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Additional material for:

Supporting information: "Statistical thermodynamics of bond torsional modes. Tests of separable, almost-separable, and improved Pitzer–Gwinn approximations"

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Table S-1 provides a glossary of acronyms used in the paper. Tables S-II to S-VIII contain partition functions for the 1-D torsional potential using a moment of inertia, *I*, calculated via the C scheme. Tables S-IX to S-XV contain partition functions for the 1-D torsional potential using R-scheme moments of inertia. Tables S-XVI to S-XXII contain partition functions for the full-D torsional potential using C-scheme moments of inertia. Tables S-XXIII to S-XXIX contain partition functions for the full-D torsional potential using R-scheme moments of inertia. Tables S-XXX to S-XXXV contain isotope ratios for the 1-D potential using C-scheme moments of inertia. Tables S-XXXVI to S-XL1 contain isotope ratios for the 1-D potential using R-scheme moments of inertia. Tables S-XLII to S-XLVII contain isotope ratios for the full-D potential using C-scheme moments of inertia. Tables S-XLVIII to S-LIII contain isotope ratios for the

full-D potential using R-scheme moments of inertia. Table S-LIV contains MU%E data for the partition function calculations while table S-LV contains MU%E data for the isotope ratios.

A great many methods exist for approximating eigenvalues—too many to properly survey here. In the main paper we only considered corrections to the harmonic estimate of the zero-point energy that made use of the accurate zero-point energy, but we alluded to an approximate scheme of McClurg, Flagan, and Goddard[12] (MFG) that was presented specifically for treating torsions represented by a single cosine 1-D potential of the form of Eq. (2). We now consider the possibility of estimating the anharmonicity correction for the accurate 1-D potential, given by Eq. (1), by fitting an approximate reference potential of the form of Eq. (2) and then calculating the MFG anharmonicity estimate of this reference potential. If we choose our reference potential by setting W equal to the mean of the two mean of the two barrier heights of the accurate 1-D potential, and use a C scheme moment of inertia, the resulting MFG ZPE corrections are given in Table LVI. We compare these to the accurate ZPE corrections of the reference 1-D potential and the accurate 1-D potential. The MFG ZPE-correction estimate predicts the accurate ZPE correction of the reference potential to within 6–8% for the 7 isotopomers studied, but this estimate is only 42% to 55% of the value of the ZPE correction of the accurate 1-D potential.

For the special case of two coaxial symmetric tops, the reduced moment of inertia takes the simple form

$$I = \frac{I_1 I_2}{I_1 + I_2}, \tag{S-1}$$

where I_1 and I_2 are the moments of inertia of the two groups about the rotation axis.

However, when the tops are not symmetric, or the system contains two or more hindered

rotators, more complicated expressions are required due, in part, to the difficulty of

decoupling the internal rotation from the overall rotation. In 1942 Pitzer and Gwinn[4]

provided an expression for the case of a single symmetric rotator attached to a rigid frame

and in 1946 Pitzer[5] presented an expression for calculating the reduced moment of inertia

for a single asymmetric top attached to a rigid frame. In our article, we refer to 1946

Pitzer procedure as the C or curvilinear reduced moment of inertia scheme; for

convenience we will reiterate the numerical details here, and will consider only the case

of a single internal rotation. When a molecule contains two or more asymmetric rotators

that are attached to a single rigid frame, Pitzer[5] presented two levels of approximation in

which the internal rotations may be nearly decoupled and reasonable effective moments

obtained. For more general problems it is still possible to rigorously decouple the overall

rotation from the internal rotations as discussed by Kilpatrick and Pitzer,[49] but the

coupling among the various internal rotators is more complicated.

Let I be the desired reduced moment of inertia for a particular internal rotation, M

be the mass of the entire molecule, and let the principal moments of inertia be defined as

I_j, where $j = 1$, 2, or 3. All of the atoms in the molecule are divided into two groups

rotating with respect to one another; one group will be designated as the top T (the

moment does not depend on the choice of which group to designate). A coordinate

system is defined such that the z axis is the chosen axis of rotation, the x axis is

perpendicular to the z axis and passes through the center of mass of the rotating top, and

the y axis is perpendicular to both x and z. It is important that the axes of the top (x, y, z)

and the axes of the full molecule (1, 2, 3) are either both right-handed or both left-

handed. The direction cosines between the axes of the top and a particular principal

moment of inertia axis j are defined as α_{jx}, α_{jy}, and α_{jz}. The vector from the full

molecule's center of mass to the origin of the (x,y,z) axes is given by $\mathbf{r}$, with its

components r_1, r_2, and r_3 on the principal moment of inertia axes.

The reduced moment of inertia for internal rotation is then given by

$$I = A - \sum_{i=1}^{3} \left\{ \frac{\left(\alpha_{iy}U\right)^2}{M} + \frac{\beta_i^2}{I_i} \right\} \tag{S-2}$$

where

$$\beta_i = \alpha_{iz}A - \alpha_{ix}B - \alpha_{iy}C + U\left(\alpha_{i-1,y}r_{i+1} - \alpha_{i+1,y}r_{i-1}\right) \tag{S-3}$$

and $i - 1 = 3$ if $i = 1$, and $i + 1 = 1$ if $i = 3$, the moment of inertia for the rotating top about

the z axis is given by

$$A = \sum_{j \in T} m_j \left(x_j^2 + y_j^2 \right), \tag{S-4}$$

where m_j is the mass of an atom located at the point (x_j, y_j, z_j) and the sum includes only

the atoms belonging to the top, the xy product of inertia is given by

$$B = \sum_{j \in T} m_j x_j z_j, \tag{S-5}$$

the yz produce of inertia is given by

$$C = \sum_{j \in T} m_j y_j z_j, \tag{S-6}$$

and the off-balance factor is given by

$$U = \sum_{j \in T} m_j x_j. \tag{S-7}$$

In equations 4–7 atoms that lie on the rotation axis, z, need not be included in the

summations.

Table S-I. Glossary of acronyms.

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AS	The method of Ayala and Schlegel;[14] see section IV.C.2
C scheme	Curvilinear moment of inertia scheme of Pitzer[5]
CAF scheme	Curvilinear-averaged-frozen scheme for effective moment of inertia; see Section IV.E
CAR scheme	Curvilinear-averaged-relaxed scheme for effective moment of inertia; see Section IV.E
CT	Chuang–Truhlar[18] interpolatory methods for obtaining the parameters of a reference model; see Section IV.B
CW	CT method that uses the C-scheme I and the barrier height to calculate the required frequency
Cω	CT method that uses the C-scheme I and the harmonic frequency
FR	Free rotator; see Eqs. (19) and (23)
HO	Harmonic oscillator
HO+T	HO for nontorsion modes and a separable anharmonic treatment of the torsion
I	The effective reduced moment of inertia associated with the torsional motion[a]
IW	CT method that uses the effective reduced moment of inertia and the barrier height to calculate the required frequency, more typically referred to as CW or RW in order to specify whether the R scheme or C scheme I has been used

Iω	CT method that uses the effective reduced moment of inertia and the harmonic frequency, more typically referred to as Cω or Rω specify whether the R scheme or C scheme I has been used
IRPG	Improved-reference Pitzer–Gwinn approximation; see section V.B
MC-HO	Multi-conformer harmonic oscillator approximation; see Eq. (9)
MPG	Modified Pitzer–Gwinn method (used here only for the torsional coordinate); see Eq. (41)
PG	The Pitzer–Gwinn approximation. This notation is reserved for calculations where the classical approximation involves all the coupling of the full-D potential.
RPG	Torsional Pitzer–Gwinn approximation using a single cosine reference potential. In the present article the reference potential is obtained by requiring the barrier height to be equal to the mean value of the barrier heights of the accurate 1-D potential.
R scheme	A "rectilinear" moment of inertia scheme[9]
RW	CT method that uses the R-scheme I and the barrier height to calculate the required frequency
Rω	Method for obtaining reference model parameters by using the R-scheme I and the harmonic frequency
SAS	Segmented Ayala–Schlegel method; see Section IV.C.3
SRC	Segmented reference classical method; see Section IV.C.3
SRPG	Segment reference Pitzer–Gwinn approximation; see Section IV.C.3
SR-TDPPI-HS	The TDPPI-HS method applied to a segmented reference potential

TDPPI-AS	Torsional displaced-points path integral method with anharmonic sampling
TDPPI-HS	Torsional displaced-points path integral method with harmonic sampling
TES	Torsional eigenvalue summation; see Section IV.D.1
TPG	Torsional Pitzer–Gwinn approximation, i.e., the PG approximation used only for the 1-D torsional potential
WK	The Wigner–Kirkwood approximation; see Eq. (40)
Z	When appended to any other method acronym this indicates that an accurate ZPE is used.
ZPE	Zero-point energy

Note: reference, equation, and section numbers used in this table refer to the references, equations, and sections in the main article.

Table S-II. Partition functions for the 1-D torsional potential of H_2O_2 using the C scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Cω	0.541	0.952	1.343	2.087	2.796	3.474	5.051	7.540	13.115
MC-HO	0.541	0.953	1.347	2.109	2.855	3.595	5.429	8.717	18.190
SAS	0.566	1.023	1.464	2.308	3.093	3.818	5.428	7.846	13.188
SRC	0.762	1.167	1.560	2.302	2.998	3.662	5.216	7.701	13.301
SR-TDPPI-HS	0.601	1.056	1.479	2.252	2.964	3.637	5.203	7.695	13.300
SRPG	0.566	1.018	1.444	2.223	2.940	3.616	5.187	7.684	13.295
CT-ωW	0.541	0.953	1.347	2.104	2.837	3.553	5.268	8.107	14.871
CT-CW	0.364	0.698	1.019	1.631	2.220	2.791	4.156	6.408	11.767
RPG	0.440	0.788	1.137	1.852	2.584	3.312	5.041	7.744	13.558
TDPPI-HS	0.642	1.114	1.554	2.358	3.094	3.786	5.381	7.891	13.488
WK	0.626	1.110	1.553	2.358	3.094	3.786	5.382	7.892	13.488
MPG	0.679	1.126	1.560	2.360	3.095	3.787	5.382	7.892	13.488
TDPPI-AS	0.609	1.105	1.550	2.357	3.094	3.786	5.381	7.891	13.488
TPG	0.591	1.065	1.510	2.324	3.067	3.763	5.365	7.880	13.483
C	0.796	1.220	1.632	2.406	3.127	3.811	5.395	7.897	13.489
CT-Cω-Z	0.636	1.061	1.457	2.204	2.912	3.588	5.162	7.643	13.200
MC-HO-Z	0.637	1.062	1.462	2.227	2.974	3.713	5.548	8.836	18.309
SRPG-Z	0.666	1.135	1.566	2.347	3.062	3.736	5.301	7.789	13.382
CT-Wω-Z	0.637	1.062	1.461	2.221	2.955	3.670	5.384	8.218	14.968
CT-CW-Z	0.428	0.778	1.105	1.722	2.312	2.883	4.247	6.496	11.843
RPG-Z	0.518	0.878	1.233	1.955	2.691	3.421	5.151	7.850	13.647
TPG-Z	0.696	1.187	1.638	2.453	3.194	3.888	5.482	7.987	13.571
TES	0.644	1.116	1.555	2.358	3.094	3.786	5.382	7.892	13.488

Table S-III. Partition functions for the 1-D torsional potential of D_2O_2 using the C scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Cω	0.845	1.385	1.903	2.900	3.857	4.778	6.928	10.330	17.966
MC-HO	0.845	1.386	1.909	2.930	3.939	4.942	7.441	11.927	24.869
SAS	0.887	1.489	2.070	3.183	4.224	5.194	7.365	10.662	18.000
SRC	1.045	1.600	2.139	3.157	4.111	5.022	7.154	10.561	18.241
SR-TDPPI-HS	0.913	1.514	2.078	3.120	4.086	5.004	7.144	10.557	18.240
SRPG	0.887	1.486	2.052	3.099	4.069	4.988	7.132	10.548	18.236
CT-ωW	0.845	1.386	1.908	2.922	3.914	4.884	7.220	11.093	20.331
CT-CW	0.613	1.055	1.479	2.296	3.089	3.863	5.723	8.802	16.142
RPG	0.690	1.150	1.615	2.581	3.576	4.568	6.931	10.631	18.598
TDPPI-HS	0.967	1.592	2.179	3.264	4.264	5.208	7.388	10.826	18.498
WK	0.959	1.590	2.179	3.264	4.264	5.208	7.388	10.826	18.498
MPG	0.979	1.597	2.182	3.265	4.265	5.208	7.388	10.826	18.498
TDPPI-AS	0.953	1.588	2.178	3.263	4.264	5.208	7.388	10.826	18.498
TPG	0.927	1.554	2.146	3.238	4.244	5.191	7.376	10.817	18.494
C	1.091	1.673	2.238	3.299	4.289	5.226	7.398	10.830	18.499
CT-Cω-Z	0.905	1.450	1.969	2.967	3.924	4.844	6.992	10.389	18.015
MC-HO-Z	0.906	1.452	1.976	2.998	4.007	5.010	7.509	11.995	24.938
SRPG-Z	0.951	1.556	2.124	3.170	4.139	5.058	7.198	10.609	18.287
CT-Wω-Z	0.906	1.451	1.974	2.990	3.982	4.952	7.287	11.156	20.388
CT-CW-Z	0.657	1.105	1.531	2.349	3.142	3.917	5.776	8.853	16.187
RPG-Z	0.739	1.204	1.672	2.641	3.638	4.632	6.995	10.692	18.649
TPG-Z	0.993	1.627	2.221	3.314	4.318	5.263	7.444	10.880	18.545
TES	0.968	1.593	2.180	3.264	4.264	5.208	7.388	10.826	18.498

Table S-IV. Partition functions for the 1-D torsional potential of HOOD using the C scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Cω	0.659	1.120	1.560	2.401	3.205	3.976	5.773	8.613	14.979
MC-HO	0.659	1.122	1.565	2.426	3.273	4.113	6.203	9.951	20.758
SAS	0.691	1.204	1.699	2.646	3.529	4.348	6.173	8.928	15.037
SRC	0.870	1.333	1.783	2.630	3.426	4.185	5.961	8.800	15.199
SR-TDPPI-HS	0.722	1.233	1.710	2.586	3.396	4.163	5.949	8.795	15.198
SRPG	0.691	1.200	1.679	2.561	3.375	4.144	5.935	8.785	15.193
CT-ωW	0.659	1.121	1.564	2.420	3.252	4.065	6.019	9.255	16.970
CT-CW	0.460	0.837	1.198	1.888	2.555	3.204	4.759	7.329	13.448
RPG	0.537	0.929	1.322	2.133	2.966	3.795	5.767	8.854	15.495
TDPPI-HS	0.768	1.299	1.796	2.707	3.544	4.333	6.153	9.019	15.413
WK	0.755	1.296	1.795	2.707	3.544	4.333	6.153	9.019	15.413
MPG	0.790	1.307	1.800	2.708	3.545	4.333	6.153	9.019	15.413
TDPPI-AS	0.745	1.293	1.793	2.706	3.544	4.333	6.153	9.019	15.413
TPG	0.722	1.255	1.757	2.677	3.520	4.312	6.138	9.009	15.408
C	0.909	1.394	1.865	2.749	3.573	4.354	6.164	9.024	15.414
CT-Cω-Z	0.737	1.207	1.650	2.492	3.296	4.066	5.860	8.693	15.046
MC-HO-Z	0.737	1.208	1.655	2.518	3.366	4.206	6.296	10.044	20.851
SRPG-Z	0.773	1.293	1.776	2.658	3.470	4.238	6.024	8.867	15.261
CT-Wω-Z	0.737	1.208	1.654	2.512	3.344	4.157	6.110	9.342	17.046
CT-CW-Z	0.514	0.902	1.266	1.960	2.627	3.276	4.830	7.397	13.508
RPG-Z	0.600	1.001	1.398	2.214	3.050	3.881	5.854	8.936	15.564
TPG-Z	0.807	1.352	1.857	2.778	3.620	4.410	6.230	9.093	15.477
TES	0.769	1.300	1.796	2.707	3.544	4.333	6.153	9.019	15.413

Table S-V. Partition functions for the 1-D torsional potential of $H_2^{18}O_2$ using the C scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Cω	0.544	0.957	1.349	2.096	2.807	3.487	5.071	7.569	13.164
MC-HO	0.544	0.958	1.354	2.118	2.867	3.609	5.451	8.751	18.262
SAS	0.569	1.027	1.471	2.317	3.104	3.832	5.447	7.874	13.235
SRC	0.764	1.171	1.566	2.310	3.009	3.675	5.235	7.729	13.349
SR-TDPPI-HS	0.604	1.060	1.485	2.261	2.975	3.651	5.222	7.723	13.348
SRPG	0.569	1.023	1.450	2.232	2.951	3.630	5.206	7.712	13.343
CT-ωW	0.544	0.958	1.353	2.113	2.849	3.567	5.290	8.139	14.930
CT-CW	0.366	0.701	1.023	1.638	2.228	2.801	4.171	6.432	11.809
RPG	0.442	0.792	1.141	1.859	2.594	3.324	5.059	7.772	13.607
TDPPI-HS	0.645	1.119	1.560	2.367	3.105	3.800	5.401	7.920	13.537
WK	0.629	1.115	1.559	2.367	3.106	3.800	5.401	7.920	13.537
MPG	0.681	1.131	1.566	2.369	3.107	3.801	5.401	7.920	13.537
TDPPI-AS	0.612	1.110	1.556	2.366	3.105	3.800	5.401	7.920	13.537
TPG	0.595	1.070	1.517	2.333	3.078	3.777	5.384	7.909	13.531
C	0.798	1.225	1.638	2.415	3.139	3.824	5.414	7.926	13.538
CT-Cω-Z	0.639	1.065	1.462	2.211	2.922	3.601	5.181	7.671	13.249
MC-HO-Z	0.639	1.066	1.467	2.235	2.985	3.727	5.569	8.869	18.380
SRPG-Z	0.669	1.139	1.571	2.355	3.072	3.748	5.319	7.816	13.429
CT-Wω-Z	0.639	1.066	1.466	2.229	2.966	3.683	5.404	8.249	15.026
CT-CW-Z	0.430	0.780	1.109	1.728	2.319	2.893	4.262	6.518	11.885
RPG-Z	0.519	0.881	1.237	1.961	2.700	3.432	5.169	7.877	13.695
TPG-Z	0.698	1.191	1.643	2.461	3.204	3.900	5.501	8.015	13.618
TES	0.647	1.121	1.561	2.367	3.106	3.800	5.401	7.920	13.537

Table S-VI. Partition functions for the 1-D torsional potential of D^{18}OOH using the C scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Cω	0.662	1.124	1.564	2.407	3.213	3.985	5.787	8.633	15.015
MC-HO	0.662	1.125	1.569	2.432	3.281	4.123	6.218	9.975	20.808
SAS	0.693	1.207	1.704	2.652	3.537	4.358	6.187	8.949	15.072
SRC	0.872	1.336	1.787	2.637	3.434	4.194	5.975	8.820	15.235
SR-TDPPI-HS	0.724	1.237	1.714	2.593	3.404	4.173	5.963	8.815	15.234
SRPG	0.693	1.204	1.684	2.567	3.383	4.154	5.949	8.806	15.229
CT-ωW	0.662	1.125	1.568	2.426	3.260	4.075	6.034	9.277	17.011
CT-CW	0.462	0.839	1.201	1.893	2.561	3.212	4.770	7.346	13.480
RPG	0.539	0.931	1.326	2.139	2.973	3.804	5.781	8.875	15.531
TDPPI-HS	0.770	1.303	1.800	2.713	3.553	4.343	6.167	9.040	15.449
WK	0.758	1.300	1.799	2.713	3.553	4.343	6.167	9.040	15.449
MPG	0.793	1.311	1.804	2.715	3.553	4.344	6.167	9.040	15.449
TDPPI-AS	0.747	1.296	1.798	2.713	3.552	4.343	6.167	9.040	15.449
TPG	0.724	1.259	1.761	2.683	3.529	4.323	6.152	9.030	15.444
C	0.911	1.397	1.869	2.756	3.582	4.365	6.179	9.045	15.450
CT-Cω-Z	0.739	1.210	1.653	2.498	3.303	4.075	5.873	8.713	15.081
MC-HO-Z	0.739	1.211	1.659	2.524	3.373	4.216	6.311	10.067	20.900
SRPG-Z	0.775	1.296	1.780	2.664	3.478	4.247	6.038	8.887	15.297
CT-Wω-Z	0.739	1.211	1.658	2.517	3.352	4.167	6.124	9.363	17.087
CT-CW-Z	0.516	0.904	1.269	1.964	2.633	3.284	4.841	7.414	13.540
RPG-Z	0.602	1.003	1.401	2.219	3.057	3.890	5.867	8.957	15.600
TPG-Z	0.809	1.355	1.861	2.784	3.628	4.420	6.244	9.114	15.513
TES	0.772	1.304	1.801	2.714	3.553	4.343	6.167	9.040	15.449

