Supplemental information for:

Computation of Entropy Values for Non-Electrolyte Solute Molecules in Solution Based on Semi-Empirical Corrections to a Polarized Continuum Model

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Table S1. Experimental gas phase and solvation entropies (J mol^{-1} K^{-1}) for various substances in solvents. The standard conditions for the gas phase values are 1 bar and 298.15 K and the solute concentration in each case is 1 mol dm^{-3} (1 M).

solute	solvent	$S°_{gas\_expt}$	$\Delta_{solv}S_{expt}$ [h]	$S°_{solute\_expt}$ [i]
1,4-Dioxane	cyclohexane	300.0 [a]	-72.0	228.0
1,4-Dioxane	ethanol	300.0 [a]	-71.5	228.5
1,4-Dioxane	*n*-Hexane	300.0 [a]	-74.1	225.9
1,4-Dioxane	toluene	300.0 [a]	-86.2	213.8
acetone	*n*-Hexane	295.5 [f]	-63.6	231.9
acetone	toluene	295.5 [f]	-77	218.5
acetone	water	295.5 [f]	-119.2	176.3
acetonitrile	cyclohexane	245.6 [g]	-60.7	184.9
acetonitrile	water	245.6 [g]	-95.8	149.8
benzene	cyclohexane	269.3 [e]	-70.7	198.6
benzene	*n*-Hexane	269.3 [e]	-74.1	195.2
butanol	benzene	362.1 [a]	-82.0	280.1
butanol	cyclohexane	362.1 [a]	-70.3	291.8
butanol	*n*-Hexane	362.1 [a]	-69.5	292.6
butanol	toluene	362.1 [a]	-90.8	271.3
butanol	water	362.1 [a]	-146.9	215.2
butanone	*n*-Hexane	339.5 [f]	-69.9	269.6
butanone	toluene	339.5 [f]	-82.8	256.7
chloroform	*n*-Hexane	295.5 [a]	-82.4	213.2
cyclohexane	benzene	298.3 [a]	-68.6	229.7
cyclohexane	water	298.3 [a]	-132.2	166.1
diethylether	cyclohexane	342.3 [a]	-61.5	280.8
diethylether	water	342.3 [a]	-131.0	211.3
ethanol	benzene	282.8 [b]	-77.8	205
ethanol	cyclohexane	282.8 [b]	-51.5	231.3
ethanol	*n*-Hexane	282.8 [b]	-53.1	229.7
ethanol	toluene	282.8 [b]	-73.6	209.2
ethanol	water	282.8 [b]	-132.2	150.6
ethylacetate	cyclohexane	342.3 [a]	-131	211.3
nitromethane	ethanol	275.1 [c]	-73.2	201.9
nitromethane	*n*-Hexane	275.1 [c]	-61.9	213.2

n-Pentane	benzene	347.9 [a]	-59	288.9
propanol	cyclohexane	322.6 [a]	-64	258.6
propanol	toluene	322.6 [a]	-79.1	243.5
propanol	water	322.6 [a]	-138.5	184.1
toluene	benzene	320.8 [d]	-78.2	242.6
toluene	cyclohexane	320.8 [d]	-75.3	245.5
toluene	ethanol	320.8 [d]	-81.2	239.6
toluene	*n*-Hexane	320.8 [d]	-73.2	247.6
Xe	ethanol	169.7	-46.9	122.8
Xe	water	169.7 [a]	-98.3	71.4

[a]Taken from Ref. 1, [b]Taken from Ref. 2, [c]Taken from ref 3, [d]Taken from Ref. 4, [e]Taken from Ref. 5, [f]Taken from Ref. 6, [g]Taken from Ref. 7, [h]Taken from Ref. 8. [i]$S°_{gas} + \Delta_{solv}S$.

Table S2. Various parameters incorporated in the proposed translational model. All values were obtained using the QM/PCM technique.

Solute	Solvent	m [g mol^{-1}]	V_{cavity} [10^{-30} m^3]	$V_{molecule}$ [10^{-30} m^3]
1,4-Dioxane	cyclohexane	88.05243	160.354	113.853
1,4-Dioxane	ethanol	88.05243	160.409	113.868
1,4-Dioxane	*n*-Hexane	88.05243	160.351	113.852
1,4-Dioxane	toluene	88.05243	160.361	113.854
acetone	*n*-Hexane	58.04186	128.629	88.814
acetone	toluene	58.04186	128.62	88.812
acetone	water	58.04186	128.632	88.822
acetonitrile	cyclohexane	41.02655	98.394	64.599
acetonitrile	water	41.02655	98.386	64.599
benzene	cyclohexane	78.04695	158.605	110.67
benzene	*n*-Hexane	78.04695	158.6	110.624
butanol	benzene	74.07317	167.984	119.403
butanol	cyclohexane	74.07317	167.985	119.407
butanol	*n*-Hexane	74.07317	167.986	119.41
butanol	toluene	74.07317	167.984	119.401
butanol	water	74.07317	167.979	119.358
butanone	*n*-Hexane	72.05751	157.839	110.612
butanone	toluene	72.05751	157.833	110.615
chloroform	*n*-Hexane	117.91438	145.52	94.536
cyclohexane	benzene	84.0939	185.077	134.976
cyclohexane	water	84.0939	185.083	134.978
diethylether	cyclohexane	74.07317	169.932	120.151
diethylether	water	88.05243	174.063	122.205
ethanol	benzene	74.07317	169.974	120.231
ethanol	cyclohexane	46.04186	109.242	74.642
ethanol	*n*-Hexane	46.04186	109.237	74.642
ethanol	toluene	46.04186	109.234	74.643
ethanol	water	46.04186	109.244	74.642
ethylacetate	cyclohexane	46.04186	109.292	74.643
nitromethane	ethanol	61.01638	107.554	71.646
nitromethane	*n*-Hexane	61.01638	107.534	71.631
n-Pentane	benzene	72.0939	183.186	131.516

propanol	cyclohexane	60.05751	138.325	96.707
propanol	toluene	60.05751	138.332	96.709
propanol	water	60.05751	138.409	96.718
toluene	benzene	92.0626	187.783	133.18
toluene	cyclohexane	92.0626	187.778	133.177
toluene	ethanol	92.0626	187.851	133.227
toluene	*n*-Hexane	92.0626	187.776	133.175
Xe	ethanol	131.9042	77.283	44.724
Xe	water	131.9042	77.283	44.724

Table S3. Various parameters incorporated in the proposed rotational model. All values were obtained using the QM/PCM technique.

solute	solvent	σ [–]	$\tilde{A}$ [GHz]	$\tilde{B}$ [GHz]	$\tilde{C}$ [GHz]	μ [debye]	μ_p [debye]	P [au]
1,4-Dioxane	cyclohexane	2	5.11023	4.7127	2.75366	0	0	58.110526
1,4-Dioxane	ethanol	2	5.09927	4.7103	2.75014	0	0	65.252405
1,4-Dioxane	*n*-Hexane	2	5.11082	4.71288	2.75386	0	0	57.717533
1,4-Dioxane	toluene	2	5.10889	4.71231	4.71231	0	0	58.993934
acetone	*n*-Hexane	2	10.18504	8.57307	4.93851	3.4566	3.188	42.298028
acetone	toluene	2	10.18291	8.57744	4.9394	3.5452	3.1934	43.153286
acetone	water	2	10.17396	8.59826	4.94378	4.0047	3.2216	47.671199
acetonitrile	cyclohexane	3	158.86526	9.28072	9.28072	4.409	4.0794	28.507709
acetonitrile	water	3	158.73632	9.28709	9.28709	4.8869	4.079	31.524576
benzene	cyclohexane	12	5.73045	5.73018	2.86516	0	0	72.066342
benzene	*n*-Hexane	12	5.73071	5.73044	2.86529	0	0	71.440589
butanol	benzene	1	18.68927	1.96378	1.86637	2.077744	1.92968	59.632693
butanol	cyclohexane	1	18.69064	1.9638	1.86638	2.058034	1.92862	58.99764
butanol	*n*-Hexane	1	18.69146	1.96381	1.86638	2.046071	1.927988	58.613709
butanol	toluene	1	18.68877	1.96378	1.86637	2.084881	1.93012	59.862961
butanol	water	1	18.67358	1.96366	1.86643	2.288663	1.939169	66.772729
butanone	*n*-Hexane	1	9.56191	3.6	2.75186	3.300261	3.026102	54.703282
butanone	toluene	1	9.55885	3.60004	2.75168	3.393036	3.03136	55.872924
chloroform	*n*-Hexane	3	3.25032	3.24933	1.68527	1.3308	1.2333	50.43084
cyclohexane	benzene	6	4.31948	4.31931	2.4674	0	0	76.145354
cyclohexane	water	6	4.31941	4.31929	2.4676	0	0	87.015282
diethylether	cyclohexane	2	18.25859	2.23537	2.09626	1.6709	1.251	67.006196
diethylether	water	1	7.39687	2.32706	2.05985	2.31308	2.138133	59.079922
ethanol	benzene	2	7.9174	1.26846	1.12372	1.3663	1.2329	59.622499
ethanol	cyclohexane	1	35.4147	9.36495	8.16486	1.918349	1.77079	33.113976
ethanol	*n*-Hexane	1	35.40934	9.36845	8.16721	1.897836	1.769532	32.810888
ethanol	toluene	1	35.40595	9.37061	8.16866	1.885459	1.768821	32.626725
ethanol	water	1	35.41656	9.36371	8.16402	1.925777	1.771237	33.223381
ethylacetate	cyclohexane	1	35.45535	9.33168	8.14203	2.147287	1.7837	36.353703
nitromethane	ethanol	1	12.55523	10.53867	5.94537	4.481914	3.902535	34.660905
nitromethane	*n*-Hexane	1	12.51837	10.57656	5.94888	4.093862	3.869036	31.266191
n-Pentane	benzene	2	17.07087	1.94466	1.84528	0.0938	0.0879	68.645628

propanol	cyclohexane	1	26.20267	3.77441	3.54196	2.046096	1.915707	45.997057
propanol	toluene	1	26.19962	3.77419	3.5418	2.072974	1.917034	46.644169
propanol	water	1	26.17803	3.77228	3.54075	2.276747	1.924657	51.658173
toluene	benzene	1	5.57312	2.52851	1.7584	0.471094	0.408941	87.906944
toluene	cyclohexane	1	5.57349	2.52867	1.75851	0.463372	0.408832	86.673616
toluene	ethanol	1	5.56664	2.5262	1.7566	0.541476	0.41099	100.464027
toluene	*n*-Hexane	1	5.57372	2.52877	1.75858	0.458764	0.408733	85.927674
Xe	ethanol	1				0	0	33.414849
Xe	water	1				0	0	33.754328

