0.51022
C	0.00010	1.23767	1.90794
O	0.00014	2.41132	2.64169
C	0.00006	0.03425	2.61905
C	-0.00002	-1.17707	1.93083
H	-0.00005	-2.11377	2.47706
C	-0.00004	-1.16869	0.53767
H	0.00002	0.01498	-1.26559
H	-0.00042	3.16534	2.02511
H	0.00009	0.04823	3.70441
H	0.00011	2.17251	-0.03879
Cl	-0.00014	-2.70719	-0.33618

Aniline|Ox.|SMD

C	0.00000	-0.00005	-0.22961
N	0.00000	0.00008	-1.56164
C	-0.00005	1.24158	0.48131
H	0.00008	2.16969	-0.08077
C	0.00005	1.22694	1.85575
H	0.00020	2.15939	2.40906
C	0.00000	0.00004	2.55210
H	0.00006	0.00001	3.63670
C	-0.00006	-1.22692	1.85580
H	-0.00022	-2.15939	2.40907
C	0.00003	-1.24166	0.48135

H	-0.00009	-2.16979	-0.08072
H	-0.00068	0.86874	-2.08635
H	0.00079	-0.86839	-2.08667

p-Methoxyaniline|Ox.|SMD

C	0.00003	-0.02725	-0.33058
N	0.00004	-0.00135	-1.66734
C	-0.00005	1.19269	0.40956
H	0.00003	2.13511	-0.12833
C	0.00002	1.17323	1.78219
H	0.00013	2.10486	2.33404
C	-0.00001	-0.07026	2.46017
O	-0.00003	-0.19888	3.79706
C	-0.00009	-1.29094	1.73256
H	-0.00028	-2.22484	2.28380
C	0.00006	-1.27448	0.36569
H	-0.00003	-2.19843	-0.20310
H	-0.00074	0.87614	-2.17375
H	0.00075	-0.85872	-2.20709
C	0.00004	1.00746	4.61521
H	0.00000	0.64610	5.64132
H	-0.90131	1.59107	4.41667
H	0.90145	1.59097	4.41671

p-Methylaniline|Ox.|SMD

C	-0.00001	0.00089	-0.29993
N	0.00011	-0.00360	-1.63286
C	-0.00004	1.23981	0.41185
H	0.00019	2.16942	-0.14809
C	-0.00002	1.23011	1.78496
H	0.00018	2.16882	2.32973
C	-0.00013	0.01280	2.51045
C	0.00005	0.00494	4.00378
C	-0.00026	-1.21351	1.79136
H	-0.00050	-2.14872	2.34273
C	-0.00011	-1.23374	0.42115
H	-0.00027	-2.16716	-0.13244
H	-0.00051	0.86282	-2.16009
H	0.00084	-0.87351	-2.15430
H	-0.00038	1.01608	4.41495
H	0.87896	-0.53225	4.38295
H	-0.87811	-0.53321	4.38328

N-Methylaniline|Ox.|SMD

C	0.00003	-0.05082	-0.32836
C	-0.00009	1.17788	0.35930
H	-0.00019	2.10672	-0.20050
C	-0.00014	1.21354	1.73706
H	-0.00037	2.16156	2.25984
C	-0.00009	-0.01415	2.46202
N	-0.00019	-0.06439	3.80643
C	0.00019	1.03860	4.75016
H	-0.00056	-0.99530	4.21781
C	0.00003	-1.25835	1.75757
H	0.00021	-2.18174	2.32868
C	0.00011	-1.26569	0.38108
H	0.00024	-2.20762	-0.15623
H	0.00058	1.99487	4.23625
H	0.88689	0.95439	5.38481
H	-0.88667	0.95507	5.38469
H	0.00002	-0.05944	-1.41305

Dimethylamine|Ox.|SMD

N	0.01522	1.34969	-0.70920
H	0.31492	2.44728	-2.44463
C	-0.14476	1.51435	-2.12230
C	0.28253	2.42316	0.19969
H	0.26847	0.64634	-2.63934
H	0.15992	3.38067	-0.30157
H	-1.22328	1.54868	-2.34754
H	-0.08733	0.41231	-0.32162
H	-0.37158	2.32881	1.07170
H	1.31629	2.32170	0.56451

Diethylamine|Ox.|SMD

N	-0.10104	0.67331	-0.24385
C	0.56420	0.95826	-1.48995
C	0.15624	1.38197	0.98440
C	-0.18265	0.55971	2.21849
C	-0.28689	0.60507	-2.70191