Table S-VII. Partition functions for the 1-D torsional potential of H^{18}OOH using the C scheme *I*

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Cω	0.542	0.954	1.346	2.092	2.801	3.480	5.060	7.554	13.138
MC-HO	0.543	0.955	1.350	2.114	2.861	3.601	5.440	8.733	18.224
SAS	0.568	1.025	1.467	2.312	3.098	3.825	5.437	7.860	13.211
SRC	0.763	1.169	1.563	2.306	3.003	3.669	5.226	7.715	13.325
SR-TDPPI-HS	0.602	1.058	1.482	2.256	2.969	3.644	5.213	7.709	13.324
SRPG	0.568	1.021	1.447	2.228	2.945	3.623	5.197	7.698	13.319
CT-ωW	0.543	0.955	1.350	2.108	2.843	3.559	5.278	8.122	14.898
CT-CW	0.365	0.699	1.021	1.635	2.224	2.796	4.164	6.420	11.788
RPG	0.441	0.790	1.139	1.856	2.589	3.318	5.050	7.758	13.583
TDPPI-HS	0.643	1.117	1.557	2.362	3.100	3.793	5.391	7.906	13.512
WK	0.628	1.113	1.556	2.362	3.100	3.793	5.391	7.906	13.512
MPG	0.680	1.129	1.563	2.364	3.101	3.794	5.391	7.906	13.512
TDPPI-AS	0.610	1.107	1.553	2.361	3.099	3.793	5.391	7.906	13.512
TPG	0.593	1.067	1.513	2.328	3.072	3.770	5.374	7.894	13.507
C	0.797	1.222	1.635	2.410	3.133	3.817	5.404	7.911	13.514
CT-Cω-Z	0.638	1.063	1.459	2.207	2.917	3.595	5.171	7.656	13.224
MC-HO-Z	0.638	1.064	1.464	2.231	2.979	3.720	5.558	8.851	18.342
SRPG-Z	0.667	1.137	1.569	2.351	3.067	3.742	5.310	7.802	13.405
CT-Wω-Z	0.638	1.064	1.463	2.225	2.960	3.676	5.393	8.232	14.995
CT-CW-Z	0.429	0.779	1.107	1.725	2.316	2.888	4.254	6.507	11.864
RPG-Z	0.518	0.880	1.235	1.958	2.695	3.427	5.160	7.864	13.671
TPG-Z	0.697	1.189	1.641	2.457	3.199	3.894	5.491	8.001	13.594
TES	0.646	1.118	1.558	2.363	3.100	3.793	5.391	7.906	13.512

Table S-VIII. Partition functions for the 1-D torsional potential of $H^{18}OOD$ using the C scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Cω	0.662	1.124	1.564	2.407	3.213	3.985	5.787	8.633	15.014
MC-HO	0.662	1.125	1.569	2.432	3.281	4.123	6.218	9.975	20.808
SAS	0.693	1.207	1.703	2.652	3.536	4.358	6.186	8.948	15.071
SRC	0.872	1.336	1.787	2.636	3.434	4.194	5.974	8.820	15.234
SR-TDPPI-HS	0.724	1.236	1.714	2.592	3.404	4.172	5.963	8.815	15.233
SRPG	0.693	1.204	1.684	2.567	3.383	4.154	5.949	8.805	15.228
CT-ωW	0.662	1.125	1.568	2.426	3.260	4.075	6.034	9.277	17.011
CT-CW	0.462	0.839	1.201	1.893	2.561	3.212	4.770	7.345	13.478
RPG	0.539	0.931	1.325	2.138	2.973	3.804	5.781	8.874	15.530
TDPPI-HS	0.770	1.303	1.800	2.713	3.552	4.343	6.167	9.039	15.448
WK	0.757	1.300	1.799	2.713	3.553	4.343	6.167	9.039	15.448
MPG	0.792	1.310	1.804	2.714	3.553	4.343	6.167	9.039	15.448
TDPPI-AS	0.747	1.296	1.797	2.712	3.552	4.343	6.167	9.039	15.448
TPG	0.724	1.259	1.761	2.683	3.528	4.322	6.152	9.029	15.443
C	0.911	1.397	1.869	2.755	3.582	4.364	6.178	9.044	15.449
CT-Cω-Z	0.739	1.210	1.653	2.498	3.303	4.075	5.873	8.713	15.080
MC-HO-Z	0.739	1.211	1.659	2.524	3.373	4.216	6.311	10.067	20.900
SRPG-Z	0.774	1.296	1.779	2.664	3.478	4.247	6.037	8.887	15.295
CT-Wω-Z	0.739	1.211	1.658	2.517	3.352	4.167	6.124	9.363	17.086
CT-CW-Z	0.516	0.904	1.269	1.964	2.633	3.284	4.841	7.413	13.538
RPG-Z	0.602	1.003	1.401	2.219	3.056	3.889	5.867	8.956	15.599
TPG-Z	0.809	1.355	1.861	2.784	3.627	4.419	6.243	9.113	15.511
TES	0.772	1.304	1.801	2.713	3.553	4.343	6.167	9.039	15.448

Table S-IX. Partition functions for the 1-D torsional potential of H_2O_2 using the R scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Rω	0.541	0.953	1.346	2.101	2.830	3.537	5.222	7.976	14.421
MC-HO	0.541	0.953	1.347	2.109	2.855	3.595	5.429	8.717	18.190
SAS	0.671	1.211	1.732	2.721	3.640	4.492	6.389	9.251	15.597
SRC	0.903	1.384	1.850	2.730	3.556	4.343	6.187	9.133	15.776
SR-TDPPI-HS	0.758	1.287	1.780	2.688	3.527	4.322	6.176	9.129	15.775
SRPG	0.671	1.208	1.712	2.637	3.487	4.289	6.152	9.114	15.768
CT-ωW	0.541	0.953	1.347	2.104	2.837	3.553	5.268	8.107	14.871
CT-RW	0.489	0.879	1.251	1.966	2.656	3.329	4.942	7.608	13.959
RPG	0.522	0.935	1.348	2.197	3.064	3.928	5.979	9.185	16.080
TDPPI-HS	0.806	1.355	1.869	2.812	3.681	4.499	6.387	9.361	15.998
WK	0.794	1.352	1.868	2.813	3.681	4.499	6.387	9.361	15.998
MPG	0.861	1.372	1.876	2.815	3.682	4.499	6.387	9.362	15.998
TDPPI-AS	0.785	1.349	1.866	2.812	3.681	4.499	6.387	9.361	15.998
TPG	0.701	1.263	1.791	2.756	3.637	4.463	6.362	9.346	15.991
C	0.944	1.447	1.935	2.853	3.709	4.519	6.398	9.366	15.999
CT-Rω-Z	0.741	1.175	1.575	2.333	3.061	3.767	5.446	8.187	14.603
MC-HO-Z	0.741	1.175	1.577	2.342	3.089	3.828	5.662	8.948	18.420
SRPG-Z	0.919	1.489	2.004	2.928	3.772	4.567	6.416	9.355	15.967
CT-Wω-Z	0.741	1.175	1.576	2.336	3.069	3.783	5.494	8.322	15.059
CT-RW-Z	0.670	1.083	1.464	2.183	2.873	3.545	5.153	7.810	14.135
RPG-Z	0.714	1.152	1.577	2.439	3.315	4.183	6.234	9.428	16.284
TPG-Z	0.960	1.557	2.096	3.060	3.934	4.752	6.635	9.594	16.193
TES	0.807	1.356	1.869	2.813	3.681	4.499	6.387	9.361	15.998

Table S-X. Partition functions for the 1-D torsional potential of D_2O_2 using the R scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Rω	0.845	1.386	1.907	2.920	3.907	4.872	7.181	10.982	19.947
MC-HO	0.845	1.386	1.909	2.930	3.939	4.942	7.441	11.927	24.869
SAS	1.074	1.800	2.499	3.832	5.079	6.243	8.856	12.839	21.731
SRC	1.264	1.936	2.589	3.820	4.975	6.077	8.656	12.779	22.073
SR-TDPPI-HS	1.151	1.864	2.537	3.789	4.954	6.062	8.649	12.776	22.072
SRPG	1.074	1.799	2.483	3.749	4.923	6.036	8.631	12.764	22.067
CT-ωW	0.845	1.386	1.908	2.922	3.914	4.884	7.220	11.093	20.331
CT-RW	0.802	1.324	1.827	2.804	3.757	4.691	6.936	10.658	19.536
RPG	0.834	1.392	1.955	3.123	4.327	5.528	8.387	12.864	22.504
TDPPI-HS	1.214	1.956	2.659	3.963	5.169	6.309	8.944	13.101	22.384
WK	1.208	1.955	2.659	3.963	5.169	6.309	8.944	13.101	22.384
MPG	1.234	1.963	2.662	3.964	5.170	6.309	8.944	13.102	22.384
TDPPI-AS	1.206	1.954	2.658	3.963	5.169	6.309	8.944	13.101	22.384
TPG	1.122	1.881	2.597	3.919	5.135	6.281	8.925	13.090	22.379
C	1.320	2.025	2.708	3.992	5.190	6.323	8.952	13.105	22.385
CT-Rω-Z	1.051	1.602	2.126	3.139	4.125	5.088	7.393	11.182	20.121
MC-HO-Z	1.051	1.603	2.128	3.150	4.159	5.161	7.659	12.145	25.087
SRPG-Z	1.335	2.079	2.768	4.031	5.198	6.304	8.884	12.998	22.260
CT-Wω-Z	1.051	1.602	2.127	3.142	4.132	5.101	7.432	11.295	20.509
CT-RW-Z	0.996	1.531	2.036	3.014	3.967	4.899	7.140	10.853	19.707
RPG-Z	1.037	1.609	2.179	3.358	4.568	5.773	8.633	13.099	22.701
TPG-Z	1.394	2.174	2.895	4.213	5.422	6.560	9.188	13.329	22.574
TES	1.214	1.957	2.659	3.963	5.169	6.309	8.944	13.101	22.384

Table S-XI. Partition functions for the 1-D torsional potential of HOOD using the R scheme *I*

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Rω	0.659	1.121	1.564	2.418	3.248	4.057	5.993	9.181	16.711
MC-HO	0.659	1.122	1.565	2.426	3.273	4.113	6.203	9.951	20.758
SAS	0.844	1.469	2.069	3.212	4.277	5.267	7.481	10.840	18.314
SRC	1.063	1.629	2.177	3.213	4.185	5.111	7.281	10.748	18.565
SR-TDPPI-HS	0.933	1.544	2.117	3.177	4.160	5.093	7.271	10.744	18.565
SRPG	0.844	1.466	2.051	3.128	4.122	5.062	7.250	10.730	18.558
CT-ωW	0.659	1.121	1.564	2.420	3.252	4.065	6.019	9.255	16.970
CT-RW	0.629	1.078	1.508	2.339	3.145	3.933	5.826	8.959	16.430
RPG	0.656	1.135	1.615	2.606	3.623	4.636	7.045	10.814	18.926
TDPPI-HS	0.988	1.623	2.220	3.323	4.341	5.301	7.520	11.018	18.827
WK	0.980	1.621	2.220	3.323	4.341	5.301	7.520	11.018	18.827
MPG	1.026	1.635	2.225	3.325	4.342	5.301	7.520	11.018	18.827
TDPPI-AS	0.975	1.619	2.219	3.323	4.341	5.301	7.520	11.018	18.827
TPG	0.881	1.533	2.146	3.269	4.300	5.268	7.497	11.004	18.820
C	1.110	1.703	2.277	3.358	4.365	5.319	7.529	11.022	18.828
CT-Rω-Z	0.874	1.353	1.801	2.657	3.485	4.293	6.223	9.399	16.900
MC-HO-Z	0.874	1.354	1.802	2.666	3.512	4.352	6.441	10.188	20.994
SRPG-Z	1.119	1.770	2.362	3.437	4.423	5.356	7.528	10.986	18.769
CT-Wω-Z	0.874	1.354	1.801	2.659	3.490	4.302	6.250	9.475	17.163
CT-RW-Z	0.834	1.302	1.737	2.569	3.375	4.162	6.049	9.173	16.616
RPG-Z	0.870	1.369	1.860	2.863	3.888	4.905	7.315	11.072	19.141
TPG-Z	1.169	1.850	2.471	3.592	4.614	5.573	7.785	11.266	19.034
TES	0.989	1.624	2.220	3.323	4.341	5.301	7.520	11.018	18.827

Table S-XII. Partition functions for the 1-D torsional potential of $H_2{}^{18}O_2$ using the R scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Rω	0.544	0.958	1.352	2.110	2.841	3.551	5.242	8.005	14.471
MC-HO	0.544	0.958	1.354	2.118	2.867	3.609	5.451	8.751	18.262
SAS	0.675	1.216	1.738	2.729	3.651	4.505	6.407	9.278	15.642
SRC	0.906	1.388	1.856	2.738	3.566	4.356	6.205	9.160	15.822
SR-TDPPI-HS	0.761	1.291	1.786	2.696	3.537	4.335	6.194	9.156	15.821
SRPG	0.675	1.213	1.718	2.645	3.498	4.302	6.171	9.141	15.814
CT-ωW	0.544	0.958	1.353	2.113	2.849	3.567	5.290	8.139	14.930
CT-RW	0.491	0.882	1.256	1.972	2.665	3.339	4.957	7.631	14.000
RPG	0.524	0.938	1.353	2.204	3.074	3.940	5.996	9.212	16.128
TDPPI-HS	0.809	1.360	1.875	2.821	3.692	4.512	6.406	9.389	16.045
WK	0.797	1.357	1.874	2.821	3.692	4.512	6.406	9.389	16.045
MPG	0.863	1.376	1.882	2.823	3.693	4.513	6.406	9.389	16.045
TDPPI-AS	0.788	1.354	1.872	2.820	3.692	4.512	6.406	9.389	16.045
TPG	0.705	1.268	1.797	2.765	3.648	4.477	6.381	9.373	16.038
C	0.946	1.451	1.941	2.862	3.720	4.533	6.417	9.394	16.046
CT-Rω-Z	0.743	1.178	1.580	2.341	3.071	3.779	5.464	8.215	14.652
MC-HO-Z	0.743	1.179	1.582	2.350	3.099	3.841	5.682	8.981	18.491
SRPG-Z	0.921	1.492	2.008	2.935	3.781	4.578	6.432	9.381	16.012
CT-Wω-Z	0.743	1.178	1.581	2.344	3.079	3.796	5.514	8.353	15.117
CT-RW-Z	0.671	1.085	1.467	2.188	2.880	3.554	5.167	7.831	14.175
RPG-Z	0.716	1.155	1.581	2.444	3.323	4.193	6.250	9.454	16.330
TPG-Z	0.962	1.560	2.100	3.067	3.944	4.764	6.652	9.620	16.239
TES	0.810	1.361	1.875	2.821	3.692	4.512	6.406	9.389	16.045

Table S-XIII. Partition functions for the 1-D torsional potential of $D^{18}OOH$ using the R scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Rω	0.662	1.125	1.568	2.425	3.256	4.067	6.008	9.202	16.750
MC-HO	0.662	1.125	1.569	2.432	3.281	4.123	6.218	9.975	20.808
SAS	0.847	1.473	2.074	3.219	4.286	5.279	7.497	10.864	18.355
SRC	1.066	1.632	2.182	3.220	4.194	5.123	7.297	10.773	18.607
SR-TDPPI-HS	0.936	1.548	2.122	3.184	4.169	5.105	7.288	10.769	18.606
SRPG	0.847	1.470	2.056	3.136	4.132	5.074	7.266	10.755	18.600
CT-ωW	0.662	1.125	1.568	2.426	3.260	4.075	6.034	9.277	17.011
CT-RW	0.631	1.081	1.512	2.344	3.153	3.943	5.839	8.980	16.467
RPG	0.658	1.138	1.619	2.612	3.631	4.647	7.061	10.839	18.969
TDPPI-HS	0.991	1.627	2.225	3.331	4.351	5.313	7.537	11.043	18.869
WK	0.983	1.625	2.225	3.331	4.351	5.313	7.537	11.043	18.869
MPG	1.028	1.639	2.231	3.332	4.352	5.313	7.537	11.043	18.869
TDPPI-AS	0.978	1.623	2.224	3.330	4.351	5.313	7.537	11.043	18.869
TPG	0.884	1.537	2.151	3.277	4.310	5.280	7.514	11.029	18.863
C	1.113	1.707	2.283	3.365	4.375	5.331	7.546	11.047	18.870
CT-Rω-Z	0.877	1.356	1.805	2.663	3.493	4.302	6.237	9.421	16.939
MC-HO-Z	0.877	1.357	1.806	2.671	3.520	4.362	6.456	10.211	21.043
SRPG-Z	1.122	1.773	2.367	3.444	4.433	5.367	7.544	11.010	18.810
CT-Wω-Z	0.877	1.357	1.805	2.664	3.498	4.311	6.264	9.497	17.203
CT-RW-Z	0.836	1.304	1.740	2.575	3.382	4.171	6.062	9.193	16.653
RPG-Z	0.872	1.372	1.863	2.869	3.896	4.915	7.330	11.096	19.183
TPG-Z	1.172	1.854	2.476	3.599	4.624	5.585	7.801	11.290	19.076
TES	0.992	1.628	2.226	3.331	4.351	5.313	7.537	11.043	18.869

Table S-XIV. Partition functions for the 1-D torsional potential of $H^{18}OOH$ using the R scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Rω	0.543	0.955	1.349	2.105	2.835	3.544	5.232	7.989	14.445
MC-HO	0.543	0.955	1.350	2.114	2.861	3.601	5.440	8.733	18.224
SAS	0.673	1.214	1.735	2.725	3.646	4.499	6.398	9.264	15.619
SRC	0.905	1.386	1.853	2.734	3.561	4.350	6.196	9.147	15.799
SR-TDPPI-HS	0.760	1.289	1.783	2.692	3.532	4.329	6.185	9.142	15.798
SRPG	0.673	1.210	1.715	2.641	3.492	4.296	6.162	9.127	15.791
CT-ωW	0.543	0.955	1.350	2.108	2.843	3.559	5.278	8.122	14.898
CT-RW	0.490	0.880	1.253	1.969	2.660	3.334	4.949	7.619	13.979
RPG	0.523	0.937	1.350	2.200	3.069	3.934	5.987	9.198	16.104
TDPPI-HS	0.807	1.357	1.872	2.817	3.686	4.505	6.396	9.375	16.021
WK	0.796	1.354	1.871	2.817	3.686	4.506	6.396	9.375	16.021
MPG	0.862	1.374	1.879	2.819	3.687	4.506	6.397	9.375	16.021
TDPPI-AS	0.787	1.351	1.869	2.816	3.686	4.505	6.396	9.375	16.021
TPG	0.703	1.265	1.794	2.760	3.643	4.470	6.372	9.360	16.014
C	0.945	1.449	1.938	2.858	3.714	4.526	6.407	9.380	16.022
CT-Rω-Z	0.742	1.176	1.577	2.337	3.066	3.773	5.454	8.200	14.627
MC-HO-Z	0.742	1.177	1.579	2.346	3.094	3.834	5.671	8.963	18.453
SRPG-Z	0.920	1.491	2.006	2.932	3.776	4.573	6.424	9.368	15.990
CT-Wω-Z	0.742	1.177	1.578	2.340	3.074	3.789	5.503	8.337	15.086
CT-RW-Z	0.670	1.085	1.466	2.185	2.877	3.550	5.160	7.820	14.155
RPG-Z	0.715	1.154	1.579	2.442	3.319	4.188	6.242	9.441	16.307
TPG-Z	0.961	1.559	2.098	3.064	3.939	4.758	6.643	9.607	16.216
TES	0.809	1.358	1.872	2.817	3.686	4.506	6.396	9.375	16.021