Table S4. Total entropies and respective entropic terms for all solutes at a concentration of 1 mol dm^{-3} investigated in this study (J mol^{-1} K^{-1}).

solute	solvent	S_{elec}	S_{trans}	S_{rot}	S_{vib}	$S_{conformer}$	$S_{configuration}$	S_{tot_calc}
1,4-Dioxane	cyclohexane	0	63.0	103.0	32.6	0.0	27.3	226.0
1,4-Dioxane	ethanol	0	63.0	103.0	32.8	0.0	27.3	226.1
1,4-Dioxane	cyclohexane	0	63.0	103.0	32.6	0.0	27.3	226.0
1,4-Dioxane	toluene	0	63.0	103.0	32.6	0.0	27.3	226.0
acetone	*n*-Hexane	0	57.8	87.0	43.6	0.0	29.3	217.7
acetone	toluene	0	57.8	84.8	43.2	0.0	29.3	215.1
acetone	water	0	57.8	77.9	44.7	0.0	29.3	209.8
acetonitrile	cyclohexane	0	54.3	62.3	10.6	0.0	31.6	158.7
acetonitrile	water	0	54.3	54.9	10.4	0.0	31.6	151.0
benzene	cyclohexane	0	62.6	86.6	20.6	0.0	27.4	197.3
benzene	*n*-Hexane	0	62.6	86.6	20.6	0.0	27.4	197.3
butanol	benzene	0	61.2	107.7	66.1	26.8	26.9	288.7
butanol	cyclohexane	0	61.2	107.9	66.1	26.7	26.9	288.8
butanol	*n*-Hexane	0	61.2	108.0	66.1	26.8	26.9	288.9
butanol	toluene	0	61.2	107.6	66.1	26.8	26.9	288.6
butanol	water	0	61.2	104.7	66.3	26.6	26.9	285.7
butanone	*n*-Hexane	0	61.3	101.3	64.3	5.7	27.5	260.0
butanone	toluene	0	61.3	99.1	63.9	6.1	27.5	257.9
chloroform	*n*-Hexane	0	71.3	104.8	23.0	0.0	28.2	227.3
cyclohexane	benzene	0	61.7	95.3	40.6	0.0	26.1	223.7
cyclohexane	water	0	61.7	95.3	40.7	0.0	26.1	223.8
diethylether	cyclohexane	0	61.6	101.6	67.5	7.4	26.8	264.8
diethylether	water	0	61.6	95.3	68.4	7.4	26.8	259.6
ethanol	benzene	0	54.2	91.0	22.4	9.1	30.7	207.4
ethanol	cyclohexane	0	54.2	91.5	22.3	9.1	30.7	207.9
ethanol	*n*-Hexane	0	54.2	91.8	22.3	9.1	30.7	208.1
ethanol	toluene	0	54.2	90.8	22.4	9.1	30.7	207.3
ethanol	water	0	54.3	85.4	22.8	9.1	30.7	202.2
ethylacetate	cyclohexane	0	64.5	110.4	88.7	8.7	26.6	298.9
nitromethane	ethanol	0	59.1	80.1	17.0	0.0	30.8	187.1
nitromethane	*n*-Hexane	0	59.1	87.9	17.0	0.0	30.8	194.8
n-Pentane	benzene	0	60.9	103.3	70.2	12.4	26.2	272.9

propanol	cyclohexane	0	58.1	100.7	42.6	18.2	28.6	248.2
propanol	toluene	0	58.1	100.2	42.7	18.0	28.6	247.6
propanol	water	0	58.1	96.3	43.3	18.1	28.6	244.4
toluene	benzene	0	65.0	112.8	44.2	0.0	25.9	248.0
toluene	cyclohexane	0	65.0	112.8	50.0	0.0	25.9	253.7
toluene	ethanol	0	65.0	112.8	44.2	0.0	25.9	247.9
toluene	*n*-Hexane	0	65.0	112.8	45.8	0.0	25.9	249.5
Xe	ethanol	0	72.8	0.0	0.0	0.0	33.6	106.5
Xe	water	0	72.8	0.0	0.0	0.0	33.6	106.5

Table S5. The standard entropies (J mol^{-1} K^{-1}) for all solute molecules in the standard state (298.15 K, 1 mol dm^{-3}) investigated in this study.

solute	solvent	$S°_{calc}$	$S°_{expt}$	$S°_{calc\text{-}IGT}$
1,4-Dioxane	cyclohexane	226.0	228.0	273.4
1,4-Dioxane	ethanol	226.1	228.5	273.5
1,4-Dioxane	*n*-Hexane	226.0	225.9	273.4
1,4-Dioxane	toluene	226.0	213.8	273.4
acetone	*n*-Hexane	217.7	231.9	271.4
acetone	toluene	215.1	218.5	271.0
acetone	water	209.8	176.3	272.5
acetonitrile	cyclohexane	158.7	184.9	216.3
acetonitrile	water	151.0	149.8	216.1
benzene	cyclohexane	197.3	198.6	264.2
benzene	*n*-Hexane	197.3	195.2	264.2
butanol	benzene	288.7	280.1	310.4
butanol	cyclohexane	288.8	291.8	310.3
butanol	*n*-Hexane	288.9	292.6	310.3
butanol	toluene	288.6	271.3	310.4
butanol	water	285.7	215.2	310.5
butanone	*n*-Hexane	260.0	269.6	306.9
butanone	toluene	257.9	256.7	303.4
chloroform	*n*-Hexane	227.3	213.2	278.7
cyclohexane	benzene	223.7	229.7	288.0
cyclohexane	water	223.8	166.1	288.1
diethylether	cyclohexane	264.8	280.8	310.8
diethylether	water	259.6	211.3	311.8
ethanol	benzene	207.4	205.0	245.4
ethanol	cyclohexane	207.9	231.3	245.4
ethanol	*n*-Hexane	208.1	229.7	245.3
ethanol	toluene	207.3	209.2	245.4
ethanol	water	202.2	150.6	245.8
ethylacetate	cyclohexane	298.9	292.6	338.5
nitromethane	ethanol	187.1	201.9	254.6
nitromethane	*n*-Hexane	194.8	213.2	254.6
n-Pentane	benzene	272.9	288.9	314.6

propanol	cyclohexane	248.2	258.6	277.5
propanol	toluene	247.6	243.5	277.6
propanol	water	244.4	184.1	278.1
toluene	benzene	248.0	242.6	301.3
toluene	cyclohexane	253.7	245.5	307.1
toluene	ethanol	247.9	239.6	301.3
toluene	*n*-Hexane	249.5	247.6	301.3
Xe	ethanol	106.5	122.8	142.9
Xe	water	106.5	71.4	142.9

Table S6. Cartesian coordination for all molecules investigated in this study.

solute	solvent	coordination			
1,4-Dioxane	cyclohexane	C	0.22632100	-0.72518600	-1.16519800
		C	0.22632100	-0.72518600	1.16519800
		C	-0.22632100	0.72518600	1.16519800
		C	-0.22632100	0.72518600	-1.16519800
		H	-0.18944700	-1.26071300	2.02052200
		H	1.32436400	-0.76996900	-1.21663500
		H	-0.18944700	-1.26071300	-2.02052200
		H	-1.32436400	0.76996900	1.21663500
		H	0.18944700	1.26071300	2.02052200
		H	-1.32436400	0.76996900	-1.21663500
		H	0.18944700	1.26071300	-2.02052200
		H	1.32436400	-0.76996900	1.21663500
		O	-0.22632100	-1.39086900	0.00000000
		O	0.22632100	1.39086900	0.00000000
1,4-Dioxane	ethanol	C	0.22680300	-0.72473600	-1.16656500
		C	0.22680300	-0.72473600	1.16656500
		C	-0.22680300	0.72473600	1.16656500
		C	-0.22680300	0.72473600	-1.16656500
		H	-0.18802200	-1.25809200	2.02333400
		H	1.32442000	-0.77026800	-1.21639200
		H	-0.18802200	-1.25809200	-2.02333400
		H	-1.32442000	0.77026800	1.21639200
		H	0.18802200	1.25809200	2.02333400
		H	-1.32442000	0.77026800	-1.21639200
		H	0.18802200	1.25809200	-2.02333400
		H	1.32442000	-0.77026800	1.21639200
		O	-0.22680300	-1.39193500	0.00000000
		O	0.22680300	1.39193500	0.00000000
1,4-Dioxane	*n*-Hexane	C	0.22629100	-0.72521400	-1.16512500
		C	0.22629100	-0.72521400	1.16512500
		C	-0.22629100	0.72521400	1.16512500
		C	-0.22629100	0.72521400	-1.16512500
		H	-0.18954300	-1.26086900	2.02036000
		H	1.32435800	-0.76995700	-1.21666900

