Mechanism of the Formation of Carboxylate from Alcohols and Water Catalyzed by a Bipyridine-Based Ruthenium Complex: A Computational Study

*Haixia Li and Michael B. Hall**

Department of Chemistry, Texas A&M University, College Station, Texas 77843-3255, United States.

mbhall@tamu.edu

Contents

1. Adjustments for the Standard-state Concentration

An adjustment for 1 atm to 1 M standard-state concentration of *RT*ln(24.5), i.e., 1.9 kcal/mol, was used for all the species in aqueous solution. Taking the gas-phase reaction (equation 1) as an example, we define the "θ" standard state for all species at 1 atm pressure and "θ′" standard state for all species in the gas phase at 1 mol/L. Two standard-state free energies can convert to each other using the equation 2. If A, B, C, and D are ideal gases, their concentration at 1 atm may be derived from the ideal gas law as (1/24.5) mol/L at 298 K. Therefore, equation 2 becomes equation 3. For the reactions involving water, an adjustment for 1 atm to 55.6 M standard-state concentration of *RT*ln(55.6), i.e., 4.3 kcal/mol, was employed.

$$aA + bB \rightarrow cC + dD \quad \text{(equation 1)}$$

$$\Delta G^{\theta'} = \Delta G^{\theta} + RT\ln\left(\frac{Q^{\theta'}}{Q^{\theta}}\right) \quad \text{(equation 2)}$$

$$\text{where } Q = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

$$\Delta G^{\theta'} = \Delta G^{\theta} + RT\ln\left(\frac{\frac{1^c \cdot 1^d}{1^a \cdot 1^b}}{\frac{24.5^a \cdot 24.5^b}{24.5^c \cdot 24.5^d}}\right)$$

$$= \Delta G^{\theta} + RT\ln(24.5)^{c+d-a-b} \quad \text{(equation 3)}$$

2. Optimized Geometries of Stationary Points Involved in Energy Profiles but not Shown in the Main Text

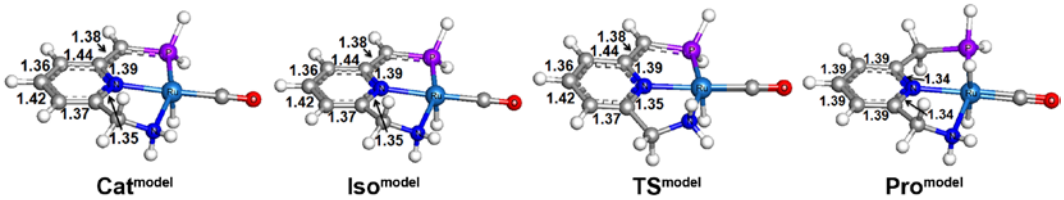

Figure S1: Optimized geometries for the intermediates and transition states using the catalyst model. Key bond lengths are given in Å and *tert*-butyl groups are omitted for clarity.

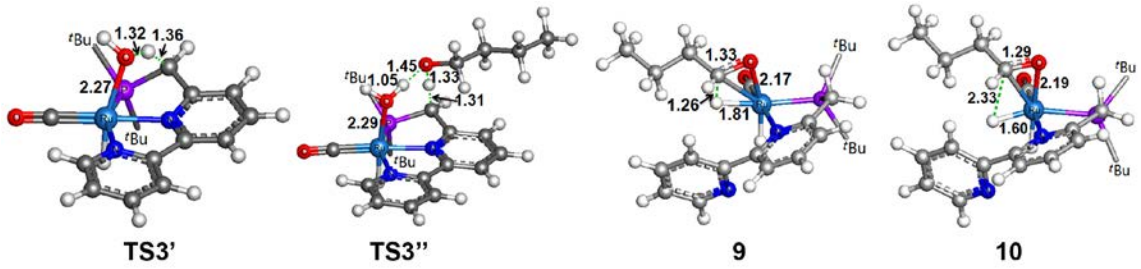

Figure S2: Optimized geometries of stationary points involved in Figure 3 but not shown in Figure 4. Key bond lengths are given in Å and *tert*-butyl groups are omitted for clarity.

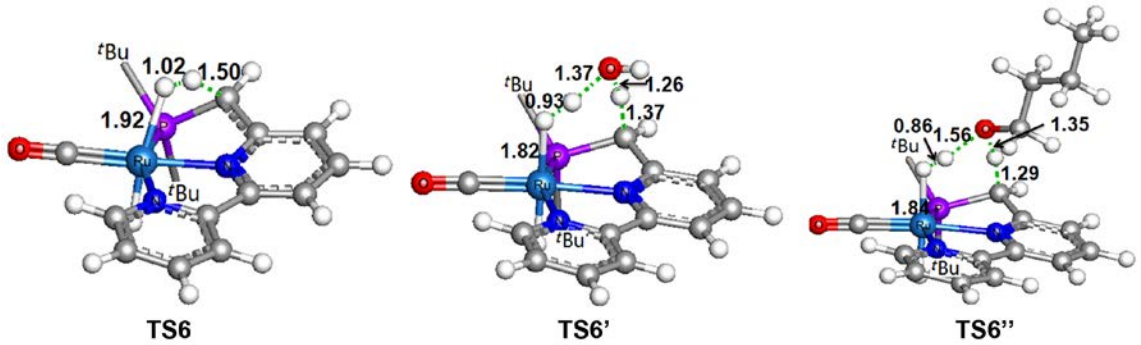

Figure S3: Optimized geometries of transition states involved in Figure 5. Key bond lengths are given in Å and *tert*-butyl groups are omitted for clarity.

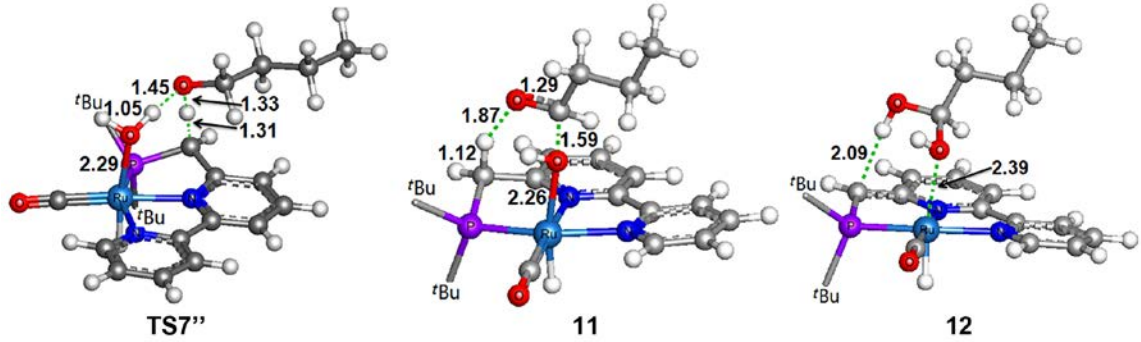

Figure S4: Optimized geometries of stationary points involved in Figure 6 but not shown in Figure 7. Key bond lengths are given in Å and *tert*-butyl groups are omitted for clarity.

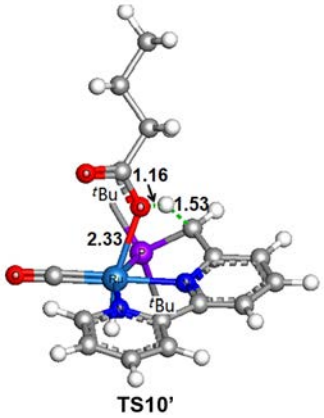

Figure S5: Optimized geometry of **TS10'** involved in Figure 10. Key bond lengths are given in Å and *tert*-butyl groups are omitted for clarity.

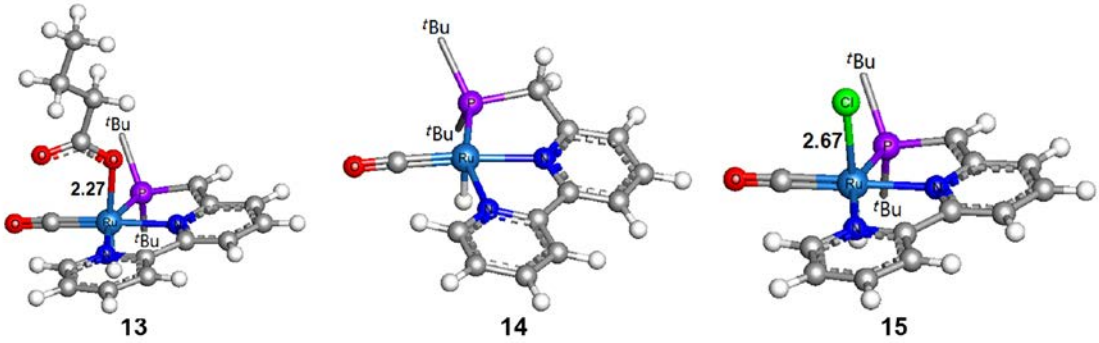

Figure S6: Optimized geometries of stationary points involved in Figure 11 and 13 but not shown in Figure 12 and 14. Key bond lengths are given in Å and *tert*-butyl groups are omitted for clarity.

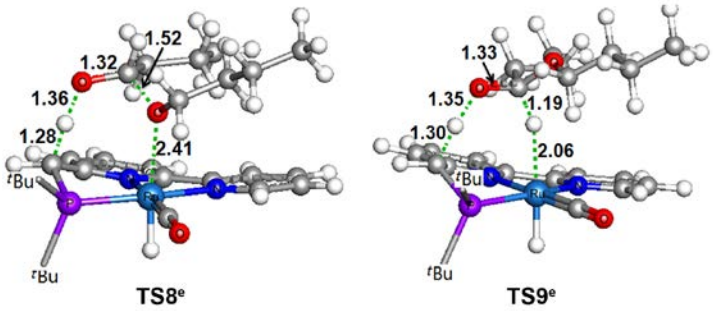

Figure S7: Optimized geometries of stationary points involved in Figure 15 but not shown in the text. Key bond lengths are given in Å and *tert*-butyl groups are omitted for clarity.

3. Unfavorable Pathways for Hydrogen Release

The direct and water-mediated pathways for hydrogen release from the complex **5**, **6**, and **8** were calculated and the optimized transition structures were shown in Figure S8. The barriers for **TS_S8-A** and **TS_S8-B** for the hydrogen release from complex **5** are 49.5[36.4] and 46.4[28.4] kcal/mol, respectively. The barriers for **TS_S8-C** and **TS_S8-D** for the hydrogen release from complex **6** are 50.2[48.4] and 47.4[41.1] kcal/mol, respectively. In the Milstein's proposed mechanism, hydrogen was released from the complex **8**. However, the barriers for **TS_S8-E** (direct transition state) and **TS_S8-F** (water-mediated transition state) for this process are 46.9[45.0] and 43.3[37.3] kcal/mol, respectively. Therefore, these pathways are unfavorable due to the high barriers.

