Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Are Thermodynamic Cycles Necessary for Continuum Solvent Calculation of p*K*as and Reduction Potentials?

Junming Ho,[1,2*]

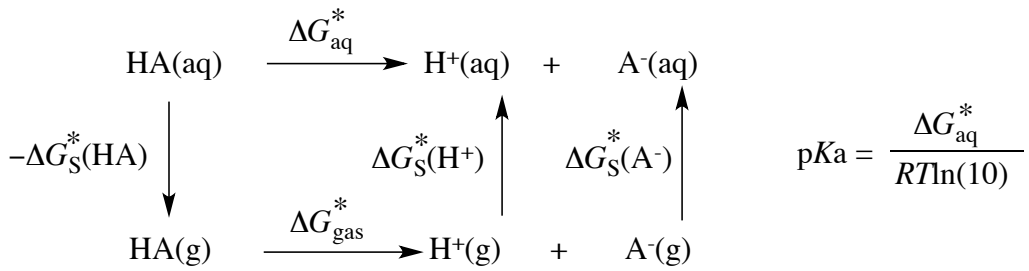
[1]*Department of Chemistry, Yale University, P. O. Box 208107, New Haven, CT 06520-8107.*

[2] *Institute of High Performance Computing, Agency for Science, Technology and Research, 1 Fusionopolis Way, #16-16, Connexis, Singapore 138632*

Email: junming.ho@yale.edu

SUPPORTING INFORMATION

S1. Procedure for calculating the dissociation free energy via a thermodynamic cycle, and directly within the SMD continuum model



$$\mathrm{p}K\mathrm{a} = \frac{\Delta G^*_{\mathrm{aq}}}{RT\ln(10)}$$

Thermodynamic cycle using free energies of solvation computed via eqn (4) in the text.

$$\Delta G^*_{\mathrm{soln}}(\mathrm{TC}) = \Delta E^{\mathrm{L}}_{\mathrm{soln}} + \Delta G^{\mathrm{soln,L}}_{\mathrm{corr}} + G^*_{\mathrm{soln}}(\mathrm{H}^+) + \Delta E^{\mathrm{H}}_{\mathrm{gas}} - \Delta E^{\mathrm{L}}_{\mathrm{gas}} \quad \text{(S1a)}$$

$$\Delta E^{\mathrm{L}}_{\mathrm{soln}} = E^{\mathrm{L}}_{\mathrm{soln}}(A^-) - E^{\mathrm{L}}_{\mathrm{soln}}(HA) \quad \text{(S1b)}$$

$$\Delta E^{\mathrm{L}}_{gas} = E^{\mathrm{L}}_{gas}(A^-) - E^{\mathrm{L}}_{gas}(HA) \quad \text{(S1c)}$$

$$\Delta G^{\mathrm{soln,L}}_{\mathrm{corr}} = G^{\mathrm{soln,L}}_{\mathrm{corr}}(A^-) - G^{\mathrm{soln,L}}_{\mathrm{corr}}(HA) \quad \text{(S1d)}$$

L and H denote that the quantities are evaluated at the low and high levels of theory, respectively. The derivation of eqn (S1) is explained in the text. The gas phase and solution phase electronic energies and thermal corrections are evaluated on geometries optimised in the respective phases. Geometries and thermal corrections were evaluated at the M06-2X/6-31G(d) level of theory, and high-level corrections (H=MP2 or G3(MP2)-RAD(+)) were carried out as single-point calculations on the optimised geometries in the gas phase.

Direct calculation of solution phase dissociation free energies:

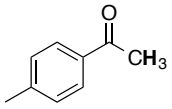
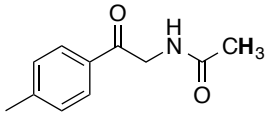
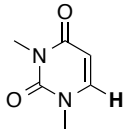
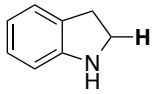
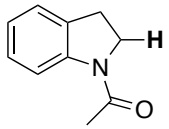
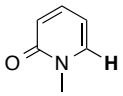
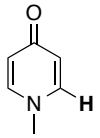
$$\Delta G^*_{\mathrm{soln}} = \Delta E^{\mathrm{H}}_{\mathrm{soln}} + \Delta G^{\mathrm{soln,L}}_{\mathrm{corr}} + G^*_{\mathrm{soln}}(\mathrm{H}^+) \quad \text{(S2a)}$$

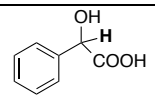
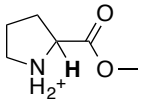
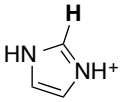
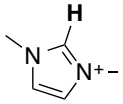
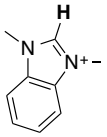
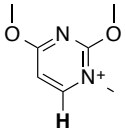
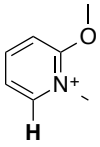
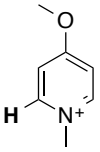
$$\Delta E^{H}_{\mathrm{soln}} = E^{H}_{\mathrm{soln}}(A^-) - E^{H}_{\mathrm{soln}}(HA) \quad \text{(S2b)}$$

The high-level single-point calculations and thermal corrections are computed directly within the SMD solvation model on the solution-phase optimised geometry.

Table S2. Aqueous p*K*a values calculated via a thermodynamic cycle[a] (with and without rovibrational corrections) and directly within the SMD model.

Acid	Alcohols	p*K*a (TC)[b]	p*K*a (TC-rovib)[c]	p*K*a (Direct)[d]	Expt[e]
1	CH_3O**H**	25.91	27.15	27.66	15.5
2	CH_3CH_2O**H**	25.15	26.45	27.29	15.9
3	CF_3CH_2O**H**	20.63	20.98	20.75	12.5
4	$C(CH_3)_3O$**H**	25.58	26.96	27.83	18
5	$C_6H_5CH_2O$**H**	23.65	24.70	25.32	15.4
6	$CH_3CH(O$**H**$)CH_3$	25.24	26.46	27.30	17.1
7	$CF_3CH(O$**H**$)CF_3$	14.04	14.31	13.96	9.3
8	C_6H_5O**H**	15.92	16.27	16.30	10
9	p-F-C_6H_4O**H**	16.11	16.41	16.20	9.95
10	p-NH_2-C_6H_4O**H**	17.53	17.74	17.69	10.3
11	p-NO_2-C_6H_4O**H**	11.11	11.07	10.53	7.15
12	p-Me-C_6H_4O**H**	16.39	16.79	16.84	10.14
13	p-MeO-C_6H_4O**H**	16.83	17.15	17.17	10.21
	Carboxylic acids				
14	HCOO**H**	6.05	6.37	6.41	3.8
15	CH_3COO**H**	7.94	8.41	8.88	4.8
16	CF_3COO**H**	-0.30	0.05	-0.32	0.5
17	CCl_3COO**H**	-0.21	0.08	-0.16	0.65
18	CH_2CHCOO**H**	6.84	7.17	7.45	4.25
19	C_6H_5COO**H**	6.26	6.87	7.27	4.2
20	CH_3COCOO**H**	3.35	3.50	3.38	2.5
	Inorganic acids				
21	**H**F	15.89	16.02	15.23	3.17
22	**H**Cl	0.59	0.65	0.01	-8
23	H_2O	25.13	25.38	26.30	14
24	**H**OOH	18.66	18.91	19.48	11.7
25	NH_3	41.58	41.93	43.29	33
26	H_2S	14.43	14.52	14.29	7
27	**H**N_3	7.09	7.17	6.66	4.72
28	**H**OCl	12.78	12.90	13.65	7.5
29	**H**NO_2	3.98	3.89	3.59	3.29
30	**H**NO_3	-3.47	-3.48	-4.21	-1.3
31	H_2SO_4	-9.57	-9.41	-9.73	-10
32	H_3PO_4	1.83	1.57	1.05	2.12

