Supplemental information for:

A Simple Heuristic Approach to Estimate the Thermochemistry of Condensed-Phase Molecules based on the Polarizable Continuum Model.

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Contents:

Appendix 1. Elicitation process for rotational partition function.

$$q_{rot,\,non-linear} = \frac{1}{\sigma}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\pi}\int_{0}^{2\pi}\int_{0}^{2\pi}\frac{1}{h^3}e^{-H_{rot}(p,q)/k_BT}\,dp_\theta dp_\phi dp_\psi d\theta d\phi d\psi$$

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

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

Integration over p_θ gives the factor:

$$\sqrt{2\pi k_BT}\left(\frac{\sin^2\psi}{I_a} - \frac{\sin^2\psi}{I_b}\right)^{-1/2}$$

Integration over p_φ gives the factor:

$$\sqrt{2\pi k_BT I_a I_b}\sin\theta\left(\frac{\sin^2\psi}{I_a} - \frac{\sin^2\psi}{I_b}\right)^{1/2}$$

Integration over p_ψ gives the factor:

$$\sqrt{2\pi k_BT I_c}$$

Integration over θ, φ, and ψ gives the factor:

$$\int_0^{\pi}\exp\left(-\frac{\mu E}{k_BT}(1-\cos\theta)\right)\sin\theta d\theta = \frac{k_BT}{\mu E}\left[1-\exp\left(-\frac{2\mu E}{k_BT}\right)\right]$$

$$\int_0^{2\pi} d\phi = 2\pi$$

$$\int_0^{2\pi} d\psi = 2\pi$$

Combining all the integrals, we finally obtain the following equation:

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

Appendix 2. Parameter study using van der Waals radii scaled with various α.

Standard enthalpies of formation and entropy were assessed for methanol (CH_3OH) using the CBS-QB3//ωB97X-D method. The conductor-like polarizable continuum model (CPCM) was used. Bondi's van der Waals radii scaled by α = 1.2, 1.25, 1.3, and 1.35 were used. The repulsion and dispersion interaction energies were evaluated using the method reported by Floris and Tomasi[42,43]. Figure S5 shows the effects of α on ΔH_{298} and S_{298} for CH_3OH. When α increases, both ΔH_{298} and S_{298} also increase to close to the experimental values. This result suggests that suitable values of α for PCMs can be obtained by inverse analysis.

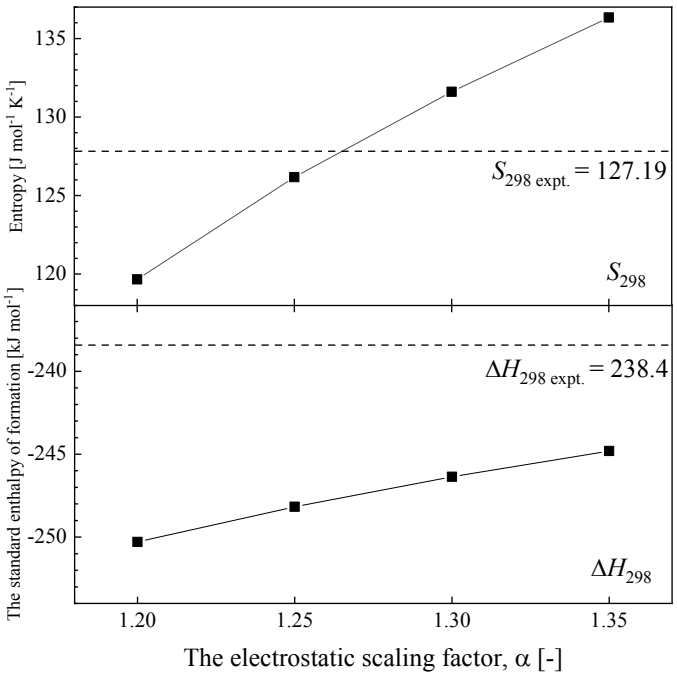

Figure S1 Standard enthalpy of formation and entropy calculated with various electrostatic scaling factors.

Appendix 3. Free volumes for liquid molecules taken from this work and previous studies based on other models.

Table S1 Free volumes for liquid molecules taken from this work and previous studies based on other models.

	V_{free} **this work** 10^{-30} m^3	V_{free} **Ref. 23** 10^{-30} m^3	V_{free} **Ref. 28** 10^{-30} m^3
H_2O	0.0993	-	0.25
CH_3OH	0.116	0.028	0.35
C_2H_5OH	0.125	-	0.30
1-C_3H_7OH	0.144	-	0.31
2-C_3H_7OH	0.148	-	-
1-C_4H_9OH	0.161	-	-
2-C_4H_9OH	0.151	-	-
***i*-C_4H_9OH**	0.152	-	-
HCOOH	0.133	-	0.39
CH_3COOH	0.164	-	0.39
CH_3CN	0.153	-	-
CH_3NO_2	0.156	-	-
Acetone	0.143	-	0.79
DMSO	0.183	-	-
THF	0.145	-	-
Benzene	0.164	0.365	1.14
CCl_4	0.292	0.386	-
C_5H_{12}	0.164	-	-
C_6H_{14}	0.180	-	-
cyc-C_6H_{12}	0.147	-	-

Appendix 4. Influence of REP and DIS options on Standard enthalpies of formation for liquid species.

Table S2 Standard enthalpies of formation (kJ mol^{-1}) for liquid species. The calculated values were obtained based on the CBS-QB3//ωB97X-D method with or without REP and DIS options.

Species	$\Delta_f H°_{liq,calc.}$ with dis,rep	$\Delta_f H°_{liq,calc.}$ without dis,rep	$\Delta_f H°_{liq,calc.}$ without dis	$\Delta_f H°_{liq,calc.}$ without rep	$\Delta_f H°_{liq,expt.}$
H_2O	-282.50	-265.96	-261.97	-286.50	-285.83
CH_3OH	-245.04	-221.46	-216.90	-249.65	-238
C_2H_5OH	-285.74	-253.53	-247.97	-291.48	-276
CH_3CN	27.28	51.41	55.90	25.27	40.56
CH_3NO_2	-139.23	-108.11	-102.24	-145.02	-113
$CH_3C(O)CH_3$	-270.18	-238.26	-233.09	-275.53	-249.4
DMSO	-235.78	-185.71	-177.39	-244.10	-203.4
THF	-240.18	-194.32	-194.32	-187.42	-216.36
Benzene	37.80	82.37	94.26	25.90	49
CCl_4	-159.40	-116.46	-107.07	-168.85	-128.1
cyc-C_6H_{12}	-173.67	-119.91	-112.50	-181.64	-157.7
(RMSD)	19.89	21.16	27.19	26.23	-

Appendix 5. Translational and rotational entropies for the liquid-phase with associated parameters under standard temperature (298.15 K) and pressure (1 atm) conditions.

Table S3 Translational entropy and associated free-volume and cavity volumes for liquid molecules.

	m	$V_{\alpha=1.2}$	$V_{\alpha=1.0}$	V_{free}	S_{trans}	$S_{trans,\ IGT.}$
	g mol^{-1}	10^{-30} m^3	10^{-30} m^3	10^{-30} m^3	J mol K^{-1}	J mol K^{-1}
H_2O	18.01	30.93	19.16	0.0993	37.36	144.80
CH_3OH	32.04	55.28	36.64	0.116	45.85	151.98
C_2H_5OH	46.05	77.98	53.66	0.125	51.01	156.51
1-C_3H_7OH	60.06	100.25	77.97	0.144	55.70	159.82
2-C_3H_7OH	60.06	100.50	69.95	0.148	46.81	159.82
1-C_4H_9OH	74.07	123.34	87.13	0.161	59.90	162.44
2-C_4H_9OH	74.07	122.05	86.83	0.151	51.64	162.44
i-C_4H_9OH	74.07	122.17	86.83	0.152	58.71	162.44
HCOOH	46.01	59.41	39.04	0.133	51.45	156.50
CH_3COOH	60.02	82.32	55.00	0.164	56.52	159.81
CH_3CN	41.03	68.88	45.26	0.153	51.25	155.07
CH_3NO_2	61.02	77.29	51.53	0.156	56.34	160.02
Acetone	58.04	94.20	65.29	0.143	55.01	159.39
DMSO	78.01	104.64	71.19	0.183	60.73	163.08
THF	72.06	108.71	76.59	0.145	57.82	162.09
Benzene	78.05	118.78	83.36	0.164	74.42	163.09
CCl_4	151.88	128.54	84.22	0.292	61.39	171.39
C_5H_{12}	72.09	134.53	95.84	0.164	58.84	162.10
C_6H_{14}	87.12	156.61	112.34	0.180	61.98	164.31
cyc-C_6H_{12}	84.09	138.74	100.50	0.147	59.83	164.02

Table S4 Rotational entropy and associated parameters required for rotational corrections of liquid molecules.

	σ	$\tilde{A}$	$\tilde{B}$	$\tilde{C}$	μ	μ_{vac}	$\mu*$	P	E	S_{rot}	$S_{rot\ IGT.}$
	-	GHz	GHz	GHz	debye	debye	debye	a.u.	10^9 N C^{-1}	J mol K^{-1}	J mol K^{-1}
H_2O	2	817.45	435.16	283.99	2.50	2.19	0.31	7.97	7.81	23.37	43.78
CH_3OH	1	128.11	24.78	23.91	2.09	1.65	0.44	22.15	4.01	67.41	79.45
C_2H_5OH	1	34.40	9.20	8.13	2.37	1.91	0.47	38.51	2.45	83.02	93.34
1-C_3H_7OH	1	26.15	3.77	3.54	2.55	1.93	0.62	53.75	2.33	91.15	101.69
2-C_3H_7OH	1	8.64	8.09	4.77	2.36	1.80	0.56	54.76	2.07	93.11	102.02
1-C_4H_9OH	1	18.65	1.96	1.87	2.28	1.76	0.52	69.77	1.51	102.34	108.50
2-C_4H_9OH	1	8.08	3.44	2.66	2.37	1.82	0.55	70.07	1.58	101.44	108.27
i-C_4H_9OH	1	7.61	3.52	2.66	2.38	1.87	0.52	70.31	1.49	102.03	108.42
HCOOH	1	77.89	12.19	10.54	2.12	1.67	0.45	23.80	3.81	74.83	87.87
CH_3COOH	1	11.46	9.50	5.37	2.28	1.85	0.43	37.47	2.32	90.11	99.68
CH_3CN	3	158.44	9.30	9.30	5.19	4.08	1.11	33.25	6.75	52.15	77.43
CH_3NO_2	1	12.59	10.52	5.95	4.73	3.92	0.81	36.97	4.41	77.46	98.43
Acetone	2	10.17	8.62	4.95	4.28	3.24	1.04	49.98	4.21	75.40	100.92
DMSO	1	6.94	6.79	4.15	6.38	4.72	1.66	63.40	5.30	79.47	104.24
THF	1	7.16	6.96	4.00	2.31	1.82	0.48	61.71	1.59	97.48	104.15
Benzene	6	5.73	5.73	2.86	0	0	0	77.45	0	92.37	92.37
CCl_4	12	1.71	1.71	1.71	0	0	0	68.05	0	98.78	98.78
C_5H_{12}	2	17.07	1.95	1.85	0.094	0.088	0.007	70.32	0.02	103.59	103.59
C_6H_{14}	2	14.64	1.14	1.10	0	0	0	84.23	0	119.17	119.17
cyc-C_6H_{12}	2	4.32	4.32	2.47	0	0	0	79.10	0	108.53	108.53

Appendix 6. Solvation entropy based on the scaled-particle theory (SPT).