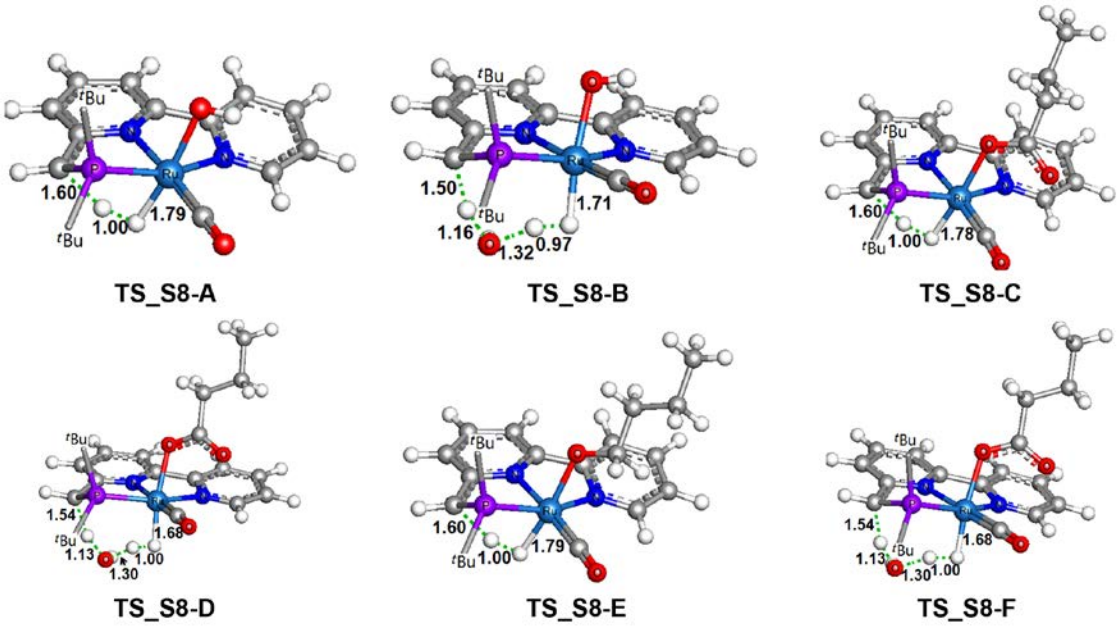

Figure S8: Optimized geometries of the transition structures for hydrogen release from the complex **5**, **6**, and **8**. Key bond lengths are given in Å and *tert*-butyl groups are omitted for clarity.

4. Unfavorable Pathways for the Formation of the Gem-diol

The pathways for the formation of the gem-diol without catalyst **3** involve the direct coupling of aldehyde and water, the water-catalyzed pathways, and the alcohol-catalyzed pathways. Optimized transition structures are shown in Figure S9. The barrier for the direct coupling transition state **TS_S9-A** is 40.1[34.4] kcal/mol higher than the separate aldehyde and water. The barriers for the water-catalyzed transition states **TS_S9-B**, **TS_S9-C**, and **TS_S9-D** are 32.7[17.5], 31.7[8.1], and 35.4[4.0]

kcal/mol, respectively. The barriers for the alcohol-catalyzed transition states **TS_S9-E** and **TS_S9-F** are 31.1[15.6] and 27.8[2.5] kcal/mol, respectively. Therefore, water and alcohol can lower the reaction barrier by acting as proton shuttles, but more water or alcohol molecule disfavor the reaction due to the entropy loss. All these barriers are very high compared to the rate-determining transition state **TS8** (6.3[–12.6] kcal/mol) in Figure 6 in the main text. Another pathway over a three-molecule transition state **TS_S9-G** involving catalyst **3**, water, and alcohol is also unfavorable, because the barrier for **TS_S9-G** is 17.9[0.0] kcal/mol, higher than the **TS8** by 11.6[12.6] kcal/mol.

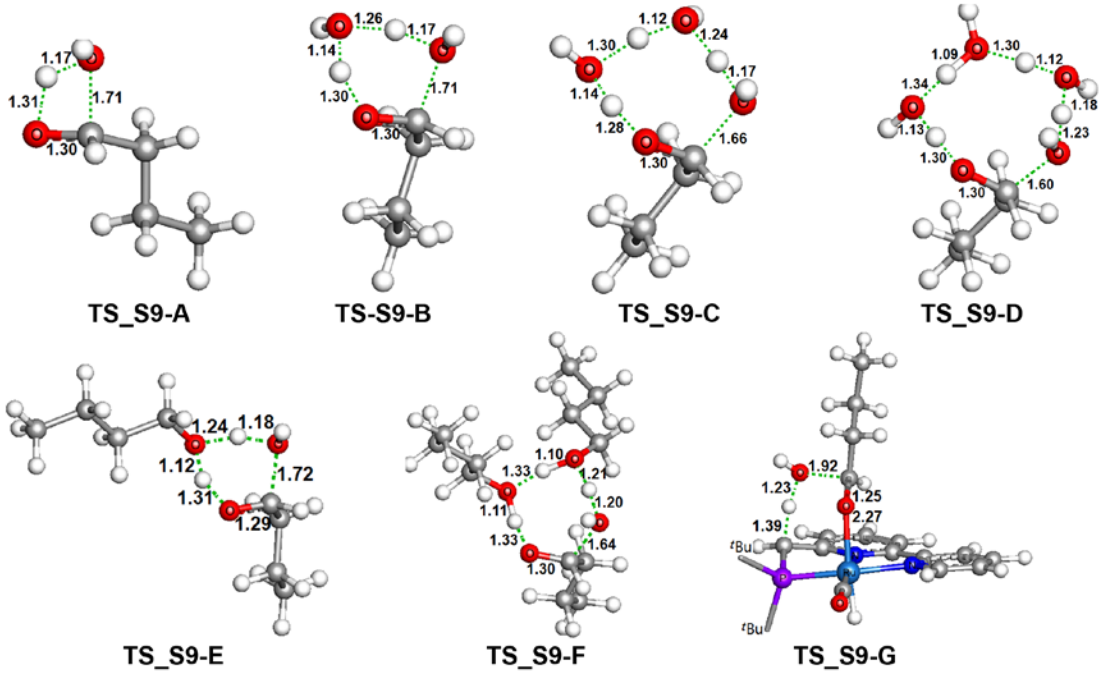

Figure S9: Optimized geometries of the transition structures for the formation of the gem-diol. Key bond lengths are given in Å and *tert*-butyl groups are omitted for clarity.

5. Unfavorable Transition-State Structures for the Dehydrogenation of the Gem-diol

The dehydrogenation of the gem-diol via alternative stepwise transition-state structures was located (Figure S10). The barrier for the rate-determining transition state **TS_S10-A** is higher than that for **TS9** (Figure 8 in the text) by 0.8[1.6] kcal/mol. Thus, the stepwise transition-state structures are unfavorable.

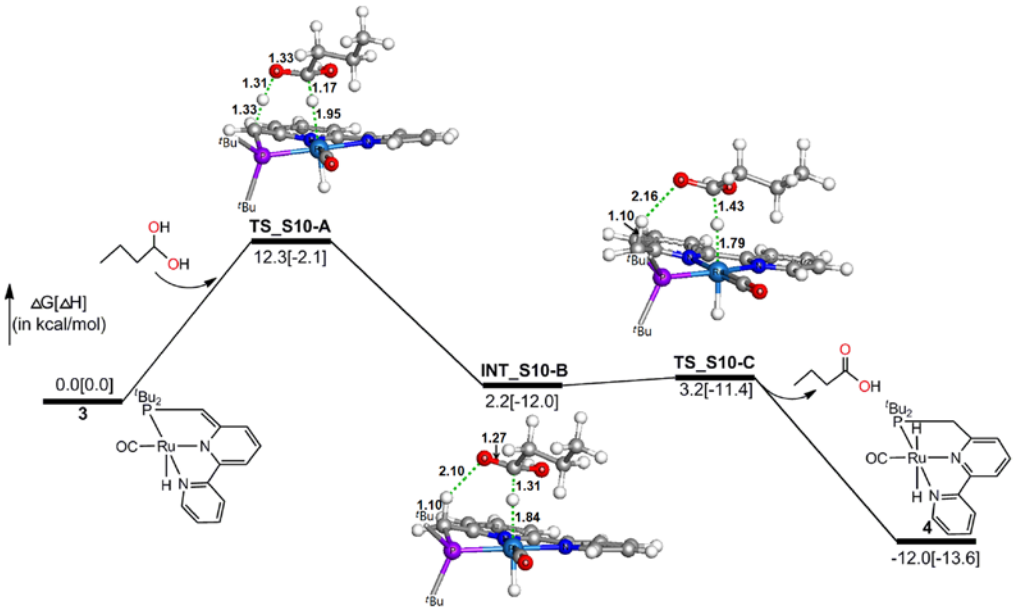

Figure S10: Energy profiles for the dehydrogenation of the gem-diol via the stepwise transition-state structures. Key bond lengths are given in Å and *tert*-butyl groups are omitted for clarity.

6. Results for the Formation of the Active Catalyst 3 from the Precursor Complex 2 under NaOH in Toluene

The pathway for the formation of catalyst **3** from complex **2** under NaOH in toluene is shown in Figure S11. Because NaOH does not dissociate in toluene, we optimize the geometries in gas phase, and then do the single-point corrections in toluene. Values shown in Figure S11 are the energies in solvent. As shown in Figure S11, the reaction starts by adding NaOH to the complex **2** to form a stable intermediate **INT_S11-A**. Over transition state **TS_S11-B** with a barrier of 1.4[1.3] kcal/mol, an intermediate **INT_S11-C** involving catalyst **3**, NaCl, and H_2O is formed. The generation of the active catalyst **3** from **INT_S11-C** by releasing $NaCl{\cdot}H_2O$ is somewhat unfavorable. However, the following transformations from catalyst **3** in the reaction drive this process to generate the catalyst **3**.

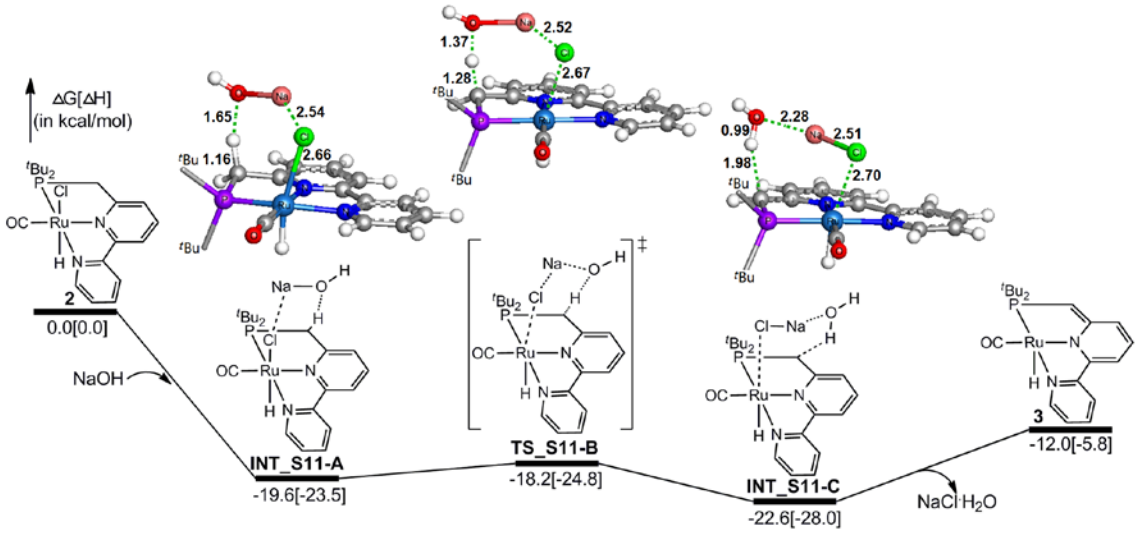

Figure S11: Energy profiles for the formation of the active catalyst **3** from the precursor complex **2** in toluene. Key bond lengths are given in Å and *tert*-butyl groups are omitted for clarity.

7. Comparison Results for M06, TPSS, and LC-ωPBE functionals

The calculation procedures here are similar to those in the text only by replacing the *ω*B97X-D functional for M06, TPSS, and LC-ωPBE functionals. Results for the rate-determining transition state **TS1** in the double hydrogen transfer mechanism and **TS4** in the β-H elimination mechanism for the dehydrogenation of the alcohol (Figure 3) are shown in Table S1. According to Table S1, the double hydrogen transfer mechanism is more favourable than the β-H elimination mechanism with the M06, TPSS, and LC-ωPBE functionals.

Table S1: Calculation results for **TS1** and **TS4** for the dehydrogenation of the alcohol. Values in kcal/mol are relative to the separate catalyst **3** and alcohol.

	TS1	**TS4**
M06	16.4[3.0]	17.8[6.3]
TPSS	22.5[9.3]	26.0[15.3]
LC-ωPBE	22.5[9.0]	23.5[12.2]

The stationary points involved in the pathways for the formation of acid and ester (Figure 15 in the text) are also calculated by using the M06, TPSS, and LC-ωPBE functionals. The calculation results are shown in Table S2. The results are consistent with the experimental observations that the reaction only produces acid.