33	$CH_3SO_3\mathbf{H}$	-5.51	-5.67	-5.40	-2.6
34	$CF_3SO_3\mathbf{H}$	-14.64	-14.47	-14.67	-14
	Carbon acids				
35	$C\mathbf{H}_3COCH_3$	26.46	27.09	27.43	19
36	$C\mathbf{H}_3COCH_2COCH_3$	13.17	13.55	14.13	9
37	$\mathbf{H}CCH$	28.00	28.22	27.46	21.7
38	$\mathbf{H}CN$	17.01	16.92	16.62	9.4
39	$C\mathbf{H}_3CN$	34.55	34.57	34.91	28.9
40	$C\mathbf{H}_3CH_2CN$	37.13	37.18	37.59	30.9
41	$C\mathbf{H}_2(CN)_2$	15.62	15.58	15.74	11.81
42	$C\mathbf{H}_3NO_2$	17.32	17.28	17.24	10.3
43	$C\mathbf{H}_3CONH_2$	33.79	33.61	34.26	28.4
44	$C\mathbf{H}_3CON(CH_3)_2$	33.69	34.16	34.77	29.4
45	$C\mathbf{H}_3CONHCH_2CONH_2$	33.77	34.09	34.39	29.1
46	$CH_3CONHC\mathbf{H}_2CONH_2$	30.10	30.52	31.14	23.9
47	$C\mathbf{H}_3COOCH_2CH_3$	30.64	31.09	31.67	25.6
48		25.08	25.54	26.01	18.7
49		20.64	20.57	21.16	14.5
50		37.75	37.52	37.37	30
51		43.22	43.87	43.83	36
52		39.68	40.17	40.06	33
53		40.91	40.98	40.76	32
54		40.19	40.16	40.09	32

55		24.98	24.83	25.20	22.6
	Cationic acids				
56	+NH_2-C**H**$_2$-COOMe	24.37	24.23	24.66	21
57	+NMe_3-C**H**$_2$-COOMe	24.38	24.18	24.43	18
58	Me_2C=NH-C**H**$_2$-COOMe	18.00	17.25	18.15	14
59		25.12	25.15	26.10	21
60		25.75	25.96	25.84	23.8
61		27.33	27.15	27.10	23
62		25.19	24.94	24.74	21.6
63		31.32	31.36	31.31	33
64		33.95	33.91	33.90	34
65		33.73	33.40	33.36	33
66	**H**+oxoguanine	-2.36	-2.90	-3.21	-0.1
67	**H**+cytosine	2.31	2.62	3.27	4.4
68	**H**+ch3nh2	9.07	9.53	10.11	10.67
69	**H**+allyamine	8.39	8.29	8.89	9.49
70	**H**+cyclohexamine	10.19	10.27	10.65	10.49
71	**H**+pyrrolidine	10.06	10.40	10.69	11.27
72	**H**+dimethylamine	9.77	10.30	10.43	10.77
73	**H**+methylsulfonylaniline	-1.45	-1.97	-1.76	1.48
74	**H**+aniline	1.63	1.30	1.79	4.61

75	**H**+guanidine	14.12	15.71	16.51	13.6
76	**H**+acetamidine	12.94	13.19	13.99	12.1
77	**H**+pyridine	3.60	4.10	4.18	5.25
78	**H**+aminopyridine	7.58	8.47	8.64	9.18
79	**H**+pyrazine	-0.90	-1.22	-1.38	1.1
80	**H**+isoquinoline	3.99	4.16	4.19	5.38
81	**H**+pyrimidine	-0.19	-0.25	-0.33	-7.7
82	**H**+morpholine	8.52	8.56	8.68	8.49
83	**H**+benzothiazole	-1.85	-1.78	-2.03	1.2

[a] Calculated using the thermodynamic cycle A shown in Figure 1.

[b] Aqueous p*K*a values calculated via the thermodynamic cycle (Figure 1 cycle A) employing G3(MP2)-RAD(+) gas phase energies with solvation free energies computed from Eq 1.

[c] Aqueous p*K*a values calculated via the thermodynamic cycle (Figure 1 cycle A) employing G3(MP2)-RAD(+) gas phase energies with solvation free energies computed from Eq 4.

[d] Aqueous p*K*a values calculated directly within the SMD continuum model via Eq 10 where high level calculations are performed at G3(MP2)-RAD(+). [d] All geometries and thermal corrections are computed at the M06-2X/6-31+G(d) level.

[e] See ref 11 for details.

Table S3. DMSO p*K*a values calculated via a thermodynamic cycle[a] (with and without rovibrational corrections) and directly within the SMD model.

	Acid	p*K*a (TC)[b]	p*K*a (TC-rovib)[c]	p*K*a (Direct)[d]	Expt[e]
1	Picric acid	0.35	0.27	-0.46	0
2	$MeSO_2OH$	-3.60	-3.74	-3.94	1.6
3	CF_3COOH	-0.90	-0.59	-0.99	3.45
4	2,4-$(NO_2)_2$-phenol	6.43	6.58	6.14	5.1
5	PhCOSH	3.25	3.40	3.62	5.2
6	$Cl_2CHCOOH$	2.55	2.87	2.66	6.4
7	p-NO_2-C_6H_4OH	9.84	9.80	9.15	10.8
8	PhCOOH	9.44	9.52	9.53	11
9	CH_3COOH	12.31	12.54	12.56	12.3
10	HCN	11.53	11.48	11.19	12.9
11	$(CH_3CO)_2CH_2$	14.78	15.07	15.20	13.3
12	C_5NH_4OH	13.68	13.68	13.04	14.8
13	$PhCH_2SH$	12.65	13.33	13.50	15.4
14	NC-NH_2	11.39	11.71	12.23	16.9
15	n-BuSH	14.16	14.58	14.61	17
16	PhOH	16.37	16.62	16.49	18
17	Imidazole	14.50	14.67	14.56	18.6
18	$PhCONHNH_2$	16.12	16.27	16.51	18.9
19	Pyrazole	14.84	15.17	15.32	19.8
20	$(NH_2)_2C=S$	16.72	18.02	17.78	21.1
21	CF_3CH_2OH	24.71	25.17	24.76	23.45
22	$H_2NCOOEt$	22.93	23.25	23.59	24.6
23	$PhCOCH_3$	26.25	26.57	26.82	24.7
24	$CH_3C(O)NH_2$	23.73	23.53	23.83	25.5
25	$CH_3C(O)CH_3$	28.74	29.07	29.19	26.5
26	$(NH_2)_2C=O$	23.65	24.00	24.25	26.95
27	CH_3OH	33.35	33.37	33.38	29
28	MeCN	29.32	29.84	30.15	31.3
29	DMSO	35.80	36.34	36.47	35
30	4-Methylpyridine	32.11	32.14	32.47	35
31	$PhNMe_2$-H+	1.44	1.04	1.15	2.4
32	Pyridine-H+	-0.06	0.04	0.08	3.4
33	$PhNH_3$+	-3.22	-3.75	-3.27	3.6
34	Et_3N-H+	8.37	8.09	8.25	9

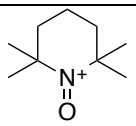
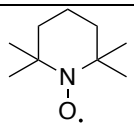
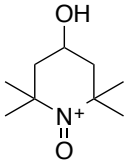
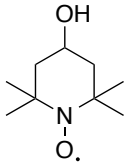
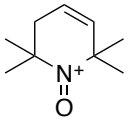
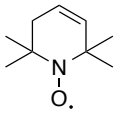
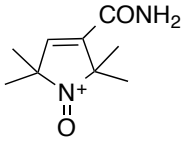
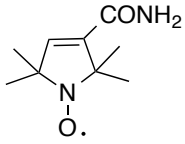
[a] Calculated using the thermodynamic cycle A shown in Figure 1.

[b] DMSO p*K*a values calculated via the thermodynamic cycle (Figure 1 cycle A) employing G3(MP2)-RAD(+) gas phase energies with solvation free energies computed from Eq 1.