Table S5 Solvation entropies based on the scaled-particle theory (SPT) with our computational and experimental entropies [J mol^{-1} K^{-1}].

	ΔS solv. SPT	ΔS solv. This work	ΔS solv. Expt.
H_2O	-70.79	-127.77	-118.89
CH_3OH	-86.37	-118.09	-112.62
C_2H_5OH	-123.35	-117.51	-120.733
CH_3CN	-115.37	-129.10	-93.647
CH_3NO_2	-132.08	-129.57	-111
$CH_3C(O)CH_3$	-136.75	-121.97	-95.26
DMSO	-193.54	-128.52	-117.6
THF	-189.21	-114.20	-97.9
Benzene	-175.61	-103.22	-95.898
CCl_4	-146.93	-99.55	-95.26
cyc-C_6H_{12}	-211.61	-123.67	-94.3

Appendix 7. Total entropies and vibrational entropic terms corrected in a manner that the lower frequencies than 100 cm^{-1} (L.F.) are raised up to 100 cm^{-1}.

Table S6 Total entropies and vibrational entropic terms corrected in a manner that the lower frequencies than 100 cm^{-1} (L.F.) are raised up to 100 cm^{-1}.

Species	$S_{vib.}$	$S_{vib.}$ L.F. raised up to 100cm-*1*	$S_{tot,\ liq.\ calc.}$	$S_{tot,\ liq.\ calc.}$ L.F. raised up to 100cm-*1*	$S_{liq.\ tot.}$ expt.
1-C_4H_9OH	64.5	63.23	251.9	250.7	225.73
CH_3COOH	31.9	27.2	174.3	169.6	158.00
CH_3NO_2	27.5	22.9	162.3	156.7	171.75
$CH_3C(O)CH_3$	47.9	42.0	178.3	172.4	200.40
THF	43.9	31.5	199.1	186.8	203.80
C_6H_{14}	96.3	96.3	286.9	286.9	296.06

Appendix 8. Temperature dependence profiles of Gibbs free energy for gaseous and liquid systems.

The liquid curves based on this study in the right-hand panels are correlated by $\Delta\Delta_{solv.}G^{\circ}_{calc.-expt.}$ compensation.

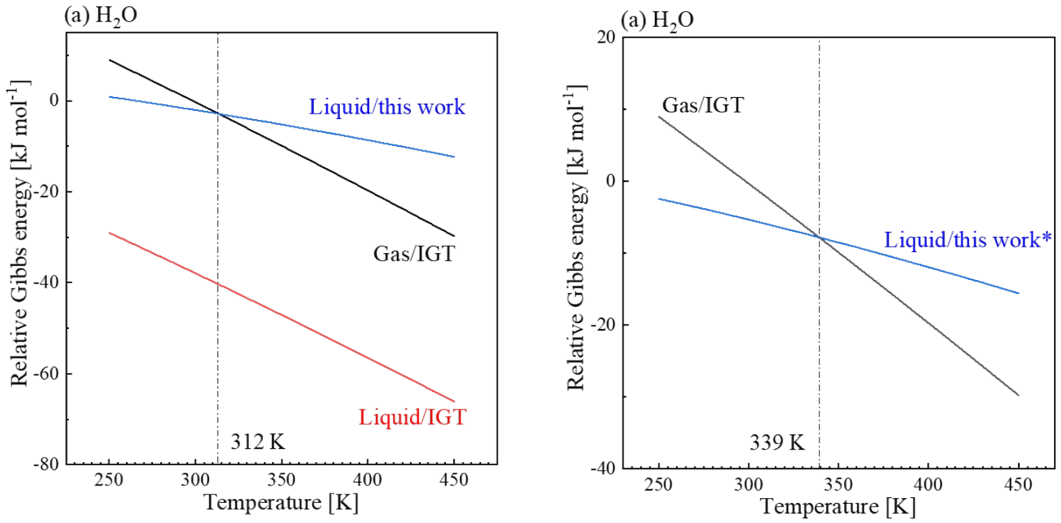

Fig. S2 H_2O.

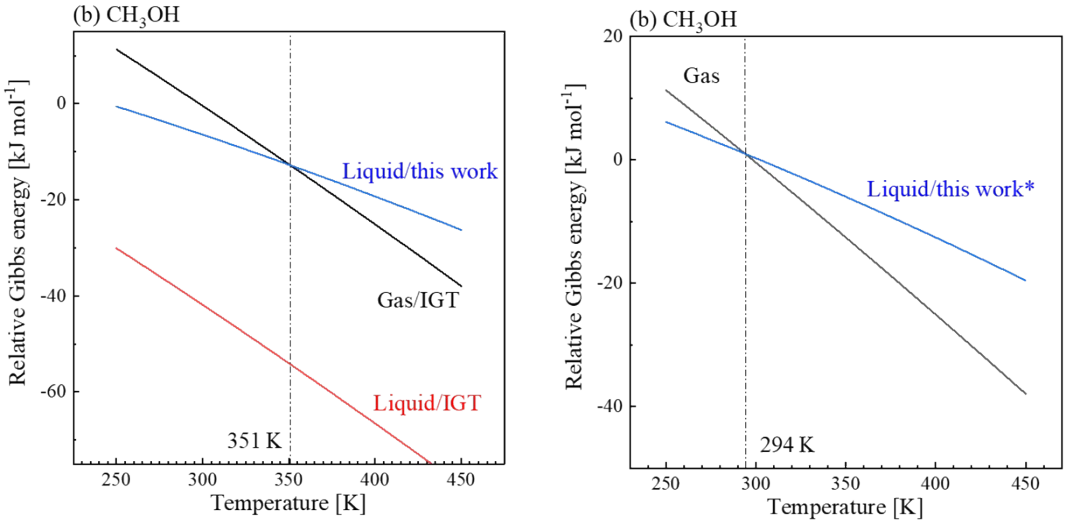

Fig. S3 CH_3OH.

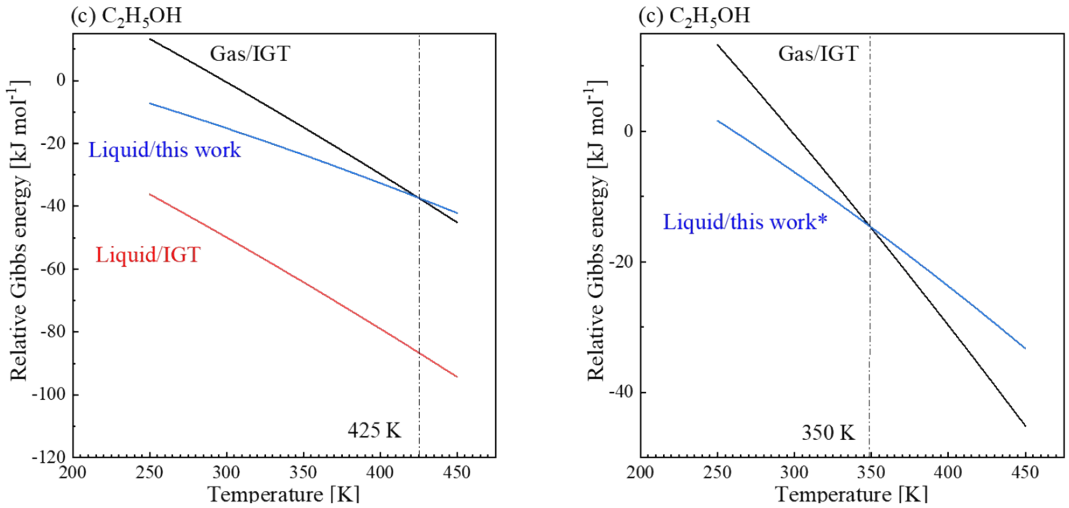

Fig. S4 C_2H_5OH.

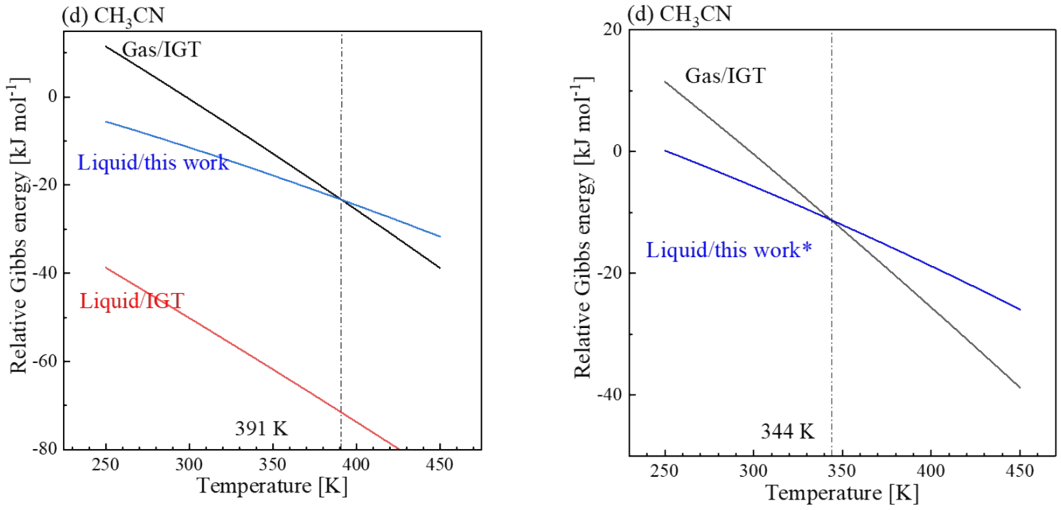

Fig. S5 CH_3CN.