Table S2: Calculation results for the stationary points involved in the pathways for the formation of acid and ester. Values in kcal/mol are relative to the separate catalyst **3**, water, and alcohol.

	TS7/TS3	**5/8**	**TS8/TS8[e]**	(**3**+) gem-diol /hemiacetal	**TS9/TS9[e]**	(**4**+) acid/ester
M06	10.0[–1.4]/ 10.8[–6.1]	–1.4[–7.2]/ 0.1[–11.9]	11.8[–7.0]/ 14.9[–12.1]	1.3[–4.1]/ 1.4[–9.7]	13.8[–5.6]/ 17.2[–9.2]	–10.8[–17.2]/ –10.6[–21.6]
TPSS	9.4[–2.3]/ 15.4[–1.8]	–1.9[–7.9]/ 3.4[–7.8]	18.2[–0.8]/ 31.2[6.0]	1.9[–2.9]/ 5.2[–5.5]	16.0[7.4]/ 33.2[8.3]	–11.0[–17.3]/ –10.0[–20.7]
LC-ωPBE	10.3[–1.4]/ 15.2[–1.8]	–3.1[–9.0]/ 2.3[–9.2]	13.0[–6.2]/ 24.4[–1.8]	–2.9[–7.6]/ 0.0[–11.0]	21.4[2.2]/ 27.7[2.1]	–14.4[–21.1]/ –12.9[–24.8]

8. Total Energies and Cartesian Coordinates of the Structures Involved in this Study

***n*-butyl alcohol**

O	2.488732	-0.301785	-0.091301
C	1.321191	0.485341	0.017936
H	1.348215	1.178783	-0.829116
H	1.334851	1.098873	0.934069
C	0.037707	-0.337734	-0.029495
H	0.043036	-0.941350	-0.945018
H	0.031512	-1.045340	0.812721
C	-1.223529	0.524187	0.026530
H	-1.217131	1.228023	-0.815469
H	-1.206541	1.136598	0.937359
C	-2.507849	-0.301898	-0.009038
H	-3.394775	0.337136	0.027958
H	-2.563359	-0.900819	-0.924063
H	-2.555235	-0.990714	0.841136
H	2.504454	-0.906286	0.655242

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –233.605157513

Thermal correction to Enthalpy= 0.146622

Thermal correction to Gibbs Free Energy= 0.108935

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –233.623552081

H_2O

O	0.000000	0.000000	0.117548
H	0.000000	0.758274	-0.470190
H	0.000000	-0.758274	-0.470190

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 76.3965824239

Thermal correction to Enthalpy= 0.025659

Thermal correction to Gibbs Free Energy= 0.004243

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 76.4231837162

***n*-propyl aldehyde**

O	2.442991	-0.146817	-0.319478
C	1.456249	0.251002	0.250353
C	0.117125	-0.442103	0.244913

H	0.174331	-1.307417	-0.421826
H	-0.063654	-0.813154	1.264423
C	-1.023412	0.504560	-0.150644
H	-0.853300	0.868658	-1.170452
H	-1.006036	1.387297	0.501010
C	-2.391677	-0.168311	-0.065581
H	-3.189095	0.520423	-0.357826
H	-2.441771	-1.040077	-0.725621
H	-2.598478	-0.509911	0.954056
H	1.484369	1.197830	0.837813

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –232.389972748

Thermal correction to Enthalpy= 0.121472

Thermal correction to Gibbs Free Energy= 0.084142

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –232.404823384

Gem-diol

O	2.044617	-0.971738	-0.073327
C	1.094532	-0.009671	0.298640
C	-0.262616	-0.530937	-0.133922
H	-0.244201	-0.615202	-1.226792
H	-0.379635	-1.543835	0.266610
C	-1.418261	0.361040	0.312350
H	-1.255126	1.370254	-0.079636
H	-1.412492	0.445847	1.407472
C	-2.774747	-0.167235	-0.149216
H	-3.589346	0.485149	0.178522
H	-2.817398	-0.233485	-1.241455
H	-2.965694	-1.168960	0.250589
H	1.111097	0.136890	1.394350
H	2.918940	-0.620813	0.115851
O	1.323385	1.227081	-0.335413
H	1.856381	1.782241	0.237307

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 308.808175169

Thermal correction to Enthalpy= 0.152298

Thermal correction to Gibbs Free Energy= 0.111130

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 308.842127700

3

Ru	0.354034	-0.745045	-0.023110
P	-1.732306	0.255158	-0.036631
O	-0.550288	-3.616481	0.028602
N	0.990494	1.244356	-0.016197
C	-1.283498	1.973742	-0.055427
C	0.062431	2.275409	-0.038846
C	0.587212	3.620257	-0.036841
H	-0.116428	4.445578	-0.048990
C	1.928696	3.843752	-0.025241
H	2.308059	4.861329	-0.025873
C	2.845783	2.759775	-0.015032
H	3.911278	2.945584	-0.009088
C	2.324130	1.488770	-0.014448
C	-0.204520	-2.504699	0.016376
C	-2.873880	-0.046951	-1.506379
C	-3.026738	-1.551968	-1.772158
H	-3.680503	-1.699624	-2.640243
H	-2.059767	-2.009327	-1.994932
H	-3.469053	-2.089101	-0.930396
C	-4.254446	0.598991	-1.327608
H	-4.812679	0.525722	-2.268499
H	-4.847468	0.097747	-0.557820
H	-4.177168	1.660542	-1.071263
C	-2.186658	0.592562	-2.725443
H	-2.111683	1.677547	-2.620860
H	-1.176566	0.197209	-2.866567
H	-2.771771	0.365975	-3.624780
C	-2.622844	-0.019844	1.611989
C	-3.338158	-1.374843	1.666758
H	-4.225693	-1.395628	1.027909
H	-2.680251	-2.197385	1.370183
H	-3.672339	-1.568260	2.693327

C	-3.600335	1.109494	1.967000
H	-4.001475	0.937169	2.973243
H	-3.093796	2.078447	1.967801
H	-4.448149	1.164239	1.281479
C	-1.487898	-0.009868	2.655647
H	-0.820776	-0.872317	2.530663
H	-0.896907	0.909774	2.587375
H	-1.911254	-0.066225	3.665720
C	3.163181	0.263607	-0.013304
C	4.558208	0.288395	-0.027450
C	3.189778	-2.064252	-0.008163
C	5.269594	-0.901153	-0.031453
H	5.082453	1.235332	-0.038118
C	4.573982	-2.105553	-0.022110
H	2.596785	-2.971198	-0.005221
H	6.354365	-0.887926	-0.043605
H	5.086385	-3.060140	-0.027094
N	2.495810	-0.915927	-0.002422
H	0.312499	-0.883053	-1.558074
H	-2.016933	2.771700	-0.085663

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 1399.19948683

Thermal correction to Enthalpy= 0.461513

Thermal correction to Gibbs Free Energy= 0.381075

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 1399.23267935

TS1

Ru	-0.224193	0.155248	-0.753761
P	1.968540	-0.056023	-0.056010
O	0.172001	2.394641	-2.719302
N	-0.502255	-1.491259	0.546814
C	1.595484	-0.897407	1.525966
C	0.475895	-1.842823	1.405666
C	0.294953	-2.975306	2.213387
H	1.081990	-3.273234	2.896081
C	-0.895364	-3.675278	2.145295
H	-1.045410	-4.552074	2.766964
C	-1.921268	-3.240548	1.304524
H	-2.870492	-3.760369	1.285453
C	-1.689406	-2.120274	0.519778
C	0.018707	1.541054	-1.946031
C	3.029840	-1.247112	-1.085051
C	3.093604	-0.772144	-2.545935
H	3.628837	-1.520085	-3.143106
H	2.089208	-0.658356	-2.961873
H	3.620250	0.176817	-2.659521
C	4.446769	-1.440116	-0.526874
H	4.948989	-2.233395	-1.093055
H	5.060719	-0.541236	-0.614348
H	4.429701	-1.747580	0.523881
C	2.331429	-2.619364	-1.064331
H	2.339025	-3.065090	-0.065453
H	1.296701	-2.553380	-1.410026
H	2.871418	-3.298410	-1.734281
C	2.969707	1.473351	0.426404
C	3.702543	2.051443	-0.793484
H	4.524586	1.419373	-1.137966
H	3.018846	2.224043	-1.630860
H	4.132056	3.020528	-0.515614
C	3.962532	1.179872	1.563638
H	4.509820	2.100237	1.798178
H	3.436412	0.872528	2.471275
H	4.699033	0.415774	1.309586
C	1.984318	2.538941	0.938605
H	1.282761	2.847689	0.158811
H	1.418861	2.177407	1.803910
H	2.559434	3.422458	1.241094
C	-2.704123	-1.464298	-0.342497
C	-4.007576	-1.937095	-0.476683
C	-3.189348	0.350411	-1.706447
C	-4.917406	-1.230492	-1.249968
H	-4.311752	-2.847549	0.024402
C	-4.503448	-0.059343	-1.872317
H	-2.815405	1.252750	-2.174977
H	-5.935538	-1.587979	-1.359777
H	-5.178911	0.531792	-2.479028
N	-2.304321	-0.331051	-0.967496

H	0.051876	-0.797735	-1.979931
O	0.067280	0.853715	2.799494
C	-0.907541	1.175846	1.947603
C	-1.491492	2.585873	2.093648
H	-1.939157	2.658408	3.092965
H	-0.671658	3.313437	2.061497
C	-2.529585	2.910443	1.022359
H	-3.320756	2.147302	1.041556
H	-2.055170	2.832826	0.034112
C	-3.151257	4.296275	1.181505
H	-3.886304	4.502100	0.396743
H	-3.656912	4.391443	2.148358
H	-2.383125	5.075321	1.133032
H	-0.529994	1.208953	0.823988
H	2.449724	-1.299766	2.073716
H	0.985883	-0.021193	2.201346
H	-1.755174	0.453527	1.909181

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 1632.80480131

Thermal correction to Enthalpy= 0.604132

Thermal correction to Gibbs Free Energy= 0.510415

Imaginary frequency: –952.8559 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 1632.8535538700

7

Ru	-0.205206	0.175195	-0.728280
P	1.984953	-0.031115	-0.069290
O	0.128024	2.586065	-2.491605
N	-0.461039	-1.540541	0.473461
C	1.715811	-1.088825	1.430420
C	0.512624	-1.972569	1.290963
C	0.335772	-3.138638	2.032699
H	1.131634	-3.488002	2.679951
C	-0.872271	-3.814877	1.953762
H	-1.028421	-4.723279	2.525876
C	-1.897251	-3.307116	1.163474
H	-2.856601	-3.807424	1.128068
C	-1.662196	-2.146119	0.436186
C	0.000199	1.658259	-1.802148
C	3.091856	-1.078740	-1.195796
C	3.109209	-0.467434	-2.606387
H	3.685720	-1.119805	-3.272921
H	2.094968	-0.379002	-3.002915
H	3.574132	0.520517	-2.628650
C	4.528793	-1.249823	-0.684286
H	5.051715	-1.965603	-1.329258
H	5.096560	-0.317138	-0.709385
H	4.559749	-1.647586	0.335384
C	2.453674	-2.477876	-1.286518
H	2.513037	-3.018249	-0.336297
H	1.407092	-2.423092	-1.596509
H	3.000337	-3.066603	-2.032007
C	2.928755	1.457628	0.610503
C	3.587202	2.233069	-0.540855
H	4.431524	1.698332	-0.983914
H	2.869141	2.468836	-1.332666
H	3.970081	3.182944	-0.151057
C	3.980084	1.080616	1.668101
H	4.468704	1.998025	2.015668
H	3.518780	0.612104	2.541717
H	4.759803	0.418820	1.289329
C	1.894514	2.377803	1.284252
H	1.184202	2.776696	0.556047
H	1.325126	1.866702	2.069956
H	2.428041	3.222294	1.737118
C	-2.678441	-1.447888	-0.386185
C	-3.991929	-1.895774	-0.514132
C	-3.146071	0.400718	-1.708329
C	-4.897407	-1.158916	-1.262557
H	-4.308495	-2.809338	-0.026626
C	-4.467438	0.015605	-1.868672
H	-2.762433	1.306478	-2.161599
H	-5.923266	-1.495136	-1.366664
H	-5.138148	0.629746	-2.457597
N	-2.265038	-0.308717	-0.990021
H	0.100829	-0.719667	-2.030641
O	-0.268200	0.576491	2.906829