[c] DMSO p*K*a values calculated via the thermodynamic cycle (Figure 1 cycle A) employing G3(MP2)-RAD(+) gas phase energies with solvation free energies computed from Eq 4.

[d] DMSO p*K*a values calculated directly within the SMD continuum model via Eq 10 where high level calculations are performed at G3(MP2)-RAD(+). [d] All geometries and thermal corrections are computed at the M06-2X/6-31+G(d) level.
[e] See ref 51 for details.

Table S4. Aqueous reduction potentials calculated via a thermodynamic cycle[a] (with and without rovibrational corrections) and directly within the SMD model.

	Ox	Red	E° (TC)[b]	E° (TC-rovib)[c]	E° (Direct)[d]	Expt[e]
1	$Me_2NH^{\cdot+}$	Me_2NH	1.24	1.25	1.24	1.27
2	$Et_2NH^{\cdot+}$	Et_2NH	1.25	1.23	1.22	1.36
3	Piperidine$^{\cdot+}$	Piperidine	1.26	1.26	1.24	1.34
4	$PhNH_2^{\cdot+}$	PhNH2	1.17	1.16	1.12	1.02
5	4OH-$PhNH_2^{\cdot+}$	4OH-$PhNH_2$	0.87	0.87	0.83	0.76
6	4NH_2-Ph-$NH_2^{\cdot+}$	4NH_2-Ph-NH_2	0.50	0.47	0.43	0.59
7	4Me-$PhNH_2^{\cdot+}$	4Me-$PhNH_2$	1.02	1.01	0.97	0.92
8	4MeO-$PhNH_2^{\cdot+}$	4MeO-$PhNH_2$	0.83	0.82	0.78	0.79
9	4COCH3-$PhNH_2^{\cdot+}$	4COCH3-$PhNH_2$	1.39	1.40	1.35	1.14
10	4CN-$PhNH_2^{\cdot+}$	4CN-$PhNH_2$	1.49	1.49	1.42	1.32
11	$Ph_2NH^{\cdot+}$	Ph_2NH	1.03	1.01	0.98	1.0
12	Indole$^{\cdot+}$	Indole	1.35	1.35	1.33	1.24
13	3-methyl-indole$^{\cdot+}$	3-methyl-indole	1.17	1.16	1.15	1.07
14	2,3-dimethyl-indole$^{\cdot+}$	2,3-dimethyl-indole	0.96	0.95	0.94	0.93
	Nitroxides					
15			0.64	0.60	0.55	0.74
16			0.71	0.75	0.70	0.825
17			0.71	0.72	0.68	0.795
18			0.84	0.86	0.81	0.955
	Alcohols					
19	PhO$^{\cdot}$	PhO^{-}	0.43	0.42	0.45	0.794
20	4F-PhO$^{\cdot}$	4F-PhO^{-}	0.35	0.35	0.40	0.76
21	4CN-PhO$^{\cdot}$	4CN-PhO^{-}	0.79	0.80	0.80	1.12
22	4$COCH_3$-PhO$^{\cdot}$	4$COCH_3$-PhO^{-}	0.76	0.75	0.76	1.00

23	$4NO_2$-PhO$^{\cdot}$	$4NO_2$-PhO^{-}	0.97	0.98	0.99	1.22
24	$4NMe_2$-PhO$^{\cdot}$	$4NMe_2$-PhO^{-}	-0.22	-0.24	-0.21	0.174
25	4MeO-PhO$^{\cdot}$	4MeO-PhO^{-}	0.13	0.12	0.14	0.54
26	4OH-PhO$^{\cdot}$	4OH-PhO^{-}	0.17	0.14	0.16	0.45
27	1-naphthol$^{\cdot}$	1-naphthol^{-}	0.22	0.21	0.24	0.59
28	PhOH$^{\cdot+}$	PhOH	1.90	1.91	1.90	1.5
29	4MeO-PhOH$^{\cdot+}$	4MeO-PhOH	1.37	1.37	1.35	1.1
30	OH-PhOH$^{\cdot+}$	OH-Ph-OH	1.41	1.44	1.41	1.1
31	PhS$^{\cdot}$	PhS^{-}	0.28	0.26	0.26	0.69
32	4MeO-PhS$^{\cdot}$	4MeO-PhS^{-}	0.10	0.07	0.08	0.57
33	$4NH_2$-PhS$^{\cdot}$	$4NH_2$-PhS^{-}	-0.09	-0.12	-0.09	0.36
34	HS$^{\cdot}$	HS^{-}	0.67	0.67	0.67	1.15
35	$CH_3S^{\cdot}$	CH_3S^{-}	0.08	0.06	0.05	0.73
36	Ascorbate$^{\cdot}$	Ascorbate^{-}	0.81	0.84	0.88	0.72
37	PhCOS$^{\cdot}$	PhCOS^{-}	1.01	0.99	0.97	1.21
38	4MePhCOS$^{\cdot}$	4MePhCOS^{-}	0.99	0.97	0.95	1.19
39	4MeOPhCOS$^{\cdot}$	4MeoPhCOS^{-}	0.97	0.96	0.94	1.17
40	EtCOS$^{\cdot}$	EtCOS^{-}	0.95	0.93	0.92	1.22
41	$Me_2COHO^{\cdot}$	Me_2COHO^{-}	0.95	0.93	0.86	1.45
42	MeHCOHO$^{\cdot}$	MeHCOHO^{-}	0.95	0.96	0.89	1.47

[a] Calculated using the thermodynamic cycle B shown in Figure 1.

[b] Aqueous E° values calculated via the thermodynamic cycle (Figure 1 cycle A) employing G3(MP2)-RAD(+) gas phase energies with solvation free energies computed from Eq 1.

[c] Aqueous E° values calculated via the thermodynamic cycle (Figure 1 cycle A) employing G3(MP2)-RAD(+) gas phase energies with solvation free energies computed from Eq 4.

[d] Aqueous E° values calculated directly within the SMD continuum model via Eq 10 where high level calculations are performed at G3(MP2)-RAD(+). [d] All geometries and thermal corrections are computed at the M06-2X/6-31+G(d) level.

[e] See ref 10 for details.

Table S5. G3(MP2)-RAD(+) electronic energies, M06-2X/6-31+G(d) zero-point vibrational energy, thermal corrections and free energies of solvation.