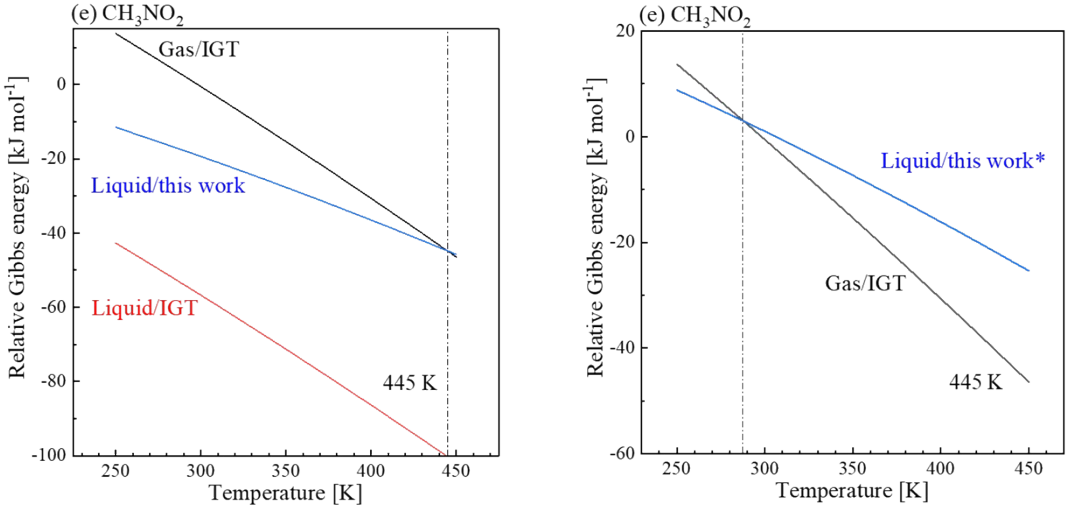

Fig. S6 CH_3NO_2.

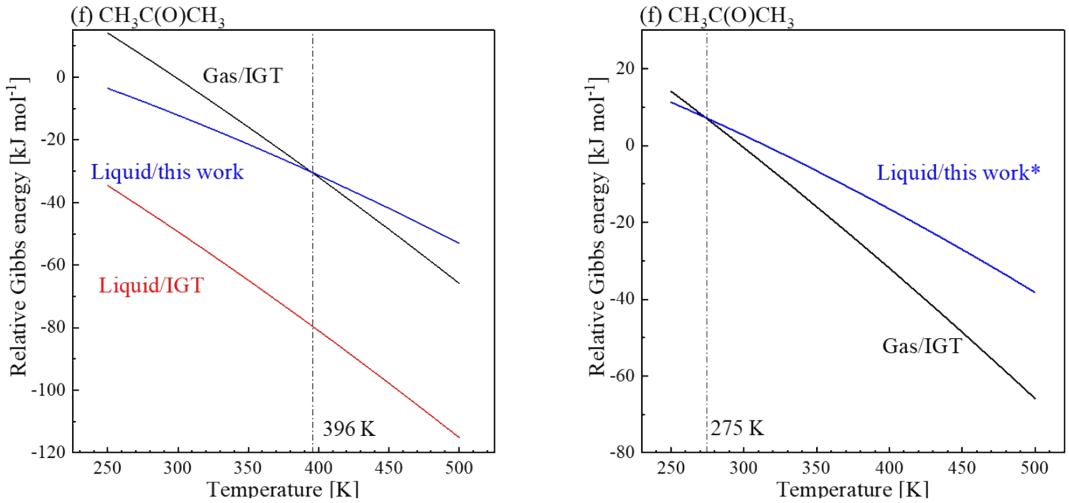

Fig. S7 $CH_3C(O)CH_3$.

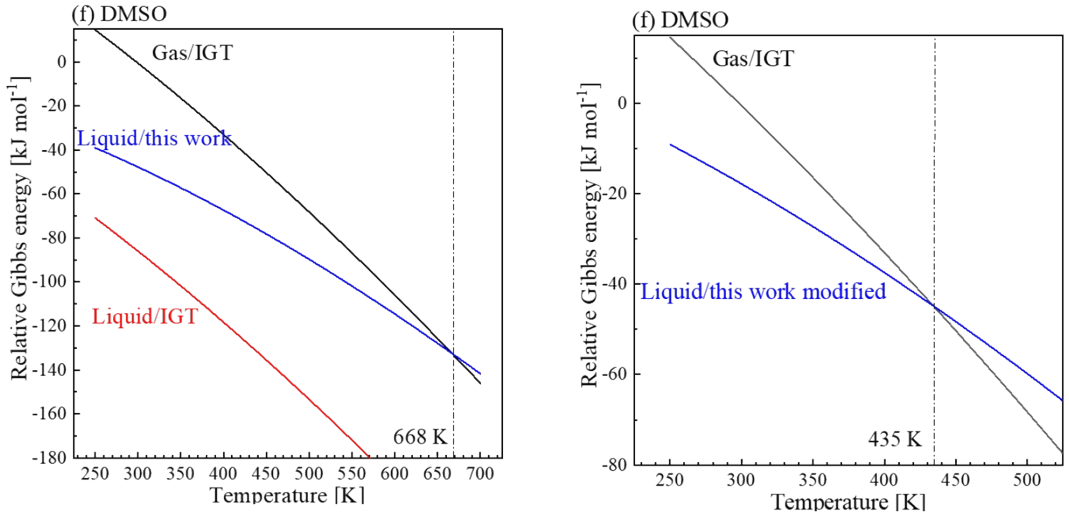

Fig. S8 DMSO.

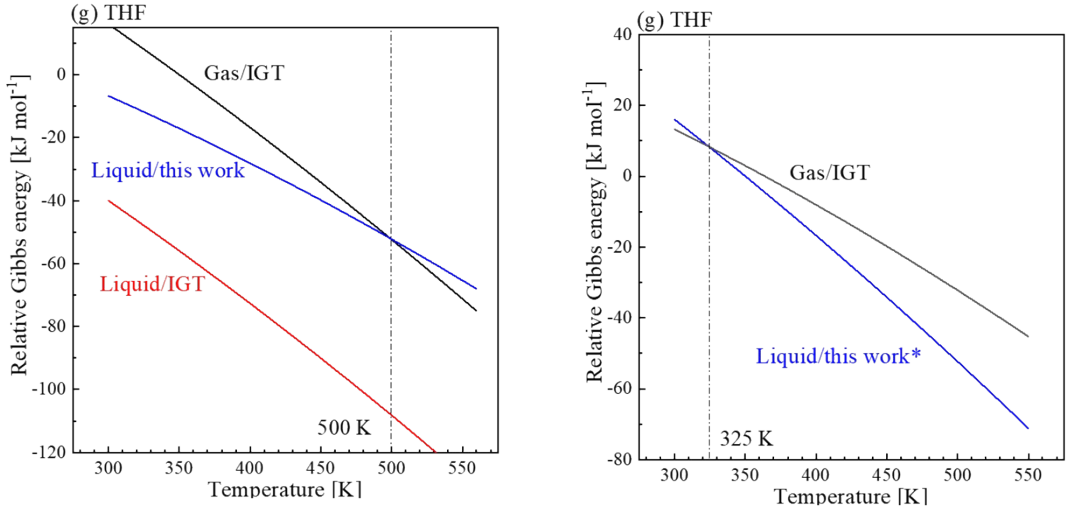

Fig. S9 THF.

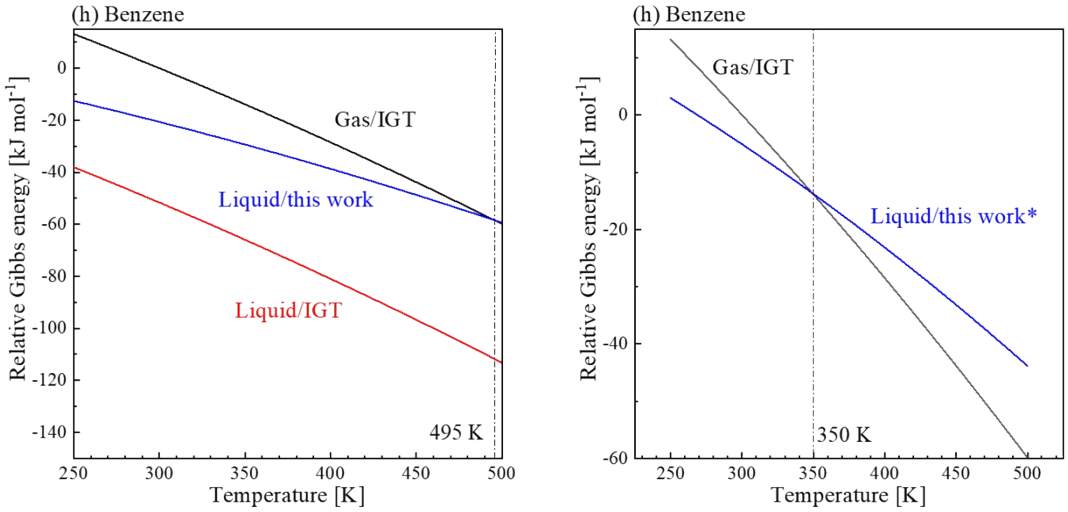

Fig. S10 Benzene.