C	-1.113195	0.986321	2.039219
C	-1.615304	2.438664	2.117027
H	-2.136817	2.532150	3.079311
H	-0.751125	3.111382	2.163004
C	-2.547308	2.837756	0.978288
H	-3.378593	2.120202	0.923806
H	-2.003831	2.751334	0.029081
C	-3.103112	4.253167	1.121697
H	-3.762815	4.514216	0.287772
H	-3.675951	4.360620	2.049176
H	-2.292083	4.988742	1.148227
H	-0.593943	1.042012	0.827866
H	2.600468	-1.641327	1.757523
H	1.399926	-0.380916	2.219049
H	-1.979746	0.312414	1.808205

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 1632.8094538900

Thermal correction to Enthalpy= 0.606776

Thermal correction to Gibbs Free Energy= 0.511760

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 1632.8642664200

TS2

Ru	-0.192430	0.167154	-0.746024
P	1.986548	-0.024390	-0.068806
O	0.128084	2.593446	-2.489627
N	-0.456517	-1.534520	0.470356
C	1.728109	-1.098335	1.426565
C	0.512561	-1.969382	1.293349
C	0.329524	-3.129833	2.040114
H	1.123250	-3.479795	2.689885
C	-0.881145	-3.803499	1.961957
H	-1.041692	-4.708859	2.537588
C	-1.900059	-3.295621	1.165958
H	-2.860802	-3.793233	1.127601
C	-1.659008	-2.138763	0.431983
C	0.007560	1.653866	-1.812743
C	3.119418	-1.059905	-1.184007
C	3.135519	-0.448420	-2.594572
H	3.722003	-1.094223	-3.258898
H	2.121011	-0.371647	-2.992765
H	3.589695	0.544787	-2.614547
C	4.556307	-1.215191	-0.668032
H	5.087954	-1.926874	-1.310459
H	5.115012	-0.276992	-0.694550
H	4.590009	-1.611015	0.352423
C	2.497118	-2.466104	-1.278626
H	2.561281	-3.008918	-0.329905
H	1.450945	-2.419471	-1.591494
H	3.051617	-3.046958	-2.024548
C	2.918783	1.465164	0.630949
C	3.563448	2.259266	-0.515875
H	4.411605	1.736900	-0.966120
H	2.839536	2.492120	-1.303113
H	3.937778	3.210362	-0.120507
C	3.980809	1.092407	1.679572
H	4.452549	2.013512	2.040668
H	3.534312	0.599937	2.547954
H	4.772179	0.452917	1.288050
C	1.880859	2.371211	1.317653
H	1.156914	2.760465	0.598741
H	1.324114	1.852168	2.105004
H	2.409066	3.218728	1.771245
C	-2.668212	-1.446347	-0.401033
C	-3.982788	-1.892099	-0.533071
C	-3.122448	0.390119	-1.744184
C	-4.881361	-1.161256	-1.294431
H	-4.304288	-2.800560	-0.039095
C	-4.442991	0.006437	-1.909250
H	-2.733022	1.289335	-2.205415
H	-5.907285	-1.495888	-1.402751
H	-5.107752	0.616014	-2.509692
N	-2.246360	-0.313959	-1.012682
H	0.118937	-0.765864	-2.053744
O	-0.362025	0.552093	2.954800
C	-1.199378	0.969276	2.125560
C	-1.655009	2.428923	2.133389
H	-2.177797	2.568374	3.090921

H	-0.773937	3.078686	2.162898
C	-2.579558	2.810483	0.982671
H	-3.412102	2.094148	0.935642
H	-2.030148	2.706614	0.040505
C	-3.131818	4.228943	1.106580
H	-3.783738	4.480193	0.264015
H	-3.712149	4.350700	2.027740
H	-2.319099	4.962752	1.128875
H	-0.567785	1.042216	0.728987
H	2.611888	-1.671764	1.719465
H	1.466474	-0.404773	2.238899
H	-2.013603	0.283948	1.789712

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 1632.8088255000

Thermal correction to Enthalpy= 0.604356

Thermal correction to Gibbs Free Energy= 0.510282

Imaginary frequency: – 359.4772 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 1632.8580320500

4

Ru	-0.385847	-0.791967	-0.047668
P	1.704267	0.113114	-0.059178
O	0.403091	-3.678036	0.244531
N	-0.988892	1.208945	-0.304047
C	1.313472	1.777024	-0.815727
C	-0.103777	2.197554	-0.538602
C	-0.519894	3.522044	-0.588199
H	0.207723	4.307253	-0.760872
C	-1.869651	3.818990	-0.428874
H	-2.212523	4.847597	-0.461830
C	-2.776795	2.786410	-0.246730
H	-3.833075	3.001728	-0.144338
C	-2.305211	1.475460	-0.192192
C	0.098768	-2.558467	0.137380
C	2.438757	0.576992	1.633890
C	2.474512	-0.681198	2.517194
H	2.814862	-0.404476	3.522308
H	1.477280	-1.120826	2.594394
H	3.159450	-1.441566	2.134240
C	3.830187	1.222155	1.594812
H	4.090506	1.559929	2.604837
H	4.608549	0.523457	1.279570
H	3.864107	2.100432	0.941328
C	1.470762	1.585792	2.281727
H	1.493050	2.559285	1.780449
H	0.446458	1.203781	2.283597
H	1.776835	1.749099	3.321428
C	3.071620	-0.544961	-1.198763
C	3.774031	-1.726426	-0.509714
H	4.396007	-1.410424	0.331506
H	3.054573	-2.469060	-0.151249
H	4.430683	-2.223527	-1.232971
C	4.109631	0.509215	-1.621881
H	4.828054	0.039587	-2.303827
H	3.649684	1.339910	-2.166011
H	4.675955	0.920534	-0.787277
C	2.403412	-1.078823	-2.478121
H	1.710550	-1.892184	-2.262658
H	1.832816	-0.307798	-3.004119
H	3.187705	-1.441287	-3.153820
C	-3.158616	0.283024	-0.031576
C	-4.548679	0.346797	0.073893
C	-3.221987	-2.031058	0.106942
C	-5.281610	-0.821542	0.199150
H	-5.054500	1.304468	0.056307
C	-4.601864	-2.035974	0.212556
H	-2.650354	-2.950668	0.115860
H	-6.362404	-0.786428	0.281991
H	-5.128223	-2.978813	0.304134
N	-2.502668	-0.902774	-0.008904
H	-0.479529	-0.608524	1.622360
H	1.391243	1.625182	-1.899304
H	2.024831	2.562342	-0.543555
H	-0.353290	-0.916105	-1.725995

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 1400.4024484900

Thermal correction to Enthalpy= 0.481352

Thermal correction to Gibbs Free Energy= 0.402054

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 1400.4432040100

TS3

Ru	0.177620	-0.112931	-0.607610
P	-2.073408	-0.267333	-0.098113
O	0.364320	-2.620733	-2.247594
N	-0.013113	1.714724	0.448701
C	-2.120067	0.922445	1.290961
C	-1.140640	1.997790	1.137728
C	-1.246726	3.244043	1.782458
H	-2.157379	3.486701	2.318260
C	-0.187615	4.127799	1.740122
H	-0.261462	5.090045	2.236928
C	0.988933	3.781953	1.071297
H	1.828282	4.464906	1.055690
C	1.039883	2.552260	0.432925
C	0.299286	-1.658453	-1.595275
C	-3.235666	0.476436	-1.410858
C	-3.057327	-0.234411	-2.762191
H	-3.665565	0.275536	-3.519089
H	-2.013508	-0.200388	-3.083704
H	-3.373586	-1.278234	-2.737068
C	-4.713598	0.457162	-0.991881
H	-5.300765	1.013359	-1.732247
H	-5.129914	-0.550555	-0.939907
H	-4.866084	0.943318	-0.022781
C	-2.836490	1.952867	-1.597616
H	-3.049292	2.547497	-0.704702
H	-1.777675	2.059391	-1.844365
H	-3.422976	2.373056	-2.422991
C	-2.816800	-1.873856	0.576639
C	-3.335548	-2.761677	-0.565685
H	-4.223070	-2.358717	-1.057473
H	-2.563972	-2.934374	-1.322932
H	-3.610339	-3.737899	-0.150168
C	-3.926468	-1.608398	1.606576
H	-4.325033	-2.569135	1.953614
H	-3.526032	-1.082818	2.477423
H	-4.761064	-1.032971	1.200742
C	-1.695256	-2.655781	1.281547
H	-0.892834	-2.905499	0.582720
H	-1.279534	-2.103074	2.126021
H	-2.116624	-3.594739	1.661679
C	2.222789	2.047171	-0.310264
C	3.409988	2.769083	-0.422446
C	3.110439	0.334517	-1.596225
C	4.470358	2.240228	-1.143718
H	3.507524	3.737913	0.050957
C	4.317327	0.999293	-1.748877
H	2.941224	-0.635125	-2.048471
H	5.399571	2.792471	-1.234360
H	5.112648	0.545700	-2.328252
N	2.089657	0.831749	-0.887942
H	-0.263364	0.577701	-1.956306
H	0.315870	-0.543791	2.200807
H	-3.111079	1.273402	1.586615
O	1.025109	-0.721750	1.432286
O	-0.720819	-0.328052	3.123816
H	-1.548631	0.292794	2.268370
H	-0.458259	0.296446	3.805665
C	1.727511	-1.908049	1.719044
H	1.096930	-2.792832	1.542107
H	1.995848	-1.913662	2.785941
C	2.988135	-2.015007	0.877275
H	2.699026	-2.061263	-0.179515
H	3.578009	-1.097883	1.005994
C	3.838062	-3.236802	1.219442
H	3.229714	-4.144180	1.115446
H	4.141945	-3.188504	2.272920
C	5.077105	-3.350382	0.333227
H	5.711669	-2.462657	0.432615
H	5.680844	-4.224803	0.593194
H	4.794417	-3.440588	-0.721431

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 1709.2517979300

Thermal correction to Enthalpy= 0.633266

Thermal correction to Gibbs Free Energy= 0.534497

Imaginary frequency: – 965.0367 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 1709.2994471900

TS3'