Solvent	Water											
Solute	EG3(gas)[a]	EG3(soln)[a]	ZPVE[b] (gas)	ZPVE[b] (soln)	Srot[c] (gas)	Srot[c] (soln)	Evib[d] (gas)	Evib[d] (soln)	Svib[e] (gas)	Svib[e] (soln)	ΔGsolv[f]	ΔGsolv[f,g] (rovib)
1	-115.6213259	-115.6282231	136.46	136.26	79.41	79.52	1.30	1.29	6.57	6.51	-23.81	-24.03
1-base	-114.9959835	-115.125741	94.81	101.82	68.30	68.73	0.18	0.16	0.70	0.62	-349.31	-342.42
2	-154.8974288	-154.9044137	212.55	211.32	93.30	93.36	3.83	4.08	19.95	21.91	-23.77	-25.36
2-base	-154.2784419	-154.4021586	171.81	177.84	92.62	92.82	2.55	2.54	12.51	12.79	-335.00	-329.13
3	-452.4161868	-452.4239393	153.98	154.17	110.59	110.63	7.67	7.78	42.39	43.14	-25.97	-25.90
3-base	-451.8250567	-451.9341206	114.53	117.05	110.55	110.42	6.77	6.89	37.09	39.19	-290.65	-288.59
4	-233.4530586	-233.4596249	360.33	359.04	107.00	107.01	10.02	9.94	52.09	51.45	-21.86	-23.03
4-base	-232.8403821	-232.9566791	320.70	326.86	106.74	106.76	8.95	8.28	45.68	41.61	-314.89	-308.17
5	-346.4107276	-346.420713	353.39	353.66	117.22	117.33	10.99	10.77	61.19	60.06	-31.77	-31.42
5-base	-345.8089224	-345.9219833	312.44	318.62	117.04	117.16	9.86	9.59	54.64	53.02	-305.90	-299.54
6	-194.1750337	-194.1819622	287.10	286.07	101.97	102.01	6.68	6.65	34.46	34.14	-23.25	-24.23
6-base	-193.560011	-193.6794673	246.65	252.54	101.59	101.69	5.58	5.37	28.20	27.22	-323.52	-317.58
7	-789.2011492	-789.2059274	167.96	167.88	123.08	123.15	15.76	15.59	91.50	90.22	-16.95	-16.84
7-base	-788.6369842	-788.7308654	129.47	130.81	123.12	123.00	15.18	14.96	88.68	87.10	-248.93	-247.30
8	-307.1471027	-307.1556171	277.34	276.79	112.51	112.55	7.04	6.93	34.27	33.53	-28.90	-29.36
8-base	-306.5775849	-306.6763935	240.66	242.12	112.29	112.28	6.28	6.12	30.74	29.88	-266.14	-264.59
9	-406.3092723	-406.3178619	255.57	254.67	116.80	116.83	9.21	9.13	46.90	46.35	-29.00	-29.83
9-base	-405.7438082	-405.8389578	219.47	220.28	116.69	116.64	8.46	8.30	43.44	42.71	-255.06	-254.17
10	-362.4540809	-362.4690459	320.72	319.93	116.72	116.76	11.18	10.94	58.22	56.42	-48.77	-49.28
10-base	-361.8797325	-361.9864018	284.79	285.12	116.62	116.55	10.54	10.40	58.25	56.58	-289.28	-288.59
11	-511.4742782	-511.4848258	285.85	284.64	122.83	122.84	13.10	12.95	73.27	72.24	-39.23	-40.28
11-base	-510.9395295	-511.017808	250.87	249.55	122.69	122.66	12.46	12.45	71.02	71.02	-214.03	-215.34
12	-346.4216584	-346.4296498	350.39	349.69	116.87	116.90	11.60	11.39	64.03	62.45	-27.42	-27.88
12-base	-345.8503387	-345.9490582	313.15	314.74	116.71	116.70	10.93	10.71	61.48	59.96	-265.93	-264.11
13	-421.5639371	-421.574521	364.52	364.20	120.36	120.41	13.64	13.44	75.19	73.91	-35.44	-35.59
13-base	-420.9910039	-421.0934468	328.00	329.79	120.24	120.23	12.70	12.66	70.54	70.73	-276.72	-275.02

14	-189.5987064	-189.6067774	90.25	89.59	87.95	88.00	0.84	0.83	3.63	3.58	-27.50	-28.17
14-base	-189.0374537	-189.1492755	54.10	55.24	86.31	86.52	0.36	0.36	1.50	1.48	-300.15	-299.07
15	-228.8814446	-228.8903637	164.72	163.00	99.74	99.74	4.34	4.33	25.36	25.26	-29.57	-31.27
15-base	-228.314374	-228.4278105	128.84	129.66	99.35	99.30	3.81	3.66	22.91	22.18	-306.63	-305.71
16	-526.3783187	-526.3841246	105.04	103.11	113.70	113.69	8.46	8.52	47.60	47.90	-20.86	-22.81
16-base	-525.8494429	-525.941696	70.20	70.07	113.61	113.49	7.90	7.76	44.82	43.92	-245.75	-245.71
17	-1606.450759	-1606.457689	90.88	90.10	122.08	122.09	11.37	11.26	65.32	64.49	-23.64	-24.28
17-base	-1605.92538	-1606.014356	55.44	56.03	122.17	122.02	11.27	10.89	65.84	63.14	-237.67	-236.60
18	-266.9160992	-266.9234176	179.40	178.42	105.43	105.47	5.62	5.53	31.05	30.21	-26.14	-26.96
18-base	-266.3549393	-266.4634102	143.24	144.10	105.17	105.14	5.24	5.09	30.12	29.23	-293.36	-292.38
19	-420.3985003	-420.4068526	307.60	305.58	119.95	119.96	10.92	11.06	60.40	61.10	-29.19	-31.28
19-base	-419.8439111	-419.94778	271.06	272.24	119.80	119.80	10.50	10.33	58.54	57.44	-282.27	-280.93
20	-342.0933751	-342.1010918	190.47	189.63	110.44	110.45	8.70	8.32	51.42	46.87	-34.55	-34.42
20-base	-341.5457898	-341.6497476	155.01	155.27	110.35	110.24	8.65	8.09	52.37	48.09	-286.50	-285.50
21	-100.3768453	-100.3835751	24.19	23.46	27.65	27.80	0.00	0.00	0.00	0.00	-22.16	-22.92
21-base	-99.77232438	-99.91309372	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-369.52	-369.52
22	-460.4067604	-460.4087644	17.83	17.51	33.16	33.26	0.00	0.00	0.00	0.00	-8.84	-9.18
22-base	-459.8704686	-459.9742132	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-272.32	-272.32
23	-76.37243245	-76.3841153	56.32	55.43	43.88	44.03	0.01	0.01	0.02	0.03	-40.21	-41.14
23-base	-75.73470295	-75.88518659	22.31	22.80	28.25	28.20	0.00	0.00	0.00	0.00	-409.90	-409.40
24	-151.4284016	-151.4421578	71.03	70.38	69.32	69.33	0.95	1.01	4.58	4.98	-44.34	-45.04
24-base	-150.8142533	-150.9559115	35.38	36.03	72.23	72.02	0.18	0.15	0.75	0.61	-383.37	-382.65
25	-56.51290365	-56.51826302	91.70	90.77	47.91	47.97	0.08	0.07	0.31	0.29	-19.76	-20.71
25-base	-55.85345497	-55.97831842	49.14	50.13	45.56	45.38	0.01	0.01	0.04	0.05	-341.33	-340.30
26	-399.0067712	-399.0085781	40.48	40.22	52.68	52.71	0.04	0.04	0.14	0.15	-7.83	-8.10
26-base	-398.4401022	-398.5392655	15.78	16.02	34.02	33.96	0.00	0.00	0.00	0.00	-262.12	-261.87
27	-164.6308749	-164.637501	57.30	56.98	78.84	78.85	0.98	0.96	4.39	4.32	-22.35	-22.67
27-base	-164.0760272	-164.1786543	16.39	16.48	59.63	59.60	0.71	0.71	3.12	3.09	-271.51	-271.40
28	-535.497349	-535.5040437	35.09	34.88	77.02	77.04	0.24	0.24	1.02	1.00	-22.99	-23.21
28-base	-534.9192757	-535.0337829	4.08	4.49	58.02	57.98	0.32	0.25	1.37	1.05	-310.34	-309.89
29	-205.530477	-205.5338492	55.25	54.98	86.38	86.24	0.87	0.76	3.82	3.26	-16.10	-16.27