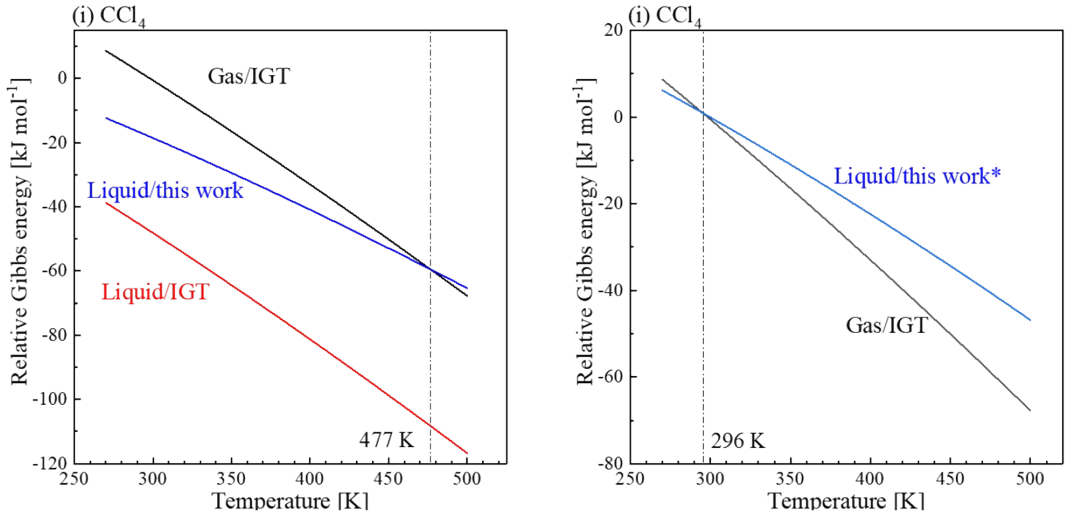

Fig. S11 CCl_4.

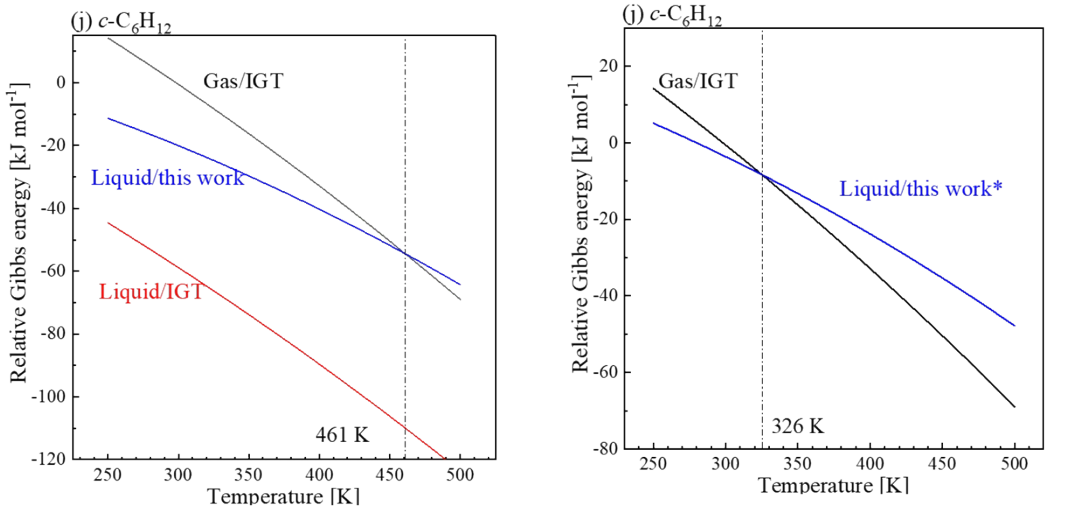

Fig. S12 *cyc*-C_6H_{12}.

Appendix 9. Specific procedure to calculate translational and rotational entropies.

1. Geometric optimization and frequency analysis are conducted using PCMs with Bondi's van der Waals radii scaled by $\alpha = 1.2$. The result provides molecular weight m, $V_{\alpha=1.2}$, the dipole-moment μ, rotational constants ($\tilde{A}$, $\tilde{B}$, $\tilde{C}$), and polarizability, P.

   Here, we consider that any molecular orbital (MO) and density functional theory (DFT) methods with PCMs can be used. It is preferable that the frequency scaling factor is obtained in advance.

2. A single point calculation is conducted using PCMs for the structure optimized in (1) with Bondi's van der Waals radii scaled by $\alpha = 1.0$. The result provides $V_{\alpha=1.0}$. The free-volume V_{free}, can then be calculated:

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

The translational entropy $S_{\text{trans.}}$, can be calculated from the corrected Sackur-Tetrode equation:

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

e.g.) H_2O

$$V_{free} = \left(V_{a=1.2}^{1/3} - V_{a=1.0}^{1/3}\right)^3 = (30.926^{1/3} - 19.159^{1/3})^3 \times 10^{-30} = 9.928 \times 10^{-32}$$

$$S_{trans.}^{liquid} = 8.314\left[\ln\left(9.928 \times 10^{-32}\left(\frac{2\pi \times \frac{18.01}{6.02 \times 10^{-23} \times 1000} \times 1.38 \times 10^{-23} \times 298.15}{(6.63 \times 10^{-34})^2}\right)^{\frac{2}{3}}\right) + \frac{5}{2}\right]$$

$= 37.4$ [J mol^{-1} K^{-1}]

3. A single point calculation is conducted for the same structure without PCMs. The result provides the dipole moment in a vacuum, μ_{vac}. The induced dipole moment μ^*, and surrounding electric field E, can then be calculated according to the following equations:

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

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

e.g.) H_2O

$$\mu^* = \mu - \mu_{vac} = (2.500[debye] - 2.92\,[debye]) \times 3.33564 \times 10^{-30} = 1.03 \times 10^{-30}[C\,m]$$

$$E = \frac{\mu^*}{P} = \frac{1.03 \times 10^{-30}[C\,m]}{7.97 \times 1.65 \times 10^{-41}} = 7.89 \times 10^{9}$$

The rotational entropy $S_{\text{rot.}}$, can be calculated by assigning the obtained values and constants to the following equations:

$$S_{rot,\ linear} = R[\ln\left\{\frac{1}{\sigma 2hc\tilde{B}}\frac{k_B T}{2\mu E}\left[1 - \exp\left(-\frac{2\mu E}{k_B T}\right)\right]\right\} - \frac{2\mu E}{k_B T}\frac{\exp\left(-\frac{2\mu E}{k_B T}\right)}{\left[1 - \exp\left(-\frac{2\mu E}{k_B T}\right)\right]} + 2] \quad (13)$$

$$S_{rot,non-linear} = R[\ln\left\{\frac{1}{\sigma}\left(\frac{k_B T}{hc}\right)^{\frac{3}{2}}\left(\frac{\pi}{\tilde{A}\tilde{B}\tilde{C}}\right)^{\frac{1}{2}}\frac{k_B T}{2\mu E}\left[1 - \exp\left(-\frac{2\mu E}{k_B T}\right)\right]\right\} - \frac{2\mu E}{k_B T}\frac{\exp\left(-\frac{2\mu E}{k_B T}\right)}{\left[1 - \exp\left(-\frac{2\mu E}{k_B T}\right)\right]} + \frac{5}{2}] \quad (14)$$

e.g.) H_2O

$$\frac{2\mu E}{k_B T} = \frac{2 \times 2.500 \times 3.33564 \times 10^{-30} \times 7.89 \times 10^{9}}{1.38 \times 10^{-23} \times 298.15} = 31.98$$

$$\tilde{A} = \frac{817.45 \times 10^{9}}{2.997 \times 10^{8}} = 2728\ [m^{-1}]$$

$$\tilde{B} = \frac{435.16 \times 10^{9}}{2.997 \times 10^{8}} = 1451\ [m^{-1}]$$

$$\tilde{C} = \frac{283.99 \times 10^{9}}{2.997 \times 10^{8}} = 947.3\ [m^{-1}]$$

$$S_{rot,non-linear} = R\left[\ln\left\{\frac{1}{2}\left(\frac{1.38 \times 10^{-23} \times 298.15}{6.63 \times 10^{-34} \times 2.997 \times 10^{8}}\right)^{\frac{3}{2}}\left(\frac{\pi}{(2728 \times 1451 \times 947.3)}\right)^{\frac{1}{2}}\frac{1}{31.98}[1 - \exp(-31.98)]\right\}\frac{1}{31.9}\right.$$

$$= 23\ [J\,K^{-1}\,mol^{-1}]$$

Appendix 10. Parameter study using various PCMs and atomic radii.

The conductor-like polarizable continuum model (CPCM), the integral equation formalism model (IEF-PCM), and the solvation model based on density (SMD) were tested. Bondi's van der Waals radii, Pauling's van der Waals radii, and UFF radii scaled by $\alpha = 1.2$ were also tested. The standard enthalpies of formation and entropy were assessed for water (H_2O) and methanol (CH_3OH) using the CBS-QB3//ωB97X-D method, as shown in the main text. Geometric optimization and frequency analysis were conducted at the ωB97X-D/6-311++G(d,p) level[37] of theory. The repulsion and dispersion interaction energy were evaluated using the method reported by Floris and Tomasi[42,43]. The results are listed in Table S4. All combinations of PCMs and radii investigated in this study provided reasonable values for ΔH_{298} and S_{298}.

Table S7 Standard enthalpy of formation and entropy calculated with various PCMs and atomic radii.

Species	States	PCMs	Radiis	$\Delta H_{298\ calc.}$	$\Delta H_{298,\ expt.}$	$S_{298\ calc.}$	$S_{298\ expt.}$
H_2O	Gas	-	-	-242.85	-241.826	188.54	188.84
	Liquid	CPCM	Bondi	-286.40	-285.83	60.75	69.95
		CPCM	Pauling	-288.83		58.34	
		CPCM	UFF	-275.25		67.10	
		IEFPCM	Bondi	-286.19		60.80	
		IEFPCM	Pauling	-288.67		58.40	
		IEFPCM	UFF	-275.16		67.15	
		SMD	smd-Coulomb.	-286.21		60.81	
		SMD	Bondi	-286.21		60.81	
		SMD	Pauling	-288.48		58.35	
		SMD	UFF	-277.18		67.13	
CH3OH	Gas	-	-	-202.47	-205	238.74	239.81
	Liquid	CPCM	Bondi	-250.29	-238.4	119.67	127.19
		CPCM	Pauling	-252.97		117.43	
		CPCM	UFF	-240.27		125.33	
		IEFPCM	Bondi	-249.99		119.89	
		IEFPCM	Pauling	-252.65		123.48	
		IEFPCM	UFF	-240.09		125.49	
		SMD	smd-Coulomb.	-249.35		121.29	
		SMD	Bondi	-248.66		120.28	
		SMD	Pauling	-252.27		117.49	
		SMD	UFF	-243.20		125.70	

Appendix 11. Geometries of all stational points investigated in this study.