Table S-XV. Partition functions for the 1-D torsional potential of H^{18}OOD using the R scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Rω	0.662	1.125	1.568	2.424	3.255	4.066	6.005	9.194	16.720
MC-HO	0.662	1.125	1.569	2.432	3.281	4.123	6.218	9.975	20.808
SAS	0.844	1.467	2.067	3.208	4.271	5.260	7.471	10.826	18.289
SRC	1.062	1.626	2.174	3.208	4.179	5.104	7.271	10.733	18.539
SR-TDPPI-HS	0.932	1.542	2.114	3.172	4.154	5.086	7.261	10.729	18.539
SRPG	0.844	1.465	2.049	3.124	4.117	5.055	7.240	10.716	18.532
CT-ωW	0.662	1.125	1.568	2.426	3.260	4.075	6.034	9.277	17.011
CT-RW	0.628	1.076	1.506	2.335	3.141	3.928	5.818	8.947	16.407
RPG	0.655	1.133	1.613	2.602	3.618	4.630	7.035	10.799	18.900
TDPPI-HS	0.986	1.621	2.217	3.318	4.335	5.294	7.509	11.003	18.800
WK	0.978	1.619	2.216	3.318	4.335	5.294	7.510	11.003	18.800
MPG	1.023	1.632	2.222	3.320	4.336	5.294	7.510	11.003	18.800
TDPPI-AS	0.973	1.617	2.215	3.318	4.335	5.293	7.509	11.003	18.800
TPG	0.881	1.532	2.143	3.265	4.294	5.260	7.487	10.989	18.794
C	1.109	1.701	2.274	3.353	4.359	5.311	7.519	11.007	18.801
CT-Rω-Z	0.874	1.354	1.802	2.660	3.490	4.298	6.232	9.409	16.907
MC-HO-Z	0.874	1.354	1.803	2.669	3.517	4.359	6.453	10.209	21.041
SRPG-Z	1.114	1.763	2.355	3.428	4.413	5.345	7.513	10.967	18.740
CT-Wω-Z	0.874	1.354	1.802	2.662	3.495	4.309	6.262	9.495	17.201
CT-RW-Z	0.829	1.296	1.731	2.562	3.367	4.153	6.038	9.157	16.590
RPG-Z	0.866	1.364	1.854	2.855	3.878	4.894	7.301	11.053	19.111
TPG-Z	1.164	1.844	2.463	3.583	4.603	5.561	7.770	11.246	19.004
TES	0.987	1.621	2.217	3.318	4.335	5.294	7.509	11.003	18.800

Table S-XVI. Full-D partition functions of H_2O_2 using the C scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Cω	1.62E-09	3.18E-06	9.11E-03	6.76E-01	1.12E+01	8.13E+02	5.18E+04
MC-HO	1.62E-09	3.19E-06	9.20E-03	6.91E-01	1.16E+01	8.74E+02	5.99E+04
SAS	1.74E-09	3.46E-06	1.01E-02	7.48E-01	1.23E+01	8.74E+02	5.39E+04
SRC	1.98E-09	3.69E-06	1.00E-02	7.25E-01	1.18E+01	8.40E+02	5.29E+04
SR-TDPPI-HS	1.79E-09	3.50E-06	9.83E-03	7.17E-01	1.17E+01	8.37E+02	5.29E+04
SRPG	1.73E-09	3.41E-06	9.70E-03	7.11E-01	1.17E+01	8.35E+02	5.28E+04
CT-ωW	1.62E-09	3.18E-06	9.18E-03	6.86E-01	1.15E+01	8.48E+02	5.57E+04
CT-CW	1.18E-09	2.41E-06	7.12E-03	5.37E-01	9.01E+00	6.69E+02	4.40E+04
RPG	1.34E-09	2.69E-06	8.08E-03	6.25E-01	1.07E+01	8.11E+02	5.32E+04
TDPPI-HS	1.89E-09	3.67E-06	1.03E-02	7.48E-01	1.22E+01	8.66E+02	5.42E+04
WK	1.88E-09	3.67E-06	1.03E-02	7.48E-01	1.22E+01	8.66E+02	5.42E+04
MPG	1.91E-09	3.69E-06	1.03E-02	7.49E-01	1.22E+01	8.66E+02	5.42E+04
TDPPI-AS	1.87E-09	3.67E-06	1.03E-02	7.48E-01	1.22E+01	8.66E+02	5.42E+04
TPG	1.81E-09	3.57E-06	1.01E-02	7.42E-01	1.21E+01	8.63E+02	5.42E+04
C	2.07E-09	3.86E-06	1.05E-02	7.56E-01	1.23E+01	8.68E+02	5.43E+04
CT-Cω-Z	2.77E-09	4.76E-06	1.19E-02	8.28E-01	1.32E+01	9.05E+02	5.54E+04
MC-HO-Z	2.77E-09	4.77E-06	1.20E-02	8.45E-01	1.36E+01	9.73E+02	6.41E+04
SRPG-Z	2.96E-09	5.11E-06	1.27E-02	8.70E-01	1.37E+01	9.30E+02	5.65E+04
CT-Wω-Z	2.77E-09	4.77E-06	1.20E-02	8.40E-01	1.35E+01	9.44E+02	5.96E+04
CT-CW-Z	2.03E-09	3.61E-06	9.32E-03	6.57E-01	1.06E+01	7.45E+02	4.71E+04
RPG-Z	2.29E-09	4.02E-06	1.06E-02	7.65E-01	1.26E+01	9.04E+02	5.69E+04
TPG-Z	3.10E-09	5.35E-06	1.33E-02	9.08E-01	1.43E+01	9.62E+02	5.79E+04
IRPG	1.96E-09	3.84E-06	1.10E-02	8.16E-01	1.36E+01	1.02E+03	7.18E+04
IRPG-Z	3.01E-09	5.30E-06	1.36E-02	9.59E-01	1.55E+01	1.12E+03	7.57E+04
accurate	3.00E-09	5.27E-06	1.35E-02	9.50E-01	1.54E+01	1.11E+03	7.52E+04

Table S-XVII. Full-D partition functions of D_2O_2 using the C scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Cω	3.01E-06	1.11E-03	6.24E-01	2.15E+01	2.31E+02	1.00E+04	4.73E+05
MC-HO	3.02E-06	1.11E-03	6.30E-01	2.19E+01	2.39E+02	1.08E+04	5.46E+05
SAS	3.24E-06	1.20E-03	6.85E-01	2.35E+01	2.51E+02	1.06E+04	4.88E+05
SRC	3.48E-06	1.24E-03	6.79E-01	2.29E+01	2.43E+02	1.03E+04	4.83E+05
SR-TDPPI-HS	3.30E-06	1.21E-03	6.71E-01	2.27E+01	2.42E+02	1.03E+04	4.83E+05
SRPG	3.24E-06	1.19E-03	6.67E-01	2.26E+01	2.41E+02	1.03E+04	4.83E+05
CT-ωW	3.02E-06	1.11E-03	6.29E-01	2.18E+01	2.36E+02	1.04E+04	5.08E+05
CT-CW	2.30E-06	8.59E-04	4.94E-01	1.72E+01	1.87E+02	8.27E+03	4.03E+05
RPG	2.50E-06	9.38E-04	5.55E-01	1.99E+01	2.21E+02	1.00E+04	4.87E+05
TDPPI-HS	3.47E-06	1.27E-03	7.02E-01	2.37E+01	2.52E+02	1.07E+04	4.96E+05
WK	3.46E-06	1.27E-03	7.02E-01	2.37E+01	2.52E+02	1.07E+04	4.96E+05
MPG	3.48E-06	1.27E-03	7.02E-01	2.37E+01	2.52E+02	1.07E+04	4.96E+05
TDPPI-AS	3.46E-06	1.27E-03	7.02E-01	2.37E+01	2.52E+02	1.07E+04	4.96E+05
TPG	3.38E-06	1.25E-03	6.97E-01	2.36E+01	2.51E+02	1.07E+04	4.95E+05
C	3.64E-06	1.30E-03	7.10E-01	2.39E+01	2.52E+02	1.07E+04	4.96E+05
CT-Cω-Z	4.04E-06	1.38E-03	7.22E-01	2.40E+01	2.52E+02	1.06E+04	4.90E+05
MC-HO-Z	4.04E-06	1.38E-03	7.30E-01	2.45E+01	2.61E+02	1.14E+04	5.66E+05
SRPG-Z	4.34E-06	1.48E-03	7.72E-01	2.53E+01	2.63E+02	1.09E+04	5.01E+05
CT-Wω-Z	4.04E-06	1.38E-03	7.28E-01	2.43E+01	2.58E+02	1.11E+04	5.27E+05
CT-CW-Z	3.08E-06	1.07E-03	5.72E-01	1.92E+01	2.04E+02	8.77E+03	4.18E+05
RPG-Z	3.35E-06	1.17E-03	6.43E-01	2.22E+01	2.41E+02	1.06E+04	5.05E+05
TPG-Z	4.53E-06	1.55E-03	8.07E-01	2.64E+01	2.74E+02	1.13E+04	5.14E+05
IRPG	3.57E-06	1.32E-03	7.47E-01	2.58E+01	2.80E+02	1.26E+04	6.55E+05
IRPG-Z	4.57E-06	1.59E-03	8.45E-01	2.83E+01	3.01E+02	1.32E+04	6.75E+05
accurate	4.51E-06	1.57E-03	8.34E-01	2.80E+01	2.98E+02	1.31E+04	6.72E+05

Table S-XVIII. Full-D partition functions of HOOD using the C scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Cω	1.39E-07	1.18E-04	1.51E-01	7.62E+00	1.02E+02	5.70E+03	3.13E+05
MC-HO	1.40E-07	1.19E-04	1.52E-01	7.78E+00	1.05E+02	6.13E+03	3.62E+05
SAS	1.50E-07	1.29E-04	1.66E-01	8.39E+00	1.11E+02	6.10E+03	3.24E+05
SRC	1.66E-07	1.35E-04	1.65E-01	8.14E+00	1.07E+02	5.89E+03	3.20E+05
SR-TDPPI-HS	1.53E-07	1.30E-04	1.62E-01	8.07E+00	1.06E+02	5.88E+03	3.20E+05
SRPG	1.49E-07	1.27E-04	1.61E-01	8.02E+00	1.06E+02	5.86E+03	3.19E+05
CT-ωW	1.40E-07	1.19E-04	1.52E-01	7.73E+00	1.04E+02	5.95E+03	3.36E+05
CT-CW	1.04E-07	9.09E-05	1.19E-01	6.07E+00	8.19E+01	4.70E+03	2.66E+05
RPG	1.16E-07	1.00E-04	1.34E-01	7.05E+00	9.71E+01	5.70E+03	3.22E+05
TDPPI-HS	1.62E-07	1.36E-04	1.70E-01	8.42E+00	1.11E+02	6.08E+03	3.28E+05
WK	1.61E-07	1.36E-04	1.70E-01	8.42E+00	1.11E+02	6.08E+03	3.28E+05
MPG	1.63E-07	1.37E-04	1.70E-01	8.43E+00	1.11E+02	6.08E+03	3.28E+05
TDPPI-AS	1.61E-07	1.36E-04	1.70E-01	8.42E+00	1.11E+02	6.08E+03	3.28E+05
TPG	1.56E-07	1.33E-04	1.68E-01	8.37E+00	1.10E+02	6.06E+03	3.27E+05
C	1.74E-07	1.42E-04	1.73E-01	8.49E+00	1.11E+02	6.09E+03	3.28E+05
CT-Cω-Z	2.11E-07	1.61E-04	1.85E-01	8.89E+00	1.15E+02	6.19E+03	3.30E+05
MC-HO-Z	2.11E-07	1.62E-04	1.87E-01	9.08E+00	1.19E+02	6.66E+03	3.81E+05
SRPG-Z	2.26E-07	1.74E-04	1.98E-01	9.36E+00	1.20E+02	6.37E+03	3.36E+05
CT-Wω-Z	2.11E-07	1.62E-04	1.87E-01	9.02E+00	1.18E+02	6.46E+03	3.54E+05
CT-CW-Z	1.57E-07	1.24E-04	1.46E-01	7.09E+00	9.27E+01	5.11E+03	2.80E+05
RPG-Z	1.75E-07	1.37E-04	1.65E-01	8.23E+00	1.10E+02	6.19E+03	3.39E+05
TPG-Z	2.36E-07	1.82E-04	2.06E-01	9.77E+00	1.25E+02	6.59E+03	3.45E+05
IRPG	1.67E-07	1.42E-04	1.81E-01	9.17E+00	1.23E+02	7.17E+03	4.34E+05
IRPG-Z	2.34E-07	1.83E-04	2.14E-01	1.04E+01	1.37E+02	7.67E+03	4.53E+05
accurate	2.32E-07	1.81E-04	2.12E-01	1.03E+01	1.35E+02	7.60E+03	4.50E+05

Table S-XIX. Full-D partition functions of $H_2^{18}O_2$ using the C scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Cω	2.26E-09	4.22E-06	1.16E-02	8.42E-01	1.38E+01	9.91E+02	6.28E+04
MC-HO	2.26E-09	4.23E-06	1.17E-02	8.60E-01	1.43E+01	1.07E+03	7.26E+04
SAS	2.42E-09	4.60E-06	1.28E-02	9.31E-01	1.52E+01	1.06E+03	6.53E+04
SRC	2.76E-09	4.89E-06	1.27E-02	9.03E-01	1.46E+01	1.02E+03	6.41E+04
SR-TDPPI-HS	2.50E-09	4.64E-06	1.25E-02	8.93E-01	1.45E+01	1.02E+03	6.40E+04
SRPG	2.41E-09	4.53E-06	1.23E-02	8.85E-01	1.44E+01	1.02E+03	6.39E+04
CT-ωW	2.26E-09	4.23E-06	1.17E-02	8.55E-01	1.41E+01	1.03E+03	6.75E+04
CT-CW	1.65E-09	3.20E-06	9.04E-03	6.69E-01	1.11E+01	8.15E+02	5.33E+04
RPG	1.87E-09	3.57E-06	1.03E-02	7.78E-01	1.32E+01	9.88E+02	6.44E+04
TDPPI-HS	2.64E-09	4.88E-06	1.31E-02	9.32E-01	1.51E+01	1.06E+03	6.57E+04
WK	2.63E-09	4.87E-06	1.31E-02	9.32E-01	1.51E+01	1.06E+03	6.57E+04
MPG	2.67E-09	4.89E-06	1.31E-02	9.32E-01	1.51E+01	1.06E+03	6.57E+04
TDPPI-AS	2.62E-09	4.86E-06	1.30E-02	9.32E-01	1.51E+01	1.06E+03	6.57E+04
TPG	2.52E-09	4.74E-06	1.29E-02	9.24E-01	1.50E+01	1.05E+03	6.56E+04
C	2.89E-09	5.12E-06	1.33E-02	9.42E-01	1.52E+01	1.06E+03	6.57E+04
CT-Cω-Z	3.83E-09	6.28E-06	1.51E-02	1.03E+00	1.62E+01	1.10E+03	6.71E+04
MC-HO-Z	3.84E-09	6.30E-06	1.52E-02	1.05E+00	1.68E+01	1.18E+03	7.75E+04
SRPG-Z	4.10E-09	6.75E-06	1.61E-02	1.08E+00	1.69E+01	1.13E+03	6.83E+04
CT-Wω-Z	3.84E-09	6.29E-06	1.52E-02	1.04E+00	1.66E+01	1.15E+03	7.21E+04
CT-CW-Z	2.81E-09	4.76E-06	1.18E-02	8.16E-01	1.30E+01	9.06E+02	5.70E+04
RPG-Z	3.17E-09	5.31E-06	1.34E-02	9.49E-01	1.54E+01	1.10E+03	6.89E+04
TPG-Z	4.29E-09	7.06E-06	1.68E-02	1.13E+00	1.75E+01	1.17E+03	7.01E+04
IRPG	2.73E-09	5.10E-06	1.39E-02	1.02E+00	1.68E+01	1.25E+03	8.71E+04
IRPG-Z	4.17E-09	7.00E-06	1.72E-02	1.19E+00	1.91E+01	1.36E+03	9.18E+04
accurate	4.16E-09	6.97E-06	1.71E-02	1.18E+00	1.89E+01	1.35E+03	9.12E+04

Table S-XX. Full-D partition functions of D^{18}OOH using the C scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Cω	1.66E-07	1.37E-04	1.70E-01	8.51E+00	1.13E+02	6.30E+03	3.44E+05
MC-HO	1.66E-07	1.38E-04	1.72E-01	8.69E+00	1.17E+02	6.77E+03	3.98E+05
SAS	1.79E-07	1.49E-04	1.88E-01	9.37E+00	1.24E+02	6.73E+03	3.57E+05
SRC	1.98E-07	1.57E-04	1.87E-01	9.10E+00	1.19E+02	6.50E+03	3.52E+05
SR-TDPPI-HS	1.83E-07	1.50E-04	1.83E-01	9.02E+00	1.18E+02	6.49E+03	3.52E+05
SRPG	1.78E-07	1.48E-04	1.82E-01	8.96E+00	1.18E+02	6.47E+03	3.51E+05
CT-ωW	1.66E-07	1.38E-04	1.72E-01	8.64E+00	1.16E+02	6.57E+03	3.70E+05
CT-CW	1.24E-07	1.05E-04	1.34E-01	6.79E+00	9.10E+01	5.19E+03	2.93E+05
RPG	1.38E-07	1.16E-04	1.51E-01	7.88E+00	1.08E+02	6.29E+03	3.54E+05
TDPPI-HS	1.93E-07	1.58E-04	1.92E-01	9.41E+00	1.23E+02	6.71E+03	3.61E+05
WK	1.92E-07	1.58E-04	1.92E-01	9.41E+00	1.23E+02	6.71E+03	3.61E+05
MPG	1.94E-07	1.58E-04	1.92E-01	9.42E+00	1.23E+02	6.71E+03	3.61E+05
TDPPI-AS	1.92E-07	1.58E-04	1.92E-01	9.41E+00	1.23E+02	6.71E+03	3.61E+05
TPG	1.86E-07	1.55E-04	1.90E-01	9.35E+00	1.23E+02	6.70E+03	3.60E+05
C	2.07E-07	1.64E-04	1.95E-01	9.49E+00	1.24E+02	6.72E+03	3.61E+05
CT-Cω-Z	2.50E-07	1.87E-04	2.09E-01	9.93E+00	1.28E+02	6.84E+03	3.62E+05
MC-HO-Z	2.51E-07	1.87E-04	2.11E-01	1.01E+01	1.32E+02	7.34E+03	4.19E+05
SRPG-Z	2.68E-07	2.01E-04	2.23E-01	1.05E+01	1.33E+02	7.03E+03	3.70E+05
CT-Wω-Z	2.51E-07	1.87E-04	2.11E-01	1.01E+01	1.31E+02	7.13E+03	3.90E+05
CT-CW-Z	1.87E-07	1.43E-04	1.64E-01	7.91E+00	1.03E+02	5.63E+03	3.08E+05
RPG-Z	2.08E-07	1.58E-04	1.86E-01	9.19E+00	1.22E+02	6.83E+03	3.73E+05
TPG-Z	2.81E-07	2.10E-04	2.33E-01	1.09E+01	1.39E+02	7.27E+03	3.79E+05
IRPG	1.99E-07	1.65E-04	2.05E-01	1.03E+01	1.37E+02	7.92E+03	4.77E+05
IRPG-Z	2.79E-07	2.12E-04	2.42E-01	1.16E+01	1.52E+02	8.47E+03	4.98E+05
accurate	2.76E-07	2.10E-04	2.39E-01	1.15E+01	1.50E+02	8.40E+03	4.94E+05