29-base	-204.9767261	-205.0827663	22.03	21.40	84.80	84.84	0.22	0.23	0.93	0.95	-283.96	-284.60
30	-280.6493143	-280.6529272	71.75	70.76	97.29	97.22	1.64	1.60	7.29	7.08	-17.20	-18.15
30-base	-280.1207328	-280.2188782	38.52	37.48	96.63	96.59	0.78	0.80	3.30	3.37	-261.26	-262.29
31	-699.6574863	-699.6796509	102.86	101.67	100.64	100.59	6.12	5.78	30.76	28.34	-67.30	-68.11
31-base	-699.1497457	-699.2578586	71.45	70.75	106.08	105.99	5.20	4.80	27.47	23.62	-291.15	-291.08
32	-643.587374	-643.6117947	127.77	126.37	107.53	107.53	9.17	8.68	52.19	46.52	-78.70	-78.90
32-base	-643.0536798	-643.1681267	98.74	96.86	107.32	107.24	7.08	7.09	37.00	36.46	-312.08	-313.77
33	-663.7607855	-663.7806393	164.07	163.54	107.27	107.27	8.03	7.33	44.57	37.97	-62.52	-61.77
33-base	-663.2426599	-663.350789	134.00	133.75	106.81	106.82	5.78	5.75	29.38	29.03	-295.80	-295.98
34	-961.2500231	-961.2599349	104.63	102.78	118.41	118.40	12.38	12.41	70.10	70.19	-31.84	-33.69
34-base	-960.7625958	-960.8500814	73.74	72.84	118.28	118.19	10.92	11.00	61.97	62.40	-234.38	-235.30
35	-192.9644657	-192.9707471	222.91	221.85	101.00	100.94	6.43	6.49	39.25	40.72	-20.91	-22.32
35-base	-192.3631871	-192.4693534	187.26	189.11	100.30	100.32	4.72	4.30	24.09	21.59	-285.09	-282.91
36	-345.4573538	-345.4676786	325.32	324.18	115.57	115.71	13.79	13.66	84.33	83.30	-33.31	-34.32
36-base	-344.9012759	-344.9944088	290.93	291.17	115.73	115.77	12.90	12.41	77.41	72.61	-254.04	-252.86
37	-77.24693029	-77.24686243	50.74	50.98	45.55	45.58	1.09	0.99	4.68	4.21	-2.47	-2.20
37-base	-76.63419781	-76.74430703	18.75	20.14	49.92	49.84	0.83	0.60	3.72	2.58	-287.39	-285.87
38	-93.33422748	-93.33705659	22.95	23.24	49.38	49.42	0.44	0.37	1.84	1.56	-9.45	-9.16
38-base	-92.76550705	-92.86654851	13.06	12.86	47.42	47.41	0.00	0.00	0.00	0.00	-265.65	-265.86
39	-132.6190953	-132.624872	120.92	120.14	86.66	86.66	2.00	1.93	9.70	9.27	-16.66	-17.38
39-base	-132.0085007	-132.1028636	80.37	79.75	83.57	83.55	2.89	2.90	15.88	15.98	-251.20	-251.83
40	-171.8898762	-171.8952407	198.04	197.51	99.91	99.89	4.78	4.69	25.53	24.90	-15.40	-15.82
40-base	-171.2747348	-171.3668494	156.76	156.93	98.86	98.82	5.53	5.75	32.17	34.14	-245.49	-245.68
41	-224.7503713	-224.7615369	119.50	119.20	105.09	105.08	5.25	5.22	28.66	28.83	-31.25	-31.63
41-base	-224.2037784	-224.2832834	83.85	83.22	103.65	103.77	4.87	4.80	26.03	25.53	-211.55	-212.14
42	-244.7929606	-244.7988216	134.30	134.50	98.47	98.48	3.51	3.11	21.45	16.62	-21.24	-20.01
42-base	-244.2099665	-244.3172315	97.01	97.87	97.72	97.85	2.27	1.94	10.20	8.44	-287.27	-286.26
43	-209.0203589	-209.035793	195.53	196.27	100.17	100.12	6.03	5.09	35.69	29.01	-46.52	-44.72
43-base	-208.4075734	-208.5174565	159.16	159.58	99.62	99.58	4.30	3.93	20.71	18.42	-298.22	-297.48
44	-287.5452262	-287.5568646	346.98	347.21	111.34	111.28	12.48	12.27	76.13	73.73	-34.30	-33.55
44-base	-286.9322259	-287.0381729	308.37	311.35	110.77	110.74	10.55	10.09	58.72	55.76	-285.40	-281.99

45	-416.8401341	-416.8641444	347.22	344.87	118.81	118.61	15.42	15.42	93.02	92.25	-73.63	-75.69
45-base	-416.2471293	-416.3457662	308.77	308.83	118.22	118.33	13.56	13.70	78.05	79.36	-271.30	-271.53
46	-416.8401322	-416.8641446	347.21	344.87	118.81	118.61	15.42	15.43	93.02	92.26	-73.63	-75.68
46-base	-416.2472854	-416.3519641	309.01	308.65	119.90	119.93	15.53	15.14	93.42	89.78	-288.92	-288.59
47	-307.4133975	-307.418582	315.25	314.13	111.91	111.94	11.50	11.18	70.53	66.67	-17.80	-18.10
47-base	-306.8046739	-306.9056356	275.98	278.04	111.46	111.54	10.59	10.20	62.79	60.59	-272.58	-270.28
48	-423.7585706	-423.7648099	439.38	438.54	123.59	123.59	17.39	17.22	102.88	101.15	-22.10	-22.60
48-base	-423.1658487	-423.2648075	401.97	403.93	123.35	123.36	16.36	16.05	95.17	93.51	-268.23	-266.09
49	-631.576824	-631.5937546	587.98	587.99	134.40	134.42	28.59	27.98	177.43	171.03	-53.23	-51.93
49-base	-631.0084888	-631.1035281	551.68	552.25	134.37	134.54	27.79	27.57	170.62	168.65	-261.67	-260.78
50	-492.9529778	-492.9684849	380.48	380.16	122.37	122.35	17.08	16.57	102.33	96.47	-47.92	-47.00
50-base	-492.3544477	-492.4422655	343.14	342.72	122.17	122.17	16.40	16.41	96.31	96.12	-236.89	-237.24
51	-363.4163907	-363.4241257	344.57	343.62	117.87	117.89	8.94	8.87	43.88	43.46	-25.31	-26.20
51-base	-362.791195	-362.8851114	306.53	309.21	117.71	117.70	8.77	8.50	43.09	41.63	-251.31	-248.47
52	-515.9238405	-515.9313517	445.43	443.82	126.81	126.82	17.19	17.25	97.10	97.23	-26.06	-27.65
52-base	-515.3174139	-515.3998798	407.24	407.99	126.68	126.70	17.29	17.12	99.22	97.11	-222.21	-221.01
53	-362.4540713	-362.4675348	323.17	324.45	116.08	116.09	10.32	9.57	56.51	49.75	-41.62	-39.08
53-base	-361.8425531	-361.9342313	285.30	287.59	115.84	115.85	9.76	9.31	52.23	48.53	-245.74	-242.82
54	-362.4360111	-362.4578307	322.29	323.49	116.40	116.35	10.98	10.46	63.42	58.12	-65.01	-62.73
54-base	-361.8241488	-361.9255091	283.92	285.94	116.16	116.13	10.57	10.41	60.20	59.45	-273.45	-271.36
55	-534.8266045	-534.8418568	394.45	394.22	125.82	125.81	17.01	17.26	98.63	100.99	-49.24	-49.92
55-base	-534.2545536	-534.3420166	356.91	355.77	126.01	126.04	17.01	17.44	95.84	98.60	-240.96	-242.50
$Me_2NH^{\cdot+}$	-134.7196307	-134.8273399	240.21	241.07	93.33	93.23	5.64	5.44	36.96	33.70	-283.30	-281.63
Me_2NH	-135.0288314	-135.0355264	246.22	247.58	93.35	93.37	3.97	3.80	20.71	19.72	-19.03	-17.55
$Et_2NH^{\cdot+}$	-213.2766162	-213.3756803	391.93	391.96	108.46	108.37	11.36	11.41	68.38	68.43	-260.51	-260.42
Et_2NH	-213.5775394	-213.5830152	397.22	398.25	108.26	108.23	10.55	10.06	62.67	57.46	-15.66	-13.56
$Piperidine^{\cdot+}$	-251.3473689	-251.4455373	419.64	419.94	109.78	109.73	7.79	7.89	38.89	40.03	-257.42	-257.35
Piperidine	-251.6453617	-251.6522024	422.94	423.16	109.77	109.78	6.97	6.84	34.28	33.43	-19.25	-18.91
$PhNH_2^{\cdot+}$	-287.0072926	-287.1005143	311.96	310.96	112.62	112.59	7.49	7.55	36.95	37.48	-246.59	-247.68
$PhNH_2$	-287.2931253	-287.300841	310.59	310.27	112.61	112.63	7.70	7.52	37.84	36.64	-25.74	-25.90