Table S8 Geometries of gasified species at ωB97X-D/6-311++G(d,p) level of theory.

Species	Coordination			
H_2O	O	0.00000000	0.00000000	0.11633200
	H	0.00000000	0.76069400	-0.46532700
	H	0.00000000	-0.76069400	-0.46532700
	vibrational temperatures (unscaled)			
	2316.51 5610.64 5767.63			
CH_3OH	C	0.04632300	0.66025700	0.00000000
	H	-0.43933300	1.07394600	0.89248400
	H	1.08942100	0.97736900	0.00000000
	H	-0.43933300	1.07394600	-0.89248400
	O	0.04632300	-0.75312400	0.00000000
	H	-0.85927300	-1.06181500	0.00000000
	vibrational temperatures (unscaled)			
	440.32 1543.06 1583.07 1700.08 1969.53			
	2143.66 2160.56 2175.44 4326.30 4407.46			
	4514.26 5661.93			
C_2H_5OH	O	1.14845000	-0.39479900	-0.00000200
	H	1.98136200	0.07673900	-0.00000200
	C	0.08513900	0.54576100	0.00000100
	H	0.14101100	1.19097900	0.88745200
	H	0.14100900	1.19098200	-0.88744800
	C	-1.21967700	-0.22147300	0.00000100
	H	-1.28796300	-0.85708300	0.88568600
	H	-2.06782500	0.46812600	0.00000300
	H	-1.28796500	-0.85708000	-0.88568600
	vibrational temperatures (unscaled)			
	388.04 432.05 619.09 1170.24 1296.51			
	1540.85 1585.40 1653.36 1847.85 1982.87			
	2023.46 2063.46 2148.01 2155.49 2191.17			
	4333.93 4370.55 4456.97 4486.62 4505.27			
	5632.29			
$1\text{-}C_3H_7OH$	C	1.89065000	-0.12778800	0.01727200
	H	2.01977400	-0.69457800	0.94437800
	H	2.03492200	-0.81928500	-0.81819400
	H	2.68578100	0.61946600	-0.02899200
	C	0.51311200	0.52680900	-0.04441500

	H	0.40521800	1.10302200	-0.96856000
	H	0.40559500	1.23702300	0.78539200
	C	-0.61432800	-0.49464400	0.02536500
	H	-0.53577300	-1.19582100	-0.80951700
	H	-0.53019200	-1.08081400	0.95239400
	O	-1.90076200	0.08699400	-0.08511300
	H	-2.01583400	0.70877300	0.63466900
	vibrational temperatures (unscaled)			
	192.21	327.57	384.90	449.03	672.28
	1104.99	1294.98	1299.55	1511.14	1577.71
	1598.68	1659.68	1800.07	1900.52	1932.01
	2002.37	2044.89	2066.66	2152.49	2164.84
	2169.90	2188.17	4314.62	4359.48	4374.92
	4430.01	4459.19	4481.34	4495.93	5633.80
2-C_3H_7OH	C	-1.18817800	-0.78642400	-0.10224100
	H	-1.19951700	-0.85056100	-1.19392300
	H	-2.13281400	-0.34081200	0.22615400
	H	-1.13900900	-1.79913500	0.30751100
	C	0.00225000	0.04322400	0.36316200
	H	-0.00581000	0.09067100	1.46229300
	C	1.32651800	-0.54324300	-0.08953800
	H	1.35893600	-0.59860900	-1.18120600
	H	2.15500900	0.08238600	0.24807100
	H	1.45998900	-1.54931300	0.31609700
	O	-0.05574200	1.36576800	-0.16220200
	H	-0.89438100	1.75788600	0.08432300
	vibrational temperatures (unscaled)			
	324.52	392.96	430.35	533.18	608.90
	705.48	1204.07	1350.06	1376.67	1416.91
	1580.76	1688.33	1724.75	1852.31	1988.62
	2010.42	2042.08	2069.67	2137.67	2144.15
	2160.96	2176.53	4308.53	4367.45	4387.06
	4474.17	4493.33	4503.46	4514.66	5637.36
1-C_4H_9OH	C	-2.38931700	-0.15163400	-0.14511100
	H	-2.77582800	0.85073000	0.06479200
	H	-3.06749800	-0.87395300	0.31604000
	H	-2.43029900	-0.30135800	-1.22864600
	C	-0.96461600	-0.31397800	0.37651100
	H	-0.60718600	-1.32877100	0.17849900
	C	0.00798600	0.68788000	-0.24129400

	H	-0.31201900	1.71066900	-0.00516000
	H	-0.02383000	0.60550700	-1.33708900
	C	1.44653700	0.51584300	0.22983400
	H	2.07117900	1.32740500	-0.16717300
	H	1.49303600	0.57026100	1.32076400
	H	-0.95426800	-0.19287600	1.46617000
	O	1.99820900	-0.74676800	-0.10808100
	H	2.01749600	-0.82213400	-1.06319100
	vibrational temperatures (unscaled)			
	122.54	211.55	346.72	359.86	453.20
	502.15	765.83	1083.49	1215.00	1239.41
	1395.98	1407.40	1526.18	1587.98	1607.72
	1655.25	1772.54	1846.68	1911.77	1931.12
	1994.14	2035.75	2044.52	2053.36	2137.62
	2157.45	2164.09	2176.39	2178.52	4325.70
	4342.81	4366.95	4374.64	4397.20	4440.67
	4457.10	4475.45	4484.60	5630.08	
$2\text{-}C_4H_9OH$	C	-1.80622600	-0.64003200	-0.00435700
	H	-1.93965600	-0.69067000	-1.08853500
	H	-2.64339000	-0.08172800	0.41874300
	H	-1.82377000	-1.65624900	0.39757100
	C	-0.49292500	0.04346100	0.32697400
	H	-0.38309000	0.09354700	1.42213400
	C	0.70885500	-0.71006500	-0.24350300
	H	0.58543700	-0.78501100	-1.32968000
	H	0.68811700	-1.73104400	0.15370500
	O	-0.58403300	1.36629100	-0.19276600
	H	0.19543800	1.85697600	0.06986100
	C	2.05290200	-0.06559900	0.08607000
	H	2.88183700	-0.67601600	-0.27903100
	H	2.15575400	0.91905300	-0.38092000
	H	2.17995000	0.05422400	1.16717400
	vibrational temperatures (unscaled)			
	165.13	326.31	347.67	368.34	405.85
	551.16	672.38	721.76	1130.72	1198.54
	1347.61	1426.81	1471.00	1529.94	1580.14
	1677.71	1704.75	1823.34	1909.74	1930.96
	2002.61	2036.27	2041.59	2070.08	2132.41
	2154.02	2158.58	2160.49	2177.24	4290.67
	4367.92	4377.11	4379.36	4437.87	4474.95

	4480.43 4496.99 4516.39 5645.33			
i-C_4H_9OH	C	1.69407000	-0.80310400	-0.00714900
	H	1.86056800	-0.83570600	1.07511500
	C	0.44072800	0.00783400	-0.33594000
	H	0.30505700	-0.00242500	-1.42744600
	C	-0.78846500	-0.65718000	0.28394000
	H	-0.82398900	-1.71598900	-0.00952500
	H	-0.71434700	-0.62185200	1.37536400
	H	1.61474200	-1.83355600	-0.36606900
	O	-2.00768700	-0.01060600	-0.03632500
	H	-2.14332900	-0.07244500	-0.98283800
	H	2.58015700	-0.35534100	-0.46430700
	C	0.57713600	1.45922800	0.11960800
	H	-0.33294100	2.02547300	-0.08775300
	H	0.76079900	1.50435100	1.19885900
	H	1.41396200	1.95166900	-0.38355200
	vibrational temperatures (unscaled)			
	180.47 317.57 346.46 354.84 390.47			
	518.25 618.65 711.82 1192.51 1338.56			
	1354.88 1390.61 1410.94 1576.09 1630.62			
	1703.01 1730.46 1827.46 1859.40 1938.51			
	1985.45 2027.79 2046.12 2102.75 2146.66			
	2148.71 2168.79 2182.79 2192.13 4291.42			
	4349.62 4361.04 4365.24 4385.88 4461.88			
	4469.81 4486.05 4515.12 5667.74			
HCOOH	C	0.13370500	0.39809700	0.00000100
	H	0.10477000	1.49496500	0.00001200
	O	-1.11116100	-0.08988000	-0.00000400
	H	-1.05122900	-1.05409400	0.00002400
	O	1.12919000	-0.26380100	-0.00000100
	vibrational temperatures (unscaled)			
	923.23 983.39 1535.41 1673.15 1892.78			
	2034.41 2672.37 4437.23 5497.76			
CH_3COOH	C	0.09044800	0.12491100	-0.00000200
	O	0.78541800	-1.03071600	0.00000000
	H	1.72162600	-0.79864800	0.00000400
	O	0.63003400	1.19816900	0.00000000
	C	-1.38982200	-0.11959400	-0.00000100
	H	-1.66649900	-0.70247700	-0.88080300
	H	-1.66650700	-0.70237600	0.88086700