Ru	0.141241	-1.017971	-0.457533
P	1.992773	0.210226	0.180941
O	1.385598	-2.675277	-2.628190
N	-0.784957	0.096472	1.090105
C	0.971553	1.638575	0.699652
C	-0.199270	1.252690	1.477346
C	-0.849795	2.046785	2.438525
H	-0.382196	2.963866	2.778198
C	-2.091559	1.660612	2.910015
H	-2.603987	2.272398	3.645863
C	-2.712328	0.510641	2.415993
H	-3.714131	0.247069	2.730555
C	-2.019528	-0.247805	1.482298
C	0.906260	-2.013987	-1.798339
C	2.950667	-0.443282	1.683677
C	3.556259	-1.819882	1.361215
H	3.981817	-2.246860	2.277337
H	2.786126	-2.502457	0.991203
H	4.356528	-1.770146	0.621766
C	4.032778	0.524303	2.181806
H	4.455607	0.140099	3.117684
H	4.858253	0.637477	1.475810
H	3.616713	1.515703	2.390456
C	1.939805	-0.641156	2.828167
H	1.523940	0.308537	3.175600
H	1.118346	-1.297284	2.530774
H	2.458938	-1.104785	3.675167
C	3.193886	0.922983	-1.100953
C	4.387580	-0.019184	-1.322264
H	5.071472	-0.053201	-0.471255
H	4.058678	-1.037891	-1.550128
H	4.959700	0.341219	-2.184842
C	3.691658	2.323383	-0.705682
H	4.420214	2.663527	-1.450981
H	2.869353	3.043783	-0.699166
H	4.181210	2.348719	0.269783
C	2.456560	1.043262	-2.447456
H	2.213899	0.059954	-2.856010
H	1.521302	1.597720	-2.367790
H	3.119901	1.551581	-3.157955
C	-2.577755	-1.406954	0.743545
C	-3.789588	-2.008203	1.074229
C	-2.334967	-2.817068	-1.081731
C	-4.279665	-3.040109	0.286910
H	-4.341071	-1.673973	1.944695
C	-3.542956	-3.445975	-0.819269
H	-1.716159	-3.110553	-1.921140
H	-5.221616	-3.518144	0.533445
H	-3.886492	-4.241962	-1.469267
N	-1.850382	-1.825859	-0.321702
H	0.526592	-2.226578	0.497194
H	0.283341	1.623975	-0.473040
H	1.470258	2.543479	1.044537
O	-0.371252	1.012499	-1.414857
C	-1.698992	1.399783	-1.601188
H	-2.391322	0.793397	-0.987851
H	-1.990416	1.228332	-2.650964
C	-1.934678	2.869723	-1.252066
H	-1.661361	3.033926	-0.200803
H	-1.258637	3.490559	-1.854336
C	-3.382367	3.306384	-1.467418
H	-4.043705	2.662875	-0.871693
H	-3.659996	3.143569	-2.516828
C	-3.624736	4.767677	-1.094395
H	-4.667771	5.057446	-1.254397
H	-3.384220	4.946470	-0.040611
H	-2.995645	5.434252	-1.693845

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 1632.8150996000

Thermal correction to Enthalpy= 0.606274

Thermal correction to Gibbs Free Energy= 0.511276

Imaginary frequency: – 1378.6587 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 1632.8473446600

TS3''

Ru	0.796908	-0.810234	-0.502872
P	-1.331266	-1.652640	-0.156383
O	2.312488	-3.275595	0.297383
N	-0.304241	0.871404	-1.180056
C	-2.249668	-0.073657	-0.146730
C	-1.644979	0.930793	-1.014998
C	-2.348990	2.023433	-1.558292
H	-3.427881	2.060199	-1.460268
C	-1.654459	3.045724	-2.170335
H	-2.188455	3.898305	-2.577628
C	-0.259744	2.996768	-2.251572
H	0.288547	3.808890	-2.710919
C	0.385320	1.878698	-1.746265
C	1.728349	-2.311920	0.004556
C	-2.047569	-2.627195	-1.626622
C	-1.155579	-3.832515	-1.965088
H	-1.542203	-4.323377	-2.866410
H	-0.129830	-3.512700	-2.164134
H	-1.132388	-4.579135	-1.169743
C	-3.496849	-3.084732	-1.402602
H	-3.880336	-3.519831	-2.333092
H	-3.589516	-3.847237	-0.626906
H	-4.150029	-2.245738	-1.141504
C	-2.053323	-1.683617	-2.844603
H	-2.766794	-0.864273	-2.719052
H	-1.065003	-1.259246	-3.035675
H	-2.356322	-2.254966	-3.729723
C	-1.790706	-2.513766	1.467115
C	-1.537872	-4.026977	1.376475
H	-2.231132	-4.540435	0.707425
H	-0.514637	-4.245126	1.053927
H	-1.666944	-4.462972	2.373686
C	-3.242855	-2.228355	1.882767
H	-3.451659	-2.751936	2.823242
H	-3.392333	-1.159837	2.059595
H	-3.974888	-2.568099	1.147503
C	-0.868788	-1.968511	2.571123
H	0.180166	-2.173450	2.342690
H	-1.000304	-0.896246	2.725229
H	-1.116464	-2.478092	3.510445
C	1.856501	1.676690	-1.781815
C	2.737546	2.625217	-2.298596
C	3.622760	0.246402	-1.322228
C	4.099175	2.360833	-2.316075
H	2.363312	3.565640	-2.682994
C	4.552770	1.143221	-1.824682
H	3.925601	-0.715269	-0.926075
H	4.793496	3.093924	-2.712492
H	5.605167	0.885566	-1.823175
N	2.309834	0.503248	-1.284947
H	0.733955	-1.468181	-1.933203
H	-0.031741	0.781676	1.681261
H	-3.334714	-0.146187	-0.245197
O	0.924540	0.532106	1.355723
O	-1.399818	1.107169	2.036719
H	-1.934076	0.476876	1.005770
C	-1.573949	2.482276	1.867448
H	-1.077360	2.842684	0.943528
H	-1.095758	3.030113	2.697192
C	-3.048267	2.879550	1.802569
H	-3.545464	2.261591	1.042657
H	-3.527037	2.634179	2.758786
C	-3.253347	4.354237	1.464367
H	-2.763413	4.569837	0.504757
H	-2.743822	4.975281	2.212675
C	-4.726044	4.751404	1.385660
H	-4.847050	5.810151	1.136506
H	-5.248489	4.165152	0.621253
H	-5.232414	4.571313	2.339821
C	1.767224	0.372807	2.474930
H	1.587453	1.201423	3.175140
H	1.536720	-0.560169	3.011072
C	3.226375	0.365366	2.054115

H	3.427440	1.268232	1.462771
H	3.393474	-0.492602	1.391896
C	4.192432	0.286786	3.234239
H	4.037253	1.150641	3.893055
H	3.964080	-0.603487	3.833796
C	5.652240	0.238810	2.786909
H	5.910490	1.127077	2.199659
H	6.334474	0.191307	3.640623
H	5.838836	-0.640192	2.160120

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 1866.4679635900

Thermal correction to Enthalpy= 0.754107

Thermal correction to Gibbs Free Energy= 0.641083

Imaginary frequency: – 1101.2538 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 1866.5087613700

8

Ru	-0.033261	-0.220500	-0.814476
P	2.026295	0.198315	0.078837
O	0.306810	1.409980	-3.311363
N	-0.264069	-1.416106	0.913922
C	1.632514	-0.234964	1.849471
C	0.580969	-1.306355	1.947813
C	0.406011	-2.093743	3.083921
H	1.106201	-2.015866	3.907981
C	-0.685152	-2.949186	3.149376
H	-0.840169	-3.571822	4.024206
C	-1.602341	-2.975901	2.105500
H	-2.484511	-3.600003	2.172578
C	-1.368731	-2.174583	0.992289
C	0.165961	0.789650	-2.335565
C	3.412088	-1.010878	-0.377931
C	3.625084	-0.981997	-1.900705
H	4.351608	-1.756037	-2.175242
H	2.687955	-1.185206	-2.424676
H	4.016159	-0.024463	-2.250726
C	4.742997	-0.752969	0.341954
H	5.440780	-1.562484	0.097827
H	5.213623	0.183260	0.034270
H	4.628928	-0.741329	1.431142
C	2.931048	-2.422707	0.007888
H	2.863917	-2.552757	1.093107
H	1.958451	-2.647259	-0.436912
H	3.656685	-3.155373	-0.363440
C	2.697222	1.961222	0.207084
C	3.509656	2.314690	-1.048667
H	4.473304	1.800824	-1.092091
H	2.951904	2.092641	-1.963844
H	3.712477	3.391716	-1.041652
C	3.545366	2.202553	1.467027
H	3.915462	3.234116	1.448198
H	2.952779	2.092198	2.379772
H	4.412639	1.544445	1.538493
C	1.475694	2.898239	0.254228
H	0.976752	2.933353	-0.717070
H	0.717817	2.572803	0.971919
H	1.817856	3.910158	0.501960
C	-2.304377	-2.027444	-0.149217
C	-3.496507	-2.741311	-0.249145
C	-2.775792	-0.894980	-2.115972
C	-4.346417	-2.507767	-1.320712
H	-3.763257	-3.471770	0.504687
C	-3.982858	-1.560781	-2.269690
H	-2.442784	-0.153769	-2.832205
H	-5.278742	-3.054848	-1.409372
H	-4.616335	-1.335867	-3.119461
N	-1.948645	-1.122141	-1.088747
H	0.574390	-1.451555	-1.672870
H	1.160881	0.672563	2.246428
H	2.508807	-0.465778	2.461805
O	-0.977246	1.119739	0.599616
C	-1.855304	2.050723	0.095822
H	-2.629064	1.597129	-0.565828
H	-1.348499	2.815547	-0.536490
C	-2.588437	2.789023	1.218750
H	-3.108415	2.046025	1.838586
H	-1.839414	3.264647	1.866900

C	-3.579994	3.836639	0.716071
H	-4.318506	3.352489	0.062845
H	-3.050369	4.565003	0.087822
C	-4.304037	4.570054	1.844116
H	-5.008640	5.313848	1.458172
H	-4.866373	3.867906	2.469635
H	-3.590711	5.089433	2.493466

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 1632.8353448600

Thermal correction to Enthalpy= 0.610207

Thermal correction to Gibbs Free Energy= 0.513804

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 1632.8812435700

9

Ru	0.098558	0.579871	0.185036
P	-2.105314	0.080039	0.042365
O	-0.276736	3.095999	1.739731
N	0.262098	-1.498366	-0.686973
C	-2.022728	-1.047792	-1.431961
C	-0.796353	-1.918735	-1.405551
C	-0.772250	-3.121075	-2.109800
H	-1.645639	-3.424597	-2.676246
C	0.369411	-3.905642	-2.080400
H	0.412548	-4.840469	-2.629652
C	1.447528	-3.483294	-1.314928
H	2.349507	-4.077973	-1.228721
C	1.351304	-2.285125	-0.616057
C	-0.119769	2.133096	1.102312
C	-2.880743	-0.945050	1.426330
C	-2.717977	-0.181575	2.751930
H	-3.071998	-0.816097	3.572837
H	-1.667216	0.060009	2.930355
H	-3.295328	0.744791	2.778575
C	-4.354689	-1.306816	1.203897
H	-4.676148	-1.993104	1.995883
H	-5.009855	-0.433342	1.247023
H	-4.516590	-1.815687	0.247589
C	-2.066238	-2.248698	1.534013
H	-2.206200	-2.896121	0.661980
H	-0.998455	-2.048870	1.658778
H	-2.415166	-2.805507	2.411237
C	-3.280537	1.431984	-0.563390
C	-3.801941	2.259628	0.621590
H	-4.514116	1.704464	1.237890
H	-2.987594	2.615062	1.259583
H	-4.324143	3.141185	0.232628
C	-4.467234	0.884707	-1.375818
H	-5.109548	1.724132	-1.665597
H	-4.138962	0.399496	-2.299489
H	-5.083633	0.178844	-0.817494
C	-2.461378	2.365135	-1.476165
H	-1.707300	2.917022	-0.913645
H	-1.927480	1.834179	-2.268122
H	-3.145760	3.085149	-1.940373
C	2.466693	-1.869093	0.287047
C	3.688227	-1.445502	-0.232492
C	3.171147	-1.562264	2.433493
C	4.673392	-1.025646	0.654194
H	3.846577	-1.420538	-1.305225
C	4.406823	-1.072223	2.016521
H	2.936635	-1.637629	3.492082
H	5.627900	-0.664034	0.285620
H	5.140532	-0.747598	2.745882
N	2.215150	-1.958459	1.595581
H	0.239048	-0.056362	1.640893
H	-1.932249	-0.374230	-2.292098
H	-2.922266	-1.654874	-1.572651
O	0.520643	1.139152	-1.866393
C	1.756665	1.205378	-1.371760
H	1.858249	0.837108	-0.174336
C	2.410674	2.586863	-1.318988
H	2.598978	2.898070	-2.354287
H	1.684378	3.292214	-0.900047
C	3.708984	2.610335	-0.516001
H	4.402604	1.861975	-0.924178
H	3.496560	2.300377	0.515707
C	4.380795	3.981695	-0.510324