		H	-0.18954300	-1.26086900	-2.02036000
		H	-1.32435800	0.76995700	1.21666900
		H	0.18954300	1.26086900	2.02036000
		H	-1.32435800	0.76995700	-1.21666900
		H	0.18954300	1.26086900	-2.02036000
		H	1.32435800	-0.76995700	1.21666900
		O	-0.22629100	-1.39079700	0.00000000
		O	0.22629100	1.39079700	0.00000000
1,4-Dioxane	toluene	C	0.22638900	-0.72512600	-1.16536200
		C	0.22638900	-0.72512600	1.16536200
		C	-0.22638900	0.72512600	1.16536200
		C	-0.22638900	0.72512600	-1.16536200
		H	-0.18923700	-1.26036800	2.02088600
		H	1.32437500	-0.76999700	-1.21656400
		H	-0.18923700	-1.26036800	-2.02088600
		H	-1.32437500	0.76999700	1.21656400
		H	0.18923700	1.26036800	2.02088600
		H	-1.32437500	0.76999700	-1.21656400
		H	0.18923700	1.26036800	-2.02088600
		H	1.32437500	-0.76999700	1.21656400
		O	-0.22638900	-1.39102700	0.00000000
		O	0.22638900	1.39102700	0.00000000
acetone	*n*-hexane	C	0.00000000	0.00000000	0.18524000
		C	0.00000000	1.28366500	-0.61176000
		H	-0.78260000	1.26230400	-1.37513400
		H	-0.14113800	2.13893100	0.04741400
		H	0.95620000	1.38230400	-1.13543500
		C	0.00000000	-1.28366500	-0.61176000
		H	-0.95620000	-1.38230400	-1.13543500
		H	0.78260000	-1.26230400	-1.37513400
		H	0.14113800	-2.13893100	0.04741400
		O	0.00000000	0.00000000	1.39449900
acetone	toluene	C	0.00000000	0.00000000	0.18488800
		C	0.00000000	1.28332200	-0.61169000
		H	-0.78305100	1.26174500	-1.37451000
		H	-0.14028200	2.13917100	0.04691700

		H	0.95578200	1.38097200	-1.13624600
		C	0.00000000	-1.28332200	-0.61169000
		H	-0.95578200	-1.38097200	-1.13624600
		H	0.78305100	-1.26174500	-1.37451000
		H	0.14028200	-2.13917100	0.04691700
		O	0.00000000	0.00000000	1.39482900
acetone	water	C	0.00000000	0.00000000	-0.18295100
		C	0.00000000	-1.28172300	0.61121000
		H	-0.79406400	-1.26392800	1.36230900
		H	-0.12411400	-2.14089500	-0.04643300
		H	0.94782800	-1.36904600	1.15127000
		C	0.00000000	1.28172300	0.61121000
		H	-0.94782800	1.36904600	1.15127000
		H	0.79406400	1.26392800	1.36230900
		H	0.12411400	2.14089500	-0.04643300
		O	0.00000000	0.00000000	-1.39638900
acetonitrile	cyclohexane	C	0.00000000	0.00000000	-1.17535100
		H	0.00000000	1.02574900	-1.54616900
		H	0.88832400	-0.51287400	-1.54616900
		H	-0.88832400	-0.51287400	-1.54616900
		C	0.00000000	0.00000000	0.28011700
		N	0.00000000	0.00000000	1.42998700
acetonitrile	water	C	0.00000000	0.00000000	-1.17521000
		H	0.00000000	1.02616500	-1.54407200
		H	0.88868500	-0.51308300	-1.54407200
		H	-0.88868500	-0.51308300	-1.54407200
		C	0.00000000	0.00000000	0.27923600
		N	0.00000000	0.00000000	1.42972300
benzene	cyclohexane	C	0.03668600	-1.39066400	0.00000000
		C	1.22273300	-0.66357600	-0.00002000
		C	1.18604100	0.72711300	0.00001000
		C	-0.03667800	1.39066300	-0.00000400
		C	-1.22273600	0.66357200	-0.00001000
		C	-1.18604600	-0.72710600	0.00001400
		H	0.06528700	-2.47414100	-0.00000300
		H	2.17533400	-1.18054300	0.00001600

		H	2.11003400	1.29362800	0.00003100
		H	-0.06527600	2.47413500	0.00002200
		H	-2.17533000	1.18053300	-0.00003000
		H	-2.11004600	-1.29362100	0.00002700
benzene	*n*-hexane	C	0.03304300	-1.39072000	0.00000000
		C	1.22096100	-0.66675900	-0.00002000
		C	1.18791100	0.72398700	0.00001000
		C	-0.03303600	1.39071900	-0.00000400
		C	-1.22096300	0.66675500	-0.00001000
		C	-1.18791600	-0.72397900	0.00001400
		H	0.05880500	-2.47426700	-0.00000300
		H	2.17220300	-1.18621900	0.00001600
		H	2.11338300	1.28807900	0.00003100
		H	-0.05879400	2.47426000	0.00002200
		H	-2.17219800	1.18620900	-0.00003000
		H	-2.11339600	-1.28807200	0.00002700
butanol	benzene	C	-1.31503900	0.48765900	0.01599000
		H	-1.34750100	1.17838200	-0.83034600
		H	-1.33711300	1.09244300	0.93361000
		C	-0.03696700	-0.33742700	-0.03091500
		H	-0.03767300	-0.93756700	-0.94767900
		H	-0.03314400	-1.04419700	0.80989300
		C	1.22309900	0.52412300	0.02876000
		H	1.20602400	1.13129700	0.94145600
		H	1.21745600	1.22969700	-0.81013800
		C	2.50532200	-0.30271300	-0.00941800
		H	2.56085200	-0.89685800	-0.92647800
		H	3.39198700	0.33481800	0.03076400
		H	2.55129800	-0.99415600	0.83747800
		O	-2.49070800	-0.30050900	-0.08853400
		H	-2.50501000	-0.91963800	0.64320400
butanol	cyclohexane	C	-1.31523700	0.48758200	0.01628100
		H	-1.34756500	1.17843200	-0.82995500
		H	-1.33733000	1.09244900	0.93393700
		C	-0.03700600	-0.33735700	-0.03057000
		H	-0.03807500	-0.93790900	-0.94704400

		H	-0.03288100	-1.04391100	0.81048600
		C	1.22311700	0.52412400	0.02850900
		H	1.20623300	1.13184700	0.94085700
		H	1.21733900	1.22928300	-0.81074100
		C	2.50535300	-0.30269400	-0.00947000
		H	2.56072600	-0.89737100	-0.92618500
		H	3.39204700	0.33482400	0.03017000
		H	2.55157000	-0.99369400	0.83777300
		O	-2.49058300	-0.30043100	-0.08874700
		H	-2.50475400	-0.92043100	0.64217300
butanol	*n*-hexane	C	-1.31535900	0.48753600	0.01645100
		H	-1.34760500	1.17845400	-0.82973300
		H	-1.33746400	1.09246200	0.93412300
		C	-0.03702900	-0.33731400	-0.03035800
		H	-0.03831400	-0.93811700	-0.94665600
		H	-0.03272800	-1.04373400	0.81085000
		C	1.22312800	0.52412400	0.02836300
		H	1.20636100	1.13217200	0.94050500
		H	1.21726600	1.22903900	-0.81109500
		C	2.50537100	-0.30268300	-0.00950400
		H	2.56065000	-0.89767100	-0.92601800
		H	3.39208400	0.33482600	0.02981400
		H	2.55173300	-0.99342300	0.83794000
		O	-2.49050400	-0.30038800	-0.08887700
		H	-2.50461400	-0.92088200	0.64157500
butanol	toluene	C	-1.31496800	0.48768700	0.01588100
		H	-1.34747800	1.17836000	-0.83049500
		H	-1.33703500	1.09244600	0.93348500
		C	-0.03695300	-0.33745200	-0.03103900
		H	-0.03752500	-0.93744400	-0.94790600
		H	-0.03324100	-1.04429900	0.80968100
		C	1.22309200	0.52412300	0.02885400
		H	1.20594900	1.13109300	0.94167800
		H	1.21749700	1.22985100	-0.80991400
		C	2.50531000	-0.30272000	-0.00940000
		H	2.56089700	-0.89666800	-0.92658800

		H	3.39196600	0.33481500	0.03098100
		H	2.55119900	-0.99432900	0.83736500
		O	-2.49075100	-0.30053900	-0.08845700
		H	-2.50511000	-0.91933600	0.64359000
butanol	water	C	-1.31305000	0.48844600	0.01210300
		H	-1.34705400	1.17687800	-0.83615800
		H	-1.33499500	1.09327400	0.92869400
		C	-0.03649100	-0.33808000	-0.03441300
		H	-0.03276300	-0.93392600	-0.95425500
		H	-0.03641600	-1.04685900	0.80397600
		C	1.22295000	0.52410600	0.03211200
		H	1.20385700	1.12436400	0.94912100
		H	1.21857400	1.23490300	-0.80235700
		C	2.50499200	-0.30293800	-0.00916500
		H	2.56240000	-0.88998000	-0.93080500
		H	3.39144700	0.33451500	0.03807600
		H	2.54797400	-1.00037500	0.83296500
		O	-2.49163500	-0.30192700	-0.08639300
		H	-2.51034300	-0.90658000	0.65806300
butanone	*n*-hexane	C	0.52728200	0.17069400	-0.02158000
		C	1.87544300	-0.51042800	0.03547500
		H	1.92035000	-1.35639200	-0.65490100
		H	2.66833500	0.20242800	-0.18694000
		H	2.02651100	-0.90737000	1.04465700
		C	-0.68143200	-0.74389100	-0.06261900
		H	-0.61855500	-1.30918300	-1.00127400
		H	-0.56136100	-1.49246400	0.72979300
		O	0.42346800	1.37549000	-0.02301900
		C	-2.01483100	-0.02184400	0.05075500
		H	-2.13430600	0.70511200	-0.75445900
		H	-2.84108100	-0.73423300	-0.00040900
		H	-2.08640300	0.52099800	0.99549700
butanone	toluene	C	0.52746300	0.17054800	-0.02170900
		C	1.87483800	-0.51110700	0.03558100
		H	1.91805900	-1.35913300	-0.65223800
		H	2.66856100	0.20001100	-0.18946600