	H	-1.91599000	0.83197000	-0.00005400
	vibrational temperatures (unscaled)			
	97.17 619.19 788.86 858.37 964.13			
	1265.15 1456.11 1545.33 1772.33 1944.84			
	2048.44 2123.18 2130.57 2678.21 4418.93			
	4525.22 4588.04 5527.91			
CH_3CN	C	0.00000000	0.00000000	-1.17534800
	H	0.00000000	1.02544200	-1.54750400
	H	-0.88805900	-0.51272100	-1.54750400
	H	0.88805900	-0.51272100	-1.54750400
	C	0.00000000	0.00000000	0.28062100
	N	0.00000000	0.00000000	1.43012500
	vibrational temperatures (unscaled)			
	554.99 555.14 1352.15 1531.23 1531.25			
	2034.48 2128.44 2128.44 3454.05 4416.87			
	4539.32 4539.33			
CH_3NO_2	C	-1.31938400	-0.00000400	-0.00289600
	H	-1.65883300	-0.90530600	-0.49794600
	H	-1.65883700	0.90526400	-0.49800600
	H	-1.62368700	0.00003300	1.04355500
	O	0.72792500	-1.07837200	0.00276900
	O	0.72791800	1.07837600	0.00276900
	N	0.17298800	0.00000000	-0.01064800
	vibrational temperatures (unscaled)			
	45.38 712.19 900.36 987.38 1384.04			
	1615.40 1648.40 2045.50 2115.08 2120.82			
	2143.33 2432.87 4449.42 4595.11 4637.53			
$CH_3C(O)CH_3$	C	0.00000000	0.18635700	0.00000000
	C	-1.28481800	-0.61195100	0.00244800
	H	-1.26501400	-1.37275600	0.78788600
	H	-2.13817200	0.04999300	0.14214200
	H	-1.38577200	-1.13822000	-0.95216300
	C	1.28481800	-0.61195100	-0.00244800
	H	1.38577200	-1.13822000	0.95216300
	H	1.26501400	-1.37275600	-0.78788600
	H	2.13817200	0.04999300	-0.14214200
	O	0.00000000	1.39340400	0.00000000
	vibrational temperatures (unscaled)			
	277.94 370.91 433.67 468.77 540.39			
	973.79 1022.12 1334.03 1383.44 1393.30			

	1475.94 1518.23 1934.26 1966.23 2064.09 2079.43 2080.66 2110.44 4408.37 4410.75 4563.78 4569.72 4581.93 4583.78			
DMSO	C	-0.25834800	-0.78378900	1.35432600
	H	0.62085500	-1.42330000	1.25896700
	H	-0.20474200	-0.21756200	2.28371900
	H	-1.17990700	-1.36831200	1.32659700
	S	-0.25834800	0.42616200	0.00000000
	C	-0.25834800	-0.78378900	-1.35432600
	H	-1.17990700	-1.36831200	-1.32659700
	H	-0.20474200	-0.21756200	-2.28371900
	H	0.62085500	-1.42330000	-1.25896700
	O	1.09516700	1.07565400	0.00000000
	vibrational temperatures (unscaled) 249.31 327.57 420.63 455.50 531.30 952.83 993.74 1303.88 1354.79 1398.52 1492.44 1569.89 1921.27 1953.49 2077.39 2097.29 2099.45 2124.55 4395.27 4397.11 4547.76 4552.41 4563.75 4565.39			
THF	C	-1.12630900	-0.46968100	0.15646200
	O	0.00002400	-1.19531600	-0.29534000
	C	1.12627400	-0.46968800	0.15668100
	C	0.77338600	1.01214100	-0.04978500
	C	-0.77336700	1.01215000	-0.04991100
	H	-1.99361100	-0.80323500	-0.41384800
	H	-1.30426900	-0.68142500	1.22192000
	H	1.30401500	-0.68141800	1.22217800
	H	1.99368800	-0.80325800	-0.41344800
	H	1.19385100	1.64026200	0.73762600
	H	1.16079600	1.37088400	-1.00483300
	H	-1.19395100	1.64025500	0.73745000
	H	-1.16061900	1.37092700	-1.00501000
	vibrational temperatures (unscaled) 21.25 411.86 942.12 945.37 1167.24 1261.58 1326.85 1368.51 1385.67 1420.17 1533.77 1641.65 1662.81 1763.90 1784.43 1822.12 1844.09 1897.07 1902.98 1969.96 2019.64 2145.54 2175.51 2179.96 2207.93 4297.20 4303.50 4423.71 4439.86 4479.12 4495.16 4500.06 4519.02			

Benzene	C	0.01056900	1.39073000	-0.00000100
	C	-1.19920800	0.70453900	0.00000400
	C	-1.20977900	-0.68623300	0.00000500
	C	-0.01056900	-1.39073000	0.00000100
	C	1.19920800	-0.70453900	-0.00000400
	C	1.20977900	0.68623300	-0.00000500
	H	0.01880600	2.47510500	-0.00000100
	H	-2.13414700	1.25393200	0.00000700
	H	-2.15295800	-1.22135500	0.00000900
	H	-0.01880600	-2.47510500	0.00000100
	H	2.13414700	-1.25393200	-0.00000700
	H	2.15295800	1.22135500	-0.00000900
	vibrational temperatures (unscaled)			
	594.93	595.11	900.56	901.57	1000.17
	1047.51	1263.20	1263.38	1443.96	1444.11
	1476.29	1477.07	1482.62	1541.12	1541.51
	1696.04	1736.44	1736.83	1930.66	1989.65
	2191.15	2191.61	2400.61	2400.93	4573.49
	4588.27	4588.88	4611.96	4612.51	4627.67
CCl_4	C	0.00000000	0.00000000	0.00000000
	Cl	1.02718500	1.02718500	1.02718500
	Cl	-1.02718500	-1.02718500	1.02718500
	Cl	-1.02718500	1.02718500	-1.02718500
	Cl	1.02718500	-1.02718500	-1.02718500
	vibrational temperatures (unscaled)			
	325.90	325.90	467.44	467.44	467.44
	673.63	1144.04	1144.04	1144.04	
C_5H_{12}	C	2.54579500	0.32476700	-0.00000500
	H	2.58584700	0.97013700	0.88297900
	H	2.58584700	0.97011900	-0.88300300
	H	3.44457600	-0.29729400	0.00000100
	C	1.27714200	-0.52355000	0.00000300
	H	1.27558600	-1.18215400	-0.87672000
	H	1.27558900	-1.18214200	0.87673400
	C	0.00000000	0.31342800	0.00000000
	H	0.00000100	0.97374700	-0.87724700
	H	-0.00000100	0.97374900	0.87724600
	C	-1.27714200	-0.52355000	-0.00000100
	H	-1.27558700	-1.18215100	0.87672300
	H	-1.27558900	-1.18214500	-0.87673100

	C	-2.54579500	0.32476700	0.00000400
	H	-2.58584700	0.97013400	-0.88298300
	H	-2.58584700	0.97012200	0.88299900
	H	-3.44457600	-0.29729400	0.00000000
	vibrational temperatures (unscaled)			
	150.33	162.57	260.45	351.93	365.34
	581.40	582.36	1058.38	1108.34	1255.68
	1273.72	1353.30	1436.77	1512.06	1532.27
	1573.52	1685.37	1735.91	1826.97	1861.89
	1913.68	1921.97	1973.79	2030.25	2037.86
	2039.57	2136.38	2140.44	2151.88	2153.04
	2154.44	2164.25	2173.17	4336.82	4354.22
	4360.75	4364.12	4365.75	4376.22	4403.71
	4423.30	4467.22	4468.74	4478.08	4478.41
C_6H_{14}	C	3.20588700	-0.20856300	0.00000300
	H	3.28980000	-0.84950300	-0.88329400
	H	3.28980500	-0.84948000	0.88331500
	H	4.05953000	0.47435200	-0.00000800
	C	1.88149000	0.55009300	-0.00000400
	H	1.83419600	1.20657200	0.87705800
	H	1.83419800	1.20655500	-0.87707900
	C	0.66542400	-0.37371600	0.00000200
	H	0.71182900	-1.03156300	0.87774200
	H	0.71182600	-1.03157100	-0.87773200
	C	-0.66542400	0.37371600	0.00000100
	H	-0.71182500	1.03156900	-0.87773500
	H	-0.71183000	1.03156400	0.87773900
	C	-1.88149000	-0.55009300	-0.00000500
	H	-1.83419600	-1.20657100	0.87705700
	H	-1.83419900	-1.20655600	-0.87707900
	C	-3.20588700	0.20856200	0.00000300
	H	-3.28980200	0.84950200	-0.88329300
	H	-4.05953000	-0.47435200	-0.00000500
	H	-3.28980400	0.84948100	0.88331500
	vibrational temperatures (unscaled)			
	104.09	144.19	192.46	213.05	350.96
	366.45	435.12	537.35	683.64	1059.98
	1082.26	1172.98	1300.81	1319.09	1321.86
	1469.34	1488.13	1537.89	1568.35	1571.19
	1683.75	1738.99	1807.58	1835.71	1892.17

	1924.02	1935.12	1935.77	2010.92	2041.44
	2043.41	2046.54	2146.07	2146.23	2154.42
	2162.62	2163.02	2163.51	2173.32	2179.63
	4337.14	4341.78	4358.96	4362.93	4366.48
	4367.19	4374.34	4391.52	4414.26	4430.13
	4471.60	4472.61	4480.65	4480.66	
cyc-C_6H_{12}	C	1.36302500	-0.52218300	-0.23041700	
	C	1.13373200	0.91930300	0.23045400	
	C	-0.22927800	1.44145700	-0.23042900	
	C	-1.36302500	0.52218300	0.23041700	
	C	-1.13373200	-0.91930300	-0.23045400	
	C	0.22927800	-1.44145700	0.23042900	
	H	-0.39101400	2.45832100	0.14050100	
	H	1.18056400	0.95728000	1.32677800	
	H	1.93349500	1.56782000	-0.14045200	
	H	1.41936600	-0.54375800	-1.32673800	
	H	2.32451700	-0.89056100	0.14052500	
	H	-1.41936600	0.54375800	1.32673800	
	H	-2.32451700	0.89056100	-0.14052600	
	H	-1.93349500	-1.56782000	0.14045300	
	H	-1.18056400	-0.95728000	-1.32677800	
	H	0.23873400	-1.50103200	1.32675400	
	H	0.39101400	-2.45832100	-0.14050100	
	H	-0.23873400	1.50103300	-1.32675400	
	vibrational temperatures (unscaled)				
	344.02	344.09	560.87	626.63	628.00
	764.63	1155.34	1155.98	1174.17	1268.45
	1268.75	1332.59	1333.15	1508.90	1515.29
	1515.87	1563.95	1612.30	1648.11	1707.42
	1861.50	1861.67	1877.49	1877.91	1943.86
	1996.29	1999.75	2000.13	2003.36	2003.79
	2139.79	2140.21	2150.09	2150.50	2156.96
	2179.65	4347.58	4347.73	4349.63	4354.14
	4354.23	4356.90	4428.71	4428.97	4432.79
	4433.01	4434.40	4443.78		

Table S9 Geometries and vibrational temperatures of liquid species

at ωB97X-D/6-311++G(d,p)/CPCM level of theory.