4OH-$PhNH_2^{\cdot+}$	-362.1848363	-362.2810651	324.89	324.00	116.67	116.65	10.11	10.07	51.84	51.81	-258.23	-259.14
4OH-$PhNH_2$	-362.4540856	-362.4690409	320.71	319.94	116.72	116.76	11.19	10.94	58.31	56.44	-48.77	-49.24
4NH_2-Ph-$NH_2^{\cdot+}$	-342.3494625	-342.4397102	358.47	355.77	116.71	116.69	10.89	11.37	55.67	58.81	-241.69	-244.84
4NH_2-Ph-NH_2	-342.599944	-342.6137825	354.02	353.34	116.79	116.81	11.97	11.67	63.51	61.21	-44.64	-44.95
4Me-$PhNH_2^{\cdot+}$	-326.2910946	-326.3796886	384.78	383.68	116.93	116.90	12.08	12.13	67.48	67.93	-234.47	-235.65
4Me-$PhNH_2$	-326.5676209	-326.5746383	383.54	382.84	116.93	116.95	12.31	12.14	68.11	66.92	-23.76	-24.28
4MeO-$PhNH_2^{\cdot+}$	-401.4464737	-401.5324013	401.03	399.79	120.38	120.36	14.00	14.00	76.84	77.26	-228.63	-229.99
4MeO-$PhNH_2$	-401.7098293	-401.7196139	397.84	397.42	120.39	120.43	14.34	14.14	79.58	77.96	-32.21	-32.37
4$COCH_3$-$PhNH_2^{\cdot+}$	-439.5012978	-439.6003605	410.58	410.01	123.52	123.48	16.47	16.11	93.90	91.16	-264.77	-264.87
4$COCH_3$-$PhNH_2$	-439.7950437	-439.8088241	410.18	408.74	123.51	123.50	16.65	16.52	94.30	93.21	-45.59	-46.83
4CN-$PhNH_2^{\cdot+}$	-379.1404768	-379.2462283	307.73	306.84	119.81	119.78	12.12	12.05	66.86	66.36	-277.77	-278.58
4CN-$PhNH_2$	-379.4455737	-379.4576145	306.93	306.05	119.77	119.77	12.41	12.26	67.75	66.63	-38.29	-38.99
$Ph_2NH^{\cdot+}$	-517.8074044	-517.8868312	526.71	525.60	130.05	130.05	18.56	18.67	105.35	106.05	-211.19	-212.40
Ph_2NH	-518.0750607	-518.0817008	524.84	524.78	130.10	130.14	19.20	18.93	109.37	107.35	-23.54	-23.28
Indole$^{\cdot+}$	-363.1292381	-363.2157139	344.54	343.31	117.89	117.87	8.91	8.90	44.13	43.87	-230.50	-231.66
Indole	-363.4163912	-363.4241229	344.57	343.63	117.87	117.89	8.94	8.87	43.86	43.49	-25.30	-26.21
3-methyl-indole$^{\cdot+}$	-402.4131063	-402.4970378	417.88	417.55	121.82	121.80	13.57	13.29	75.07	72.10	-223.97	-223.68
3-methyl-indole	-402.692238	-402.6991008	418.05	417.78	121.81	121.83	13.55	13.17	72.78	69.37	-22.77	-22.40
2,3-dimethyl-indole$^{\cdot+}$	-441.7009326	-441.7824409	490.38	489.19	124.85	124.82	18.35	18.19	106.87	104.94	-217.58	-218.35
2,3-dimethyl-indole	-441.97015	-441.9770723	491.08	490.47	124.88	124.90	18.34	17.99	104.91	101.69	-22.66	-22.67
tempo-cation	-482.9820849	-483.0618599	701.21	699.96	124.86	124.80	23.21	23.41	127.96	131.32	-208.62	-210.64
tempo-radical	-483.2346119	-483.2405999	697.65	699.83	124.83	124.84	23.25	22.76	127.71	124.80	-19.18	-16.62
OH-tempo-cation	-558.1379982	-558.2283332	711.45	713.65	127.80	127.76	26.68	25.74	148.98	141.42	-240.30	-236.77
OH-tempo-radical	-558.3949203	-558.409607	708.52	708.00	127.77	127.78	26.60	26.40	147.70	146.29	-46.58	-46.88
tempene-cation	-481.7475782	-481.8268985	636.38	636.21	124.44	124.39	22.71	22.47	125.44	124.12	-208.11	-208.11

tempene-radical	-482.0021651	-482.007861	633.04	631.60	124.46	124.49	22.89	22.88	127.08	126.98	-19.37	-20.80
tcpo-cation	-611.0268462	-611.1176231	628.62	628.93	129.61	129.60	29.50	28.94	170.64	167.02	-242.31	-241.47
tcpo-radical	-611.2853718	-611.3031178	625.97	624.18	129.67	129.68	29.82	29.66	174.39	172.81	-56.15	-57.64
$PhO^{\cdot}$	-306.494203	-306.500741	242.64	243.12	106.46	106.48	6.39	6.46	31.56	32.14	-27.15	-26.78
PhO^{-}	-306.5775828	-306.6763942	240.67	242.11	106.53	106.52	6.28	6.12	30.75	29.86	-266.14	-264.60
4F-$PhO^{\cdot}$	-405.6599331	-405.6656281	221.67	221.97	110.78	110.78	8.42	8.48	43.58	44.22	-25.01	-24.85
4F-PhO^{-}	-405.7438056	-405.8389568	219.48	220.27	110.93	110.87	8.46	8.30	43.45	42.66	-255.06	-254.18
4CN-$PhO^{\cdot}$	-398.6414926	-398.650298	238.70	238.91	113.81	113.80	11.07	11.03	61.58	61.33	-29.54	-29.29
4CN-PhO^{-}	-398.7568763	-398.8392588	238.97	238.99	113.84	113.80	10.84	10.75	60.18	59.74	-221.93	-221.85
4$COCH_3$-$PhO^{\cdot}$	-458.9923773	-459.0030673	342.29	341.90	123.32	123.31	15.25	15.17	87.36	86.68	-37.86	-38.12
4$COCH_3$-PhO^{-}	-459.1008283	-459.1900729	341.89	341.86	123.37	123.33	15.27	15.02	88.49	86.76	-243.76	-243.51
4NO_2-$PhO^{\cdot}$	-510.8156704	-510.8220788	249.95	249.51	116.88	116.88	12.65	12.67	71.98	72.21	-26.17	-26.65
4NO_2-PhO^{-}	-510.9395256	-511.0177996	250.85	249.54	116.93	116.89	12.46	12.46	71.06	71.10	-214.02	-215.34
4NMe_2-$PhO^{\cdot}$	-440.3376442	-440.3564617	440.16	441.19	123.53	123.53	17.33	17.39	101.24	101.95	-57.82	-56.94
4NMe_2-PhO^{-}	-440.4065676	-440.5069338	434.10	436.63	123.48	123.43	16.64	16.27	94.73	92.14	-269.59	-266.65
4MeO-$PhO^{\cdot}$	-420.9189494	-420.9299858	331.78	332.20	120.14	120.16	12.70	12.63	70.38	69.91	-38.75	-38.26
4MeO-PhO^{-}	-420.9910039	-421.0934468	328.00	329.79	120.23	120.23	12.69	12.66	70.53	70.73	-276.72	-275.03
4OH-$PhO^{\cdot}$	-381.6627571	-381.6789642	255.06	255.69	116.40	116.40	9.19	9.04	47.39	46.95	-55.79	-55.18
4OH-PhO^{-}	-381.7356803	-381.8427386	250.30	252.25	116.53	116.51	10.39	9.48	57.84	49.15	-292.09	-288.45
1-$naphthol^{\cdot}$	-459.9719084	-459.9799572	367.67	368.10	124.07	124.08	12.97	12.96	68.96	68.91	-30.69	-30.27
1-$naphthol^{-}$	-460.0567973	-460.1475495	365.21	366.61	124.11	124.13	12.83	12.73	67.58	67.18	-244.81	-243.38
$PhOH^{\cdot+}$	-306.8316744	-306.9269493	277.52	278.34	112.56	112.54	7.12	6.95	35.33	34.38	-255.53	-254.60
PhOH	-307.1471039	-307.1556192	277.35	276.78	112.51	112.55	7.03	6.93	34.16	33.54	-28.90	-29.39
4MeO-$PhOH^{\cdot+}$	-421.2787618	-421.3665232	367.12	366.98	120.38	120.35	13.44	13.22	74.16	72.66	-236.12	-236.03
4MeO-PhOH	-421.5639378	-421.5745254	364.52	364.19	120.36	120.41	13.64	13.44	75.17	73.90	-35.44	-35.61
OH-$PhOH^{\cdot+}$	-382.0153134	-382.1145766	291.03	292.21	116.62	116.62	9.51	9.16	49.05	46.87	-268.84	-267.37
OH-Ph-OH	-382.3082106	-382.3240508	287.38	286.30	110.90	110.94	10.46	10.29	53.80	52.56	-52.08	-52.98
$PhS^{\cdot}$	-629.1532948	-629.1568652	240.29	240.04	110.18	110.18	7.11	7.18	36.36	36.81	-12.23	-12.55
PhS^{-}	-629.2407109	-629.3252533	237.61	238.99	110.31	110.34	7.12	7.08	36.16	36.08	-225.23	-223.86
4MeO-$PhS^{\cdot}$	-743.5763567	-743.582539	328.39	327.36	122.99	123.01	13.46	13.64	75.59	77.08	-21.06	-22.36