H	3.715696	4.737738	-0.080259
H	5.303779	3.974258	0.077453
H	4.632367	4.301374	-1.527276
H	2.462617	0.459510	-1.792457

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 1632.8036041600

Thermal correction to Enthalpy= 0.607992

Thermal correction to Gibbs Free Energy= 0.510241

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 1632.8539051600

TS4

Ru	0.135635	0.613038	0.169837
P	-2.112753	0.058842	0.062188
O	-0.163720	3.164893	1.680680
N	0.286433	-1.476019	-0.694758
C	-2.019970	-1.064010	-1.415168
C	-0.774295	-1.909142	-1.404263
C	-0.740787	-3.109227	-2.112901
H	-1.615871	-3.421468	-2.671970
C	0.409461	-3.880892	-2.096165
H	0.458821	-4.813199	-2.649212
C	1.487224	-3.449939	-1.335162
H	2.395246	-4.036123	-1.254516
C	1.382865	-2.254876	-0.632334
C	-0.040405	2.185757	1.061262
C	-2.836725	-0.993886	1.453372
C	-2.671855	-0.229008	2.778200
H	-2.986001	-0.876984	3.604906
H	-1.626391	0.048657	2.935095
H	-3.279759	0.676972	2.820477
C	-4.302916	-1.398262	1.256747
H	-4.591190	-2.096104	2.051543
H	-4.981574	-0.543654	1.314396
H	-4.466687	-1.907631	0.301006
C	-1.982253	-2.272905	1.545795
H	-2.110328	-2.919505	0.671382
H	-0.919595	-2.042855	1.662396
H	-2.305941	-2.844853	2.423035
C	-3.339565	1.373366	-0.522873
C	-3.850543	2.187502	0.675673
H	-4.534569	1.615018	1.307842
H	-3.027343	2.557378	1.294512
H	-4.401305	3.058873	0.303385
C	-4.529986	0.800518	-1.310388
H	-5.192864	1.625249	-1.596627
H	-4.208088	0.312430	-2.234978
H	-5.123108	0.088045	-0.735457
C	-2.562138	2.327591	-1.449656
H	-1.791451	2.875701	-0.905697
H	-2.057244	1.811693	-2.270041
H	-3.267529	3.049618	-1.877991
C	2.496774	-1.838219	0.271421
C	3.714141	-1.400582	-0.245735
C	3.199891	-1.545412	2.419129
C	4.696246	-0.980283	0.643896
H	3.871908	-1.365875	-1.318539
C	4.430562	-1.040018	2.005817
H	2.967457	-1.632474	3.477315
H	5.647908	-0.608153	0.278208
H	5.161578	-0.714741	2.737572
N	2.247197	-1.943608	1.578753
H	0.297957	0.003797	1.628634
H	-1.955453	-0.387086	-2.274942
H	-2.905072	-1.693639	-1.549480
O	0.421530	1.152407	-1.941488
C	1.617023	1.225259	-1.436949
H	1.797574	0.781192	0.065294
C	2.291304	2.587184	-1.340861
H	2.542097	2.875635	-2.371263
H	1.558169	3.314555	-0.977414
C	3.551315	2.604302	-0.480493
H	4.233163	1.812352	-0.820112
H	3.281238	2.353760	0.552185
C	4.270542	3.951006	-0.514861
H	3.613992	4.750910	-0.157047
H	5.162994	3.943223	0.118040
H	4.582675	4.208190	-1.532904

H	2.324568	0.428842	-1.737160

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 1632.8008089200

Thermal correction to Enthalpy= 0.605109

Thermal correction to Gibbs Free Energy= 0.507484

Imaginary frequency: – 686.3950 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 1632.8473469700

10

Ru	0.201193	0.631480	0.257681
P	-2.112502	0.018079	0.072659
O	-0.019091	3.208636	1.739431
N	0.354960	-1.408747	-0.738394
C	-1.958881	-0.995699	-1.470962
C	-0.686869	-1.803146	-1.498635
C	-0.616472	-2.940890	-2.301958
H	-1.476630	-3.223020	-2.898956
C	0.548181	-3.689668	-2.329956
H	0.624200	-4.572263	-2.956709
C	1.605676	-3.301651	-1.519161
H	2.525243	-3.873199	-1.472434
C	1.466049	-2.169849	-0.724667
C	0.064924	2.213316	1.143772
C	-2.771648	-1.166760	1.390547
C	-2.655374	-0.490818	2.768170
H	-2.933724	-1.214300	3.543390
H	-1.628815	-0.165373	2.955089
H	-3.315078	0.372547	2.872451
C	-4.214008	-1.634396	1.155625
H	-4.466870	-2.399396	1.898868
H	-4.938753	-0.824239	1.265640
H	-4.345414	-2.085562	0.166350
C	-1.857236	-2.407166	1.404983
H	-1.948530	-2.998756	0.488387
H	-0.806744	-2.141464	1.549222
H	-2.162083	-3.050913	2.238024
C	-3.413844	1.303562	-0.408240
C	-3.968733	1.983822	0.852472
H	-4.619646	1.324976	1.432777
H	-3.165691	2.345290	1.502571
H	-4.566486	2.851821	0.552083
C	-4.568086	0.731140	-1.247505
H	-5.276118	1.537656	-1.470914
H	-4.215259	0.339196	-2.205908
H	-5.120789	-0.058611	-0.736739
C	-2.696681	2.379153	-1.245061
H	-1.935264	2.899325	-0.661052
H	-2.194260	1.970402	-2.123849
H	-3.440381	3.112194	-1.579813
C	2.557992	-1.802279	0.224628
C	3.742295	-1.228822	-0.231531
C	3.243165	-1.720313	2.395103
C	4.696553	-0.855097	0.706464
H	3.890083	-1.049031	-1.291040
C	4.437916	-1.093063	2.050618
H	3.019105	-1.944899	3.434735
H	5.619938	-0.378583	0.393273
H	5.147637	-0.809702	2.819827
N	2.315865	-2.077761	1.508290
H	0.266704	-0.036179	1.696528
H	-1.898069	-0.257124	-2.278127
H	-2.819845	-1.643251	-1.664327
O	0.120797	1.232253	-1.843182
C	1.348733	1.321938	-1.456551
H	1.728322	0.605403	0.730129
C	2.029527	2.673839	-1.376708
H	2.248640	2.975913	-2.412745
H	1.322492	3.410674	-0.980788
C	3.326691	2.673416	-0.572608
H	3.979521	1.871103	-0.943528
H	3.098285	2.421748	0.468205
C	4.063927	4.008914	-0.641531
H	3.437384	4.819175	-0.253913
H	4.984354	3.987725	-0.050119
H	4.333355	4.262621	-1.672828
H	2.031997	0.503323	-1.744692

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 1632.8112278400

Thermal correction to Enthalpy= 0.607223

Thermal correction to Gibbs Free Energy= 0.510465

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 1632.8525576200

TS6

Ru	-0.370652	-0.812529	-0.099903
P	1.737677	0.147830	-0.024434
O	0.430649	-3.711474	-0.011356
N	-0.986824	1.180513	-0.277510
C	1.204542	1.551583	-1.064858
C	-0.080358	2.092647	-0.717044
C	-0.511167	3.421093	-0.933119
H	0.208291	4.166321	-1.253239
C	-1.835858	3.746025	-0.743542
H	-2.172319	4.765607	-0.902913
C	-2.765269	2.758066	-0.382218
H	-3.819128	2.995254	-0.307837
C	-2.299160	1.473974	-0.172596
C	0.125800	-2.588614	-0.052410
C	2.301174	0.772668	1.674728
C	2.369482	-0.409535	2.657582
H	2.601306	-0.026095	3.658585
H	1.410121	-0.930828	2.701142
H	3.141873	-1.134880	2.396332
C	3.636076	1.528566	1.661807
H	3.803558	1.972143	2.650353
H	4.485815	0.873935	1.452860
H	3.633085	2.343004	0.930372
C	1.213835	1.738622	2.180540
H	1.182646	2.660085	1.593096
H	0.225807	1.272572	2.157737
H	1.440517	2.008708	3.218415
C	3.189982	-0.603994	-0.978116
C	3.896580	-1.650127	-0.101922
H	4.447498	-1.197644	0.726170
H	3.189045	-2.379608	0.304541
H	4.621139	-2.197547	-0.715307
C	4.201235	0.448967	-1.462182
H	5.014169	-0.062075	-1.991575
H	3.741977	1.146118	-2.168135
H	4.650002	1.023646	-0.652151
C	2.649095	-1.324937	-2.226673
H	1.951772	-2.123192	-1.970148
H	2.140908	-0.638473	-2.907412
H	3.498793	-1.765579	-2.761738
C	-3.150333	0.286952	0.056238
C	-4.517708	0.362400	0.317642
C	-3.242034	-2.031312	0.070859
C	-5.255752	-0.803403	0.448444
H	-4.995387	1.328874	0.424227
C	-4.606342	-2.025860	0.312364
H	-2.689974	-2.958368	-0.025334
H	-6.320298	-0.758378	0.651843
H	-5.139073	-2.965372	0.400003
N	-2.518567	-0.908325	-0.049634
H	-0.518344	-0.912397	1.487523
H	0.558197	0.455748	-1.853151
H	1.937537	2.267275	-1.433740
H	-0.036368	-0.371210	-1.940566

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 1400.3559093100

Thermal correction to Enthalpy= 0.476448

Thermal correction to Gibbs Free Energy= 0.397448

Imaginary frequency: – 1450.5333 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 1400.3775095000

TS6'

Ru	-0.391447	-0.844773	-0.050753
P	1.706924	0.127336	0.052042
O	0.470565	-3.698114	0.350830

N	-0.996374	1.178481	-0.160216
C	1.264255	1.728716	-0.712007
C	-0.077218	2.156333	-0.350205
C	-0.505859	3.498851	-0.323412
H	0.224843	4.288703	-0.455936
C	-1.841489	3.788601	-0.138428
H	-2.175357	4.821170	-0.114768
C	-2.772977	2.755776	0.008228
H	-3.824353	2.981066	0.131923
C	-2.306742	1.450844	-0.010004
C	0.137526	-2.598598	0.176273
C	2.311762	0.548553	1.809238
C	2.379672	-0.720061	2.675146
H	2.649981	-0.439718	3.700455
H	1.408644	-1.220567	2.702120
H	3.124608	-1.435711	2.324284
C	3.660823	1.282504	1.830207
H	3.871408	1.610628	2.855027
H	4.495062	0.652684	1.515163
H	3.643488	2.176300	1.197880
C	1.272530	1.493124	2.442681
H	1.266411	2.473810	1.959147
H	0.264969	1.072530	2.401505
H	1.534939	1.645027	3.496159
C	3.148808	-0.560116	-0.971679
C	3.925448	-1.618380	-0.171264
H	4.485169	-1.199580	0.667287
H	3.262151	-2.402498	0.207471
H	4.651158	-2.097370	-0.838311
C	4.094778	0.552621	-1.451697
H	4.900675	0.102839	-2.043508
H	3.567963	1.260971	-2.096823
H	4.557636	1.106832	-0.633251
C	2.583831	-1.267096	-2.217277
H	1.927224	-2.096730	-1.945545
H	2.026584	-0.590820	-2.865789
H	3.426761	-1.673391	-2.789636
C	-3.171499	0.249798	0.097230
C	-4.555672	0.319259	0.246906
C	-3.260334	-2.069217	0.084668
C	-5.298820	-0.849867	0.314756
H	-5.049759	1.280721	0.310481
C	-4.639249	-2.069865	0.228309
H	-2.697857	-2.992657	0.018770
H	-6.376322	-0.807392	0.432007
H	-5.175230	-3.010465	0.273045
N	-2.536956	-0.943691	0.022873
H	-0.464636	-0.753760	1.548251
H	0.925367	1.327358	-1.980895
H	2.013481	2.520615	-0.670686
H	-0.489749	-1.045527	-1.855459
O	0.376875	0.769627	-2.967489
H	-0.150678	-0.269938	-2.243352
H	-0.348432	1.328521	-3.265863