Species	Coordination and vibrational temperatures				
H_2O	coordination				
	O	0.00000000	0.00000000	0.11753600	
	H	0.00000000	0.75906000	-0.47014500	
	H	0.00000000	-0.75906000	-0.47014500	
	vibrational temperatures (unscaled)				
	2318.99	5577.85	5708.79		
CH_3OH	C	0.04724500	0.66479800	0.00000000	
	H	-0.44397800	1.06865300	0.89146800	
	H	1.08912500	0.98590100	0.00000000	
	H	-0.44397800	1.06865300	-0.89146800	
	O	0.04724500	-0.75657300	0.00000000	
	H	-0.86259900	-1.05940800	0.00000000	
	vibrational temperatures (unscaled)				
	428.36	1522.10	1563.45	1699.84	1969.63
	2130.62	2139.72	2161.53	4349.36	4440.90
	4516.46	5626.34			
C_2H_5OH	O	-1.15603000	-0.39526500	-0.00000200	
	H	-1.98421100	0.08872100	0.00001200	
	C	-0.08160000	0.54423700	-0.00000100	
	H	-0.14411400	1.18648200	-0.88656500	
	H	-0.14411500	1.18648300	0.88656300	
	C	1.22369700	-0.22155000	0.00000100	
	H	1.30073700	-0.85478300	-0.88768300	
	H	2.06661800	0.47387500	0.00000000	
	H	1.30073600	-0.85478000	0.88768700	
	vibrational temperatures (unscaled)				
	384.29	431.68	623.48	1169.12	1292.37
	1541.70	1557.40	1637.45	1847.99	1981.88
	2015.58	2051.50	2129.46	2133.05	2176.63
	4360.02	4373.58	4461.01	4490.53	4496.82
	5601.16	5615.30			
1-C_3H_7OH	C	1.89024700	-0.12805500	0.02212400	
	H	2.01259500	-0.68658500	0.95506200	
	H	2.03554800	-0.82619000	-0.80781800	
	H	2.68478700	0.61986000	-0.02667300	
	C	0.51378400	0.52868300	-0.04919900	

	H	0.41476000	1.09932000	-0.97842400
	H	0.39844600	1.23960100	0.77752000
	C	-0.60916200	-0.49593700	0.01955000
	H	-0.53207600	-1.19500000	-0.81726000
	H	-0.52861300	-1.07829900	0.94689300
	O	-1.90371400	0.08948900	-0.08318300
	H	-2.02494800	0.68323600	0.66131600
	vibrational temperatures (unscaled)			
	193.24	324.67	367.66	427.86	671.61
	1101.17	1292.28	1298.16	1499.23	1555.46
	1591.00	1652.07	1796.75	1898.62	1930.63
	2002.12	2029.08	2058.23	2127.66	2143.24
	2153.77	2174.73	4341.17	4367.48	4371.25
	4424.23	4458.57	4475.06	4490.85	5601.39
$2\text{-}C_3H_7OH$	C	-1.34299800	-0.50839200	-0.08834200
	H	-1.38077300	-0.57103300	-1.18019100
	H	-2.15868600	0.13308300	0.25335800
	H	-1.49696200	-1.50984600	0.32045800
	C	-0.00229600	0.04144500	0.36129100
	H	0.00992300	0.09781400	1.45790300
	C	1.16388700	-0.82047300	-0.10218000
	H	1.16535100	-0.90321000	-1.19322200
	H	2.11817200	-0.39040300	0.21591500
	H	1.08806400	-1.82474800	0.32337100
	O	0.10030000	1.36905500	-0.16663200
	H	0.94095200	1.74042000	0.11084900
	vibrational temperatures (unscaled)			
	329.17	397.83	422.78	537.81	613.49
	707.28	1199.40	1351.02	1374.44	1404.90
	1581.84	1667.90	1711.36	1845.50	1984.12
	2003.67	2030.03	2058.39	2122.25	2127.70
	2145.28	2153.82	4339.40	4368.65	4378.76
	4481.29	4488.58	4493.61	4505.41	5602.76
$1\text{-}C_4H_9OH$	C	-2.39606600	-0.14181900	-0.13789300
	H	-2.76839900	0.85816900	0.10632000
	H	-3.07549700	-0.87153100	0.31034700
	H	-2.44779100	-0.25928200	-1.22497800
	C	-0.96668900	-0.33063400	0.36300800
	H	-0.62743100	-1.34540000	0.13223600
	C	0.00588700	0.67786400	-0.24428800

	H	-0.32072800	1.69649100	-0.00117900
	H	-0.01514300	0.60033100	-1.33956500
	C	1.44103600	0.52123200	0.23732400
	H	2.05942800	1.33629200	-0.15765000
	H	1.47991700	0.57245600	1.32877200
	H	-0.94266800	-0.23553600	1.45518600
	O	2.01596500	-0.73766900	-0.10679600
	H	2.02558500	-0.81049600	-1.06402400
	vibrational temperatures (unscaled)			
	123.82 208.77 345.73 358.23 430.86			
	500.30 761.31 1078.59 1213.58 1236.24			
	1388.29 1401.17 1520.14 1586.83 1589.11			
	1645.93 1771.68 1845.97 1904.54 1925.22			
	1990.05 2024.48 2032.01 2050.18 2117.86			
	2136.95 2141.96 2160.26 2164.61 4341.49			
	4358.81 4363.13 4367.77 4402.96 4433.73			
	4455.58 4467.45 4476.91 5599.19			
$2\text{-}C_4H_9OH$	C	-1.80395700	-0.64705100	-0.00058900
	H	-1.94189200	-0.70793000	-1.08445000
	H	-2.64601300	-0.09836600	0.42732900
	H	-1.81002600	-1.66143800	0.40520500
	C	-0.49261800	0.04305700	0.32487200
	H	-0.37937100	0.10373800	1.41679400
	C	0.70922800	-0.70633300	-0.24776300
	H	0.58687300	-0.77954100	-1.33481400
	H	0.68289200	-1.72813900	0.14604100
	O	-0.58579100	1.37288100	-0.19915900
	H	0.17068700	1.87864600	0.10506900
	C	2.05488500	-0.06817000	0.08840900
	H	2.87961800	-0.68048200	-0.28355200
	H	2.15985100	0.92234200	-0.36475900
	H	2.17847800	0.03911000	1.17083600
	vibrational temperatures (unscaled)			
	161.21 328.95 334.64 373.48 419.52			
	559.95 680.39 713.59 1121.37 1195.98			
	1343.43 1419.74 1466.17 1496.08 1583.68			
	1665.69 1715.03 1830.67 1872.50 1921.69			
	2009.31 2018.44 2030.62 2072.19 2114.13			
	2126.89 2142.73 2145.39 2165.62 4323.31			
	4366.65 4370.19 4379.53 4431.89 4470.29			

	4485.44 4490.52 4506.38 5613.45			
i-C_4H_9OH	C	1.68842100	-0.80934600	-0.00845200
	H	1.85589400	-0.84082100	1.07385900
	C	0.43897100	0.00860900	-0.33664500
	H	0.29925100	-0.00088900	-1.42640200
	C	-0.78759400	-0.65576300	0.28593700
	H	-0.82878400	-1.71049200	-0.01516200
	H	-0.71135000	-0.62300900	1.37735000
	H	1.59952000	-1.83905200	-0.36692200
	O	-2.01357600	-0.00782500	-0.03595000
	H	-2.13114500	-0.04751800	-0.98789000
	H	2.57443500	-0.36584800	-0.47016800
	C	0.58753700	1.45833000	0.12158600
	H	-0.30433100	2.04370300	-0.11316300
	H	0.74650800	1.50169200	1.20508900
	H	1.44460500	1.93385400	-0.36355100
	vibrational temperatures (unscaled)			
	182.47 318.59 342.36 386.82 414.14			
	515.38 625.29 718.54 1197.79 1311.22			
	1348.47 1384.33 1408.48 1541.44 1615.17			
	1666.03 1731.05 1809.94 1919.32 1978.79			
	2000.91 2020.05 2027.68 2055.56 2128.01			
	2133.60 2147.36 2156.49 2163.36 4338.68			
	4345.17 4358.70 4363.19 4439.44 4461.60			
	4465.88 4482.25 4494.19 5600.70			
HCOOH	C	-0.12777600	0.39942200	-0.00008300
	H	-0.10678500	1.49446800	-0.00051200
	O	1.10690000	-0.08987900	0.00020400
	H	1.06904700	-1.05749100	-0.00119400
	O	-1.13135000	-0.26431000	0.00007200
	vibrational temperatures (unscaled)			
	916.34 950.36 1552.98 1667.16 1890.47			
	2042.50 2578.05 4471.82 5453.81			
CH_3COOH	C	0.08935800	0.11976200	-0.00002800
	O	0.78594500	-1.02670500	-0.00004400
	H	1.72762500	-0.81041700	-0.00019700
	O	0.62954600	1.20001200	-0.00018800
	C	-1.38964200	-0.12006500	0.00022300
	H	-1.66577800	-0.70229500	-0.88111400
	H	-1.66552400	-0.70188900	0.88190900