		H	2.02610400	-0.90534100	1.04579200
		C	-0.68134600	-0.74312100	-0.06291500
		H	-0.61828900	-1.30797800	-1.00176500
		H	-0.56088800	-1.49207400	0.72898000
		O	0.42438700	1.37602200	-0.02303400
		C	-2.01510800	-0.02191000	0.05095200
		H	-2.13606400	0.70448800	-0.75460400
		H	-2.84057000	-0.73518900	0.00020600
		H	-2.08709500	0.52058000	0.99590900
chloroform	*n*-hexane	C	-0.00005800	0.00014300	0.45450600
		H	0.00007100	0.00034200	1.53786300
		Cl	1.39599800	0.95387000	-0.08363700
		Cl	-1.52421800	0.73180400	-0.08363700
		Cl	0.12823600	-1.68574500	-0.08360200
cyclohexane	benzene	C	-1.12041500	0.58517500	0.76533500
		C	-1.12034900	0.58534200	-0.76535000
		C	0.30536700	0.58461100	-1.32234600
		C	1.12041500	-0.58517500	-0.76533500
		C	1.12034900	-0.58534200	0.76535000
		C	-0.30536700	-0.58461100	1.32234600
		H	-0.79778900	-1.52722300	1.04923200
		H	-0.28517500	-0.54594000	2.41594000
		H	0.28517500	0.54594000	-2.41594000
		H	0.79778900	1.52722300	-1.04923200
		H	-0.68657700	1.52781000	1.12424400
		H	-2.14641000	0.54698100	1.14444800
		H	-1.64621100	-0.30923600	-1.12422500
		H	-1.67513000	1.44927400	-1.14442600
		H	1.67513000	-1.44927400	1.14442600
		H	1.64621100	0.30923600	1.12422500
		H	0.68657700	-1.52781000	-1.12424400
		H	2.14641000	-0.54698100	-1.14444800
cyclohexane	water	C	-1.12034400	0.58534300	0.76538900
		C	-1.12042300	0.58521400	-0.76540000
		C	0.30544700	0.58473700	-1.32228600
		C	1.12034400	-0.58534300	-0.76538900

		C	1.12042300	-0.58521400	0.76540000
		C	-0.30544700	-0.58473700	1.32228600
		H	-0.79774900	-1.52716700	1.04822100
		H	-0.28511600	-0.54591300	2.41597200
		H	0.28511600	0.54591300	-2.41597200
		H	0.79774900	1.52716700	-1.04822100
		H	-0.68564500	1.52777400	1.12384300
		H	-2.14646000	0.54692100	1.14443700
		H	-1.64562100	-0.30995300	-1.12384800
		H	-1.67512200	1.44933200	-1.14443700
		H	1.67512200	-1.44933200	1.14443700
		H	1.64562100	0.30995300	1.12384800
		H	0.68564500	-1.52777400	-1.12384300
		H	2.14646000	-0.54692100	-1.14443700
diethylether	cyclohexane	C	-1.17652100	-0.51514700	0.00002100
		H	-1.19275800	-1.16775000	-0.88635700
		H	-1.19276300	-1.16768600	0.88644600
		C	-2.37537000	0.40901100	-0.00001200
		H	-2.36787800	1.04734900	-0.88629400
		H	-3.30065600	-0.17262200	0.00028800
		H	-2.36757900	1.04777500	0.88596300
		O	0.00000000	0.26243700	0.00000100
		C	1.17652100	-0.51514700	-0.00002200
		H	1.19276000	-1.16774800	0.88635700
		H	1.19276100	-1.16768800	-0.88644600
		C	2.37537100	0.40901100	0.00001000
		H	2.36774000	1.04751900	0.88616900
		H	3.30065600	-0.17262200	-0.00002900
		H	2.36771900	1.04760500	-0.88608800
diethylether	water	C	-1.17760200	-0.51339800	0.00001600
		H	-1.19048000	-1.16512400	-0.88606000
		H	-1.19049100	-1.16508400	0.88612200
		C	-2.38015100	0.40558300	-0.00001100
		H	-2.37924200	1.04311200	-0.88727700
		H	-3.30139400	-0.18199100	0.00027400
		H	-2.37896100	1.04351600	0.88696500

		O	0.00000000	0.26811600	0.00000700
		C	1.17760200	-0.51339800	-0.00001700
		H	1.19048700	-1.16513000	0.88605400
		H	1.19048300	-1.16507700	-0.88612800
		C	2.38015100	0.40558300	0.00000600
		H	2.37911300	1.04327800	0.88715300
		H	3.30139400	-0.18199100	-0.00003000
		H	2.37909000	1.04334900	-0.88708900
ethanol	benzene	C	1.22111400	-0.22133600	0.00002700
		H	1.29288900	-0.85602300	-0.88627300
		H	1.29281500	-0.85621300	0.88619900
		H	2.06723100	0.47055500	0.00013600
		C	-0.08420300	0.54482600	0.00005500
		H	-0.14190700	1.18920200	0.88719200
		H	-0.14183300	1.18939200	-0.88694800
		O	-1.15108700	-0.39490100	-0.00009100
		H	-1.98196700	0.08135300	-0.00007300
ethanol	cyclohexane	C	1.22094200	-0.22134500	0.00002700
		H	1.29229300	-0.85614000	-0.88619800
		H	1.29221900	-0.85632900	0.88612300
		H	2.06729800	0.47028100	0.00013600
		C	-0.08432900	0.54492600	0.00005500
		H	-0.14180200	1.18939800	0.88724000
		H	-0.14172700	1.18958800	-0.88699700
		O	-1.15075900	-0.39488400	-0.00009100
		H	-1.98188800	0.08079300	-0.00007300
ethanol	*n*-Hexane	C	1.22083500	-0.22135200	0.00002700
		H	1.29192600	-0.85621100	-0.88615300
		H	1.29185300	-0.85640100	0.88607800
		H	2.06733900	0.47010900	0.00013600
		C	-0.08440500	0.54499000	0.00005500
		H	-0.14173800	1.18951900	0.88726900
		H	-0.14166400	1.18970900	-0.88702600
		O	-1.15055700	-0.39487500	-0.00009100
		H	-1.98183900	0.08044600	-0.00007300
ethanol	toluene	C	1.22117500	-0.22133200	0.00002700

		H	1.29310100	-0.85598200	-0.88630100
		H	1.29302800	-0.85617100	0.88622600
		H	2.06720700	0.47065200	0.00013600
		C	-0.08415800	0.54479100	0.00005500
		H	-0.14194500	1.18913300	0.88717400
		H	-0.14187100	1.18932300	-0.88693100
		O	-1.15120400	-0.39490700	-0.00009100
		H	-1.98199500	0.08155300	-0.00007300
ethanol	water	C	1.22269800	-0.22130800	0.00002800
		H	1.29858300	-0.85485600	-0.88719400
		H	1.29851100	-0.85504400	0.88712100
		H	2.06664200	0.47287400	0.00013600
		C	-0.08285700	0.54405000	0.00005500
		H	-0.14309500	1.18745300	0.88662100
		H	-0.14302000	1.18764400	-0.88637600
		O	-1.15424000	-0.39515100	-0.00009200
		H	-1.98274200	0.08667900	-0.00007200
ethylacetate	cyclohexane	C	2.12637200	-0.88877800	0.00000900
		H	2.03178700	-1.52664900	0.88099100
		H	2.03200800	-1.52639600	-0.88117900
		H	3.09577900	-0.39550600	0.00020100
		C	1.03467400	0.14395600	0.00000300
		O	-0.17536400	-0.43023300	-0.00003400
		O	1.20136400	1.33769100	0.00001600
		C	-1.31034600	0.45338200	-0.00002500
		H	-1.25678600	1.09439600	0.88316600
		H	-1.25683000	1.09435200	-0.88324900
		C	-2.55566600	-0.40232000	0.00002700
		H	-2.59208900	-1.03827900	0.88697900
		H	-3.43994300	0.23930700	0.00003000
		H	-2.59213000	-1.03832900	-0.88688600
nitromethane	ethanol	C	-1.32241000	-0.00078800	-0.00268900
		H	-1.66094400	-0.90550000	-0.49813100
		H	-1.62490700	-0.00026600	1.04408700
		H	-1.66164500	0.90302800	-0.49930500
		O	0.73306100	-1.07503000	0.00256700

		O	0.73124200	1.07596900	0.00257600
		N	0.16678900	-0.00000700	-0.01023700
nitromethane	*n*-Hexane	C	-1.32059200	0.00003900	-0.00282200
		H	-1.65993400	-0.90467200	-0.49851200
		H	-1.62431300	-0.00028600	1.04376000
		H	-1.65990500	0.90505400	-0.49797300
		O	0.72954500	-1.07723200	0.00269800
		O	0.72962500	1.07719100	0.00269800
		N	0.17062000	0.00000100	-0.01050200
n-Pentane	benzene	C	2.54570100	0.32495600	0.00000100
		H	3.44444900	-0.29747200	0.00000000
		H	2.58467900	0.96990000	0.88356400
		H	2.58467900	0.96990400	-0.88356100
		C	1.27702900	-0.52374300	-0.00000100
		H	1.27535600	-1.18154400	0.87738100
		H	1.27535600	-1.18154100	-0.87738500
		C	0.00000000	0.31355400	0.00000000
		H	0.00000000	0.97281400	-0.87811500
		H	0.00000000	0.97281300	0.87811700
		C	-1.27702900	-0.52374300	0.00000000
		H	-1.27535600	-1.18154300	0.87738300
		H	-1.27535600	-1.18154300	-0.87738300
		C	-2.54570100	0.32495600	0.00000000
		H	-2.58467900	0.96990200	-0.88356300
		H	-3.44444900	-0.29747200	0.00000000
		H	-2.58467900	0.96990200	0.88356200
propanol	cyclohexane	C	-1.89054300	-0.12783300	0.01796500
		H	-2.68519600	0.61986400	-0.02882600
		H	-2.01869900	-0.69304000	0.94611400
		H	-2.03502900	-0.82032900	-0.81663800
		C	-0.51319300	0.52721600	-0.04514500
		H	-0.40440100	1.23747400	0.78405700
		H	-0.40703200	1.10227500	-0.97028600
		C	0.61296200	-0.49506100	0.02460400
		H	0.53421200	-1.19644800	-0.81007000
		H	0.53022900	-1.07962600	0.95215500