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 1476.7754287400

Thermal correction to Enthalpy= 0.501701

Thermal correction to Gibbs Free Energy= 0.419451

Imaginary frequency: – 1588.5840 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 1476.8133805100

TS6’’

Ru	0.356348	-1.018258	-0.631397
P	1.935006	0.488059	0.154479
O	2.004775	-2.159400	-2.875163
N	-0.692110	-0.356253	1.082650
C	0.802434	1.507547	1.176615
C	-0.238491	0.693410	1.802350
C	-0.862574	1.001269	3.026209
H	-0.485623	1.827692	3.617734
C	-1.950767	0.264249	3.441785
H	-2.439007	0.496077	4.382787
C	-2.440540	-0.774583	2.643321
H	-3.308909	-1.340146	2.955675
C	-1.778752	-1.058215	1.460839
C	1.357081	-1.704875	-2.025628
C	3.203247	-0.238205	1.372395

C	3.992917	-1.378693	0.709501
H	4.662776	-1.828721	1.452044
H	3.316859	-2.156128	0.345104
H	4.608763	-1.041095	-0.125259
C	4.163751	0.814533	1.946371
H	4.773110	0.349317	2.730099
H	4.850403	1.219440	1.200702
H	3.621614	1.647596	2.405571
C	2.424240	-0.834914	2.559972
H	1.940193	-0.059507	3.159930
H	1.666856	-1.550693	2.231831
H	3.130908	-1.363171	3.210417
C	2.791189	1.695545	-1.030498
C	4.100482	1.095614	-1.568364
H	4.879978	1.006025	-0.809244
H	3.936684	0.111693	-2.019385
H	4.486831	1.754659	-2.353968
C	3.053977	3.055544	-0.363269
H	3.555229	3.712219	-1.083828
H	2.114759	3.536646	-0.077601
H	3.693371	2.986394	0.518934
C	1.873707	1.934533	-2.244014
H	1.703025	1.010425	-2.802227
H	0.904935	2.350221	-1.961646
H	2.375078	2.644356	-2.913228
C	-2.188129	-2.113107	0.501986
C	-3.326355	-2.898408	0.675970
C	-1.721202	-3.184486	-1.503554
C	-3.656301	-3.850535	-0.276999
H	-3.954049	-2.763050	1.547762
C	-2.838806	-3.997165	-1.390939
H	-1.050761	-3.259403	-2.351191
H	-4.540520	-4.466149	-0.151753
H	-3.055555	-4.724716	-2.163962
N	-1.396775	-2.264891	-0.585690
H	1.041517	-2.133798	0.276240
H	0.071628	2.040268	0.256689
H	1.272889	2.222187	1.853677
H	-0.588036	0.052075	-1.798797
O	-0.791269	2.205569	-0.763221
H	-0.551848	0.775345	-1.339256
C	-2.105920	2.230258	-0.326087
H	-2.161906	2.353537	0.775306
H	-2.610211	1.261465	-0.540945
C	-2.918469	3.349278	-0.975260
H	-2.429223	4.306508	-0.754103
H	-2.874829	3.221290	-2.064299
C	-4.373268	3.384142	-0.510363
H	-4.403062	3.501075	0.581474
H	-4.845808	2.416163	-0.725631
C	-5.184729	4.501777	-1.163468
H	-6.222316	4.505692	-0.814792
H	-4.751305	5.482219	-0.938479
H	-5.197068	4.390040	-2.252970

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 1633.9912905500

Thermal correction to Enthalpy= 0.622733

Thermal correction to Gibbs Free Energy= 0.525705

Imaginary frequency: – 1133.9874 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 1634.0271798500

TS7

Ru	0.386906	-0.822009	-0.072507
P	-1.721286	0.120235	-0.122526
O	-0.470273	-3.673879	-0.456041
N	0.974242	1.210370	0.036211
C	-1.298923	1.756228	0.581639
C	0.053798	2.182120	0.221147
C	0.471558	3.524976	0.195039
H	-0.263986	4.310911	0.323531
C	1.808612	3.821526	0.020604
H	2.137888	4.855570	-0.002277
C	2.744817	2.793500	-0.111859
H	3.796042	3.023699	-0.227236
C	2.284670	1.485573	-0.093944
C	-0.135585	-2.571667	-0.285969
C	-2.389319	0.495723	-1.865877

C	-2.469208	-0.790566	-2.703958
H	-2.772574	-0.534631	-3.726380
H	-1.495051	-1.283460	-2.750058
H	-3.196177	-1.505665	-2.315907
C	-3.749136	1.210126	-1.856593
H	-4.002355	1.507074	-2.881258
H	-4.561391	0.577786	-1.493190
H	-3.723374	2.121218	-1.249882
C	-1.384029	1.442317	-2.549539
H	-1.368689	2.428827	-2.077600
H	-0.370787	1.033919	-2.540120
H	-1.686555	1.579708	-3.594210
C	-3.118698	-0.561538	0.962753
C	-3.917026	-1.639910	0.212916
H	-4.513518	-1.241548	-0.610102
H	-3.262175	-2.425205	-0.178367
H	-4.611283	-2.112814	0.916927
C	-4.049843	0.551383	1.469751
H	-4.839689	0.101941	2.083346
H	-3.501135	1.255603	2.100659
H	-4.534506	1.105763	0.663739
C	-2.488708	-1.240982	2.192255
H	-1.847272	-2.074814	1.892306
H	-1.918924	-0.535054	2.800113
H	-3.298141	-1.647898	2.810938
C	3.159213	0.288718	-0.192440
C	4.547549	0.369547	-0.279818
C	3.260828	-2.027835	-0.237517
C	5.299887	-0.794408	-0.346491
H	5.039665	1.334016	-0.290182
C	4.645346	-2.019161	-0.322779
H	2.701434	-2.955532	-0.220868
H	6.381340	-0.743271	-0.413520
H	5.188587	-2.955501	-0.369439
N	2.530791	-0.908576	-0.175814
H	0.378399	-0.748843	-1.651975
H	0.219787	0.082793	2.597137
H	-2.050720	2.538471	0.456787
O	0.766762	-0.729598	2.173510
H	0.426105	-1.515119	2.606617
O	-0.625563	1.113550	3.033546
H	-1.080520	1.513161	1.833906
H	-0.132465	1.826612	3.447942

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = – 1552.0401933800

Thermal correction to Enthalpy= 0.513186

Thermal correction to Gibbs Free Energy= 0.428532

Imaginary frequency: – 963.1360 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = – 1552.0903726200

TS7'

Ru	-0.361374	-0.816083	-0.026712
P	1.732935	0.158102	0.027366
O	0.457882	-3.692025	0.236824
N	-0.981782	1.201262	-0.194599
C	1.206376	1.538386	-1.048627
C	-0.085720	2.100434	-0.656298
C	-0.505888	3.424729	-0.864411
H	0.209367	4.166168	-1.201701
C	-1.835094	3.752224	-0.666274
H	-2.170875	4.771634	-0.828882
C	-2.760044	2.769832	-0.305330
H	-3.813697	3.007008	-0.229325
C	-2.287568	1.481728	-0.094383
C	0.142937	-2.576086	0.119133
C	2.288547	0.812107	1.722558
C	2.365398	-0.348055	2.729862
H	2.560666	0.060070	3.728893
H	1.420024	-0.895771	2.760601
H	3.164679	-1.055680	2.503999
C	3.616074	1.580771	1.692418
H	3.783178	2.044293	2.671903
H	4.473147	0.933169	1.493101
H	3.602018	2.382336	0.946426
C	1.198418	1.781339	2.215913
H	1.137803	2.679041	1.594252
H	0.216435	1.302990	2.240022

H	1.449441	2.098655	3.234774
C	3.210685	-0.605148	-0.883461
C	3.930330	-1.610389	0.029234
H	4.468986	-1.123289	0.844930
H	3.233482	-2.339042	0.455198
H	4.668942	-2.163416	-0.562309
C	4.206528	0.444513	-1.404831
H	5.023058	-0.071000	-1.924492
H	3.733152	1.115409	-2.126887
H	4.651426	1.048491	-0.614154
C	2.690967	-1.382676	-2.105345
H	1.979060	-2.160121	-1.819103
H	2.222211	-0.718474	-2.834409
H	3.542487	-1.866389	-2.598115
C	-3.139117	0.290403	0.138542
C	-4.504328	0.370330	0.403111
C	-3.234950	-2.025660	0.157883
C	-5.245535	-0.794479	0.538559
H	-4.980562	1.337791	0.507264
C	-4.600048	-2.017536	0.402840
H	-2.684222	-2.953810	0.063525
H	-6.309225	-0.746879	0.745761
H	-5.135565	-2.955283	0.492400
N	-2.510579	-0.905846	0.034620
H	-0.467679	-0.842632	1.562329
H	0.639261	0.688083	-1.938981
H	1.944209	2.276474	-1.361634
O	-0.244806	-0.249497	-2.222004
H	0.139342	-0.940038	-2.765813

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1475.6021614100

Thermal correction to Enthalpy= 0.485971

Thermal correction to Gibbs Free Energy= 0.405217

Imaginary frequency: –1345.7015 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1475.6416109900

TS7''

Ru	-1.166279	0.849684	-0.236892
P	-1.188489	-1.407310	0.261271
O	-3.930942	1.001597	-1.399047
N	0.715537	0.745583	0.733355
C	0.603888	-1.637328	0.528750
C	1.241214	-0.448741	1.087233
C	2.434983	-0.471461	1.833387
H	2.846471	-1.424085	2.146690
C	3.079938	0.713176	2.123995
H	4.007346	0.703009	2.687662
C	2.552548	1.928152	1.677790
H	3.069659	2.856267	1.883851
C	1.353077	1.903752	0.982930
C	-2.850901	0.943228	-0.968211
C	-2.001784	-1.854411	1.922877
C	-3.465471	-1.385467	1.950738
H	-3.886200	-1.580453	2.944587
H	-3.532192	-0.312199	1.756467
H	-4.090920	-1.904274	1.222412
C	-1.915352	-3.350005	2.262142
H	-2.283652	-3.504925	3.283171
H	-2.521192	-3.973894	1.602176
H	-0.882894	-3.713003	2.229275
C	-1.239343	-1.094573	3.025140
H	-0.217962	-1.467566	3.142515
H	-1.198692	-0.021162	2.826038
H	-1.759264	-1.244861	3.978421
C	-1.668771	-2.688023	-1.051466
C	-3.179596	-2.967407	-1.015822
H	-3.495823	-3.507525	-0.121349
H	-3.761405	-2.042816	-1.088835
H	-3.441648	-3.589335	-1.879419
C	-0.869962	-3.993409	-0.905879
H	-1.188523	-4.694013	-1.686873
H	0.199437	-3.810798	-1.042002
H	-1.021173	-4.483888	0.057394
C	-1.351176	-2.099905	-2.438137
H	-1.926548	-1.186709	-2.616316
H	-0.286092	-1.894722	-2.562040
H	-1.644169	-2.834156	-3.198463

C	0.671716	3.108854	0.444360
C	1.205922	4.391426	0.549445
C	-1.167129	3.936099	-0.701998
C	0.519654	5.467519	0.005252
H	2.154359	4.549008	1.047481
C	-0.691158	5.237301	-0.635110
H	-2.107908	3.702969	-1.186189
H	0.927325	6.469967	0.079635
H	-1.263218	6.044102	-1.077631
N	-0.509851	2.895233	-0.178167
H	-1.879992	1.091443	1.150807
H	0.788384	-0.027996	-2.054621
H	0.904022	-2.568269	1.013961
O	0.132845	0.786481	-2.118796
H	-0.396562	0.627215	-2.902911
O	1.624364	-1.192222	-1.847544
H	1.119864	-1.549850	-0.675895
C	2.947508	-0.783291	-1.669976
H	3.014142	0.094831	-0.995623
H	3.375683	-0.454286	-2.631781
C	3.827721	-1.892646	-1.094595
H	3.350242	-2.286003	-0.186938
H	3.864784	-2.725573	-1.807844
C	5.238027	-1.416952	-0.753980
H	5.169162	-0.584663	-0.039909
H	5.713138	-1.006882	-1.654729
C	6.116921	-2.520098	-0.167961
H	7.119488	-2.153605	0.073332
H	5.677016	-2.923260	0.751251
H	6.224309	-3.351809	-0.872247