Table S-XXI. Full-D partition functions of $H^{18}OOH$ using the C scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Cω	3.81E-09	7.30E-06	2.05E-02	1.51E+00	2.48E+01	1.79E+03	1.14E+05
MC-HO	3.81E-09	7.32E-06	2.07E-02	1.54E+00	2.57E+01	1.92E+03	1.32E+05
SAS	4.09E-09	7.96E-06	2.26E-02	1.67E+00	2.73E+01	1.92E+03	1.18E+05
SRC	4.66E-09	8.47E-06	2.26E-02	1.61E+00	2.62E+01	1.85E+03	1.16E+05
SR-TDPPI-HS	4.22E-09	8.03E-06	2.21E-02	1.60E+00	2.60E+01	1.84E+03	1.16E+05
SRPG	4.07E-09	7.85E-06	2.18E-02	1.58E+00	2.58E+01	1.84E+03	1.16E+05
CT-ωW	3.81E-09	7.32E-06	2.06E-02	1.53E+00	2.54E+01	1.87E+03	1.22E+05
CT-CW	2.79E-09	5.54E-06	1.60E-02	1.20E+00	1.99E+01	1.47E+03	9.67E+04
RPG	3.15E-09	6.18E-06	1.82E-02	1.39E+00	2.37E+01	1.79E+03	1.17E+05
TDPPI-HS	4.46E-09	8.44E-06	2.31E-02	1.67E+00	2.71E+01	1.91E+03	1.19E+05
WK	4.44E-09	8.44E-06	2.31E-02	1.67E+00	2.71E+01	1.91E+03	1.19E+05
MPG	4.50E-09	8.48E-06	2.31E-02	1.67E+00	2.71E+01	1.91E+03	1.19E+05
TDPPI-AS	4.42E-09	8.42E-06	2.31E-02	1.67E+00	2.71E+01	1.91E+03	1.19E+05
TPG	4.26E-09	8.21E-06	2.28E-02	1.65E+00	2.69E+01	1.90E+03	1.19E+05
C	4.88E-09	8.86E-06	2.36E-02	1.68E+00	2.72E+01	1.91E+03	1.19E+05
CT-Cω-Z	6.59E-09	1.10E-05	2.69E-02	1.85E+00	2.93E+01	2.00E+03	1.22E+05
MC-HO-Z	6.60E-09	1.11E-05	2.72E-02	1.89E+00	3.03E+01	2.15E+03	1.41E+05
SRPG-Z	7.05E-09	1.18E-05	2.87E-02	1.94E+00	3.05E+01	2.05E+03	1.24E+05
CT-Wω-Z	6.60E-09	1.10E-05	2.71E-02	1.88E+00	2.99E+01	2.08E+03	1.31E+05
CT-CW-Z	4.83E-09	8.36E-06	2.11E-02	1.47E+00	2.35E+01	1.64E+03	1.04E+05
RPG-Z	5.45E-09	9.32E-06	2.39E-02	1.71E+00	2.79E+01	1.99E+03	1.25E+05
TPG-Z	7.37E-09	1.24E-05	3.00E-02	2.03E+00	3.17E+01	2.12E+03	1.27E+05
IRPG	4.61E-09	8.83E-06	2.47E-02	1.82E+00	3.02E+01	2.25E+03	1.58E+05
IRPG-Z	7.16E-09	1.23E-05	3.08E-02	2.14E+00	3.44E+01	2.46E+03	1.67E+05
accurate	7.02E-09	1.21E-05	3.03E-02	2.11E+00	3.40E+01	2.43E+03	1.65E+05

Table S-XXII. Full-D partition functions of H^{18}OOD using the C scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Cω	1.65E-07	1.37E-04	1.70E-01	8.50E+00	1.13E+02	6.30E+03	3.44E+05
MC-HO	1.65E-07	1.37E-04	1.72E-01	8.68E+00	1.17E+02	6.77E+03	3.98E+05
SAS	1.77E-07	1.49E-04	1.87E-01	9.36E+00	1.23E+02	6.73E+03	3.57E+05
SRC	1.96E-07	1.56E-04	1.86E-01	9.09E+00	1.19E+02	6.50E+03	3.52E+05
SR-TDPPI-HS	1.81E-07	1.50E-04	1.83E-01	9.01E+00	1.18E+02	6.49E+03	3.52E+05
SRPG	1.77E-07	1.47E-04	1.81E-01	8.95E+00	1.18E+02	6.47E+03	3.51E+05
CT-ωW	1.65E-07	1.37E-04	1.71E-01	8.63E+00	1.15E+02	6.56E+03	3.70E+05
CT-CW	1.23E-07	1.05E-04	1.34E-01	6.78E+00	9.10E+01	5.19E+03	2.93E+05
RPG	1.37E-07	1.16E-04	1.51E-01	7.87E+00	1.08E+02	6.29E+03	3.54E+05
TDPPI-HS	1.91E-07	1.57E-04	1.91E-01	9.40E+00	1.23E+02	6.71E+03	3.61E+05
WK	1.91E-07	1.57E-04	1.91E-01	9.40E+00	1.23E+02	6.71E+03	3.61E+05
MPG	1.92E-07	1.57E-04	1.92E-01	9.40E+00	1.23E+02	6.71E+03	3.61E+05
TDPPI-AS	1.90E-07	1.57E-04	1.91E-01	9.40E+00	1.23E+02	6.71E+03	3.61E+05
TPG	1.85E-07	1.54E-04	1.89E-01	9.34E+00	1.22E+02	6.69E+03	3.60E+05
C	2.05E-07	1.63E-04	1.94E-01	9.48E+00	1.24E+02	6.72E+03	3.61E+05
CT-Cω-Z	2.48E-07	1.86E-04	2.08E-01	9.91E+00	1.28E+02	6.83E+03	3.62E+05
MC-HO-Z	2.49E-07	1.86E-04	2.11E-01	1.01E+01	1.32E+02	7.34E+03	4.19E+05
SRPG-Z	2.66E-07	2.00E-04	2.22E-01	1.04E+01	1.33E+02	7.03E+03	3.70E+05
CT-Wω-Z	2.49E-07	1.86E-04	2.10E-01	1.01E+01	1.31E+02	7.13E+03	3.90E+05
CT-CW-Z	1.86E-07	1.43E-04	1.64E-01	7.90E+00	1.03E+02	5.63E+03	3.08E+05
RPG-Z	2.06E-07	1.57E-04	1.85E-01	9.17E+00	1.22E+02	6.83E+03	3.73E+05
TPG-Z	2.78E-07	2.09E-04	2.32E-01	1.09E+01	1.38E+02	7.27E+03	3.79E+05
IRPG	1.97E-07	1.64E-04	2.04E-01	1.02E+01	1.37E+02	7.92E+03	4.77E+05
IRPG-Z	2.76E-07	2.11E-04	2.41E-01	1.16E+01	1.52E+02	8.47E+03	4.98E+05
accurate	2.74E-07	2.09E-04	2.39E-01	1.15E+01	1.50E+02	8.39E+03	4.95E+05

Table S-XXIII. Full-D partition functions of H_2O_2 using the R scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Rω	1.62E-09	3.18E-06	9.17E-03	6.84E-01	1.14E+01	8.41E+02	5.48E+04
MC-HO	1.62E-09	3.19E-06	9.20E-03	6.91E-01	1.16E+01	8.74E+02	5.99E+04
SAS	2.06E-09	4.09E-06	1.19E-02	8.80E-01	1.45E+01	1.03E+03	6.36E+04
SRC	2.35E-09	4.37E-06	1.19E-02	8.60E-01	1.40E+01	9.96E+02	6.28E+04
SR-TDPPI-HS	2.18E-09	4.21E-06	1.17E-02	8.53E-01	1.39E+01	9.94E+02	6.27E+04
SRPG	2.05E-09	4.05E-06	1.15E-02	8.43E-01	1.38E+01	9.90E+02	6.26E+04
CT-ωW	1.62E-09	3.18E-06	9.18E-03	6.86E-01	1.15E+01	8.48E+02	5.57E+04
CT-RW	1.49E-09	2.96E-06	8.58E-03	6.43E-01	1.07E+01	7.95E+02	5.23E+04
RPG	1.59E-09	3.19E-06	9.58E-03	7.41E-01	1.27E+01	9.62E+02	6.31E+04
TDPPI-HS	2.30E-09	4.42E-06	1.23E-02	8.90E-01	1.45E+01	1.03E+03	6.43E+04
WK	2.29E-09	4.42E-06	1.23E-02	8.90E-01	1.45E+01	1.03E+03	6.43E+04
MPG	2.33E-09	4.44E-06	1.23E-02	8.91E-01	1.45E+01	1.03E+03	6.43E+04
TDPPI-AS	2.29E-09	4.41E-06	1.23E-02	8.90E-01	1.45E+01	1.03E+03	6.43E+04
TPG	2.14E-09	4.23E-06	1.20E-02	8.80E-01	1.44E+01	1.02E+03	6.42E+04
C	2.46E-09	4.58E-06	1.24E-02	8.97E-01	1.46E+01	1.03E+03	6.44E+04
CT-Rω-Z	2.77E-09	4.77E-06	1.20E-02	8.38E-01	1.34E+01	9.36E+02	5.86E+04
MC-HO-Z	2.77E-09	4.77E-06	1.20E-02	8.45E-01	1.36E+01	9.73E+02	6.41E+04
SRPG-Z	3.51E-09	6.06E-06	1.51E-02	1.03E+00	1.63E+01	1.10E+03	6.70E+04
CT-Wω-Z	2.77E-09	4.77E-06	1.20E-02	8.40E-01	1.35E+01	9.44E+02	5.96E+04
CT-RW-Z	2.55E-09	4.43E-06	1.12E-02	7.86E-01	1.26E+01	8.86E+02	5.59E+04
RPG-Z	2.72E-09	4.77E-06	1.25E-02	9.07E-01	1.49E+01	1.07E+03	6.75E+04
TPG-Z	3.67E-09	6.34E-06	1.57E-02	1.08E+00	1.69E+01	1.14E+03	6.87E+04
IRPG	2.00E-09	3.89E-06	1.10E-02	8.19E-01	1.37E+01	1.02E+03	7.18E+04
IRPG-Z	2.79E-09	4.98E-06	1.30E-02	9.26E-01	1.51E+01	1.09E+03	7.48E+04
accurate	3.00E-09	5.27E-06	1.35E-02	9.50E-01	1.54E+01	1.11E+03	7.52E+04

Table S-XXIV. Full-D partition functions of D_2O_2 using the R scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Rω	3.02E-06	1.11E-03	6.28E-01	2.17E+01	2.35E+02	1.04E+04	5.03E+05
MC-HO	3.02E-06	1.11E-03	6.30E-01	2.19E+01	2.39E+02	1.08E+04	5.46E+05
SAS	3.92E-06	1.45E-03	8.25E-01	2.83E+01	3.02E+02	1.28E+04	5.88E+05
SRC	4.21E-06	1.50E-03	8.22E-01	2.77E+01	2.94E+02	1.25E+04	5.85E+05
SR-TDPPI-HS	4.06E-06	1.47E-03	8.15E-01	2.76E+01	2.93E+02	1.25E+04	5.85E+05
SRPG	3.92E-06	1.44E-03	8.07E-01	2.74E+01	2.92E+02	1.25E+04	5.84E+05
CT-ωW	3.02E-06	1.11E-03	6.29E-01	2.18E+01	2.36E+02	1.04E+04	5.08E+05
CT-RW	2.88E-06	1.06E-03	6.03E-01	2.09E+01	2.27E+02	1.00E+04	4.88E+05
RPG	3.03E-06	1.14E-03	6.72E-01	2.41E+01	2.67E+02	1.21E+04	5.89E+05
TDPPI-HS	4.26E-06	1.54E-03	8.53E-01	2.88E+01	3.05E+02	1.29E+04	6.00E+05
WK	4.26E-06	1.54E-03	8.53E-01	2.88E+01	3.05E+02	1.29E+04	6.00E+05
MPG	4.27E-06	1.55E-03	8.53E-01	2.88E+01	3.05E+02	1.29E+04	6.00E+05
TDPPI-AS	4.25E-06	1.54E-03	8.53E-01	2.88E+01	3.05E+02	1.29E+04	6.00E+05
TPG	4.09E-06	1.51E-03	8.43E-01	2.86E+01	3.03E+02	1.29E+04	5.99E+05
C	4.41E-06	1.57E-03	8.59E-01	2.89E+01	3.05E+02	1.29E+04	6.00E+05
CT-Rω-Z	4.04E-06	1.38E-03	7.27E-01	2.43E+01	2.57E+02	1.10E+04	5.21E+05
MC-HO-Z	4.04E-06	1.38E-03	7.30E-01	2.45E+01	2.61E+02	1.14E+04	5.66E+05
SRPG-Z	5.25E-06	1.80E-03	9.34E-01	3.06E+01	3.18E+02	1.32E+04	6.06E+05
CT-Wω-Z	4.04E-06	1.38E-03	7.28E-01	2.43E+01	2.58E+02	1.11E+04	5.27E+05
CT-RW-Z	3.86E-06	1.32E-03	6.98E-01	2.33E+01	2.47E+02	1.06E+04	5.06E+05
RPG-Z	4.06E-06	1.41E-03	7.78E-01	2.69E+01	2.92E+02	1.29E+04	6.11E+05
TPG-Z	5.49E-06	1.88E-03	9.76E-01	3.19E+01	3.31E+02	1.37E+04	6.22E+05
IRPG	3.62E-06	1.33E-03	7.49E-01	2.58E+01	2.80E+02	1.26E+04	6.55E+05
IRPG-Z	4.20E-06	1.48E-03	8.07E-01	2.73E+01	2.93E+02	1.30E+04	6.67E+05
accurate	4.51E-06	1.57E-03	8.34E-01	2.80E+01	2.98E+02	1.31E+04	6.72E+05

Table S-XXV. Full-D partition functions of HOOD using the R scheme *I*

T(K)	300	400	600	800	1000	1500	2400
CT-Rω	1.40E-07	1.19E-04	1.52E-01	7.72E+00	1.04E+02	5.92E+03	3.34E+05
MC-HO	1.40E-07	1.19E-04	1.52E-01	7.78E+00	1.05E+02	6.13E+03	3.62E+05
SAS	1.83E-07	1.57E-04	2.02E-01	1.02E+01	1.35E+02	7.39E+03	3.94E+05
SRC	2.03E-07	1.65E-04	2.02E-01	9.95E+00	1.31E+02	7.19E+03	3.91E+05
SR-TDPPI-HS	1.92E-07	1.61E-04	1.99E-01	9.89E+00	1.30E+02	7.18E+03	3.90E+05
SRPG	1.82E-07	1.56E-04	1.96E-01	9.80E+00	1.29E+02	7.16E+03	3.90E+05
CT-ωW	1.40E-07	1.19E-04	1.52E-01	7.73E+00	1.04E+02	5.95E+03	3.36E+05
CT-RW	1.34E-07	1.14E-04	1.47E-01	7.48E+00	1.01E+02	5.76E+03	3.26E+05
RPG	1.41E-07	1.23E-04	1.64E-01	8.61E+00	1.19E+02	6.96E+03	3.93E+05
TDPPI-HS	2.02E-07	1.69E-04	2.09E-01	1.03E+01	1.36E+02	7.43E+03	4.00E+05
WK	2.02E-07	1.68E-04	2.09E-01	1.03E+01	1.36E+02	7.43E+03	4.00E+05
MPG	2.03E-07	1.69E-04	2.09E-01	1.03E+01	1.36E+02	7.43E+03	4.00E+05
TDPPI-AS	2.02E-07	1.68E-04	2.09E-01	1.03E+01	1.36E+02	7.43E+03	4.00E+05
TPG	1.91E-07	1.63E-04	2.05E-01	1.02E+01	1.35E+02	7.41E+03	4.00E+05
C	2.12E-07	1.73E-04	2.11E-01	1.04E+01	1.36E+02	7.44E+03	4.01E+05
CT-Rω-Z	2.11E-07	1.62E-04	1.87E-01	9.01E+00	1.17E+02	6.43E+03	3.51E+05
MC-HO-Z	2.11E-07	1.62E-04	1.87E-01	9.08E+00	1.19E+02	6.66E+03	3.81E+05
SRPG-Z	2.76E-07	2.12E-04	2.41E-01	1.14E+01	1.47E+02	7.78E+03	4.11E+05
CT-Wω-Z	2.11E-07	1.62E-04	1.87E-01	9.02E+00	1.18E+02	6.46E+03	3.54E+05
CT-RW-Z	2.03E-07	1.56E-04	1.80E-01	8.73E+00	1.14E+02	6.25E+03	3.43E+05
RPG-Z	2.13E-07	1.67E-04	2.01E-01	1.01E+01	1.34E+02	7.56E+03	4.14E+05
TPG-Z	2.88E-07	2.22E-04	2.52E-01	1.19E+01	1.52E+02	8.04E+03	4.21E+05
IRPG	1.71E-07	1.44E-04	1.82E-01	9.20E+00	1.24E+02	7.18E+03	4.34E+05
IRPG-Z	2.14E-07	1.70E-04	2.04E-01	1.00E+01	1.32E+02	7.51E+03	4.47E+05
accurate	2.32E-07	1.81E-04	2.12E-01	1.03E+01	1.35E+02	7.60E+03	4.50E+05

Table S-XXVI. Full-D partition functions of $H_2^{18}O_2$ using the R scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Rω	2.26E-09	4.23E-06	1.16E-02	8.52E-01	1.41E+01	1.02E+03	6.64E+04
MC-HO	2.26E-09	4.23E-06	1.17E-02	8.60E-01	1.43E+01	1.07E+03	7.26E+04
SAS	2.87E-09	5.43E-06	1.51E-02	1.10E+00	1.79E+01	1.25E+03	7.69E+04
SRC	3.27E-09	5.80E-06	1.51E-02	1.07E+00	1.73E+01	1.21E+03	7.59E+04
SR-TDPPI-HS	3.04E-09	5.58E-06	1.49E-02	1.06E+00	1.72E+01	1.21E+03	7.59E+04
SRPG	2.86E-09	5.37E-06	1.46E-02	1.05E+00	1.70E+01	1.21E+03	7.58E+04
CT-ωW	2.26E-09	4.23E-06	1.17E-02	8.55E-01	1.41E+01	1.03E+03	6.75E+04
CT-RW	2.08E-09	3.92E-06	1.09E-02	7.99E-01	1.32E+01	9.68E+02	6.33E+04
RPG	2.21E-09	4.23E-06	1.22E-02	9.22E-01	1.56E+01	1.17E+03	7.64E+04
TDPPI-HS	3.20E-09	5.86E-06	1.56E-02	1.11E+00	1.79E+01	1.25E+03	7.78E+04
WK	3.20E-09	5.86E-06	1.56E-02	1.11E+00	1.79E+01	1.25E+03	7.78E+04
MPG	3.24E-09	5.88E-06	1.56E-02	1.11E+00	1.79E+01	1.25E+03	7.78E+04
TDPPI-AS	3.19E-09	5.85E-06	1.56E-02	1.11E+00	1.79E+01	1.25E+03	7.78E+04
TPG	2.99E-09	5.62E-06	1.53E-02	1.09E+00	1.77E+01	1.25E+03	7.77E+04
C	3.42E-09	6.07E-06	1.58E-02	1.12E+00	1.80E+01	1.25E+03	7.79E+04
CT-Rω-Z	3.84E-09	6.29E-06	1.52E-02	1.04E+00	1.65E+01	1.14E+03	7.09E+04
MC-HO-Z	3.84E-09	6.30E-06	1.52E-02	1.05E+00	1.68E+01	1.18E+03	7.75E+04
SRPG-Z	4.86E-09	7.99E-06	1.90E-02	1.28E+00	2.00E+01	1.34E+03	8.10E+04
CT-Wω-Z	3.84E-09	6.29E-06	1.52E-02	1.04E+00	1.66E+01	1.15E+03	7.21E+04
CT-RW-Z	3.53E-09	5.84E-06	1.42E-02	9.75E-01	1.55E+01	1.08E+03	6.76E+04
RPG-Z	3.76E-09	6.29E-06	1.58E-02	1.13E+00	1.83E+01	1.30E+03	8.16E+04
TPG-Z	5.08E-09	8.36E-06	1.99E-02	1.34E+00	2.08E+01	1.39E+03	8.30E+04
IRPG	2.80E-09	5.17E-06	1.40E-02	1.02E+00	1.68E+01	1.25E+03	8.71E+04
IRPG-Z	3.86E-09	6.58E-06	1.65E-02	1.15E+00	1.85E+01	1.33E+03	9.07E+04
accurate	4.16E-09	6.97E-06	1.71E-02	1.18E+00	1.89E+01	1.35E+03	9.12E+04