		O	1.90178600	0.08718700	-0.08485600
		H	2.01627100	0.70640400	0.63780000
propanol	toluene	C	-1.89052000	-0.12785300	0.01817000
		H	-2.68510500	0.61990400	-0.02874400
		H	-2.01840000	-0.69265500	0.94659200
		H	-2.03508100	-0.82064000	-0.81618200
		C	-0.51322300	0.52730600	-0.04535600
		H	-0.40411900	1.23760800	0.78368100
		H	-0.40748000	1.10209800	-0.97073300
		C	0.61270100	-0.49512200	0.02436600
		H	0.53398100	-1.19646700	-0.81034900
		H	0.53017200	-1.07945700	0.95195600
		O	1.90196600	0.08727200	-0.08477200
		H	2.01655500	0.70544700	0.63886900
propanol	water	C	-1.89034700	-0.12808600	0.02077000
		H	-2.68467800	0.61986500	-0.02718600
		H	-2.01488600	-0.68845900	0.95221200
		H	-2.03621900	-0.82434500	-0.81051700
		C	-0.51362100	0.52802100	-0.04804000
		H	-0.40125500	1.23912100	0.77916300
		H	-0.41219500	1.10024300	-0.97578200
		C	0.61081600	-0.49540400	0.02120700
		H	0.53336100	-1.19523500	-0.81501200
		H	0.52882800	-1.07927500	0.94814900
		O	1.90317200	0.08856200	-0.08340500
		H	2.02058300	0.69239700	0.65259600
toluene	benzene	C	1.19616400	-1.20072200	0.00213600
		C	-0.19414700	-1.19782100	-0.00916900
		C	-0.90999700	0.00000200	-0.01175200
		C	-0.19414500	1.19782200	-0.00914500
		C	1.19616700	1.20072000	0.00216100
		C	1.89732700	-0.00000100	0.00847000
		H	1.73279700	-2.14328300	0.00225500
		H	-0.73286100	-2.14053300	-0.01774500
		H	-0.73285600	2.14053600	-0.01770100
		H	1.73280200	2.14328000	0.00229800

		H	2.98150800	-0.00000300	0.01449700
		C	-2.41658600	0.00000100	0.00929400
		H	-2.78865400	-0.00009100	1.03878000
		H	-2.82071800	0.88495000	-0.48710100
		H	-2.82071800	-0.88486200	-0.48725600
toluene	cyclohexane	C	1.19612500	-1.20067700	0.00213200
		C	-0.19413000	-1.19777500	-0.00916500
		C	-0.90993600	0.00000200	-0.01175200
		C	-0.19412700	1.19777700	-0.00914000
		C	1.19612800	1.20067500	0.00215600
		C	1.89724700	-0.00000100	0.00845700
		H	1.73276200	-2.14322900	0.00224400
		H	-0.73285200	-2.14048400	-0.01773000
		H	-0.73284700	2.14048700	-0.01768600
		H	1.73276700	2.14322600	0.00228800
		H	2.98142200	-0.00000300	0.01447300
		C	-2.41652000	0.00000100	0.00932500
		H	-2.78862000	-0.00009100	1.03880400
		H	-2.82067900	0.88490100	-0.48715700
		H	-2.82067900	-0.88481300	-0.48731300
toluene	ethanol	C	1.19675500	-1.20147200	0.00213200
		C	-0.19449400	-1.19862700	-0.00904500
		C	-0.91094300	0.00000200	-0.01153400
		C	-0.19449200	1.19862900	-0.00902800
		C	1.19675900	1.20147000	0.00214900
		C	1.89855500	-0.00000200	0.00850000
		H	1.73328600	-2.14415900	0.00227700
		H	-0.73308800	-2.14138300	-0.01772200
		H	-0.73308300	2.14138700	-0.01769200
		H	1.73329200	2.14415600	0.00230700
		H	2.98280400	-0.00000300	0.01450700
		C	-2.41756800	0.00000100	0.00869600
		H	-2.78921900	-0.00011700	1.03828000
		H	-2.82071200	0.88589700	-0.48648300
		H	-2.82071100	-0.88578500	-0.48668200
toluene	*n*-hexane	C	1.19610200	-1.20065000	0.00212800

		C	-0.19411900	-1.19774800	-0.00916100
		C	-0.90989900	0.00000200	-0.01175200
		C	-0.19411700	1.19775000	-0.00913600
		C	1.19610500	1.20064800	0.00215300
		C	1.89719800	-0.00000100	0.00844800
		H	1.73274100	-2.14319600	0.00223800
		H	-0.73284600	-2.14045400	-0.01772000
		H	-0.73284100	2.14045700	-0.01767600
		H	1.73274600	2.14319300	0.00228100
		H	2.98137000	-0.00000300	0.01445800
		C	-2.41648000	0.00000100	0.00934300
		H	-2.78860200	-0.00009200	1.03881700
		H	-2.82065500	0.88487300	-0.48719100
		H	-2.82065500	-0.88478400	-0.48734800
Xe	ethanol	Xe	0.00000000	0.00000000	0.00000000
Xe	water	Xe	0.00000000	0.00000000	0.00000000

References

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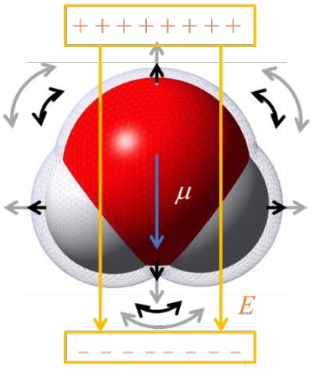
Appendix 1. a model of the restricted rotation of a dipole in an electrostatic field.

With regard to these equations, a rotational term was modeled based on the restricted rotation of a dipole in an electrostatic field as depicted in the figure below.



The orientation of a rigid rotor can be specified using the Euler angles θ, ϕ and ψ, which have ranges of 0 to π, 0 to 2π, and 0 to 2π, respectively. The rotational Hamiltonian for the kinetic energy of such a rotor can be written in terms of these angles and their conjugate momenta (p_θ, p_ϕ and p_ψ). Assuming that the dipole moment lies along the molecule-fixed *z*-axis and the external electric field is collinear, neither ψ nor ϕ will be included in the Hamiltonian. In this case, the electrostatic restriction on rotation will be along the angle θ and the Hamiltonian for a linear, non-linear and polar molecule having dipole moment μ in an electric field (E_f) can be represented as

$$\mathcal{H}_{\text{rot.,linear}} = \frac{1}{2I}\left(p_\theta^2 + \frac{1}{\sin^2\theta}p_\varphi^2\right) + \mu E(1-\cos\theta) \quad \text{(A1)}$$

and

$$\mathcal{H}_{\text{rot.,non-linear}} = \frac{\sin^2\psi}{2I_a}\left(p_\theta - \frac{\cos\psi}{\sin\theta\sin\psi}\left(p_\phi - \cos\theta p_\psi\right)\right)^2$$

$$+\frac{\cos^2\psi}{2I_b}\left(p_\theta - \frac{\cos\psi}{\sin\theta\sin\psi}\left(p_\phi - \cos\theta p_\psi\right)\right)^2 + \frac{1}{2I_c}{p_\psi}^2 + \mu E(1-\cos\theta) \quad \text{(A2)}$$

The last term in both Eqs. (A1) and (A2) represents the potential energy associated with the molecular dipole in the electric field. In the case that the Hamiltonian is defined, we can obtain classical partition functions based on the integrals

$$q_{\text{rot.,linear}} = \frac{1}{\sigma}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_0^{\pi}\int_0^{2\pi}\frac{1}{h^2}e^{-\mathcal{H}_{rot}(p,q)/k_BT}\mathrm{d}p_\theta\mathrm{d}p_\phi\mathrm{d}\theta\mathrm{d}\phi \quad \text{(A3)}$$

and

$$q_{\text{rot,non linear}} = \frac{1}{\sigma}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_0^{\pi}\int_0^{2\pi}\int_0^{2\pi}\frac{1}{h^3}e^{-\mathcal{H}_{rot}(p,q)/k_BT}\mathrm{d}p_\theta\mathrm{d}p_\phi\mathrm{d}p_\psi\mathrm{d}\theta\mathrm{d}\phi\mathrm{d}\psi \quad \text{(A4)}$$

These integrals can be used to calculate q_{rot} as

$$q_{\mathrm{rot.,linear}} = \frac{1}{\sigma}\frac{k_{\mathrm{B}}T}{2hc\tilde{B}}\frac{k_BT}{2\mu E}\left[1-\exp(-\frac{2\mu E_{\mathrm{f}}}{k_{\mathrm{B}}T})\right] \qquad \text{(A5)}$$

and

$$q_{\mathrm{rot,non\ linear}} = \frac{1}{\sigma}\left(\frac{k_{\mathrm{B}}T}{hc}\right)^{\frac{3}{2}}\left(\frac{\pi}{\tilde{A}\tilde{B}\tilde{C}}\right)^{\frac{1}{2}}\frac{k_BT}{2\mu E}\left[1-\exp(-\frac{2\mu E_{\mathrm{f}}}{k_{\mathrm{B}}T})\right] \qquad \text{(A6)}$$