H	-0.46620	2.29347	0.94683
H	0.88171	2.00457	-1.46780
H	-0.03647	1.18364	3.10341
H	0.46729	-0.31542	2.29715
H	0.30811	0.76935	-3.60342
H	-0.58920	-0.44606	-2.67680
H	-0.79530	-0.07692	-0.23092
H	-1.22648	0.23266	2.19809
H	-1.17854	1.23507	-2.75126
H	1.19546	1.72445	0.95841
H	1.48856	0.35385	-1.48616

PyrrolidinelOx.lSMD

C	-0.24822	-2.37882	-0.90566
C	-0.95534	-2.58684	-2.24903
C	-0.80139	-1.21948	-2.94389
C	-0.89599	-0.22393	-1.78283
N	-0.40343	-0.96867	-0.65127
H	-0.18570	-0.53789	0.24616
H	0.83457	-2.58116	-0.96696
H	-0.62218	-2.95548	-0.05469
H	-2.01081	-2.81459	-2.07453
H	-0.50960	-3.40505	-2.81494
H	-1.56998	-1.03460	-3.69454
H	0.18052	-1.13516	-3.41825
H	-1.93819	0.05901	-1.55736
H	-0.33811	0.71137	-1.88596

PiperidinelOx.lSMD

C	-4.83330	1.31274	0.27325
C	-4.78016	-0.17382	-0.22301
C	-3.49613	-0.84103	0.26397
C	-2.25793	-0.05898	-0.16766
C	-2.36218	1.42557	0.32696
N	-3.61540	1.95865	-0.12234
H	-4.88334	1.30603	1.36654
H	-5.68199	1.84736	-0.14705
H	-1.54828	2.03593	-0.05745
H	-2.35897	1.42139	1.42141
H	-4.84017	-0.17998	-1.31523
H	-5.67545	-0.66021	0.17418
H	-3.44077	-1.85519	-0.15113
H	-3.51563	-0.93759	1.35607
H	-2.14951	-0.05769	-1.25618
H	-1.34025	-0.46222	0.26956
H	-3.62685	2.58219	-0.92744

AnisolelOx.lSMD

C	-0.00001	-0.06509	-0.41550
C	0.00001	1.16982	0.28328
H	0.00003	2.09787	-0.27650
C	0.00003	1.19507	1.65530
H	0.00013	2.13151	2.19832
C	0.00005	-0.04924	2.35191
C	-0.00004	-1.29940	1.64966
H	-0.00014	-2.21440	2.23072
C	-0.00006	-1.29447	0.27796
H	-0.00008	-2.22671	-0.27437
H	0.00003	-0.06028	-1.49975
O	0.00021	-0.15805	3.66811
C	-0.00002	1.04371	4.50840
H	0.00016	0.66137	5.52527
H	-0.90330	1.62014	4.30588
H	0.90290	1.62066	4.30578

IndolelOx.lSMD

C	2.14941	-0.66765	0.00000
C	2.16510	0.72882	0.00000
C	0.97274	1.45786	0.00000
C	-0.24760	0.74909	0.00002
C	-0.22672	-0.67302	0.00003
C	0.93617	-1.40333	0.00004
H	0.98064	2.54260	0.00000
H	3.08664	-1.21371	-0.00008
H	3.11487	1.25204	0.00001
C	-1.60260	1.14385	0.00005
H	-2.00583	2.14620	0.00001
C	-2.37947	-0.04984	0.00003
N	-1.56602	-1.10358	-0.00001
H	-3.45280	-0.16433	-0.00007

H	-1.86823	-2.07168	-0.00006
H	0.94101	-2.48752	0.00010

p-Methoxyphenol|Ox.|SMD

C	0.04825	0.23637	-0.16239
C	0.13258	1.38224	0.68462
H	0.24123	2.35838	0.22617
C	0.07556	1.23010	2.04165
H	0.13728	2.08392	2.70833
C	-0.06750	-0.07455	2.58291
O	-0.12971	-0.29468	3.89983
H	-0.06354	0.54799	4.39304
C	-0.15216	-1.21854	1.74315
H	-0.26103	-2.19567	2.19939
C	-0.09520	-1.06890	0.38312
H	-0.15880	-1.93454	-0.26351
O	0.11408	0.49406	-1.46563
C	0.03657	-0.61139	-2.42043
H	0.11332	-0.13602	-3.39495
H	0.87218	-1.29332	-2.25556
H	-0.92342	-1.11850	-2.31198

p-Methylphenol|Ox.|SMD

C	0.00011	0.09542	-0.23262
C	-0.00001	1.28829	0.43993
C	0.00003	1.27125	1.86492
O	0.00003	2.38986	2.57959
C	-0.00001	0.04657	2.59494
C	0.00008	-1.13112	1.90191
H	0.00008	-2.07587	2.43518
C	0.00013	-1.14311	0.47292
C	0.00001	-2.43764	-0.25317
H	-0.00003	0.08197	-1.31710
H	0.00004	3.17818	1.99718
H	-0.00015	0.08327	3.67818
H	-0.00027	2.24075	-0.08033
H	0.00005	-2.30574	-1.33556
H	-0.87565	-3.03300	0.04101
H	0.87543	-3.03330	0.04111