Table S-XXVII. Full-D partition functions of D^{18}OOH using the R scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Rω	1.66E-07	1.38E-04	1.72E-01	8.63E+00	1.15E+02	6.54E+03	3.67E+05
MC-HO	1.66E-07	1.38E-04	1.72E-01	8.69E+00	1.17E+02	6.77E+03	3.98E+05
SAS	2.18E-07	1.82E-04	2.28E-01	1.14E+01	1.50E+02	8.16E+03	4.33E+05
SRC	2.41E-07	1.91E-04	2.28E-01	1.11E+01	1.45E+02	7.94E+03	4.30E+05
SR-TDPPI-HS	2.29E-07	1.86E-04	2.25E-01	1.10E+01	1.45E+02	7.93E+03	4.30E+05
SRPG	2.18E-07	1.80E-04	2.22E-01	1.09E+01	1.44E+02	7.91E+03	4.29E+05
CT-ωW	1.66E-07	1.38E-04	1.72E-01	8.64E+00	1.16E+02	6.57E+03	3.70E+05
CT-RW	1.60E-07	1.33E-04	1.66E-01	8.35E+00	1.12E+02	6.35E+03	3.58E+05
RPG	1.68E-07	1.42E-04	1.85E-01	9.62E+00	1.32E+02	7.68E+03	4.32E+05
TDPPI-HS	2.41E-07	1.95E-04	2.36E-01	1.15E+01	1.51E+02	8.20E+03	4.40E+05
WK	2.40E-07	1.95E-04	2.36E-01	1.15E+01	1.51E+02	8.20E+03	4.40E+05
MPG	2.42E-07	1.96E-04	2.36E-01	1.15E+01	1.51E+02	8.20E+03	4.40E+05
TDPPI-AS	2.40E-07	1.95E-04	2.36E-01	1.15E+01	1.51E+02	8.20E+03	4.40E+05
TPG	2.27E-07	1.89E-04	2.32E-01	1.14E+01	1.50E+02	8.18E+03	4.40E+05
C	2.53E-07	2.00E-04	2.38E-01	1.16E+01	1.51E+02	8.21E+03	4.41E+05
CT-Rω-Z	2.51E-07	1.87E-04	2.11E-01	1.01E+01	1.30E+02	7.10E+03	3.86E+05
MC-HO-Z	2.51E-07	1.87E-04	2.11E-01	1.01E+01	1.32E+02	7.34E+03	4.19E+05
SRPG-Z	3.28E-07	2.45E-04	2.72E-01	1.28E+01	1.63E+02	8.58E+03	4.52E+05
CT-Wω-Z	2.51E-07	1.87E-04	2.11E-01	1.01E+01	1.31E+02	7.13E+03	3.90E+05
CT-RW-Z	2.41E-07	1.80E-04	2.04E-01	9.74E+00	1.26E+02	6.90E+03	3.77E+05
RPG-Z	2.54E-07	1.93E-04	2.27E-01	1.12E+01	1.49E+02	8.34E+03	4.55E+05
TPG-Z	3.43E-07	2.57E-04	2.85E-01	1.33E+01	1.69E+02	8.88E+03	4.63E+05
IRPG	2.03E-07	1.67E-04	2.06E-01	1.03E+01	1.37E+02	7.92E+03	4.77E+05
IRPG-Z	2.54E-07	1.97E-04	2.30E-01	1.12E+01	1.47E+02	8.29E+03	4.91E+05
accurate	2.76E-07	2.10E-04	2.39E-01	1.15E+01	1.50E+02	8.40E+03	4.94E+05

Table S-XXVIII. Full-D partition functions of H^{18}OOH using the R scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Rω	3.81E-09	7.32E-06	2.06E-02	1.52E+00	2.53E+01	1.85E+03	1.20E+05
MC-HO	3.81E-09	7.32E-06	2.07E-02	1.54E+00	2.57E+01	1.92E+03	1.32E+05
SAS	4.84E-09	9.41E-06	2.67E-02	1.96E+00	3.21E+01	2.26E+03	1.40E+05
SRC	5.53E-09	1.00E-05	2.68E-02	1.91E+00	3.10E+01	2.19E+03	1.38E+05
SR-TDPPI-HS	5.14E-09	9.67E-06	2.63E-02	1.90E+00	3.09E+01	2.19E+03	1.38E+05
SRPG	4.83E-09	9.30E-06	2.59E-02	1.88E+00	3.06E+01	2.18E+03	1.37E+05
CT-ωW	3.81E-09	7.32E-06	2.06E-02	1.53E+00	2.54E+01	1.87E+03	1.22E+05
CT-RW	3.51E-09	6.80E-06	1.93E-02	1.43E+00	2.38E+01	1.75E+03	1.15E+05
RPG	3.74E-09	7.32E-06	2.15E-02	1.65E+00	2.81E+01	2.12E+03	1.39E+05
TDPPI-HS	5.41E-09	1.01E-05	2.76E-02	1.98E+00	3.21E+01	2.26E+03	1.41E+05
WK	5.40E-09	1.01E-05	2.76E-02	1.98E+00	3.21E+01	2.26E+03	1.41E+05
MPG	5.48E-09	1.02E-05	2.76E-02	1.98E+00	3.21E+01	2.26E+03	1.41E+05
TDPPI-AS	5.39E-09	1.01E-05	2.76E-02	1.98E+00	3.21E+01	2.26E+03	1.41E+05
TPG	5.05E-09	9.73E-06	2.70E-02	1.96E+00	3.19E+01	2.25E+03	1.41E+05
C	5.78E-09	1.05E-05	2.80E-02	2.00E+00	3.23E+01	2.27E+03	1.41E+05
CT-Rω-Z	6.59E-09	1.10E-05	2.71E-02	1.87E+00	2.98E+01	2.07E+03	1.29E+05
MC-HO-Z	6.60E-09	1.11E-05	2.72E-02	1.89E+00	3.03E+01	2.15E+03	1.41E+05
SRPG-Z	8.36E-09	1.40E-05	3.40E-02	2.31E+00	3.61E+01	2.43E+03	1.47E+05
CT-Wω-Z	6.60E-09	1.10E-05	2.71E-02	1.88E+00	2.99E+01	2.08E+03	1.31E+05
CT-RW-Z	6.08E-09	1.03E-05	2.54E-02	1.76E+00	2.80E+01	1.95E+03	1.23E+05
RPG-Z	6.47E-09	1.11E-05	2.83E-02	2.03E+00	3.31E+01	2.36E+03	1.48E+05
TPG-Z	8.74E-09	1.47E-05	3.55E-02	2.41E+00	3.76E+01	2.52E+03	1.51E+05
IRPG	4.72E-09	8.94E-06	2.48E-02	1.82E+00	3.02E+01	2.26E+03	1.58E+05
IRPG-Z	6.64E-09	1.15E-05	2.94E-02	2.07E+00	3.35E+01	2.42E+03	1.65E+05
accurate	7.02E-09	1.21E-05	3.03E-02	2.11E+00	3.40E+01	2.43E+03	1.65E+05

Table S-XXIX. Full-D partition functions of $H^{18}OOD$ using the R scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Rω	1.65E-07	1.37E-04	1.71E-01	8.61E+00	1.15E+02	6.53E+03	3.67E+05
MC-HO	1.65E-07	1.37E-04	1.72E-01	8.68E+00	1.17E+02	6.77E+03	3.98E+05
SAS	2.15E-07	1.80E-04	2.26E-01	1.13E+01	1.49E+02	8.13E+03	4.32E+05
SRC	2.39E-07	1.90E-04	2.26E-01	1.11E+01	1.45E+02	7.91E+03	4.28E+05
SR-TDPPI-HS	2.26E-07	1.84E-04	2.24E-01	1.10E+01	1.44E+02	7.90E+03	4.28E+05
SRPG	2.15E-07	1.79E-04	2.20E-01	1.09E+01	1.43E+02	7.88E+03	4.27E+05
CT-ωW	1.65E-07	1.37E-04	1.71E-01	8.63E+00	1.15E+02	6.56E+03	3.70E+05
CT-RW	1.58E-07	1.31E-04	1.65E-01	8.31E+00	1.11E+02	6.33E+03	3.57E+05
RPG	1.66E-07	1.41E-04	1.84E-01	9.57E+00	1.31E+02	7.65E+03	4.31E+05
TDPPI-HS	2.38E-07	1.93E-04	2.34E-01	1.15E+01	1.50E+02	8.17E+03	4.39E+05
WK	2.38E-07	1.93E-04	2.34E-01	1.15E+01	1.50E+02	8.17E+03	4.39E+05
MPG	2.40E-07	1.94E-04	2.34E-01	1.15E+01	1.50E+02	8.17E+03	4.39E+05
TDPPI-AS	2.37E-07	1.93E-04	2.34E-01	1.15E+01	1.50E+02	8.17E+03	4.39E+05
TPG	2.25E-07	1.87E-04	2.30E-01	1.14E+01	1.49E+02	8.15E+03	4.38E+05
C	2.50E-07	1.98E-04	2.37E-01	1.15E+01	1.50E+02	8.18E+03	4.39E+05
CT-Rω-Z	2.49E-07	1.86E-04	2.10E-01	1.00E+01	1.30E+02	7.09E+03	3.86E+05
MC-HO-Z	2.49E-07	1.86E-04	2.11E-01	1.01E+01	1.32E+02	7.34E+03	4.19E+05
SRPG-Z	3.24E-07	2.43E-04	2.71E-01	1.27E+01	1.62E+02	8.55E+03	4.50E+05
CT-Wω-Z	2.49E-07	1.86E-04	2.10E-01	1.01E+01	1.31E+02	7.13E+03	3.90E+05
CT-RW-Z	2.38E-07	1.79E-04	2.02E-01	9.69E+00	1.26E+02	6.87E+03	3.76E+05
RPG-Z	2.51E-07	1.91E-04	2.25E-01	1.12E+01	1.48E+02	8.31E+03	4.53E+05
TPG-Z	3.39E-07	2.54E-04	2.83E-01	1.33E+01	1.69E+02	8.84E+03	4.61E+05
IRPG	2.02E-07	1.66E-04	2.05E-01	1.03E+01	1.37E+02	7.92E+03	4.78E+05
IRPG-Z	2.52E-07	1.96E-04	2.29E-01	1.12E+01	1.47E+02	8.29E+03	4.91E+05
accurate	2.74E-07	2.09E-04	2.39E-01	1.15E+01	1.50E+02	8.39E+03	4.95E+05

Table S-XXX. H_2O_2/D_2O_2 isotope ratio for the 1-D torsional potential using the C scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Cω	0.640	0.687	0.706	0.720	0.725	0.727	0.729	0.730	0.730
MC-HO	0.640	0.688	0.706	0.720	0.725	0.727	0.730	0.731	0.731
SAS	0.638	0.687	0.707	0.725	0.732	0.735	0.737	0.736	0.733
SRC	0.729	0.729	0.729	0.729	0.729	0.729	0.729	0.729	0.729
SR-TDPPI-HS	0.658	0.697	0.712	0.722	0.725	0.727	0.728	0.729	0.729
SRPG	0.638	0.685	0.704	0.717	0.723	0.725	0.727	0.728	0.729
CT-ωW	0.640	0.688	0.706	0.720	0.725	0.727	0.730	0.731	0.731
CT-CW	0.594	0.662	0.689	0.710	0.719	0.722	0.726	0.728	0.729
RPG	0.638	0.685	0.704	0.718	0.723	0.725	0.727	0.728	0.729
TDPPI-HS	0.664	0.700	0.713	0.722	0.726	0.727	0.728	0.729	0.729
WK	0.653	0.698	0.713	0.722	0.726	0.727	0.728	0.729	0.729
MPG	0.694	0.705	0.715	0.723	0.726	0.727	0.728	0.729	0.729
TDPPI-AS	0.639	0.696	0.712	0.722	0.726	0.727	0.728	0.729	0.729
TPG	0.638	0.685	0.704	0.718	0.723	0.725	0.727	0.728	0.729
C	0.730	0.729	0.729	0.729	0.729	0.729	0.729	0.729	0.729
CT-Cω-Z	0.703	0.732	0.740	0.743	0.742	0.741	0.738	0.736	0.733
MC-HO-Z	0.703	0.731	0.740	0.743	0.742	0.741	0.739	0.737	0.734
SRPG-Z	0.700	0.729	0.737	0.740	0.740	0.739	0.736	0.734	0.732
CT-Wω-Z	0.703	0.732	0.740	0.743	0.742	0.741	0.739	0.737	0.734
CT-CW-Z	0.651	0.704	0.722	0.733	0.736	0.736	0.735	0.734	0.732
RPG-Z	0.701	0.729	0.737	0.740	0.740	0.739	0.736	0.734	0.732
TPG-Z	0.701	0.730	0.738	0.740	0.740	0.739	0.736	0.734	0.732
TES	0.665	0.701	0.713	0.722	0.726	0.727	0.728	0.729	0.729

Table S-XXXI. H_2O_2 / HOOD isotope ratio for the 1-D torsional potential using the C scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Cω	0.821	0.850	0.861	0.869	0.872	0.874	0.875	0.875	0.876
MC-HO	0.821	0.849	0.861	0.869	0.872	0.874	0.875	0.876	0.876
SAS	0.819	0.850	0.862	0.872	0.876	0.878	0.879	0.879	0.877
SRC	0.876	0.875	0.875	0.875	0.875	0.875	0.875	0.875	0.875
SR-TDPPI-HS	0.832	0.856	0.865	0.871	0.873	0.874	0.875	0.875	0.875
SRPG	0.819	0.848	0.860	0.868	0.871	0.873	0.874	0.875	0.875
CT-ωW	0.821	0.850	0.861	0.869	0.872	0.874	0.875	0.876	0.876
CT-CW	0.791	0.834	0.851	0.864	0.869	0.871	0.873	0.874	0.875
RPG	0.819	0.848	0.860	0.868	0.871	0.873	0.874	0.875	0.875
TDPPI-HS	0.836	0.858	0.865	0.871	0.873	0.874	0.875	0.875	0.875
WK	0.829	0.856	0.865	0.871	0.873	0.874	0.875	0.875	0.875
MPG	0.859	0.862	0.867	0.871	0.873	0.874	0.875	0.875	0.875
TDPPI-AS	0.817	0.855	0.864	0.871	0.873	0.874	0.875	0.875	0.875
TPG	0.819	0.849	0.859	0.868	0.871	0.873	0.874	0.875	0.875
C	0.876	0.875	0.875	0.875	0.875	0.875	0.875	0.875	0.875
CT-Cω-Z	0.863	0.879	0.883	0.884	0.883	0.882	0.881	0.879	0.877
MC-HO-Z	0.864	0.879	0.883	0.884	0.884	0.883	0.881	0.880	0.878
SRPG-Z	0.862	0.878	0.882	0.883	0.882	0.882	0.880	0.878	0.877
CT-Wω-Z	0.864	0.879	0.883	0.884	0.884	0.883	0.881	0.880	0.878
CT-CW-Z	0.833	0.863	0.873	0.879	0.880	0.880	0.879	0.878	0.877
RPG-Z	0.863	0.877	0.882	0.883	0.882	0.881	0.880	0.878	0.877
TPG-Z	0.862	0.878	0.882	0.883	0.882	0.882	0.880	0.878	0.877
TES	0.837	0.858	0.866	0.871	0.873	0.874	0.875	0.875	0.875

Table S-XXXII. $H_2O_2/H_2{}^{18}O_2$ isotope ratio for the 1-D torsional potential using the C scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Cω	0.994	0.995	0.996	0.996	0.996	0.996	0.996	0.996	0.996
MC-HO	0.994	0.995	0.995	0.996	0.996	0.996	0.996	0.996	0.996
SAS	0.995	0.996	0.995	0.996	0.996	0.996	0.997	0.996	0.996
SRC	0.997	0.997	0.996	0.997	0.996	0.996	0.996	0.996	0.996
SR-TDPPI-HS	0.995	0.996	0.996	0.996	0.996	0.996	0.996	0.996	0.996
SRPG	0.995	0.995	0.996	0.996	0.996	0.996	0.996	0.996	0.996
CT-ωW	0.994	0.995	0.996	0.996	0.996	0.996	0.996	0.996	0.996
CT-CW	0.995	0.996	0.996	0.996	0.996	0.996	0.996	0.996	0.996
RPG	0.995	0.995	0.996	0.996	0.996	0.996	0.996	0.996	0.996
TDPPI-HS	0.995	0.996	0.996	0.996	0.996	0.996	0.996	0.996	0.996
WK	0.995	0.996	0.996	0.996	0.996	0.996	0.996	0.996	0.996
MPG	0.997	0.996	0.996	0.996	0.996	0.996	0.996	0.996	0.996
TDPPI-AS	0.995	0.995	0.996	0.996	0.996	0.996	0.996	0.996	0.996
TPG	0.993	0.995	0.995	0.996	0.996	0.996	0.996	0.996	0.996
C	0.997	0.996	0.996	0.996	0.996	0.997	0.996	0.996	0.996
CT-Cω-Z	0.995	0.996	0.997	0.997	0.997	0.996	0.996	0.996	0.996
MC-HO-Z	0.997	0.996	0.997	0.996	0.996	0.996	0.996	0.996	0.996
SRPG-Z	0.996	0.996	0.997	0.997	0.997	0.997	0.997	0.997	0.997
CT-Wω-Z	0.997	0.996	0.997	0.996	0.996	0.996	0.996	0.996	0.996
CT-CW-Z	0.995	0.997	0.996	0.997	0.997	0.997	0.996	0.997	0.996
RPG-Z	0.998	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.996
TPG-Z	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.997
TES	0.995	0.996	0.996	0.996	0.996	0.996	0.996	0.996	0.996

Table S-XXXIII. $H_2O_2/D^{18}OOH$ isotope ratio for the 1-D torsional potential using the C scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Cω	0.817	0.847	0.859	0.867	0.870	0.872	0.873	0.873	0.873
MC-HO	0.817	0.847	0.859	0.867	0.870	0.872	0.873	0.874	0.874
SAS	0.817	0.848	0.859	0.870	0.874	0.876	0.877	0.877	0.875
SRC	0.874	0.874	0.873	0.873	0.873	0.873	0.873	0.873	0.873
SR-TDPPI-HS	0.830	0.854	0.863	0.868	0.871	0.872	0.873	0.873	0.873
SRPG	0.817	0.846	0.857	0.866	0.869	0.870	0.872	0.873	0.873
CT-ωW	0.817	0.847	0.859	0.867	0.870	0.872	0.873	0.874	0.874
CT-CW	0.788	0.832	0.848	0.862	0.867	0.869	0.871	0.872	0.873
RPG	0.816	0.846	0.857	0.866	0.869	0.871	0.872	0.873	0.873
TDPPI-HS	0.834	0.855	0.863	0.869	0.871	0.872	0.873	0.873	0.873
WK	0.826	0.854	0.863	0.869	0.871	0.872	0.873	0.873	0.873
MPG	0.856	0.859	0.865	0.869	0.871	0.872	0.873	0.873	0.873
TDPPI-AS	0.815	0.853	0.862	0.869	0.871	0.872	0.873	0.873	0.873
TPG	0.816	0.846	0.857	0.866	0.869	0.870	0.872	0.873	0.873
C	0.874	0.873	0.873	0.873	0.873	0.873	0.873	0.873	0.873
CT-Cω-Z	0.861	0.877	0.881	0.882	0.882	0.880	0.879	0.877	0.875
MC-HO-Z	0.862	0.877	0.881	0.882	0.882	0.881	0.879	0.878	0.876
SRPG-Z	0.859	0.876	0.880	0.881	0.880	0.880	0.878	0.876	0.875
CT-Wω-Z	0.862	0.877	0.881	0.882	0.882	0.881	0.879	0.878	0.876
CT-CW-Z	0.829	0.861	0.871	0.877	0.878	0.878	0.877	0.876	0.875
RPG-Z	0.860	0.875	0.880	0.881	0.880	0.879	0.878	0.876	0.875
TPG-Z	0.860	0.876	0.880	0.881	0.880	0.880	0.878	0.876	0.875
TES	0.834	0.856	0.863	0.869	0.871	0.872	0.873	0.873	0.873

Table S-XXXIV. $H_2O_2/H^{18}OOH$ isotope ratio for the 1-D torsional potential using the C scheme *I*

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Cω	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
MC-HO	0.996	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
SAS	0.996	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
SRC	0.999	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
SR-TDPPI-HS	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
SRPG	0.996	0.997	0.998	0.998	0.998	0.998	0.998	0.998	0.998
CT-ωW	0.996	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
CT-CW	0.997	0.999	0.998	0.998	0.998	0.998	0.998	0.998	0.998
RPG	0.998	0.997	0.998	0.998	0.998	0.998	0.998	0.998	0.998
TDPPI-HS	0.998	0.997	0.998	0.998	0.998	0.998	0.998	0.998	0.998
WK	0.997	0.997	0.998	0.998	0.998	0.998	0.998	0.998	0.998
MPG	0.999	0.997	0.998	0.998	0.998	0.998	0.998	0.998	0.998
TDPPI-AS	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
TPG	0.997	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
C	0.999	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
CT-Cω-Z	0.997	0.998	0.999	0.999	0.998	0.998	0.998	0.998	0.998
MC-HO-Z	0.998	0.998	0.999	0.998	0.998	0.998	0.998	0.998	0.998
SRPG-Z	0.999	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
CT-Wω-Z	0.998	0.998	0.999	0.998	0.998	0.998	0.998	0.998	0.998
CT-CW-Z	0.998	0.999	0.998	0.998	0.998	0.998	0.998	0.998	0.998
RPG-Z	1.000	0.998	0.998	0.998	0.999	0.998	0.998	0.998	0.998
TPG-Z	0.999	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
TES	0.997	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998