Based on statistical thermodynamics, the rotational entropy ($S_{\mathrm{rot.}}$) is calculated as

$$S_{\mathrm{rot.}} = \frac{d}{dT}(-RT\ln q_{\mathrm{rot.}}) \qquad \text{(A8)}$$

The entropy value can then be obtained according to the equations

$$S_{\mathrm{rot,linear}} =$$
$$R[\ln\left\{\frac{1}{\sigma}\frac{k_{\mathrm{B}}T}{2hc\tilde{B}X}[1-\exp(-\mathrm{X})]\right\} - \frac{X\exp(-\mathrm{X})}{[1-\exp(-\mathrm{X})]} + 2] \qquad (12)$$

and

$$S_{\mathrm{rot,non-linear}} =$$
$$R[\ln\left\{\frac{1}{\sigma}\left(\frac{k_{\mathrm{B}}T}{hc}\right)^{\frac{3}{2}}\left(\frac{\pi}{\tilde{A}\tilde{B}\tilde{C}}\right)^{\frac{1}{2}}\frac{1}{\mathrm{X}}[1-\exp(-\mathrm{X})]\right\} - \frac{X\exp(-\mathrm{X})}{[1-\exp(-\mathrm{X})]} + \frac{5}{2}] \qquad (13)$$

Where

$$X = \frac{2\mu E_{\mathrm{f}}}{k_{\mathrm{B}}T} \qquad (14)$$

A molecule with a polarizability of *P* has an induced dipole moment μ_{i}, by the surrounding electric field E_{f}, according to:

$$E = \frac{\mu_{\mathrm{i}}}{P} \qquad (15)$$

μ_{i} is estimated by the difference between μ and the permanent dipole moment (the dipole moment without a cavity), μ_{p}:

$$\mu_{\mathrm{i}} = \mu - \mu_{\mathrm{p}} \qquad (16)$$

Appendix 2. Specific procedure to calculate translational and rotational entropies using Gaussian program.

Sample input file for H_2O.

```
% chk=h2o.chk
#p opt freq wb97xd/6-311++g(d,p) scrf=(solvent=ch3oh,read)

Title Card Required

0 1
 O                  1.20207250   -1.15544040    0.00000000
 H                  2.16207250   -1.15544040    0.00000000
 H                  0.88161792   -0.25050457    0.00000000

alpha=1.2

--Link1--
% chk=h2o.chk
#p wb97xd/6-311++g(d,p) scrf=(solvent=ch3oh,read)
geom=allcheck guess=(read,only)

alpha=1.0

--Link1--
% chk=h2o.chk
# wb97xd/6-311++g(d,p) geom=allcheck guess=read
```

---

*The route section "#p" is required to display the cavity size in the results.

1. Geometric optimization and a frequency analysis were conducted using PCMs with van der Waals radii (employing UFF in the case of this sample) scaled by α = 1.2 (as opposed to the default value of 1.1 in Gaussian 16). The results provided the molecular weight, *m*, $V_{\alpha=1.2}$, the dipole-moment, μ, rotational constants ($\tilde{A}$, $\tilde{B}$, $\tilde{C}$) (or rotational temperatures Θ_A, Θ_B, Θ_C) and the polarizability, *P*.

```
Electronic spatial extent (au):  <R**2>=             19.8013↓
Charge=              0.0000 electrons↓
Dipole moment (field-independent basis, Debye):↓
   X=              -0.0000    Y=              0.0000    Z=             -2.3841  Tot=              2.3841↓
Quadrupole moment (field-independent basis, Debye-Ang):↓
  XX=              -7.7480   YY=             -4.2910   ZZ=             -6.4225↓
  XY=               0.0000   XZ=              0.0000   YZ=             -0.0000↓
Traceless Quadrupole moment (field-independent basis, Debye-Ang):↓
  XX=              -1.5942   YY=              1.8628   ZZ=             -0.2687↓
  XY=               0.0000   XZ=              0.0000   YZ=             -0.0000↓
Octapole moment (field-independent basis, Debye-Ang**2):↓
 XXX=               0.0000  YYY=              0.0000  ZZZ=             -1.8211  XYY=              0.0000↓
 XXY=               0.0000  XXZ=             -0.5318  XZZ=              0.0000  YZZ=              0.0000↓
 YYZ=              -1.5331  XYZ=             -0.0000↓
Hexadecapole moment (field-independent basis, Debye-Ang**3):↓
XXXX=              -7.4420 YYYY=             -6.0940 ZZZZ=             -7.7541 XXXY=             -0.0000↓
XXXZ=              -0.0000 YYYX=             -0.0000 YYYZ=              0.0000 ZZZX=             -0.0000↓
ZZZY=               0.0000 XXYY=             -2.5620 XXZZ=             -2.5905 YYZZ=             -1.9600↓
XXYZ=               0.0000 YYXZ=              0.0000 ZZXY=              0.0000↓
N-N= 9.179198186609D+00 E-N=-1.992617609858D+02  KE= 7.620288742827D+01↓
Symmetry A1   KE= 6.800900246256D+01↓
Symmetry A2   KE= 4.372579497471D-34↓
Symmetry B1   KE= 4.498325644477D+00↓
Symmetry B2   KE= 3.695559321232D+00↓
 Exact polarizability:   7.391   0.000   8.603   0.000   0.000   7.101↓
Approx polarizability:   5.366   0.000   7.611   0.000  -0.000   5.967↓
```

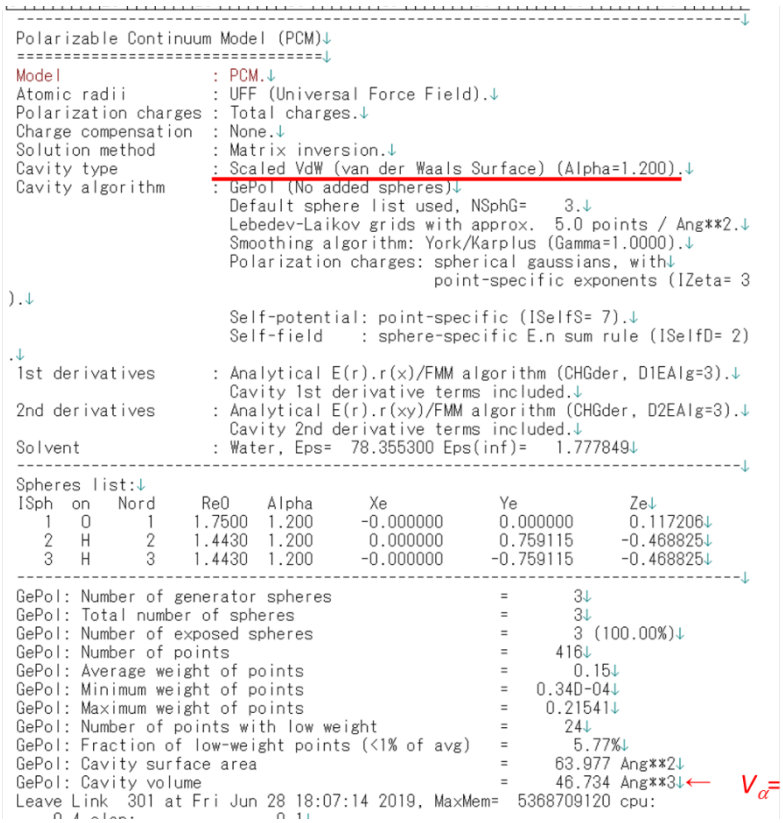
μ

Avg.→P = 7.698143

```
 ------------------↓
 - Thermochemistry -↓
 ------------------↓
 Temperature   298.150 Kelvin.  Pressure   1.00000 Atm.↓
 Atom     1 has atomic number  8 and mass  15.99491↓
 Atom     2 has atomic number  1 and mass   1.00783↓
 Atom     3 has atomic number  1 and mass   1.00783↓
 Molecular mass:    18.01056 amu.↓
 Principal axes and moments of inertia in atomic units:↓
                          1         2         3↓
    Eigenvalues --     2.19538   4.14790   6.34328↓
           X          -0.00000   0.00000   1.00000↓
           Y           1.00000   0.00000  -0.00000↓
           Z          -0.00000   1.00000   0.00000↓
 This molecule is an asymmetric top.↓
 Rotational symmetry number  2.↓
 Rotational temperatures (Kelvin)     39.45283    20.88140    13.65444↓
 Rotational constants (GHZ):         822.06359   435.09774   284.51242↓
 Zero-point vibrational energy      56742.8 (Joules/Mol)↓
                                   13.56186 (Kcal/Mol)↓
 Vibrational temperatures:   2325.97  5592.28  5730.92↓
          (Kelvin)↓
 ↓
 Zero-point correction=                           0.021612 (Hartree/Particle)↓
 Thermal correction to Energy=                    0.024448↓
 Thermal correction to Enthalpy=                  0.025392↓
 Thermal correction to Gibbs Free Energy=         0.003977↓
 Sum of electronic and zero-point Energies=           -76.417016↓
 Sum of electronic and thermal Energies=              -76.414180↓
 Sum of electronic and thermal Enthalpies=            -76.413236↓
 Sum of electronic and thermal Free Energies=         -76.434651↓
```

← $\Theta_A, \Theta_B, \Theta_C$

← $\tilde{A}, \tilde{B}, \tilde{C}$



It was considered that any molecular orbital and density functional theory method could be employed with PCMs and that the frequency scaling factor was preferably obtained in advance.

