

Supplementary material for

Accurate vibrational-rotational partition functions and standard-state free energy values for H₂O₂ from Monte Carlo path-integral calculations

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This supplementary material contains an extended table of extrapolated partition functions and extended tables of the vibrational and rotational partition functions at ten temperatures ranging from 298 K – 2400 K.

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TABLE S-I. Extended table of accurate quantum mechanical partition functions.

$T(\text{K})$	Q^{ESPE}	2σ
300	2.995×10^{-9}	$\pm 1.3 \times 10^{-11}$
400	5.2746×10^{-6}	$\pm 5.9 \times 10^{-9}$
500	5.4396×10^{-4}	$\pm 4.7 \times 10^{-7}$
600	1.3501×10^{-2}	$\pm 1.1 \times 10^{-5}$
700	0.146754	± 0.000076
800	0.94972	± 0.00030
900	4.3237	± 0.0029
1000	15.354	± 0.012
1100	45.285	± 0.024
1200	116.234	± 0.065
1300	267.32	± 0.13
1400	563.17	± 0.25
1500	1105.11	± 0.40
1600	2042.24	± 0.94
1700	3593.4	± 2.8
1800	6057.5	± 4.4
1900	9859.4	± 6.6
2000	15548.8	± 9.8
2100	23830	± 19
2200	35695	± 27
2300	52275	± 38
2400	75152	± 58

TABLE S-II. Classical mechanical and quantum mechanical values of Q_{vib} at various temperatures^a

$T(\text{K})$	$Q_{\text{vib}}^{\text{CHO}}$	$Q_{\text{vib}}^{\text{HO}}$	$Q_{\text{vib}}^{\text{HO-Z}}$	$Q_{\text{vib}}^{\text{HO-ZF}}$	$Q_{\text{vib}}^{\text{HO-F}}$
298	8.21(-6)	7.01(-13)	1.20(-12)	1.22(-12)	2.47(-12)
300	8.52(-6)	8.36(-13)	1.43(-12)	1.45(-12)	2.92(-12)
400	4.79(-5)	1.07(-9)	1.60(-9)	1.64(-9)	2.77(-9)
600	5.45(-4)	1.68(-6)	2.20(-6)	2.29(-6)	3.25(-6)
800	3.06(-3)	8.21(-5)	1.00(-4)	1.06(-4)	1.38(-4)
1000	1.17(-2)	9.86(-4)	1.16(-3)	1.24(-3)	1.53(-3)
1200	3.49(-2)	5.82(-3)	6.66(-3)	7.22(-3)	8.60(-3)
1500	1.33(-1)	4.04(-2)	4.50(-2)	4.96(-2)	5.71(-2)
2000	7.48(-1)	3.74(-1)	4.05(-1)	4.56(-1)	5.07(-1)
2400	2.23	1.37	1.47	1.67	1.82

^a Powers of ten are in parentheses.

TABLE S-III. Classical mechanical and quantum mechanical values of $Q_{\text{rot}}(T)$ at various temperatures

$T(\text{K})$	$Q_{\text{rot,CM}}^{\text{asym,e}}$	$Q_{\text{rot,CM}}^{\text{sym,e}}$	$Q_{\text{rot}}^{\text{sym,e}}$	$Q_{\text{rot,CM}}^{\text{sym,0}}$	$Q_{\text{rot}}^{\text{sym,0}}$
298	956.3	956.4	957.7	974.6	975.9
300	965.3	965.3	966.6	983.6	985.0
400	1486.1	1486.2	1487.7	1514.4	1515.9
600	2730.2	2730.4	2732.2	2782.2	2784.0
800	4203.3	4203.7	4205.8	4283.4	4285.6
1000	5874.4	5874.8	5877.2	5986.3	5988.7
1200	7722.0	7722.7	7725.3	7869.2	7871.8
1500	10791.9	10792.8	10795.7	10997.5	11000.4
2000	16615.2	16616.6	16620.0	16931.8	16935.2
2400	21841.2	21843.1	21846.8	22257.4	22261.1