Table S-XXXV. H$_2$O$_2$/H^{18}OOD isotope ratio for the 1-D torsional potential using the C scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Cω	0.817	0.847	0.859	0.867	0.870	0.872	0.873	0.873	0.874
MC-HO	0.817	0.847	0.859	0.867	0.870	0.872	0.873	0.874	0.874
SAS	0.817	0.848	0.860	0.870	0.875	0.876	0.877	0.877	0.875
SRC	0.874	0.874	0.873	0.873	0.873	0.873	0.873	0.873	0.873
SR-TDPPI-HS	0.830	0.854	0.863	0.869	0.871	0.872	0.873	0.873	0.873
SRPG	0.817	0.846	0.857	0.866	0.869	0.870	0.872	0.873	0.873
CT-ωW	0.817	0.847	0.859	0.867	0.870	0.872	0.873	0.874	0.874
CT-CW	0.788	0.832	0.848	0.862	0.867	0.869	0.871	0.872	0.873
RPG	0.816	0.846	0.858	0.866	0.869	0.871	0.872	0.873	0.873
TDPPI-HS	0.834	0.855	0.863	0.869	0.871	0.872	0.873	0.873	0.873
WK	0.827	0.854	0.863	0.869	0.871	0.872	0.873	0.873	0.873
MPG	0.857	0.860	0.865	0.870	0.871	0.872	0.873	0.873	0.873
TDPPI-AS	0.815	0.853	0.863	0.869	0.871	0.872	0.873	0.873	0.873
TPG	0.816	0.846	0.857	0.866	0.869	0.871	0.872	0.873	0.873
C	0.874	0.873	0.873	0.873	0.873	0.873	0.873	0.873	0.873
CT-Cω-Z	0.861	0.877	0.881	0.882	0.882	0.880	0.879	0.877	0.875
MC-HO-Z	0.862	0.877	0.881	0.882	0.882	0.881	0.879	0.878	0.876
SRPG-Z	0.860	0.876	0.880	0.881	0.880	0.880	0.878	0.876	0.875
CT-Wω-Z	0.862	0.877	0.881	0.882	0.882	0.881	0.879	0.878	0.876
CT-CW-Z	0.829	0.861	0.871	0.877	0.878	0.878	0.877	0.876	0.875
RPG-Z	0.860	0.875	0.880	0.881	0.881	0.880	0.878	0.877	0.875
TPG-Z	0.860	0.876	0.880	0.881	0.881	0.880	0.878	0.876	0.875
TES	0.834	0.856	0.863	0.869	0.871	0.872	0.873	0.873	0.873

Table S-XXXVI. H_2O_2/D_2O_2 isotope ratio for the 1-D torsional potential using the R scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Rω	0.640	0.688	0.706	0.720	0.724	0.726	0.727	0.726	0.723
MC-HO	0.640	0.688	0.706	0.720	0.725	0.727	0.730	0.731	0.731
SAS	0.625	0.673	0.693	0.710	0.717	0.720	0.721	0.721	0.718
SRC	0.714	0.715	0.715	0.715	0.715	0.715	0.715	0.715	0.715
SR-TDPPI-HS	0.659	0.690	0.702	0.709	0.712	0.713	0.714	0.715	0.715
SRPG	0.625	0.671	0.689	0.703	0.708	0.711	0.713	0.714	0.715
CT-ωW	0.640	0.688	0.706	0.720	0.725	0.727	0.730	0.731	0.731
CT-RW	0.610	0.664	0.685	0.701	0.707	0.710	0.713	0.714	0.715
RPG	0.626	0.672	0.690	0.703	0.708	0.711	0.713	0.714	0.715
TDPPI-HS	0.664	0.693	0.703	0.710	0.712	0.713	0.714	0.715	0.715
WK	0.657	0.692	0.703	0.710	0.712	0.713	0.714	0.715	0.715
MPG	0.698	0.699	0.705	0.710	0.712	0.713	0.714	0.715	0.715
TDPPI-AS	0.651	0.690	0.702	0.710	0.712	0.713	0.714	0.715	0.715
TPG	0.625	0.671	0.690	0.703	0.708	0.711	0.713	0.714	0.715
C	0.715	0.715	0.715	0.715	0.715	0.715	0.715	0.715	0.715
CT-Rω-Z	0.705	0.733	0.741	0.743	0.742	0.740	0.737	0.732	0.726
MC-HO-Z	0.705	0.733	0.741	0.743	0.743	0.742	0.739	0.737	0.734
SRPG-Z	0.688	0.716	0.724	0.726	0.726	0.724	0.722	0.720	0.717
CT-Wω-Z	0.705	0.733	0.741	0.743	0.743	0.742	0.739	0.737	0.734
CT-RW-Z	0.673	0.707	0.719	0.724	0.724	0.724	0.722	0.720	0.717
RPG-Z	0.689	0.716	0.724	0.726	0.726	0.725	0.722	0.720	0.717
TPG-Z	0.689	0.716	0.724	0.726	0.726	0.724	0.722	0.720	0.717
TES	0.665	0.693	0.703	0.710	0.712	0.713	0.714	0.715	0.715

Table S-XXXVII. H_2O_2/HOOD isotope ratio for the 1-D torsional potential using the R scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Rω	0.821	0.850	0.861	0.869	0.871	0.872	0.871	0.869	0.863
MC-HO	0.821	0.849	0.861	0.869	0.872	0.874	0.875	0.876	0.876
SAS	0.795	0.824	0.837	0.847	0.851	0.853	0.854	0.853	0.852
SRC	0.849	0.850	0.850	0.850	0.850	0.850	0.850	0.850	0.850
SR-TDPPI-HS	0.812	0.834	0.841	0.846	0.848	0.849	0.849	0.850	0.850
SRPG	0.795	0.824	0.835	0.843	0.846	0.847	0.849	0.849	0.850
CT-ωW	0.821	0.850	0.861	0.869	0.872	0.874	0.875	0.876	0.876
CT-RW	0.777	0.815	0.830	0.841	0.845	0.846	0.848	0.849	0.850
RPG	0.796	0.824	0.835	0.843	0.846	0.847	0.849	0.849	0.850
TDPPI-HS	0.816	0.835	0.842	0.846	0.848	0.849	0.849	0.850	0.850
WK	0.810	0.834	0.841	0.847	0.848	0.849	0.849	0.850	0.850
MPG	0.839	0.839	0.843	0.847	0.848	0.849	0.849	0.850	0.850
TDPPI-AS	0.805	0.833	0.841	0.846	0.848	0.849	0.849	0.850	0.850
TPG	0.796	0.824	0.835	0.843	0.846	0.847	0.849	0.849	0.850
C	0.850	0.850	0.850	0.850	0.850	0.850	0.850	0.850	0.850
CT-Rω-Z	0.848	0.868	0.875	0.878	0.878	0.877	0.875	0.871	0.864
MC-HO-Z	0.848	0.868	0.875	0.878	0.880	0.880	0.879	0.878	0.877
SRPG-Z	0.821	0.841	0.848	0.852	0.853	0.853	0.852	0.852	0.851
CT-Wω-Z	0.848	0.868	0.875	0.879	0.879	0.879	0.879	0.878	0.877
CT-RW-Z	0.803	0.832	0.843	0.850	0.851	0.852	0.852	0.851	0.851
RPG-Z	0.821	0.841	0.848	0.852	0.853	0.853	0.852	0.852	0.851
TPG-Z	0.821	0.842	0.848	0.852	0.853	0.853	0.852	0.852	0.851
TES	0.816	0.835	0.842	0.847	0.848	0.849	0.849	0.850	0.850

Table S-XXXVIII. $H_2O_2/H_2{}^{18}O_2$ isotope ratio for the 1-D torsional potential using the R scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Rω	0.994	0.995	0.996	0.996	0.996	0.996	0.996	0.996	0.997
MC-HO	0.994	0.995	0.995	0.996	0.996	0.996	0.996	0.996	0.996
SAS	0.994	0.996	0.997	0.997	0.997	0.997	0.997	0.997	0.997
SRC	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.997
SR-TDPPI-HS	0.996	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.997
SRPG	0.994	0.996	0.997	0.997	0.997	0.997	0.997	0.997	0.997
CT-ωW	0.994	0.995	0.996	0.996	0.996	0.996	0.996	0.996	0.996
CT-RW	0.996	0.997	0.996	0.997	0.997	0.997	0.997	0.997	0.997
RPG	0.996	0.997	0.996	0.997	0.997	0.997	0.997	0.997	0.997
TDPPI-HS	0.996	0.996	0.997	0.997	0.997	0.997	0.997	0.997	0.997
WK	0.996	0.996	0.997	0.997	0.997	0.997	0.997	0.997	0.997
MPG	0.998	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.997
TDPPI-AS	0.996	0.996	0.997	0.997	0.997	0.997	0.997	0.997	0.997
TPG	0.994	0.996	0.997	0.997	0.997	0.997	0.997	0.997	0.997
C	0.998	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.997
CT-Rω-Z	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.997
MC-HO-Z	0.997	0.997	0.997	0.997	0.997	0.997	0.996	0.996	0.996
SRPG-Z	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.997	0.997
CT-Wω-Z	0.997	0.997	0.997	0.997	0.997	0.997	0.996	0.996	0.996
CT-RW-Z	0.999	0.998	0.998	0.998	0.998	0.997	0.997	0.997	0.997
RPG-Z	0.997	0.997	0.997	0.998	0.998	0.998	0.997	0.997	0.997
TPG-Z	0.998	0.998	0.998	0.998	0.997	0.997	0.997	0.997	0.997
TES	0.996	0.996	0.997	0.997	0.997	0.997	0.997	0.997	0.997

Table S-XXXIX. $H_2O_2/D^{18}OOH$ isotope ratio for the 1-D torsional potential using the R scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Rω	0.817	0.847	0.858	0.866	0.869	0.870	0.869	0.867	0.861
MC-HO	0.817	0.847	0.859	0.867	0.870	0.872	0.873	0.874	0.874
SAS	0.792	0.822	0.835	0.845	0.849	0.851	0.852	0.852	0.850
SRC	0.847	0.848	0.848	0.848	0.848	0.848	0.848	0.848	0.848
SR-TDPPI-HS	0.810	0.831	0.839	0.844	0.846	0.847	0.847	0.848	0.848
SRPG	0.792	0.822	0.833	0.841	0.844	0.845	0.847	0.847	0.848
CT-ωW	0.817	0.847	0.859	0.867	0.870	0.872	0.873	0.874	0.874
CT-RW	0.775	0.813	0.827	0.839	0.842	0.844	0.846	0.847	0.848
RPG	0.793	0.822	0.833	0.841	0.844	0.845	0.847	0.847	0.848
TDPPI-HS	0.813	0.833	0.840	0.844	0.846	0.847	0.847	0.848	0.848
WK	0.808	0.832	0.840	0.844	0.846	0.847	0.847	0.848	0.848
MPG	0.838	0.837	0.841	0.845	0.846	0.847	0.847	0.848	0.848
TDPPI-AS	0.803	0.831	0.839	0.844	0.846	0.847	0.847	0.848	0.848
TPG	0.793	0.822	0.833	0.841	0.844	0.845	0.847	0.847	0.848
C	0.848	0.848	0.848	0.848	0.848	0.848	0.848	0.848	0.848
CT-Rω-Z	0.845	0.867	0.873	0.876	0.876	0.876	0.873	0.869	0.862
MC-HO-Z	0.845	0.866	0.873	0.877	0.878	0.878	0.877	0.876	0.875
SRPG-Z	0.819	0.840	0.847	0.850	0.851	0.851	0.850	0.850	0.849
CT-Wω-Z	0.845	0.866	0.873	0.877	0.877	0.878	0.877	0.876	0.875
CT-RW-Z	0.801	0.831	0.841	0.848	0.849	0.850	0.850	0.850	0.849
RPG-Z	0.819	0.840	0.846	0.850	0.851	0.851	0.850	0.850	0.849
TPG-Z	0.819	0.840	0.847	0.850	0.851	0.851	0.851	0.850	0.849
TES	0.814	0.833	0.840	0.844	0.846	0.847	0.847	0.848	0.848

Table S-XL. $H_2O_2/H^{18}OOH$ isotope ratio for the 1-D torsional potential using the R scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Rω	0.996	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
MC-HO	0.996	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
SAS	0.997	0.998	0.998	0.999	0.998	0.998	0.999	0.999	0.999
SRC	0.998	0.999	0.998	0.999	0.999	0.998	0.999	0.998	0.999
SR-TDPPI-HS	0.997	0.998	0.998	0.999	0.999	0.998	0.999	0.999	0.999
SRPG	0.997	0.998	0.998	0.998	0.999	0.998	0.998	0.999	0.999
CT-ωW	0.996	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
CT-RW	0.998	0.999	0.998	0.998	0.998	0.999	0.999	0.999	0.999
RPG	0.998	0.998	0.999	0.999	0.998	0.998	0.999	0.999	0.999
TDPPI-HS	0.999	0.999	0.998	0.998	0.999	0.999	0.999	0.999	0.999
WK	0.997	0.999	0.998	0.999	0.999	0.998	0.999	0.999	0.999
MPG	0.999	0.999	0.998	0.999	0.999	0.998	0.998	0.999	0.999
TDPPI-AS	0.997	0.999	0.998	0.999	0.999	0.999	0.999	0.999	0.999
TPG	0.997	0.998	0.998	0.999	0.998	0.998	0.998	0.999	0.999
C	0.999	0.999	0.998	0.998	0.999	0.998	0.999	0.999	0.999
CT-Rω-Z	0.999	0.999	0.999	0.998	0.998	0.998	0.999	0.998	0.998
MC-HO-Z	0.999	0.998	0.999	0.998	0.998	0.998	0.998	0.998	0.998
SRPG-Z	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999
CT-Wω-Z	0.999	0.998	0.999	0.998	0.998	0.998	0.998	0.998	0.998
CT-RW-Z	1.000	0.998	0.999	0.999	0.999	0.999	0.999	0.999	0.999
RPG-Z	0.999	0.998	0.999	0.999	0.999	0.999	0.999	0.999	0.999
TPG-Z	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999
TES	0.998	0.999	0.998	0.999	0.999	0.998	0.999	0.999	0.999

Table S-XLI. $H_2O_2/H^{18}OOD$ isotope ratio for the 1-D torsional potential using the R scheme I

T(K)	200	300	400	600	800	1000	1500	2400	5000
CT-Rω	0.817	0.847	0.858	0.867	0.869	0.870	0.870	0.868	0.863
MC-HO	0.817	0.847	0.859	0.867	0.870	0.872	0.873	0.874	0.874
SAS	0.795	0.825	0.838	0.848	0.852	0.854	0.855	0.855	0.853
SRC	0.850	0.851	0.851	0.851	0.851	0.851	0.851	0.851	0.851
SR-TDPPI-HS	0.813	0.835	0.842	0.847	0.849	0.850	0.851	0.851	0.851
SRPG	0.795	0.825	0.836	0.844	0.847	0.848	0.850	0.851	0.851
CT-ωW	0.817	0.847	0.859	0.867	0.870	0.872	0.873	0.874	0.874
CT-RW	0.779	0.817	0.831	0.842	0.846	0.848	0.849	0.850	0.851
RPG	0.797	0.825	0.836	0.844	0.847	0.848	0.850	0.851	0.851
TDPPI-HS	0.817	0.836	0.843	0.847	0.849	0.850	0.851	0.851	0.851
WK	0.812	0.835	0.843	0.848	0.849	0.850	0.850	0.851	0.851
MPG	0.842	0.841	0.844	0.848	0.849	0.850	0.850	0.851	0.851
TDPPI-AS	0.807	0.834	0.842	0.847	0.849	0.850	0.851	0.851	0.851
TPG	0.796	0.824	0.836	0.844	0.847	0.848	0.850	0.850	0.851
C	0.851	0.851	0.851	0.851	0.851	0.851	0.851	0.851	0.851
CT-Rω-Z	0.848	0.868	0.874	0.877	0.877	0.876	0.874	0.870	0.864
MC-HO-Z	0.848	0.868	0.875	0.877	0.878	0.878	0.877	0.876	0.875
SRPG-Z	0.825	0.845	0.851	0.854	0.855	0.854	0.854	0.853	0.852
CT-Wω-Z	0.848	0.868	0.875	0.878	0.878	0.878	0.877	0.876	0.875
CT-RW-Z	0.808	0.836	0.846	0.852	0.853	0.854	0.853	0.853	0.852
RPG-Z	0.824	0.845	0.851	0.854	0.855	0.855	0.854	0.853	0.852
TPG-Z	0.825	0.844	0.851	0.854	0.855	0.855	0.854	0.853	0.852
TES	0.818	0.837	0.843	0.848	0.849	0.850	0.851	0.851	0.851

Table S-XLII. H_2O_2/D_2O_2 isotope ratio for full-D partition functions using the C scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Cω	5.36E-04	2.87E-03	1.46E-02	3.15E-02	4.86E-02	8.12E-02	1.10E-01
MC-HO	5.36E-04	2.87E-03	1.46E-02	3.15E-02	4.86E-02	8.13E-02	1.10E-01
SAS	5.35E-04	2.88E-03	1.47E-02	3.18E-02	4.91E-02	8.21E-02	1.11E-01
SRC	5.68E-04	2.97E-03	1.48E-02	3.17E-02	4.87E-02	8.12E-02	1.09E-01
SR-TDPPI-HS	5.43E-04	2.90E-03	1.46E-02	3.15E-02	4.86E-02	8.11E-02	1.09E-01
SRPG	5.34E-04	2.86E-03	1.45E-02	3.14E-02	4.84E-02	8.10E-02	1.09E-01
CT-ωW	5.36E-04	2.87E-03	1.46E-02	3.15E-02	4.86E-02	8.13E-02	1.10E-01
CT-CW	5.15E-04	2.80E-03	1.44E-02	3.12E-02	4.83E-02	8.09E-02	1.09E-01
RPG	5.34E-04	2.86E-03	1.45E-02	3.14E-02	4.84E-02	8.10E-02	1.09E-01
TDPPI-HS	5.46E-04	2.90E-03	1.46E-02	3.15E-02	4.86E-02	8.11E-02	1.09E-01
WK	5.44E-04	2.90E-03	1.46E-02	3.15E-02	4.86E-02	8.11E-02	1.09E-01
MPG	5.50E-04	2.91E-03	1.47E-02	3.15E-02	4.86E-02	8.11E-02	1.09E-01
TDPPI-AS	5.42E-04	2.90E-03	1.46E-02	3.15E-02	4.86E-02	8.11E-02	1.09E-01
TPG	5.34E-04	2.86E-03	1.45E-02	3.14E-02	4.84E-02	8.10E-02	1.09E-01
C	5.68E-04	2.97E-03	1.48E-02	3.17E-02	4.87E-02	8.12E-02	1.09E-01
CT-Cω-Z	6.85E-04	3.45E-03	1.65E-02	3.45E-02	5.23E-02	8.53E-02	1.13E-01
MC-HO-Z	6.85E-04	3.45E-03	1.65E-02	3.45E-02	5.23E-02	8.54E-02	1.13E-01
SRPG-Z	6.83E-04	3.44E-03	1.65E-02	3.44E-02	5.21E-02	8.51E-02	1.13E-01
CT-Wω-Z	6.85E-04	3.45E-03	1.65E-02	3.45E-02	5.23E-02	8.54E-02	1.13E-01
CT-CW-Z	6.59E-04	3.37E-03	1.63E-02	3.42E-02	5.20E-02	8.49E-02	1.13E-01
RPG-Z	6.83E-04	3.44E-03	1.65E-02	3.44E-02	5.21E-02	8.51E-02	1.13E-01
TPG-Z	6.83E-04	3.44E-03	1.65E-02	3.44E-02	5.21E-02	8.51E-02	1.13E-01
IRPG	5.48E-04	2.91E-03	1.47E-02	3.16E-02	4.87E-02	8.14E-02	1.10E-01
IRPG-Z	6.58E-04	3.34E-03	1.61E-02	3.39E-02	5.15E-02	8.45E-02	1.12E-01
accurate	6.64E-04	3.37E-03	1.62E-02	3.40E-02	5.16E-02	8.43E-02	1.12E-01