2. A single point calculation was conducted using PCMs for the structure optimized in step (1) with the same van der Waals radii scaled by α = 1.0. The result provided $V_{\alpha=1.0}$ after which the free volume, V_{free}, could be calculated as

$$V_{\text{free}} = \left(V_{a=1.2}^{1/3} - V_{a=1.0}^{1/3}\right)^3.$$

```
------------------------------------------------------------------------------
Polarizable Continuum Model (PCM)
=================================
Model                : PCM.
Atomic radii         : UFF (Universal Force Field).
Polarization charges : Total charges.
Charge compensation  : None.
Solution method      : On-the-fly selection.
Cavity type          : VdW (van der Waals Surface) (Alpha=1.000).
Cavity algorithm     : GePol (No added spheres)
                       Default sphere list used, NSphG=    3.
                       Lebedev-Laikov grids with approx.  5.0 points / Ang**2.
                       Smoothing algorithm: York/Karplus (Gamma=1.0000).
                       Polarization charges: spherical gaussians, with
                                             point-specific exponents (IZeta= 3).
                       Self-potential: point-specific (ISelfS= 7).
                       Self-field    : sphere-specific E.n sum rule (ISelfD= 2).
Solvent              : Methanol, Eps=  32.613000 Eps(inf)=   1.765709
------------------------------------------------------------------------------
Spheres list:
ISph  on   Nord     ReO    Alpha      Xe           Ye           Ze
   1   O       1    1.7500  1.000     -0.000000     0.000000     0.117144
   2   H       2    1.4430  1.000     -0.000000     0.759098    -0.468575
   3   H       3    1.4430  1.000     -0.000000    -0.759098    -0.468575
------------------------------------------------------------------------------
GePol: Number of generator spheres                =       3
GePol: Total number of spheres                    =       3
GePol: Number of exposed spheres                  =       3 (100.00%)
GePol: Number of points                           =     298
GePol: Average weight of points                   =       0.16
GePol: Minimum weight of points                   =    0.24D-06
GePol: Maximum weight of points                   =    0.22001
GePol: Number of points with low weight           =      12
GePol: Fraction of low-weight points (<1% of avg) =       4.03%
GePol: Cavity surface area                        =      47.589 Ang**2
GePol: Cavity volume                              =      29.309 Ang**3   <-- V_α=1.0
Leave Link  301 at Wed Oct  5 15:36:20 2022, MaxMem=   104857600 cpu:
(Enter /usr/local/Gaussian16_b01_AVX2/g16/l302.exe)
```

The translational entropy, $S_{\text{trans.}}$, was calculated using the corrected Sackur-Tetrode equation, written as

$$S_{\text{trans.}}^{\text{liquid}} = R\left[\ln\left(V_{\text{free}}\left(\frac{2\pi m k_B T}{h^2}\right)^{\frac{3}{2}}\right) + \frac{5}{2}\right].$$

Taking H_2O as an example, these calculations become

$$V_{\text{free}} = \left(V_{a=1.2}^{1/3} - V_{a=1.0}^{1/3}\right)^3 = (46.734^{1/3} - 29.309^{1/3})^3 \times 10^{-30} = 1.396 \times 10^{-31}$$

and

$$S_{\text{trans.}}^{\text{liquid}} = 8.314\left[\ln\left(1.396 \times 10^{-31}\left(\frac{2\pi \times \frac{18.01}{6.02 \times 10^{-23} \times 1000} \times 1.38 \times 10^{-23} \times 298.15}{(6.63 \times 10^{-34})^2}\right)^{\frac{3}{2}}\right) + \frac{5}{2}\right]$$

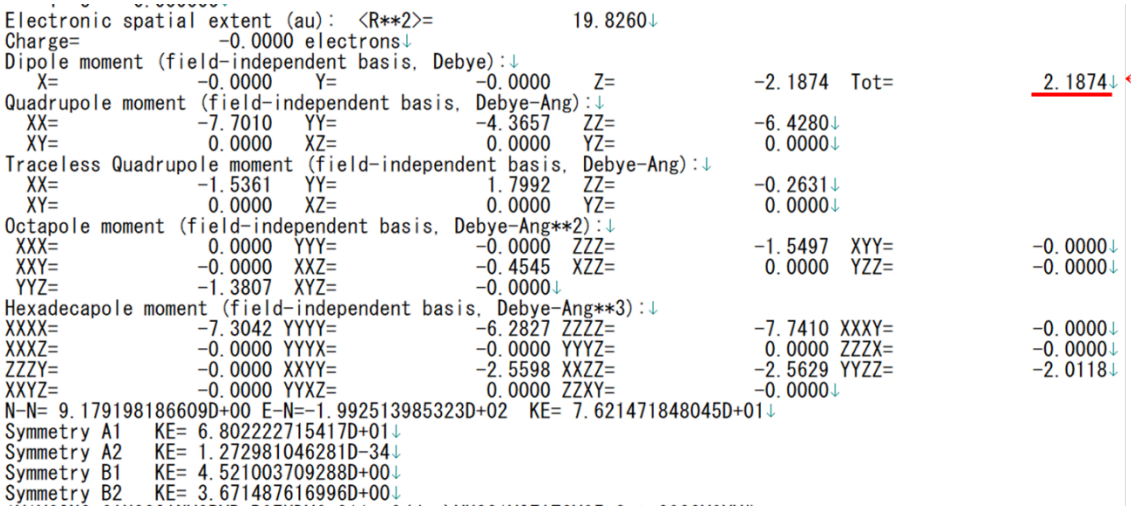
$$= 55.4 \ [\text{J mol}^{-1}\ \text{K}^{-1}].$$

3. A single-point calculation was conducted for the same structure without PCMs and the result provided the dipole moment in a vacuum, μ_{vac}. The induced dipole moment, μ^*, and surrounding electric field, *E*, were then calculated using the equations

$$\mu^* = \mu - \mu_{\mathrm{vac}}$$

and

$$E = \frac{\mu^*}{P}.$$



In the case of H_2O, these calculations are

$$\mu^* = \mu - \mu_{vac} = (2.3841[\text{debye}] - 2.1874\,[\text{debye}]) \times 3.33564 \times 10^{-30} = 6.56 \times 10^{-31}[\text{C m}]$$

and

$$E = \frac{\mu^*}{P} = \frac{6.34\times10^{-31}[\text{C m}]}{7.97\times1.65\times10^{-41}[\text{C}^2\ \text{m}^2\ \text{J}^{-1}]} = 5.15 \times 10^{9}\ [\text{J m}^{-1}\ \text{C}^{-1}].$$

Units

Units in GaussView	SI
Dipole moment: 1 [Debye]	3.33564 x 10^{-30} [C m]
Polarizability: 1 [au]	1.648777 x 10^{-41} [C^2 m^2 J^{-1}]

The rotational entropy, $S_{\text{rot.}}$, could be calculated by inserting the values obtained according to the procedures noted above along with the relevant constants into the equations

$$S_{\text{rot,linear}} = R[\ln\left\{\frac{1}{\sigma}\frac{k_{\text{B}}T}{2hc\tilde{B}X}[1-\exp(-X)]\right\} - \frac{X\exp(-X)}{[1-\exp(-X)]} + 2]$$

$$= R[\ln\left\{\frac{1}{\sigma}\frac{T}{\Theta_{\text{B}}}\frac{k_B T}{2\mu E}[1-\exp(-X)]\right\} - \frac{X\exp(-\frac{2\mu E}{k_{\text{B}}T})}{\left[1-\exp(-\frac{2\mu E}{k_{\text{B}}T})\right]} + 2]$$

and

$$S_{\text{rot,non-linear}} = R[\ln\left\{\frac{1}{\sigma}\left(\frac{k_{\text{B}}T}{hc}\right)^{\frac{3}{2}}\left(\frac{\pi}{\tilde{A}\tilde{B}\tilde{C}}\right)^{\frac{1}{2}}\frac{1}{X}[1-\exp(-X)]\right\} - \frac{X\exp(-X)}{[1-\exp(-X)]} + \frac{5}{2}]$$

$$= R[\ln\left\{\frac{1}{\sigma}\left(\frac{T^3}{\Theta_{\text{A}}\Theta_{\text{B}}\Theta_{\text{C}}}\right)^{1/2}\frac{1}{X}\left[1-\exp(-\frac{2\mu E}{k_{\text{B}}T})\right]\right\} - \frac{X\exp(-X)}{[1-\exp(-X)]} + \frac{5}{2}].$$

Taking H_2O as an example, these calculations are

$\Theta_{\text{A}} = 39.45283$ [K]

$\Theta_{\text{B}} = 20.88140$ [K]

$\Theta_{\text{C}} = 13.65444$ [K]

$$X = \frac{2\mu E}{k_B T} = \frac{2\times 2.39\times 3.33564\times 10^{-30}\times 5.15\times 10^{9}}{1.381\times 10^{-23}\times 298.15} = 19.90\ [-]$$

and

$S_{\text{rot,non-linear}} =$

$$8.314\left[\ln\left\{\frac{3.14^{0.5}}{2}\left(\frac{298.15^3}{39.452\times 20.881\times 13.654}\right)^{0.5}\frac{1}{19.90}[1-\exp(-19.90)]\right\} - \frac{20.58\exp(-19.90)}{[1-\exp(-19.90)]} + \frac{5}{2}\right]$$

$= 27.2$ [J K^{-1} mol^{-1}].

4. The vibrational entropy could be obtained from the thermochemistry output file.

   In the case of H_2O, this file was as follows.

$$S_{\mathrm{vib}} = 1.101\ [\mathrm{cal\ mol^{-1}\ K^{-1}}] = 0.004\ [\mathrm{kJ\ mol^{-1}\ K^{-1}}]$$

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	19.022	8.007	54.148
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	36.503
Rotational	0.889	2.981	16.544
Vibrational	17.244	2.045	1.101
Vibration 1	0.763	1.479	0.978

5. The configurational entropy at a concentration of C was calculated from V_{cav} and V_{solute}. As an example, for a solute at a concentration of 1 mol dm^{-3} in a solvent volume of 1 dm^3, we have the following.