4MeO-PhS$^-$	-743.656792	-743.7444018	325.24	326.34	123.13	123.17	13.51	13.49	76.13	76.06	-234.20	-233.11
4NH$_2$-PhS$^\cdot$	-684.4687459	-684.4824344	283.98	283.75	119.60	119.61	11.18	11.39	59.64	61.87	-46.08	-46.77
4NH$_2$-PhS$^-$	-684.5450299	-684.6381792	281.35	282.52	119.77	119.79	11.58	11.05	65.84	59.74	-251.76	-249.31
HS$^\cdot$	-398.3536307	-398.3555123	16.31	16.29	33.93	33.94	0.00	0.00	0.00	0.00	-6.74	-6.76
HS$^-$	-398.4401027	-398.539265	15.79	16.01	34.02	33.96	0.00	0.00	0.00	0.00	-262.12	-261.88
CH$_3$S$^\cdot$	-437.6248881	-437.6268943	94.57	94.05	83.57	83.56	1.04	1.10	4.61	4.94	-6.36	-6.91
CH$_3$S$^-$	-437.6949606	-437.7904545	96.17	97.30	74.75	74.76	0.57	0.55	2.37	2.31	-252.69	-251.56
Ascorbate$^\cdot$	-683.5205597	-683.5516965	366.28	364.18	127.18	127.05	22.58	22.81	133.76	135.45	-101.13	-103.47
Ascorbate$^-$	-683.6531607	-683.7432224	367.62	363.53	128.51	128.51	20.70	22.15	120.01	130.56	-252.38	-258.16
PhCOS$^\cdot$	-742.3728209	-742.377214	266.67	265.82	122.83	122.81	11.88	11.95	67.18	67.86	-16.72	-17.70
PhCOS$^-$	-742.4855931	-742.5729485	265.80	266.68	122.89	122.87	11.30	11.26	63.00	63.12	-235.97	-235.15
4MePhCOS$^\cdot$	-781.6490172	-781.6532216	339.84	338.88	126.02	126.01	16.49	16.49	98.45	98.47	-16.23	-17.19
4MePhCOS$^-$	-781.7601219	-781.8480594	338.53	339.15	126.09	126.07	15.97	15.81	94.53	93.22	-237.88	-237.02
4MeOPhCOS$^\cdot$	-856.794468	-856.8010952	354.14	353.44	128.91	128.91	18.39	18.25	108.08	106.81	-23.74	-24.19
4MeoPhCOS$^-$	-856.9049071	-856.9953188	353.10	353.50	128.97	128.96	17.79	17.68	103.94	102.94	-245.28	-244.70
EtCOS$^\cdot$	-590.1256956	-590.1302694	201.08	199.87	110.72	110.64	7.87	7.85	45.48	45.20	-16.10	-17.23
EtCOS$^-$	-590.2322379	-590.3236779	199.99	200.06	110.41	110.42	7.53	7.38	43.44	42.22	-245.29	-245.00
Me$_2$COHO$^\cdot$	-268.6690155	-268.6792603	262.39	262.45	105.98	106.02	9.00	8.58	47.74	44.46	-31.96	-31.36
Me$_2$COHO$^-$	-268.7562318	-268.8702254	259.79	261.82	106.20	106.19	8.42	7.95	43.00	40.03	-311.48	-309.03
MeHCOHO$^\cdot$	-229.3903898	-229.4009669	187.90	188.86	100.55	100.62	5.37	5.11	27.87	25.94	-33.53	-32.27
MeHCOHO$^-$	-229.4755764	-229.5923587	186.44	187.69	100.75	100.79	5.01	5.31	25.20	28.08	-318.73	-318.06

Solvent	**DMSO**											
1	-920.1086522	-920.1238547	301.99	301.17	136.55	136.55	25.20	25.20	152.16	152.18	-46.89	-47.71
1-base	-919.6061957	-919.6687406	267.24	266.19	136.57	136.54	25.22	25.33	153.67	154.82	-167.03	-168.31
2	-663.760782	-663.7783096	164.08	163.86	107.27	107.28	8.02	7.32	44.39	37.78	-51.06	-50.01
2-base	-663.2426863	-663.3335102	134.01	134.13	106.81	106.82	5.79	5.64	29.41	28.35	-242.34	-242.05
3	-526.3783129	-526.3851581	105.16	103.59	113.70	113.69	8.42	8.48	47.40	47.60	-20.49	-22.07
3-base	-525.8494446	-525.93224	70.20	70.24	113.61	113.54	7.90	7.79	44.82	44.05	-217.63	-217.46
4	-715.8005542	-715.8123514	294.83	293.35	130.56	130.56	18.62	18.80	108.54	109.91	-36.10	-37.80