Table S-XLIII. H_2O_2/HOOD isotope ratio for full-D partition functions using the C scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Cω	1.16E-02	2.68E-02	6.04E-02	8.88E-02	1.10E-01	1.43E-01	1.66E-01
MC-HO	1.16E-02	2.68E-02	6.04E-02	8.88E-02	1.10E-01	1.43E-01	1.66E-01
SAS	1.16E-02	2.68E-02	6.06E-02	8.92E-02	1.11E-01	1.43E-01	1.66E-01
SRC	1.19E-02	2.73E-02	6.08E-02	8.91E-02	1.10E-01	1.43E-01	1.66E-01
SR-TDPPI-HS	1.17E-02	2.69E-02	6.05E-02	8.88E-02	1.10E-01	1.42E-01	1.66E-01
SRPG	1.16E-02	2.68E-02	6.04E-02	8.87E-02	1.10E-01	1.42E-01	1.65E-01
CT-ωW	1.16E-02	2.68E-02	6.04E-02	8.88E-02	1.10E-01	1.43W-01	1.66E-01
CT-CW	1.14E-02	2.65E-02	6.01E-02	8.84E-02	1.10E-01	1.42E-01	1.65E-01
RPG	1.16E-02	2.68E-02	6.04E-02	8.87E-02	1.10E-01	1.42E-01	1.65E-01
TDPPI-HS	1.17E-02	2.70E-02	6.06E-02	8.88E-02	1.10E-01	1.42E-01	1.66E-01
WK	1.17E-02	2.70E-02	6.06E-02	8.88E-02	1.10E-01	1.42E-01	1.66E-01
MPG	1.17E-02	2.70E-02	6.06E-02	8.89E-02	1.10E-01	1.42E-01	1.66E-01
TDPPI-AS	1.17E-02	2.69E-02	6.05E-02	8.88E-02	1.10E-01	1.42E-01	1.66E-01
TPG	1.16E-02	2.68E-02	6.04E-02	8.87E-02	1.10E-01	1.42E-01	1.65E-01
C	1.19E-02	2.73E-02	6.08E-02	8.91E-02	1.10E-01	1.43E-01	1.66E-01
CT-Cω-Z	1.31E-02	2.95E-02	6.44E-02	9.31E-02	1.14E-01	1.46E-01	1.68E-01
MC-HO-Z	1.31E-02	2.95E-02	6.44E-02	9.31E-02	1.15E-01	1.46E-01	1.68E-01
SRPG-Z	1.31E-02	2.94E-02	6.43E-02	9.29E-02	1.14E-01	1.46E-01	1.68E-01
CT-Wω-Z	1.31E-02	2.95E-02	6.44E-02	9.31E-02	1.15E-01	1.46E-01	1.68E-01
CT-CW-Z	1.29E-02	2.91E-02	6.40E-02	9.27E-02	1.14E-01	1.46E-01	1.68E-01
RPG-Z	1.31E-02	2.94E-02	6.43E-02	9.29E-02	1.14E-01	1.46E-01	1.68E-01
TPG-Z	1.31E-02	2.94E-02	6.43E-02	9.29E-02	1.14E-01	1.46E-01	1.68E-01
IRPG	1.17E-02	2.70E-02	6.07E-02	8.90E-02	1.10E-01	1.43E-01	1.65E-01
IRPG-Z	1.28E-02	2.89E-02	6.35E-02	9.21E-02	1.14E-01	1.45E-01	1.67E-01
accurate	1.29E-02	2.91E-02	6.36E-02	9.22E-02	1.14E-01	1.45E-01	1.67E-01

Table S-XLIV. $H_2O_2/H_2^{18}O_2$ isotope ratio for full-D partition functions using the C scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Cω	7.16E-01	7.53E-01	7.88E-01	8.03E-01	8.11E-01	8.21E-01	8.26E-01
MC-HO	7.16E-01	7.53E-01	7.88E-01	8.03E-01	8.11E-01	8.21E-01	8.26E-01
SAS	7.17E-01	7.53E-01	7.88E-01	8.03E-01	8.12E-01	8.21E-01	8.26E-01
SRC	7.17E-01	7.54E-01	7.88E-01	8.03E-01	8.11E-01	8.21E-01	8.26E-01
SR-TDPPI-HS	7.17E-01	7.53E-01	7.88E-01	8.03E-01	8.11E-01	8.21E-01	8.26E-01
SRPG	7.16E-01	7.53E-01	7.88E-01	8.03E-01	8.11E-01	8.21E-01	8.26E-01
CT-ωW	7.16E-01	7.53E-01	7.88E-01	8.03E-01	8.11E-01	8.21E-01	8.26E-01
CT-CW	7.16E-01	7.53E-01	7.88E-01	8.03E-01	8.11E-01	8.21E-01	8.26E-01
RPG	7.16E-01	7.53E-01	7.88E-01	8.03E-01	8.11E-01	8.21E-01	8.26E-01
TDPPI-HS	7.17E-01	7.53E-01	7.88E-01	8.03E-01	8.11E-01	8.21E-01	8.26E-01
WK	7.17E-01	7.53E-01	7.88E-01	8.03E-01	8.11E-01	8.21E-01	8.26E-01
MPG	7.17E-01	7.53E-01	7.88E-01	8.03E-01	8.11E-01	8.21E-01	8.26E-01
TDPPI-AS	7.17E-01	7.53E-01	7.88E-01	8.03E-01	8.11E-01	8.21E-01	8.26E-01
TPG	7.17E-01	7.53E-01	7.88E-01	8.03E-01	8.11E-01	8.21E-01	8.26E-01
C	7.17E-01	7.54E-01	7.88E-01	8.03E-01	8.12E-01	8.21E-01	8.26E-01
CT-Cω-Z	7.22E-01	7.58E-01	7.91E-01	8.05E-01	8.13E-01	8.22E-01	8.27E-01
MC-HO-Z	7.22E-01	7.58E-01	7.91E-01	8.05E-01	8.13E-01	8.22E-01	8.27E-01
SRPG-Z	7.22E-01	7.58E-01	7.91E-01	8.06E-01	8.13E-01	8.22E-01	8.27E-01
CT-Wω-Z	7.22E-01	7.58E-01	7.91E-01	8.05E-01	8.13E-01	8.22E-01	8.27E-01
CT-CW-Z	7.22E-01	7.58E-01	7.91E-01	8.06E-01	8.13E-01	8.22E-01	8.27E-01
RPG-Z	7.22E-01	7.58E-01	7.91E-01	8.06E-01	8.13E-01	8.22E-01	8.27E-01
TPG-Z	7.22E-01	7.58E-01	7.91E-01	8.06E-01	8.13E-01	8.22E-01	8.27E-01
IRPG	7.16E-01	7.53E-01	7.87E-01	8.03E-01	8.11E-01	8.20E-01	8.24E-01
IRPG-Z	7.21E-01	7.57E-01	7.90E-01	8.05E-01	8.13E-01	8.21E-01	8.25E-01
accurate	7.20E-01	7.57E-01	7.91E-01	8.04E-01	8.12E-01	8.21E-01	8.24E-01

Table S-XLV. H$_2$O$_2$/D^{18}OOH isotope ratio for full-D partition functions using the C scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Cω	9.72E-03	2.31E-02	5.35E-02	7.94E-02	9.92E-02	1.29E-01	1.51E-01
MC-HO	9.72E-03	2.31E-02	5.35E-02	7.94E-02	9.92E-02	1.29E-01	1.51E-01
SAS	9.71E-03	2.32E-02	5.37E-02	7.98E-02	9.97E-02	1.30E-01	1.51E-01
SRC	1.00E-02	2.35E-02	5.38E-02	7.97E-02	9.94E-02	1.29E-01	1.50E-01
SR-TDPPI-HS	9.79E-03	2.32E-02	5.36E-02	7.95E-02	9.92E-02	1.29E-01	1.50E-01
SRPG	9.70E-03	2.31E-02	5.34E-02	7.93E-02	9.91E-02	1.29E-01	1.50E-01
CT-ωW	9.72E-03	2.31E-02	5.35E-02	7.94E-02	9.92E-02	1.29W-01	1.51E-01
CT-CW	9.53E-03	2.29E-02	5.31E-02	7.91E-02	9.89E-02	1.29E-01	1.50E-01
RPG	9.70E-03	2.31E-02	5.34E-02	7.93E-02	9.91E-02	1.29E-01	1.50E-01
TDPPI-HS	9.81E-03	2.33E-02	5.36E-02	7.95E-02	9.92E-02	1.29E-01	1.50E-01
WK	9.80E-03	2.33E-02	5.36E-02	7.95E-02	9.92E-02	1.29E-01	1.50E-01
MPG	9.86E-03	2.33E-02	5.36E-02	7.95E-02	9.92E-02	1.29E-01	1.50E-01
TDPPI-AS	9.78E-03	2.32E-02	5.36E-02	7.95E-02	9.92E-02	1.29E-01	1.50E-01
TPG	9.70E-03	2.31E-02	5.34E-02	7.93E-02	9.91E-02	1.29E-01	1.50E-01
C	1.00E-02	2.35E-02	5.39E-02	7.97E-02	9.94E-02	1.29E-01	1.50E-01
CT-Cω-Z	1.10E-02	2.55E-02	5.70E-02	8.34E-02	1.03E-01	1.32E-01	1.53E-01
MC-HO-Z	1.10E-02	2.55E-02	5.70E-02	8.34E-02	1.03E-01	1.33E-01	1.53E-01
SRPG-Z	1.10E-02	2.54E-02	5.70E-02	8.33E-02	1.03E-01	1.32E-01	1.53E-01
CT-Wω-Z	1.11E-02	2.55E-02	5.70E-02	8.34E-02	1.03E-01	1.33E-01	1.53E-01
CT-CW-Z	1.08E-02	2.52E-02	5.67E-02	8.30E-02	1.03E-01	1.32E-01	1.53E-01
RPG-Z	1.10E-02	2.54E-02	5.70E-02	8.32E-02	1.03E-01	1.32E-01	1.53E-01
TPG-Z	1.10E-02	2.54E-02	5.70E-02	8.32E-02	1.03E-01	1.32E-01	1.53E-01
IRPG	9.83E-03	2.33E-02	5.37E-02	7.96E-02	9.94E-02	1.29E-01	1.50E-01
IRPG-Z	1.08E-02	2.50E-02	5.62E-02	8.25E-02	1.02E-01	1.32E-01	1.52E-01
accurate	1.09E-02	2.51E-02	5.64E-02	8.25E-02	1.02E-01	1.32E-01	1.52E-01

Table S-XLVI. $H_2O_2/H^{18}OOH$ isotope ratio for full-D partition functions using the C scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Cω	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54E-01	4.56E-01
MC-HO	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54E-01	4.56E-01
SAS	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.52E-01	4.54E-01	4.56E-01
SRC	4.25E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54E-01	4.56E-01
SR-TDPPI-HS	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54E-01	4.56E-01
SRPG	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54E-01	4.56E-01
CT-ωW	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54W-01	4.56E-01
CT-CW	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54E-01	4.56E-01
RPG	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54E-01	4.56E-01
TDPPI-HS	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54E-01	4.56E-01
WK	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54E-01	4.56E-01
MPG	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54E-01	4.56E-01
TDPPI-AS	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54E-01	4.56E-01
TPG	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54E-01	4.56E-01
C	4.25E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54E-01	4.56E-01
CT-Cω-Z	4.20E-01	4.32E-01	4.43E-01	4.47E-01	4.50E-01	4.53E-01	4.55E-01
MC-HO-Z	4.20E-01	4.32E-01	4.43E-01	4.47E-01	4.50E-01	4.53E-01	4.55E-01
SRPG-Z	4.20E-01	4.32E-01	4.43E-01	4.47E-01	4.50E-01	4.53E-01	4.55E-01
CT-Wω-Z	4.20E-01	4.32E-01	4.43E-01	4.47E-01	4.50E-01	4.53E-01	4.55E-01
CT-CW-Z	4.20E-01	4.32E-01	4.43E-01	4.47E-01	4.50E-01	4.53E-01	4.55E-01
RPG-Z	4.20E-01	4.32E-01	4.43E-01	4.47E-01	4.50E-01	4.53E-01	4.55E-01
TPG-Z	4.20E-01	4.32E-01	4.43E-01	4.47E-01	4.50E-01	4.53E-01	4.55E-01
IRPG	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.52E-01	4.54E-01	4.54E-01
IRPG-Z	4.20E-01	4.31E-01	4.42E-01	4.47E-01	4.50E-01	4.53E-01	4.53E-01
accurate	4.27E-01	4.37E-01	4.46E-01	4.49E-01	4.52E-01	4.54E-01	4.55E-01

Table S-XLVII. H$_2$O$_2$/H^{18}OOD isotope ratio for full-D partition functions using the C scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Cω	9.80E-03	2.33E-02	5.36E-02	7.95E-02	9.93E-02	1.29E-01	1.51E-01
MC-HO	9.80E-03	2.33E-02	5.36E-02	7.96E-02	9.93E-02	1.29E-01	1.51E-01
SAS	9.79E-03	2.33E-02	5.38E-02	7.99E-02	9.98E-02	1.30E-01	1.51E-01
SRC	1.01E-02	2.37E-02	5.40E-02	7.98E-02	9.95E-02	1.29E-01	1.50E-01
SR-TDPPI-HS	9.87E-03	2.34E-02	5.37E-02	7.96E-02	9.93E-02	1.29E-01	1.50E-01
SRPG	9.78E-03	2.32E-02	5.36E-02	7.94E-02	9.92E-02	1.29E-01	1.50E-01
CT-ωW	9.80E-03	2.33E-02	5.36E-02	7.96E-02	9.93E-02	1.29W-01	1.51E-01
CT-CW	9.61E-03	2.30E-02	5.33E-02	7.92E-02	9.90E-02	1.29E-01	1.50E-01
RPG	9.78E-03	2.32E-02	5.36E-02	7.95E-02	9.92E-02	1.29E-01	1.50E-01
TDPPI-HS	9.89E-03	2.34E-02	5.37E-02	7.96E-02	9.93E-02	1.29E-01	1.50E-01
WK	9.88E-03	2.34E-02	5.37E-02	7.96E-02	9.93E-02	1.29E-01	1.50E-01
MPG	9.94E-03	2.34E-02	5.38E-02	7.96E-02	9.93E-02	1.29E-01	1.50E-01
TDPPI-AS	9.86E-03	2.34E-02	5.37E-02	7.96E-02	9.93E-02	1.29E-01	1.50E-01
TPG	9.78E-03	2.32E-02	5.36E-02	7.95E-02	9.92E-02	1.29E-01	1.50E-01
C	1.01E-02	2.37E-02	5.40E-02	7.98E-02	9.95E-02	1.29E-01	1.50E-01
CT-Cω-Z	1.11E-02	2.56E-02	5.72E-02	8.35E-02	1.03E-01	1.32E-01	1.53E-01
MC-HO-Z	1.11E-02	2.56E-02	5.72E-02	8.35E-02	1.03E-01	1.33E-01	1.53E-01
SRPG-Z	1.11E-02	2.56E-02	5.71E-02	8.34E-02	1.03E-01	1.32E-01	1.53E-01
CT-Wω-Z	1.11E-02	2.56E-02	5.72E-02	8.35E-02	1.03E-01	1.33E-01	1.53E-01
CT-CW-Z	1.09E-02	2.53E-02	5.68E-02	8.31E-02	1.03E-01	1.32E-01	1.53E-01
RPG-Z	1.11E-02	2.56E-02	5.71E-02	8.34E-02	1.03E-01	1.32E-01	1.53E-01
TPG-Z	1.11E-02	2.56E-02	5.71E-02	8.34E-02	1.03E-01	1.32E-01	1.53E-01
IRPG	9.91E-03	2.34E-02	5.38E-02	7.97E-02	9.95E-02	1.29E-01	1.50E-01
IRPG-Z	1.09E-02	2.51E-02	5.64E-02	8.26E-02	1.02E-01	1.32E-01	1.52E-01
accurate	1.10E-02	2.53E-02	5.66E-02	8.27E-02	1.02E-01	1.32E-01	1.52E-01

Table S-XLVIII. H_2O_2/D_2O_2 isotope ratio for full-D partition functions using the R scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Rω	5.36E-04	2.87E-03	1.46E-02	3.15E-02	4.85E-02	8.10E-02	1.09E-01
MC-HO	5.36E-04	2.87E-03	1.46E-02	3.15E-02	4.86E-02	8.13E-02	1.10E-01
SAS	5.24E-04	2.82E-03	1.44E-02	3.11E-02	4.81E-02	8.03E-02	1.08E-01
SRC	5.57E-04	2.91E-03	1.45E-02	3.11E-02	4.77E-02	7.96E-02	1.07E-01
SR-TDPPI-HS	5.38E-04	2.85E-03	1.44E-02	3.09E-02	4.76E-02	7.95E-02	1.07E-01
SRPG	5.23E-04	2.81E-03	1.43E-02	3.08E-02	4.75E-02	7.94E-02	1.07E-01
CT-ωW	5.36E-04	2.87E-03	1.46E-02	3.15E-02	4.86E-02	8.13E-02	1.10E-01
CT-RW	5.17E-04	2.79E-03	1.42E-02	3.07E-02	4.74E-02	7.93E-02	1.07E-01
RPG	5.23E-04	2.81E-03	1.43E-02	3.08E-02	4.75E-02	7.94E-02	1.07E-01
TDPPI-HS	5.40E-04	2.86E-03	1.44E-02	3.09E-02	4.76E-02	7.95E-02	1.07E-01
WK	5.39E-04	2.86E-03	1.44E-02	3.09E-02	4.76E-02	7.95E-02	1.07E-01
MPG	5.45E-04	2.87E-03	1.44E-02	3.09E-02	4.76E-02	7.95E-02	1.07E-01
TDPPI-AS	5.38E-04	2.86E-03	1.44E-02	3.09E-02	4.76E-02	7.95E-02	1.07E-01
TPG	5.23E-04	2.81E-03	1.43E-02	3.08E-02	4.75E-02	7.94E-02	1.07E-01
C	5.57E-04	2.91E-03	1.45E-02	3.11E-02	4.77E-02	7.96E-02	1.07E-01
CT-Rω-Z	6.85E-04	3.45E-03	1.65E-02	3.45E-02	5.22E-02	8.51E-02	1.12E-01
MC-HO-Z	6.85E-04	3.45E-03	1.65E-02	3.45E-02	5.23E-02	8.54E-02	1.13E-01
SRPG-Z	6.69E-04	3.38E-03	1.61E-02	3.37E-02	5.11E-02	8.34E-02	1.11E-01
CT-Wω-Z	6.85E-04	3.45E-03	1.65E-02	3.45E-02	5.23E-02	8.54E-02	1.13E-01
CT-RW-Z	6.62E-04	3.35E-03	1.61E-02	3.37E-02	5.10E-02	8.33E-02	1.11E-01
RPG-Z	6.69E-04	3.38E-03	1.61E-02	3.38E-02	5.11E-02	8.34E-02	1.11E-01
TPG-Z	6.69E-04	3.38E-03	1.61E-02	3.38E-02	5.11E-02	8.34E-02	1.11E-01
IRPG	5.53E-04	2.93E-03	1.47E-02	3.17E-02	4.88E-02	8.14E-02	1.10E-01
IRPG-Z	6.63E-04	3.36E-03	1.61E-02	3.39E-02	5.15E-02	8.44E-02	1.12E-01
accurate	6.64E-04	3.37E-03	1.62E-02	3.40E-02	5.16E-02	8.43E-02	1.12E-01