$C = 1\ [\mathrm{mol\ dm^{-3}}]$,

$V_{\mathrm{solution}} = 1\ [\mathrm{dm^3}]$,

$N_{\mathrm{solute}} = c \cdot N_{\mathrm{A}} \cdot V_{\mathrm{solution}} = 1\ [\mathrm{mol\ dm^{-3}}] \times 6.02 \times 10^{23}[\mathrm{mol^{-1}}] \times 1\ [\mathrm{dm^3}] = 6.02 \times 10^{23}$,

$N_{\mathrm{cells}} = \frac{V_{\mathrm{solution}}}{V_{\mathrm{cav}}} = \frac{1\times10^{27}\ [\mathrm{Å^3}]}{46.734[\mathrm{Å^3}]} = 2.140 \times 10^{25}$

and

$S_{\mathrm{configuration}} = k_{\mathrm{B}}[N_{\mathrm{cells}} \ln N_{\mathrm{cells}} - \{N_{\mathrm{solute}} \ln N_{\mathrm{solute}} + (N_{\mathrm{cells}} - N_{\mathrm{solute}}) \ln(N_{\mathrm{cells}} - N_{\mathrm{solute}})\}]$
$= 1.381 \times 10^{-23}[2.140 \times 10^{25} \ln 2.140 \times 10^{25} - \{6.02 \times 10^{23} \ln 6.02 \times 10^{23} +$
$(2.140 \times 10^{25} - 6.02 \times 10^{23}) \ln(2.140 \times 10^{25} - 6.02 \times 10^{23})\}] = 37.9.$

6. Finally, the entropic terms obtained as noted above are summed.

   Using H_2O as an example, this summation would be

$S = S_{\mathrm{elec}} + S_{\mathrm{trans}} + S_{\mathrm{rot}} + S_{\mathrm{vib}} + S_{\mathrm{conformer}} + S_{\mathrm{configuration}} + S_{\mathrm{orientation}}$

$= 0 + 55.4 + 27.2 + 0.0 + 0 + 37.9 + 0 = 120.4$

Appendix 3. The procedure used to calculate $S_{\text{conformer}}$ using 1-propanol in water as an example.

The 1-propanol molecule has five conformers (Figure A1) and the associated potential energies are listed in Table A1.

$$S_{\text{conformer}} = R \ln q_{\text{CD}} + \frac{N_{\text{A}}}{T} \sum_i (\varepsilon_i - \varepsilon_0) \cdot \frac{g_i \exp\left(-\frac{(\varepsilon_i - \varepsilon_0)}{k_{\text{B}} T}\right)}{q_{\text{CD}}} = 18.0 \ [\text{J mol}^{-1}\ \text{K}^{-1}]$$

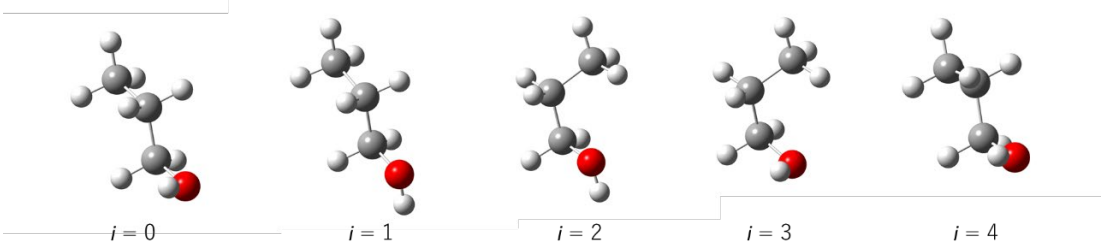


Figure A1. The conformers of 1-propanol.

Table A1. Potential energies for the conformers of 1-propnanol and the associated partition function and entropy values.

i	g_i	EE+ZPE [hartree]	$e_i - e_0$ [hartree]	$e_i - e_0$ [kJ mol^{-1}]	$q_{\text{CD}\_i} = g_i \exp(-(\varepsilon_i - \varepsilon_0)/k_{\text{B}}T)$
0	2	-194.2518	0.0000	0	2
1	1	-194.2516	0.0002	7.0×10^{-22}	0.844
2	2	-194.2513	0.0005	2.2×10^{-21}	1.17
3	2	-194.2516	0.0002	8.9×10^{-22}	1.61
4	2	-194.2515	0.0003	1.30×10^{-21}	1.46
				$q_{\text{CD}} = \Sigma q_{\text{CD}\_i}$	7.09
				$S_{\text{conformer}}$	18.0

Appendix 4. Derivation Eqn (8) from Eqn (7)

$$S_{\text{configuration}} = k_{\text{B}}[N_{\text{cell}} \ln N_{\text{cell}} - \{N_{\text{solute}} \ln N_{\text{solute}} + (N_{\text{cell}} - N_{\text{solute}}) \ln(N_{\text{cell}} - N_{\text{solute}})\}]$$

$$= k_{\text{B}} \left[N_{\text{cell}} \ln N_{\text{cell}} - \left\{N_{\text{solute}} \ln N_{\text{solute}} + N_{\text{solute}} \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right) \ln N_{\text{solute}} \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right)\right\}\right]$$

$$= k_{\text{B}} \left[N_{\text{cell}} \ln N_{\text{cell}} - N_{\text{solute}} \ln N_{\text{solute}} - N_{\text{solute}} \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right) \ln N_{\text{solute}} \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right)\right]$$

$$= k_{\text{B}} N_{\text{solute}} \left[\frac{N_{\text{cell}}}{N_{\text{solute}}} \ln N_{\text{cell}} - \ln N_{\text{solute}} - \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right) \ln N_{\text{solute}} \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right)\right]$$

$$= k_{\text{B}} N_{\text{solute}} \left[\frac{N_{\text{cell}}}{N_{\text{solute}}} \ln N_{\text{cell}} - \ln N_{\text{solute}} - \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right) \ln N_{\text{solute}} - \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right) \ln \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right)\right]$$

$$= k_{\text{B}} N_{\text{solute}} \left[\frac{N_{\text{cell}}}{N_{\text{solute}}} \ln N_{\text{cell}} - \ln N_{\text{solute}} - \frac{N_{\text{cell}}}{N_{\text{solute}}} \ln N_{\text{solute}} + \ln N_{\text{solute}} - \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right) \ln \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right)\right]$$

$$= k_{\text{B}} N_{\text{solute}} \left[\frac{N_{\text{cell}}}{N_{\text{solute}}} \ln N_{\text{cell}} - \frac{N_{\text{cell}}}{N_{\text{solute}}} \ln N_{\text{solute}} - \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right) \ln \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right)\right]$$

$$= k_{\text{B}} N_{\text{solute}} \left[\frac{N_{\text{cell}}}{N_{\text{solute}}} \ln \frac{N_{\text{cell}}}{N_{\text{solute}}} - \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right) \ln \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right)\right]$$

Appendix 5. Derivation Eqn (9) from Eqn (8)

$$S_{\text{configuration}} = R\left\{\frac{N_{\text{cell}}}{N_{\text{solute}}}\ln\frac{N_{\text{cell}}}{N_{\text{solute}}} - \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right)\ln\left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right)\right\}$$

$$= R\left\{\frac{N_{\text{cell}}}{N_{\text{solute}}}\ln\frac{N_{\text{cell}}}{N_{\text{solute}}} + \frac{N_{\text{cell}}}{N_{\text{solute}}} - \frac{N_{\text{cell}}}{N_{\text{solute}}} - \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right)\ln\left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right) + \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right) - \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right)\right\}$$

$$= R\left\{\frac{N_{\text{cell}}}{N_{\text{solute}}}\ln\frac{N_{\text{cell}}}{N_{\text{solute}}} - \frac{N_{\text{cell}}}{N_{\text{solute}}} - \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right)\ln\left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right) + \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right) + \frac{N_{\text{cell}}}{N_{\text{solute}}} - \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right)\right\} \quad (8)'$$

For $N_{\text{solute}}/N_{\text{cell}} \ll 1$, applying the approximation ($N \ln N - N \approx \ln N!$) to Eq. (8)' gives

$$S_{\text{configuration}} = R\left\{\ln\frac{N_{\text{cell}}}{N_{\text{solute}}}! - \ln\left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right)! + \frac{N_{\text{cell}}}{N_{\text{solute}}} - \left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right)\right\}$$

$$= R\left\{\ln\frac{N_{\text{cell}}}{N_{\text{solute}}}! - \ln\left(\frac{N_{\text{cell}}}{N_{\text{solute}}} - 1\right)! + 1\right\} = R\left(\ln\frac{N_{\text{cell}}}{N_{\text{solute}}} + 1\right) \quad (8)''$$

Considering Eqs (3) and (4), Eq. (8)'' can be rewritten as

$$S_{\text{configuration}} = R\left(\ln\frac{N_{\text{cell}}}{N_{\text{solute}}} + 1\right) = R\left(\ln\frac{V_{\text{solution}}/V_{\text{cavity}}}{N_{\text{A}}C\,V_{\text{solution}}} + 1\right) = R\left(\ln\frac{1}{N_{\text{A}}C\,V_{\text{cavity}}} + 1\right) \quad (8)'''$$

The entropy change derived from the concentration change can be calculated as

$$S - S^{\circ} = S_{\text{configuration}} - S^{\circ}_{\text{configuration}}$$

$$= R\left(\ln\frac{1}{N_{\text{A}}C\,V_{\text{cavity}}} + 1\right) - R\left(\ln\frac{1}{N_{\text{A}}C_0\,V_{\text{cavity}}} + 1\right) = R\ln\frac{N_{\text{A}}C_0\,V_{\text{cavity}}}{N_{\text{A}}C\,V_{\text{cavity}}} = R\ln\frac{C_0}{C} \quad (9)'$$

Transposing S° gives Eq. (9). This derivation process implies that Eq. (9) becomes invalid as $N_{\text{solute}}/N_{\text{cell}}$ increases (i.e., at high concentration).

$$S - S^{\circ} = R\ln\frac{C_0}{C}$$

$$\leftrightarrow S = S^{\circ} + R\ln\frac{C_0}{C} \quad (9)$$