Phenol|Ox.|SMD

C	-0.00011	-0.00005	-0.24652
H	-0.00016	-0.00004	-1.33083
C	0.00003	1.23472	0.44818
H	0.00010	2.16303	-0.11135
C	0.00008	1.25103	1.81855
H	0.00025	2.16902	2.39437
C	-0.00005	0.00014	2.52449
O	-0.00022	0.00015	3.81037
H	-0.00008	-0.00058	4.77797
C	-0.00018	-1.25084	1.81862
H	0.00052	-2.16878	2.39448
C	-0.00014	-1.23474	0.44824
H	0.00004	-2.16310	-0.11123

p-Cyanophenol|Ox.|SMD

C	0.01235	0.01767	-0.25912
C	0.00162	1.21436	0.40002
C	-0.00441	1.21165	1.82921
O	-0.01446	2.32901	2.52477
C	0.00008	-0.00283	2.58540
C	0.01099	-1.19527	1.91845
H	0.01489	-2.13645	2.45299
C	0.01715	-1.19448	0.49392
C	0.02822	-2.43106	-0.19388
H	0.01713	-0.02624	-1.34072
H	-0.01692	3.11779	1.94013
H	-0.00525	0.05482	3.66698
H	-0.00243	2.15983	-0.13112
N	0.03527	-3.45249	-0.75808

Dimethylsulfide|Ox.|SMD

S	-0.21283	0.22140	0.56693
C	0.21454	1.38969	-0.70737
C	0.21334	1.10056	2.05581
H	-0.02005	0.92846	-1.66531
H	-0.36879	2.30275	-0.54927
H	-0.37455	2.02369	2.09286
H	-0.01635	0.44874	2.89711
H	1.27978	1.34616	2.01928

H	1.28236	1.61762	-0.62390

Dimethyldisulfide|Ox.|SMD

S	0.17245	0.44105	-1.07072
S	-0.18544	0.00100	0.85974
C	0.14639	1.60519	1.63618
C	-0.16654	-1.16121	-1.84804
H	-0.55845	2.34549	1.25758
H	-0.01897	1.42506	2.69972
H	0.51809	-1.91123	-1.45193
H	0.02440	-0.98797	-2.90844
H	1.18137	1.89309	1.45165
H	-1.20972	-1.43179	-1.68454

Thioanisole|Ox.|SMD

C	-0.00006	-0.05434	-0.50104
C	0.00013	1.13193	0.25792
H	0.00022	2.09317	-0.24388
C	0.00020	1.07804	1.63717
H	0.00040	1.98956	2.22176
C	0.00010	-0.18858	2.27215
C	0.00005	-1.38855	1.50466
H	-0.00001	-2.34769	2.01178
C	-0.00010	-1.31018	0.12654
H	-0.00025	-2.21650	-0.46844
H	-0.00020	0.00497	-1.58418
S	0.00021	-0.42066	3.97093
C	-0.00013	1.22504	4.70118
H	0.00023	1.05278	5.77770
H	-0.90344	1.76138	4.40535
H	0.90256	1.76214	4.40485

p-Chloroaniline|Ox.|SMD

C	-0.00004	-0.02177	-0.22913
C	0.00003	1.17111	0.44813
C	-0.00002	1.17589	1.87775
C	-0.00008	-0.05865	2.59870
C	0.00003	-1.24736	1.91414
H	0.00016	-2.19314	2.44190
C	0.00001	-1.22718	0.50364
H	-0.00018	-0.04662	-1.31191
H	-0.00002	-0.03897	3.68324
H	-0.00007	2.11578	-0.08497
Cl	0.00003	-2.72660	-0.35376
N	0.00001	2.33185	2.53876
H	0.00044	3.21818	2.04538
H	-0.00035	2.35621	3.55286

p-Chlorophenol|Ox.|SMD

C	-0.00002	0.05012	-0.19801
C	-0.00003	1.24182	0.47530
C	0.00004	1.23028	1.89996
O	0.00017	2.35048	2.60946
C	-0.00007	0.01099	2.63881
C	0.00001	-1.17771	1.96149
H	0.00002	-2.12415	2.48719
C	0.00005	-1.15885	0.54422
H	-0.00011	0.01620	-1.28017
H	0.00015	3.13783	2.02560
H	-0.00021	0.05298	3.72151
H	-0.00018	2.18982	-0.05208
Cl	0.00014	-2.64438	-0.30115