Table S-XLIX. H_2O_2/HOOD isotope ratio for full-D partition functions using the R scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Rω	1.16E-02	2.68E-02	6.04E-02	8.87E-02	1.10E-01	1.42E-01	1.64E-01
MC-HO	1.16E-02	2.68E-02	6.04E-02	8.88E-02	1.10E-01	1.43E-01	1.66E-01
SAS	1.12E-02	2.61E-02	5.89E-02	8.66E-02	1.08E-01	1.39E-01	1.61E-01
SRC	1.16E-02	2.65E-02	5.91E-02	8.65E-02	1.07E-01	1.38E-01	1.61E-01
SR-TDPPI-HS	1.14E-02	2.62E-02	5.88E-02	8.63E-02	1.07E-01	1.38E-01	1.61E-01
SRPG	1.12E-02	2.60E-02	5.86E-02	8.61E-02	1.07E-01	1.38E-01	1.61E-01
CT-ωW	1.16E-02	2.68E-02	6.04E-02	8.88E-02	1.10E-01	1.43E-01	1.66E-01
CT-RW	1.11E-02	2.58E-02	5.84E-02	8.59E-02	1.07E-01	1.38E-01	1.61E-01
RPG	1.12E-02	2.60E-02	5.86E-02	8.61E-02	1.07E-01	1.38E-01	1.61E-01
TDPPI-HS	1.14E-02	2.62E-02	5.88E-02	8.63E-02	1.07E-01	1.38E-01	1.61E-01
WK	1.14E-02	2.62E-02	5.88E-02	8.63E-02	1.07E-01	1.38E-01	1.61E-01
MPG	1.14E-02	2.63E-02	5.89E-02	8.63E-02	1.07E-01	1.38E-01	1.61E-01
TDPPI-AS	1.14E-02	2.62E-02	5.88E-02	8.63E-02	1.07E-01	1.38E-01	1.61E-01
TPG	1.12E-02	2.60E-02	5.86E-02	8.61E-02	1.07E-01	1.38E-01	1.61E-01
C	1.16E-02	2.65E-02	5.91E-02	8.65E-02	1.07E-01	1.38E-01	1.61E-01
CT-Rω-Z	1.31E-02	2.95E-02	6.43E-02	9.29E-02	1.14E-01	1.46E-01	1.67E-01
MC-HO-Z	1.31E-02	2.95E-02	6.44E-02	9.31E-02	1.15E-01	1.46E-01	1.68E-01
SRPG-Z	1.27E-02	2.86E-02	6.24E-02	9.02E-02	1.11E-01	1.42E-01	1.63E-01
CT-Wω-Z	1.31E-02	2.95E-02	6.44E-02	9.31E-02	1.15E-01	1.46E-01	1.68E-01
CT-RW-Z	1.26E-02	2.84E-02	6.22E-02	9.01E-02	1.11E-01	1.42E-01	1.63E-01
RPG-Z	1.27E-02	2.86E-02	6.24E-02	9.02E-02	1.11E-01	1.42E-01	1.63E-01
TPG-Z	1.27E-02	2.86E-02	6.24E-02	9.02E-02	1.11E-01	1.42E-01	1.63E-01
IRPG	1.17E-02	2.70E-02	6.07E-02	8.90E-02	1.10E-01	1.43E-01	1.65E-01
IRPG-Z	1.30E-02	2.92E-02	6.40E-02	9.26E-02	1.14E-01	1.46E-01	1.67E-01
accurate	1.29E-02	2.91E-02	6.36E-02	9.22E-02	1.14E-01	1.45E-01	1.67E-01

Table S-L. $H_2O_2/H_2{}^{18}O_2$ isotope ratio for full-D partition functions using the R scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Rω	7.16E-01	7.53E-01	7.88E-01	8.03E-01	8.11E-01	8.21E-01	8.26E-01
MC-HO	7.16E-01	7.53E-01	7.88E-01	8.03E-01	8.11E-01	8.21E-01	8.26E-01
SAS	7.17E-01	7.54E-01	7.88E-01	8.04E-01	8.12E-01	8.21E-01	8.27E-01
SRC	7.18E-01	7.54E-01	7.89E-01	8.04E-01	8.12E-01	8.21E-01	8.27E-01
SR-TDPPI-HS	7.17E-01	7.54E-01	7.88E-01	8.04E-01	8.12E-01	8.21E-01	8.27E-01
SRPG	7.17E-01	7.54E-01	7.88E-01	8.04E-01	8.12E-01	8.21E-01	8.27E-01
CT-ωW	7.16E-01	7.53E-01	7.88E-01	8.03E-01	8.11E-01	8.21E-01	8.26E-01
CT-RW	7.17E-01	7.54E-01	7.88E-01	8.04E-01	8.12E-01	8.21E-01	8.27E-01
RPG	7.17E-01	7.54E-01	7.88E-01	8.04E-01	8.12E-01	8.21E-01	8.27E-01
TDPPI-HS	7.17E-01	7.54E-01	7.89E-01	8.04E-01	8.12E-01	8.21E-01	8.27E-01
WK	7.17E-01	7.54E-01	7.88E-01	8.04E-01	8.12E-01	8.21E-01	8.27E-01
MPG	7.18E-01	7.54E-01	7.88E-01	8.04E-01	8.12E-01	8.21E-01	8.27E-01
TDPPI-AS	7.17E-01	7.54E-01	7.88E-01	8.04E-01	8.12E-01	8.21E-01	8.27E-01
TPG	7.17E-01	7.54E-01	7.88E-01	8.04E-01	8.12E-01	8.21E-01	8.27E-01
C	7.18E-01	7.54E-01	7.89E-01	8.04E-01	8.12E-01	8.21E-01	8.27E-01
CT-Rω-Z	7.22E-01	7.58E-01	7.91E-01	8.05E-01	8.13E-01	8.22E-01	8.27E-01
MC-HO-Z	7.22E-01	7.58E-01	7.91E-01	8.05E-01	8.13E-01	8.22E-01	8.27E-01
SRPG-Z	7.23E-01	7.58E-01	7.92E-01	8.06E-01	8.14E-01	8.23E-01	8.28E-01
CT-Wω-Z	7.22E-01	7.58E-01	7.91E-01	8.05E-01	8.13E-01	8.22E-01	8.27E-01
CT-RW-Z	7.23E-01	7.58E-01	7.92E-01	8.06E-01	8.14E-01	8.23E-01	8.28E-01
RPG-Z	7.23E-01	7.58E-01	7.92E-01	8.06E-01	8.14E-01	8.23E-01	8.28E-01
TPG-Z	7.23E-01	7.58E-01	7.92E-01	8.06E-01	8.14E-01	8.23E-01	8.28E-01
IRPG	7.16E-01	7.53E-01	7.87E-01	8.03E-01	8.11E-01	8.20E-01	8.24E-01
IRPG-Z	7.21E-01	7.57E-01	7.90E-01	8.05E-01	8.13E-01	8.21E-01	8.25E-01
accurate	7.20E-01	7.57E-01	7.91E-01	8.04E-01	8.12E-01	8.21E-01	8.24E-01

Table S-LI. $H_2O_2/D^{18}OOH$ isotope ratio for full-D partition functions using the R scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Rω	9.72E-03	2.31E-02	5.34E-02	7.93E-02	9.90E-02	1.29E-01	1.49E-01
MC-HO	9.72E-03	2.31E-02	5.35E-02	7.94E-02	9.92E-02	1.29E-01	1.51E-01
SAS	9.43E-03	2.25E-02	5.21E-02	7.75E-02	9.69E-02	1.26E-01	1.47E-01
SRC	9.72E-03	2.28E-02	5.23E-02	7.74E-02	9.65E-02	1.25E-01	1.46E-01
SR-TDPPI-HS	9.53E-03	2.26E-02	5.21E-02	7.72E-02	9.64E-02	1.25E-01	1.46E-01
SRPG	9.42E-03	2.24E-02	5.19E-02	7.70E-02	9.62E-02	1.25E-01	1.46E-01
CT-ωW	9.72E-03	2.31E-02	5.35E-02	7.94E-02	9.92E-02	1.29W-01	1.51E-01
CT-RW	9.32E-03	2.23E-02	5.17E-02	7.69E-02	9.61E-02	1.25E-01	1.46E-01
RPG	9.42E-03	2.24E-02	5.19E-02	7.70E-02	9.62E-02	1.25E-01	1.46E-01
TDPPI-HS	9.55E-03	2.26E-02	5.21E-02	7.72E-02	9.64E-02	1.25E-01	1.46E-01
WK	9.54E-03	2.26E-02	5.21E-02	7.72E-02	9.64E-02	1.25E-01	1.46E-01
MPG	9.60E-03	2.27E-02	5.21E-02	7.72E-02	9.64E-02	1.25E-01	1.46E-01
TDPPI-AS	9.53E-03	2.26E-02	5.21E-02	7.72E-02	9.64E-02	1.25E-01	1.46E-01
TPG	9.42E-03	2.24E-02	5.19E-02	7.70E-02	9.62E-02	1.25E-01	1.46E-01
C	9.72E-03	2.28E-02	5.23E-02	7.74E-02	9.65E-02	1.25E-01	1.46E-01
CT-Rω-Z	1.10E-02	2.55E-02	5.70E-02	8.32E-02	1.03E-01	1.32E-01	1.52E-01
MC-HO-Z	1.10E-02	2.55E-02	5.70E-02	8.34E-02	1.03E-01	1.33E-01	1.53E-01
SRPG-Z	1.07E-02	2.47E-02	5.53E-02	8.08E-02	1.00E-01	1.28E-01	1.48E-01
CT-Wω-Z	1.11E-02	2.55E-02	5.70E-02	8.34E-02	1.03E-01	1.33E-01	1.53E-01
CT-RW-Z	1.06E-02	2.46E-02	5.51E-02	8.07E-02	9.99E-02	1.28E-01	1.48E-01
RPG-Z	1.07E-02	2.47E-02	5.53E-02	8.08E-02	1.00E-01	1.28E-01	1.48E-01
TPG-Z	1.07E-02	2.47E-02	5.53E-02	8.08E-02	1.00E-01	1.28E-01	1.48E-01
IRPG	9.85E-03	2.33E-02	5.37E-02	7.96E-02	9.94E-02	1.29E-01	1.50E-01
IRPG-Z	1.10E-02	2.53E-02	5.66E-02	8.29E-02	1.03E-01	1.32E-01	1.52E-01
accurate	1.09E-02	2.51E-02	5.64E-02	8.25E-02	1.02E-01	1.32E-01	1.52E-01

Table S-LII. $H_2O_2/H^{18}OOH$ isotope ratio for full-D partition functions using the R scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Rω	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54E-01	4.56E-01
MC-HO	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54E-01	4.56E-01
SAS	4.25E-01	4.35E-01	4.45E-01	4.49E-01	4.52E-01	4.54E-01	4.56E-01
SRC	4.25E-01	4.35E-01	4.45E-01	4.49E-01	4.52E-01	4.54E-01	4.56E-01
SR-TDPPI-HS	4.25E-01	4.35E-01	4.45E-01	4.49E-01	4.52E-01	4.54E-01	4.56E-01
SRPG	4.25E-01	4.35E-01	4.45E-01	4.49E-01	4.52E-01	4.54E-01	4.56E-01
CT-ωW	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.51E-01	4.54W-01	4.56E-01
CT-RW	4.25E-01	4.35E-01	4.45E-01	4.49E-01	4.52E-01	4.54E-01	4.56E-01
RPG	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.52E-01	4.54E-01	4.56E-01
TDPPI-HS	4.25E-01	4.35E-01	4.45E-01	4.49E-01	4.52E-01	4.54E-01	4.56E-01
WK	4.25E-01	4.35E-01	4.45E-01	4.49E-01	4.52E-01	4.54E-01	4.56E-01
MPG	4.25E-01	4.35E-01	4.45E-01	4.49E-01	4.52E-01	4.54E-01	4.56E-01
TDPPI-AS	4.25E-01	4.35E-01	4.45E-01	4.49E-01	4.52E-01	4.54E-01	4.56E-01
TPG	4.25E-01	4.35E-01	4.45E-01	4.49E-01	4.52E-01	4.54E-01	4.56E-01
C	4.25E-01	4.35E-01	4.45E-01	4.49E-01	4.52E-01	4.54E-01	4.56E-01
CT-Rω-Z	4.20E-01	4.32E-01	4.43E-01	4.47E-01	4.50E-01	4.53E-01	4.55E-01
MC-HO-Z	4.20E-01	4.32E-01	4.43E-01	4.47E-01	4.50E-01	4.53E-01	4.55E-01
SRPG-Z	4.20E-01	4.32E-01	4.43E-01	4.48E-01	4.50E-01	4.53E-01	4.55E-01
CT-Wω-Z	4.20E-01	4.32E-01	4.43E-01	4.47E-01	4.50E-01	4.53E-01	4.55E-01
CT-RW-Z	4.20E-01	4.32E-01	4.43E-01	4.48E-01	4.50E-01	4.53E-01	4.55E-01
RPG-Z	4.20E-01	4.32E-01	4.43E-01	4.48E-01	4.50E-01	4.53E-01	4.55E-01
TPG-Z	4.20E-01	4.32E-01	4.43E-01	4.48E-01	4.50E-01	4.53E-01	4.55E-01
IRPG	4.24E-01	4.35E-01	4.45E-01	4.49E-01	4.52E-01	4.54E-01	4.54E-01
IRPG-Z	4.20E-01	4.31E-01	4.42E-01	4.47E-01	4.50E-01	4.53E-01	4.53E-01
accurate	4.27E-01	4.37E-01	4.46E-01	4.49E-01	4.52E-01	4.54E-01	4.55E-01

Table S-LIII. $H_2O_2/H^{18}OOD$ isotope ratio for full-D partition functions using the R scheme I

T(K)	300	400	600	800	1000	1500	2400
CT-Rω	9.80E-03	2.33E-02	5.36E-02	7.95E-02	9.91E-02	1.29E-01	1.49E-01
MC-HO	9.80E-03	2.33E-02	5.36E-02	7.96E-02	9.93E-02	1.29E-01	1.51E-01
SAS	9.54E-03	2.27E-02	5.25E-02	7.79E-02	9.73E-02	1.26E-01	1.47E-01
SRC	9.84E-03	2.31E-02	5.26E-02	7.78E-02	9.69E-02	1.26E-01	1.47E-01
SR-TDPPI-HS	9.65E-03	2.28E-02	5.24E-02	7.76E-02	9.68E-02	1.26E-01	1.47E-01
SRPG	9.54E-03	2.26E-02	5.22E-02	7.74E-02	9.67E-02	1.26E-01	1.47E-01
CT-ωW	9.80E-03	2.33E-02	5.36E-02	7.96E-02	9.93E-02	1.29W-01	1.51E-01
CT-RW	9.44E-03	2.25E-02	5.21E-02	7.73E-02	9.66E-02	1.26E-01	1.47E-01
RPG	9.53E-03	2.26E-02	5.22E-02	7.74E-02	9.67E-02	1.26E-01	1.47E-01
TDPPI-HS	9.67E-03	2.28E-02	5.24E-02	7.76E-02	9.68E-02	1.26E-01	1.47E-01
WK	9.66E-03	2.28E-02	5.24E-02	7.76E-02	9.68E-02	1.26E-01	1.47E-01
MPG	9.72E-03	2.29E-02	5.24E-02	7.76E-02	9.68E-02	1.26E-01	1.47E-01
TDPPI-AS	9.65E-03	2.28E-02	5.24E-02	7.76E-02	9.68E-02	1.26E-01	1.47E-01
TPG	9.54E-03	2.26E-02	5.22E-02	7.74E-02	9.67E-02	1.26E-01	1.47E-01
C	9.84E-03	2.31E-02	5.26E-02	7.78E-02	9.69E-02	1.26E-01	1.47E-01
CT-Rω-Z	1.11E-02	2.56E-02	5.72E-02	8.34E-02	1.03E-01	1.32E-01	1.52E-01
MC-HO-Z	1.11E-02	2.56E-02	5.72E-02	8.35E-02	1.03E-01	1.33E-01	1.53E-01
SRPG-Z	1.08E-02	2.49E-02	5.57E-02	8.12E-02	1.00E-01	1.29E-01	1.49E-01
CT-Wω-Z	1.11E-02	2.56E-02	5.72E-02	8.35E-02	1.03E-01	1.33E-01	1.53E-01
CT-RW-Z	1.07E-02	2.48E-02	5.55E-02	8.11E-02	1.00E-01	1.29E-01	1.49E-01
RPG-Z	1.08E-02	2.49E-02	5.57E-02	8.13E-02	1.00E-01	1.29E-01	1.49E-01
TPG-Z	1.08E-02	2.49E-02	5.57E-02	8.13E-02	1.00E-01	1.29E-01	1.49E-01
IRPG	9.94E-03	2.35E-02	5.39E-02	7.98E-02	9.95E-02	1.29E-01	1.50E-01
IRPG-Z	1.10E-02	2.54E-02	5.68E-02	8.29E-02	1.03E-01	1.32E-01	1.52E-01
accurate	1.10E-02	2.53E-02	5.66E-02	8.27E-02	1.02E-01	1.32E-01	1.52E-01

Table S-LIV. MU%E for various methods

T(K)	1-D C scheme	1-D R scheme	Full-D C scheme	Full-D R scheme
CT-Iω	9.4	23.3	30.8	29.3
MC-HO	12.3	22.1	27.7	27.7
SAS	3.4	4.6	25.1	10.4
SRC	3.8	3.2	24.9	9.6
SR-TDPPI-HS	4.0	3.9	26.6	11.0
SRPG	5.3	6.2	27.3	12.5
CT-ωW	9.1	22.8	29.1	29.1
CT-IW	27.7	26.8	44.8	32.5
RPG	16.1	16.8	35.7	22.6
TDPPI-HS	0.1	0.0	23.5	7.7
WK	0.3	0.2	23.5	7.7
MPG	0.5	0.6	23.4	7.5
TDPPI-AS	0.5	0.3	23.6	7.7
TPG	1.8	2.7	24.4	9.2
C	3.9	2.7	21.9	6.5
CT-Iω-Z	5.3	15.4	14.9	13.3
MC-HO-Z	8.9	14.3	11.5	11.5
SRPG-Z	1.5	3.9	10.5	10.6
CT-Wω-Z	5.3	14.9	13.0	13.0
CT-IW-Z	24.7	19.3	32.5	17.3
RPG-Z	12.6	9.0	21.7	5.8
TPG-Z	2.8	7.7	7.8	14.3
IRPG	NA	NA	14.2	13.7
IRPG-Z	NA	NA	1.0	3.2

Table S-LV. MU%E of isotope ratios for various methods

T(K)	1-D C scheme	1-D R scheme	Full-D C scheme	Full-D R scheme
CT-Iω	0.35	1.17	3.95	4.08
MC-HO	0.37	1.37	3.93	3.93
SAS	0.47	0.55	3.67	5.31
SRC	0.71	0.58	3.32	4.96
SR-TDPPI-HS	0.08	0.07	3.81	5.35
SRPG	0.39	0.49	4.05	5.66
CT-ωW	0.33	1.30	3.93	3.93
CT-IW	0.95	0.77	4.46	5.85
RPG	0.38	0.48	4.05	5.66
TDPPI-HS	0.03	0.01	3.77	5.31
WK	0.10	0.06	3.78	5.32
MPG	0.25	0.28	3.70	5.24
TDPPI-AS	0.22	0.12	3.82	5.34
TPG	0.38	0.49	4.04	5.66
C	0.71	0.59	3.32	4.96
CT-Iω-Z	0.99	1.98	0.95	0.83
MC-HO-Z	1.02	2.18	0.96	0.96
SRPG-Z	0.90	0.54	0.84	1.22
CT-Wω-Z	1.02	2.18	0.96	0.96
CT-IW-Z	0.42	0.40	0.44	1.40
RPG-Z	0.92	0.53	0.84	1.22
TPG-Z	0.92	0.54	0.84	1.22
IRPG	NA	NA	3.67	3.59
IRPG-Z	NA	NA	0.31	0.37

Table S-LVI. A comparison of ΔZPE[a] in cm^{-1} for various 1-D potentials and methods when I is calculated via the C scheme

	MFG/ref. PES[b]	exact/ref. PES[c]	exact/acc. PES[d]
H_2O_2	−9.6	−10.4	−23.0
D_2O_2	−5.1	−5.5	−9.4
HOOD	−7.4	−7.9	−15.6
$H_2^{18}O_2$	−9.5	−10.4	−22.7
$D^{18}OOH$	−7.3	−7.9	−15.5
$H^{18}OOH$	−9.5	−10.4	−22.8
$H^{18}OOD$	−7.3	−7.9	−15.5

[a] ΔZPE = ZPE − harmonic ZPE.

[b] The MFG estimate of ΔZPE for a reference potential of the form of Eq. (8) with W equal to the average of the two barrier heights. This is given by Eqs. (20), (21), and (23) with the C scheme for I.

[c] The exact value of ΔZPE (obtained via direct diagonalization with the C scheme for I) for a reference potential of the form of Eq. (8) with W equal to the average of the two barrier heights

[d] The exact value of ΔZPE (obtained via direct diagonalization with the C scheme for I) for the accurate 1-D potential of the form of Eq. (1)