	H	-1.91854400	0.82995900	0.00009000
	vibrational temperatures (unscaled)			
	81.90 630.71 789.30 858.18 939.01			
	1272.13 1458.46 1541.08 1761.29 1940.93			
	2039.52 2101.08 2109.62 2600.62 4419.84			
	4527.92 4587.37 5496.28			
CH_3CN	C	0.00000000	0.00000000	-1.17494800
	H	0.00000000	1.02709300	-1.54086400
	H	-0.88948900	-0.51354700	-1.54086400
	H	0.88948900	-0.51354700	-1.54086400
	C	0.00000000	0.00000000	0.27816800
	N	0.00000000	0.00000000	1.42903900
	vibrational temperatures (unscaled)			
	573.50 574.93 1344.27 1523.21 1523.33			
	2018.32 2092.66 2094.06 3428.08 4425.03			
	4554.55 4555.70			
CH_3NO_2	C	-0.00067300	-1.32366000	0.00000000
	H	0.49506800	-1.66291100	0.90418900
	H	0.49506800	-1.66291100	-0.90418900
	H	-1.04910600	-1.62105400	0.00000000
	O	-0.00067300	0.73383500	1.07379800
	O	-0.00067300	0.73383500	-1.07379800
	N	0.01054000	0.16392500	0.00000000
	vibrational temperatures (unscaled)			
	72.77 713.57 905.27 983.67 1383.51			
	1620.38 1653.76 2042.77 2084.59 2104.17			
	2147.55 2337.71 4454.99 4603.92 4652.51			
$CH_3C(O)CH_3$	C	-0.00000100	0.18152500	-0.00000200
	C	-1.28013200	-0.61107700	0.00234700
	H	-1.25487800	-1.36682900	0.79126600
	H	-2.14054500	0.04331500	0.13389000
	H	-1.36754200	-1.14479900	-0.94883100
	C	1.28012500	-0.61108700	-0.00234800
	H	1.36756100	-1.14475900	0.94885600
	H	1.25484400	-1.36687600	-0.79122900
	H	2.14054100	0.04329000	-0.13394500
	O	0.00000800	1.39756100	0.00000000
	vibrational temperatures (unscaled)			
	69.92 174.56 569.57 721.96 781.14			
	1164.14 1271.77 1308.11 1564.52 1610.77			

	1799.90 1988.69 2009.58 2084.33 2087.40 2096.33 2121.46 2564.07 4390.73 4397.45 4494.71 4502.40 4558.16 4560.24			
DMSO	C	-0.26211100	-0.77105600	1.36061900
	H	0.60780500	-1.42279200	1.26739000
	H	-0.21642400	-0.19752600	2.28565400
	H	-1.18933000	-1.34433600	1.32267200
	S	-0.26211100	0.41469800	0.00000000
	C	-0.26211100	-0.77105600	-1.36061900
	H	-1.18933000	-1.34433600	-1.32267200
	H	-0.21642400	-0.19752600	-2.28565400
	H	0.60780500	-1.42279200	-1.26739000
	O	1.11687400	1.06835100	0.00000000
	vibrational temperatures (unscaled) 247.62 361.74 438.51 462.75 542.70 974.45 1020.94 1332.17 1379.77 1389.02 1474.45 1519.10 1929.63 1966.25 2064.77 2079.22 2081.35 2112.85 4402.23 4407.17 4557.66 4566.38 4573.76 4576.89			
THF	C	-1.13370300	-0.46328900	0.15325900
	O	-0.00314900	-1.19912700	-0.29560300
	C	1.12840800	-0.47048200	0.16161400
	C	0.77785700	1.00740400	-0.05628600
	C	-0.76902900	1.01530700	-0.04512200
	H	-1.99923600	-0.78849400	-0.42433000
	H	-1.31483600	-0.68019400	1.21544100
	H	1.29345900	-0.67847900	1.22834700
	H	1.99852600	-0.80873200	-0.40140700
	H	1.20666500	1.63865400	0.72345200
	H	1.15990400	1.35462000	-1.01779800
	H	-1.17846900	1.63576900	0.75348300
	H	-1.16201800	1.38623500	-0.99315300
	vibrational temperatures (unscaled) 32.29 408.67 938.44 946.15 1164.07 1257.61 1325.25 1369.86 1371.85 1402.34 1529.55 1612.41 1655.42 1756.79 1783.18 1818.02 1836.84 1898.90 1901.12 1970.93 2016.68 2136.04 2159.82 2168.21 2189.30 4319.22 4322.93 4424.23 4440.64 4483.15			
Benzene	C	-0.00092000	-1.39161500	0.00000000

	C	1.20478700	-0.69663500	-0.00002000
	C	1.20570100	0.69502800	0.00001000
	C	0.00092600	1.39161400	-0.00000400
	C	-1.20478900	0.69663200	-0.00001000
	C	-1.20570500	-0.69502200	0.00001400
	H	-0.00165900	-2.47549600	-0.00000300
	H	2.14307400	-1.23919000	0.00001600
	H	2.14468500	1.23637900	0.00003100
	H	0.00166900	2.47548900	0.00002200
	H	-2.14307000	1.23918000	-0.00002900
	H	-2.14469600	-1.23637300	0.00002600
	vibrational temperatures (unscaled)			
	594.27	595.13	898.58	899.63	994.69
	1048.95	1263.72	1263.91	1452.04	1452.06
	1473.00	1474.51	1492.59	1536.80	1537.00
	1687.81	1727.47	1727.83	1924.06	1987.02
	2186.54	2186.74	2394.81	2395.04	4583.16
	4596.68	4597.49	4619.24	4619.97	4634.91
CCl_4	C	0.00000000	0.00000000	0.00000000
	Cl	1.02718500	1.02718500	1.02718500
	Cl	-1.02718500	-1.02718500	1.02718500
	Cl	-1.02718500	1.02718500	-1.02718500
	Cl	1.02718500	-1.02718500	-1.02718500
	vibrational temperatures (unscaled)			
	324.70	324.70	466.17	466.17	466.17
	673.24	1127.51	1127.51	1127.51	
C_5H_{12}	C	2.54504900	-0.32490800	-0.00003400
	H	2.58447300	-0.97007600	-0.88333500
	H	2.58443100	-0.97034000	0.88307300
	H	3.44413400	0.29698900	0.00007600
	C	1.27678600	0.52366900	0.00005400
	H	1.27499700	1.18228100	0.87672200
	H	1.27495100	1.18239100	-0.87653100
	C	0.00000000	-0.31339300	0.00002700
	H	-0.00003800	-0.97359900	0.87726500
	H	0.00003800	-0.97365700	-0.87716600
	C	-1.27678600	0.52366900	-0.00005100
	H	-1.27496800	1.18226200	-0.87673400
	H	-1.27498000	1.18241000	0.87652000
	C	-2.54504900	-0.32490800	0.00001000

	H	-2.58447200	-0.97011600	0.88328000
	H	-2.58443300	-0.97030000	-0.88312800
	H	-3.44413400	0.29698900	-0.00007400
	vibrational temperatures (unscaled)			
	150.33	162.57	260.45	351.93	365.34
	581.40	582.36	1058.38	1108.34	1255.68
	1273.72	1353.30	1436.77	1512.06	1532.27
	1573.52	1685.37	1735.91	1826.97	1861.89
	1913.68	1921.97	1973.79	2030.25	2037.86
	2039.57	2136.38	2140.44	2151.88	2153.04
	2154.44	2164.25	2173.17	4336.82	4354.22
	4360.75	4364.12	4365.75	4376.22	4403.71
	4423.30	4467.22	4468.74	4478.08	4478.41
C_6H_{14}	C	-3.20588700	0.20856300	0.00000300
	H	-3.28980000	0.84950300	-0.88329400
	H	-3.28980500	0.84948000	0.88331500
	H	-4.05953000	-0.47435200	-0.00000800
	C	-1.88149000	-0.55009300	-0.00000400
	H	-1.83419600	-1.20657200	0.87705800
	H	-1.83419800	-1.20655500	-0.87707900
	C	-0.66542400	0.37371600	0.00000200
	H	-0.71182900	1.03156300	0.87774200
	H	-0.71182600	1.03157100	-0.87773200
	C	0.66542400	-0.37371600	0.00000100
	H	0.71182500	-1.03156900	-0.87773500
	H	0.71183000	-1.03156400	0.87773900
	C	1.88149000	0.55009300	-0.00000500
	H	1.83419600	1.20657100	0.87705700
	H	1.83419900	1.20655600	-0.87707900
	C	3.20588700	-0.20856200	0.00000300
	H	3.28980200	-0.84950200	-0.88329300
	H	4.05953000	0.47435200	-0.00000500
	H	3.28980400	-0.84948100	0.88331500
	vibrational temperatures (unscaled)			
	103.00	141.78	192.21	212.93	347.17
	363.18	434.52	536.81	682.53	1057.26
	1079.90	1170.46	1299.01	1315.73	1319.31
	1466.44	1486.69	1536.25	1566.95	1568.40
	1681.32	1733.96	1805.04	1833.71	1888.46
	1920.21	1928.91	1932.08	2005.55	2033.63

	2035.51	2043.25	2135.23	2136.52	2144.63
	2152.41	2152.73	2155.26	2166.31	2172.84
	4336.42	4340.41	4357.29	4359.92	4365.00
	4365.92	4372.98	4390.40	4412.52	4426.37
	4468.70	4469.32	4478.29	4478.31	
cyc-C_6H_{12}	C	-1.41142200	-0.37205700	-0.23060600	
	C	-0.38349100	-1.40829500	0.23059200	
	C	1.02792900	-1.03627000	-0.23060300	
	C	1.41142300	0.37205900	0.23060300	
	C	0.38348900	1.40829500	-0.23059200	
	C	-1.02792900	1.03626900	0.23060600	
	H	1.75302900	-1.76735100	0.14051900	
	H	-0.39908800	-1.46552000	1.32700000	
	H	-0.65402800	-2.40184600	-0.14043000	
	H	-1.46889300	-0.38717200	-1.32701000	
	H	-2.40707300	-0.63456000	0.14054200	
	H	1.46889900	0.38717700	1.32700700	
	H	2.40707200	0.63456100	-0.14055100	
	H	0.65402600	2.40184700	0.14042900	
	H	0.39908300	1.46552100	-1.32700000	
	H	-1.06973100	1.07839600	1.32701200	
	H	-1.75303000	1.76735000	-0.14051000	
	H	1.06973500	-1.07840400	-1.32700900	
	vibrational temperatures (unscaled)				
	344.02	345.70	559.73	628.02	628.57
	763.21	1155.59	1155.72	1173.55	1266.75
	1268.89	1331.05	1331.27	1505.74	1511.09
	1511.94	1562.13	1608.84	1643.12	1703.84
	1855.80	1856.02	1870.67	1871.30	1942.04
	1994.11	1996.86	1997.25	1997.88	1998.20
	2132.99	2133.20	2143.00	2143.13	2144.60
	2168.59	4346.01	4346.13	4348.25	4351.58
	4351.68	4353.55	4426.70	4426.74	4430.78
		4430.83	4432.86	4439.52	