4-base	-715.2759667	-715.3429683	259.26	258.46	130.55	130.53	18.74	18.77	111.38	111.70	-178.54	-179.39
5	-743.0219627	-743.0322012	292.38	292.16	123.01	123.02	12.55	12.48	69.81	69.34	-30.20	-30.35
5-base	-742.4856461	-742.5722988	265.77	266.52	122.89	122.90	11.30	11.31	63.00	63.16	-232.11	-231.41
6	-1147.26337	-1147.275113	118.44	117.68	117.82	117.81	8.55	8.55	49.98	49.89	-34.05	-34.77
6-base	-1146.728377	-1146.814123	83.27	84.13	117.91	117.80	8.19	7.98	48.67	47.17	-227.11	-225.98
7	-511.4742356	-511.4878977	285.82	285.29	122.83	122.84	13.10	13.02	73.23	73.02	-41.93	-42.48
7-base	-510.9395288	-511.0120935	250.84	250.20	122.70	122.69	12.46	12.53	71.05	71.67	-192.88	-193.63
8	-420.3984997	-420.4096461	307.31	306.23	119.95	119.96	10.97	11.00	60.67	60.77	-32.92	-33.99
8-base	-419.8438589	-419.9335022	271.05	272.18	114.04	119.81	10.50	10.44	58.51	58.32	-239.08	-239.67
9	-228.881446	-228.890897	164.68	163.81	99.74	99.73	4.35	4.24	25.41	24.08	-26.98	-27.56
9-base	-228.3143765	-228.4080497	128.82	129.51	99.36	99.31	3.80	3.72	22.90	22.47	-248.22	-247.47
10	-93.33422792	-93.33953501	22.95	23.37	49.38	49.39	0.44	0.38	1.84	1.59	-16.07	-15.63
10-base	-92.76550608	-92.86911895	13.07	13.23	47.41	47.36	0.00	0.00	0.00	0.00	-272.54	-272.37
11	-345.4573542	-345.4713488	325.36	324.49	109.81	115.72	13.77	13.68	84.17	83.57	-39.13	-41.67
11-base	-344.9012759	-344.9830517	290.92	290.31	115.73	115.75	12.91	13.04	77.49	78.82	-217.82	-218.71
12	-323.1710837	-323.1935985	248.40	248.65	106.48	106.45	6.75	6.44	34.09	32.35	-65.52	-65.04
12-base	-322.6237877	-322.7092416	212.20	212.70	106.16	106.16	5.73	5.76	28.28	28.56	-227.13	-226.68
13	-669.0619282	-669.072142	341.14	340.15	120.72	120.75	11.52	12.03	65.10	69.41	-30.33	-32.10
13-base	-668.4965391	-668.5913245	313.23	315.25	120.56	120.62	10.52	10.40	60.21	59.37	-253.31	-251.18
14	-148.6439417	-148.6626575	90.89	89.45	83.23	83.16	1.88	1.98	8.81	9.32	-53.50	-54.98
14-base	-148.0754601	-148.1809835	54.64	54.85	79.67	79.42	1.07	1.04	4.82	4.68	-284.42	-284.12
15	-556.0880186	-556.0943513	351.41	349.78	112.45	112.44	11.39	11.55	68.75	69.83	-18.14	-19.92
15-base	-555.5154248	-555.6106425	323.43	323.98	112.23	112.20	10.10	10.11	61.84	61.68	-251.69	-251.07
16	-307.1471024	-307.1571247	277.37	277.04	112.51	112.52	7.02	6.95	34.12	33.69	-30.36	-30.64
16-base	-306.5775819	-306.6654527	240.68	241.81	112.29	112.29	6.28	6.19	30.73	30.30	-234.00	-232.84
17	-225.9846662	-226.0023678	189.86	189.98	100.83	100.83	2.29	2.17	9.81	9.24	-50.46	-50.29
17-base	-225.4160531	-225.5149162	153.71	154.83	100.34	100.35	1.74	1.70	7.29	7.13	-262.96	-261.84
18	-455.7963574	-455.8177372	384.21	383.81	123.51	123.54	15.83	15.93	91.99	93.16	-63.20	-63.86
18-base	-455.2388906	-455.3271451	349.08	349.52	123.17	123.21	14.02	14.16	78.67	79.72	-240.13	-239.88
19	-225.9671338	-225.9778036	190.19	190.19	100.86	100.88	2.22	2.12	9.48	8.98	-31.40	-31.36
19-base	-225.3899993	-225.4881113	151.68	153.52	100.46	100.47	1.89	1.77	7.98	7.41	-261.85	-259.96

20	-547.6953301	-547.7180465	162.11	157.95	98.66	104.49	5.20	6.90	25.17	39.37	-67.82	-76.26
20-base	-547.1334453	-547.227346	130.39	129.45	104.24	104.24	3.58	3.67	16.75	17.14	-253.32	-254.29
21	-452.4161912	-452.4234965	153.98	152.51	110.59	110.61	7.67	7.82	42.43	43.00	-22.17	-23.66
21-base	-451.8250583	-451.9133762	114.52	115.60	110.56	110.47	6.78	6.72	37.16	36.87	-232.56	-231.42
22	-323.4624909	-323.4738092	287.00	285.33	111.49	111.52	10.77	10.77	62.95	63.19	-32.76	-34.52
22-base	-322.8741253	-322.9674449	251.15	251.28	111.24	111.28	9.19	9.16	54.51	54.54	-249.99	-249.90
23	-384.4825976	-384.4939436	366.61	365.99	120.25	120.26	12.75	12.66	71.68	70.80	-33.29	-33.74
23-base	-383.891623	-383.9801081	329.28	330.63	119.97	119.99	11.70	11.57	63.83	63.31	-237.25	-235.87
24	-209.02036	-209.0340076	195.55	195.68	100.17	100.15	6.03	5.45	35.66	31.25	-39.22	-38.35
24-base	-208.431642	-208.5270734	161.38	161.58	99.68	99.67	3.97	4.07	21.91	23.88	-255.67	-255.95
25	-192.9644658	-192.9732452	222.91	222.15	101.00	100.96	6.42	6.38	39.24	38.92	-25.12	-25.81
25-base	-192.3631855	-192.455557	187.27	188.21	100.30	100.29	4.72	4.50	24.11	22.62	-245.30	-244.13
26	-225.0692718	-225.0876763	169.39	166.91	99.37	99.35	4.03	4.39	18.77	20.75	-54.17	-56.87
26-base	-224.4794077	-224.5802611	134.77	134.07	98.93	98.89	2.85	2.91	13.13	13.39	-272.04	-272.74
27	-115.6213313	-115.6260432	136.47	135.80	79.42	79.49	1.31	1.38	6.62	7.11	-14.58	-15.34
27-base	-114.9959761	-115.0966716	94.80	96.91	68.29	77.49	0.18	0.19	0.70	0.73	-266.64	-267.28
28	-132.6190956	-132.6275108	120.90	120.51	77.53	86.65	2.00	1.91	9.70	9.15	-23.68	-26.71
28-base	-132.0084993	-132.104098	80.36	80.27	83.57	83.56	2.89	2.87	15.86	15.70	-254.35	-254.41
29	-552.6785487	-552.6907707	211.63	210.33	104.22	104.23	7.19	7.54	38.86	42.82	-38.39	-40.53
29-base	-552.0671371	-552.1563244	174.20	174.92	103.70	103.71	6.46	6.26	33.08	31.65	-241.22	-240.28
30	-287.2868345	-287.2951485	308.92	308.60	112.52	112.54	8.19	8.16	45.36	45.17	-24.19	-24.48
30-base	-286.683332	-286.7679797	269.99	270.14	112.18	112.20	7.30	7.48	36.35	37.99	-226.52	-226.67
31	-366.1877113	-366.2851997	500.61	501.89	120.60	120.56	14.52	14.32	81.14	79.96	-258.34	-256.91
31-base	-365.8155151	-365.824362	461.88	461.02	120.41	120.43	14.66	14.69	83.60	83.60	-26.20	-27.04
32	-248.3759267	-248.4744611	272.94	272.36	101.47	101.44	4.01	4.03	18.20	18.25	-260.86	-261.42
32-base	-248.0101602	-248.0179221	235.81	235.82	101.06	101.08	3.75	3.75	17.00	17.01	-22.77	-22.76
33	-287.6410938	-287.7543067	348.99	350.46	113.06	113.03	8.51	7.96	46.55	41.08	-299.97	-297.42
33-base	-287.293113	-287.3038296	310.57	309.98	112.61	112.64	7.72	7.59	37.91	37.05	-33.62	-34.08
34	-292.4995572	-292.5942173	587.64	587.66	118.37	118.28	17.23	16.95	103.60	101.01	-248.33	-247.80
34-base	-292.112916	-292.117777	547.11	545.62	117.99	118.03	17.03	16.84	102.64	100.59	-13.51	-14.59

[a] G3(MP2)-RAD(+) electronic energies in Hartrees. [b] Zero-point vibrational energy in kJ mol^{-1}. [c] Rotational entropy in J mol^{-1} K^{-1}.

[d] Vibrational energy in kJ mol^{-1}. [e] Vibrational entropy in J mol^{-1} K^{-1}. [f] SMD free energy of solvation in kJ mol^{-1} computed at the M06-2X/6-31+G(d) level of theory. [g] SMD free energy of solvation in kJ mol^{-1} computed at the M06-2X/6-31+G(d) level of theory and including rovibrational corrections.