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1709.2559329500

Thermal correction to Enthalpy= 0.633539

Thermal correction to Gibbs Free Energy= 0.534435

Imaginary frequency: –1096.2608 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1709.2996527600

5

Ru	-0.359742	-0.777284	0.033899
P	1.734461	0.129027	0.007759
O	0.467436	-3.643815	0.348181
N	-0.964075	1.238589	-0.174570
C	1.313010	1.735685	-0.839237
C	-0.087839	2.188061	-0.529543
C	-0.507562	3.506768	-0.689484
H	0.211443	4.273869	-0.954125
C	-1.853296	3.809280	-0.533506
H	-2.202178	4.829448	-0.654531
C	-2.759705	2.792085	-0.260651
H	-3.817828	3.010855	-0.192091
C	-2.279152	1.496102	-0.098480
C	0.143830	-2.531128	0.218184
C	2.442910	0.679830	1.678202
C	2.551870	-0.540572	2.607527
H	2.853450	-0.204370	3.606759
H	1.587974	-1.048988	2.688972
H	3.295989	-1.262546	2.264959
C	3.798710	1.394147	1.590118
H	4.068239	1.767186	2.585142
H	4.604061	0.732287	1.264502
H	3.767913	2.258277	0.917955
C	1.432198	1.661625	2.301298
H	1.379862	2.605602	1.748905
H	0.432132	1.224431	2.352381
H	1.756143	1.899303	3.321093
C	3.104464	-0.583036	-1.085377
C	3.910691	-1.639503	-0.313629
H	4.557022	-1.206007	0.453686
H	3.255724	-2.379478	0.156915
H	4.554728	-2.173994	-1.021425
C	4.051188	0.486276	-1.655931
H	4.828833	-0.012062	-2.246328
H	3.527852	1.171056	-2.329303
H	4.551545	1.076389	-0.886728
C	2.406626	-1.292941	-2.261164
H	1.930729	-2.216064	-1.921164
H	1.616218	-0.686636	-2.712316

H	3.159742	-1.551258	-3.015403
C	-3.134273	0.302788	0.110594
C	-4.519074	0.376330	0.246386
C	-3.205408	-2.007552	0.267232
C	-5.255733	-0.790384	0.390135
H	-5.021171	1.335952	0.237637
C	-4.586703	-2.007896	0.393174
H	-2.636409	-2.929332	0.274623
H	-6.334493	-0.747686	0.494721
H	-5.117435	-2.947209	0.494292
N	-2.489367	-0.885089	0.137238
H	-0.375953	-0.703565	1.654411
H	1.304802	1.479509	-1.905726
H	2.043550	2.533903	-0.679584
O	-0.593575	-0.504577	-2.102705
H	-0.588054	-1.366953	-2.523745

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1475.6215766100

Thermal correction to Enthalpy= 0.490424

Thermal correction to Gibbs Free Energy= 0.407924

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1475.6757822000

11

Ru	-0.054897	-0.126223	0.935575
P	-2.104452	0.122145	-0.086102
O	-0.765485	1.191836	3.538943
N	0.369772	-1.241063	-0.817368
C	-1.591526	-0.266787	-1.823084
C	-0.481907	-1.265617	-1.854511
C	-0.243450	-2.119622	-2.932391
H	-0.937720	-2.137777	-3.764339
C	0.889250	-2.916852	-2.926933
H	1.086580	-3.591644	-3.753204
C	1.790171	-2.832473	-1.868532
H	2.690502	-3.433775	-1.868952
C	1.505814	-1.962816	-0.824825
C	-0.481785	0.700690	2.524118
C	-3.385535	-1.217765	0.330212
C	-3.647652	-1.233884	1.845262
H	-4.336816	-2.053536	2.080903
H	-2.719803	-1.396911	2.398321
H	-4.102380	-0.308545	2.203942
C	-4.712921	-1.070405	-0.428516
H	-5.339892	-1.944048	-0.215450
H	-5.278459	-0.186445	-0.127975
H	-4.564295	-1.034209	-1.512597
C	-2.783950	-2.580502	-0.064065
H	-2.688639	-2.687016	-1.148948
H	-1.805047	-2.740941	0.393396
H	-3.455720	-3.373356	0.284250
C	-2.950007	1.810212	-0.222542
C	-3.839330	2.062462	1.005378
H	-4.735927	1.438767	1.021879
H	-3.289657	1.907390	1.939517
H	-4.169658	3.107213	0.988937
C	-3.762040	1.969474	-1.518698
H	-4.224142	2.963396	-1.522894
H	-3.116907	1.908737	-2.399217
H	-4.562930	1.235997	-1.621290
C	-1.847029	2.883839	-0.228249
H	-1.329491	2.904720	0.737463
H	-1.116002	2.727560	-1.031320
H	-2.320102	3.863481	-0.367202
C	2.413410	-1.694299	0.318066
C	3.709992	-2.197412	0.389996
C	2.719807	-0.519988	2.293467
C	4.522953	-1.840567	1.456864
H	4.090698	-2.845393	-0.389642
C	4.021341	-0.981912	2.425991
H	2.282450	0.156067	3.017870
H	5.536871	-2.220214	1.522055
H	4.621823	-0.665491	3.270440
N	1.929944	-0.869071	1.272981
H	-0.636793	-1.449748	1.585656
O	0.417479	1.804763	-2.208252
C	1.474920	1.600109	-1.501425
H	-2.412092	-0.530124	-2.494699

O	1.139683	1.574075	0.053391
H	-1.065622	0.661041	-2.160503
H	0.634535	2.386329	0.160040
C	2.589768	2.652724	-1.601780
H	2.856901	2.717435	-2.664324
H	2.170123	3.630917	-1.328923
C	3.831779	2.343267	-0.769583
H	3.556270	2.332024	0.290328
H	4.173246	1.324576	-1.004931
C	4.975037	3.329036	-1.004441
H	5.286244	3.329339	-2.055015
H	4.668448	4.350558	-0.753879
H	1.949649	0.589925	-1.568760
H	5.851932	3.085421	-0.395311

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1708.0390676300

Thermal correction to Enthalpy= 0.615749

Thermal correction to Gibbs Free Energy= 0.517791

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1708.0962523500

TS8

Ru	0.025762	-0.447905	-0.887440
P	2.054256	0.073701	0.089679
O	0.834965	-0.001265	-3.746410
N	-0.482647	-0.916250	1.109150
C	1.425903	0.368413	1.785150
C	0.320267	-0.530564	2.124839
C	-0.025194	-0.891817	3.438824
H	0.623645	-0.599951	4.256397
C	-1.196280	-1.584469	3.669597
H	-1.473395	-1.862703	4.681293
C	-2.044120	-1.905820	2.605917
H	-2.982103	-2.413724	2.789723
C	-1.652414	-1.546113	1.326576
C	0.512692	-0.151905	-2.638778
C	3.263259	-1.389066	0.240659
C	3.606170	-1.952410	-1.148380
H	4.224278	-2.850245	-1.027934
H	2.698105	-2.233302	-1.687558
H	4.167086	-1.249642	-1.765963
C	4.548322	-1.040113	1.006437
H	5.129085	-1.956712	1.163364
H	5.189540	-0.339579	0.468152
H	4.328909	-0.619378	1.993153
C	2.551044	-2.501627	1.033757
H	2.376241	-2.212922	2.073968
H	1.596001	-2.777033	0.580591
H	3.192553	-3.390432	1.041233
C	3.009227	1.641607	-0.385477
C	3.995140	1.356268	-1.529422
H	4.836130	0.728826	-1.227889
H	3.496152	0.885911	-2.382878
H	4.410059	2.309233	-1.876838
C	3.740209	2.255868	0.819701
H	4.280138	3.150610	0.488175
H	3.028993	2.566938	1.589327
H	4.469560	1.580065	1.270009
C	2.005368	2.687947	-0.901791
H	1.498922	2.331395	-1.805443
H	1.269078	2.943695	-0.134031
H	2.559945	3.594842	-1.171653
C	-2.480412	-1.739078	0.109355
C	-3.736596	-2.341141	0.131982
C	-2.677728	-1.340274	-2.167639
C	-4.473502	-2.434124	-1.040105
H	-4.139691	-2.730268	1.058596
C	-3.937753	-1.918478	-2.213329
H	-2.211718	-0.929440	-3.055108
H	-5.453467	-2.899062	-1.034161
H	-4.477631	-1.960779	-3.151759
N	-1.960117	-1.254367	-1.041612
H	0.572430	-1.908955	-1.105328
O	-0.082907	2.514938	1.435753
C	-1.238843	2.131335	0.914069
H	2.177865	0.448970	2.572647
O	-1.070112	1.553336	-0.474556
H	0.768308	1.451982	1.660617

H	-0.583899	2.232854	-0.954084
C	-2.253933	3.268246	0.781079
H	-2.372712	3.702298	1.780855
H	-1.808047	4.053882	0.155027
C	-3.611365	2.842034	0.227069
H	-3.473888	2.425302	-0.776524
H	-4.008904	2.024621	0.844863
C	-4.622400	3.986377	0.185016
H	-4.795693	4.396418	1.186008
H	-4.260976	4.805076	-0.446796
H	-1.729705	1.277550	1.424645
H	-5.587169	3.657657	-0.214186

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1708.0361211100

Thermal correction to Enthalpy= 0.611805

Thermal correction to Gibbs Free Energy= 0.515699

Imaginary frequency: –834.8554 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1708.0839233700

12

Ru	0.098951	-0.516906	-0.823509
P	2.112129	0.110778	0.140777
O	0.931521	-0.237035	-3.698958
N	-0.428110	-0.796055	1.198543
C	1.542826	0.405477	1.812466
C	0.377663	-0.277877	2.185137
C	-0.070219	-0.432231	3.538851
H	0.559192	-0.059042	4.339124
C	-1.274233	-1.019866	3.806377
H	-1.607172	-1.124146	4.834723
C	-2.100962	-1.484325	2.759476
H	-3.070252	-1.913807	2.974489
C	-1.628769	-1.349188	1.471000
C	0.597936	-0.327169	-2.586321
C	3.379095	-1.311398	0.281442
C	3.697312	-1.916743	-1.094669
H	4.350594	-2.787743	-0.961187
H	2.783731	-2.250759	-1.592535
H	4.212591	-1.221364	-1.758933
C	4.674147	-0.895587	0.994246
H	5.283732	-1.788058	1.179640
H	5.283203	-0.206194	0.405164
H	4.465779	-0.434028	1.965122
C	2.719694	-2.407517	1.140213
H	2.559944	-2.071038	2.167720
H	1.758148	-2.723057	0.728836
H	3.383444	-3.279808	1.166655
C	3.006253	1.681667	-0.439415
C	3.944714	1.387651	-1.619775
H	4.817214	0.798488	-1.331550
H	3.423699	0.865608	-2.428614
H	4.314306	2.337458	-2.023847
C	3.777794	2.362985	0.701761
H	4.256399	3.272957	0.320294
H	3.101294	2.655522	1.509537
H	4.560983	1.730283	1.122300
C	1.949451	2.678425	-0.945917
H	1.418014	2.274120	-1.814320
H	1.233599	2.947160	-0.166468
H	2.454572	3.597501	-1.266224
C	-2.413212	-1.718690	0.264103
C	-3.652182	-2.355867	0.326076
C	-2.545110	-1.638474	-2.054072
C	-4.345523	-2.627854	-0.843680
H	-4.067703	-2.641100	1.284303
C	-3.785498	-2.257230	-2.060646
H	-2.056990	-1.340203	-2.974249
H	-5.309660	-3.123724	-0.804551
H	-4.289738	-2.446434	-3.000834
N	-1.870182	-1.375968	-0.927469
H	0.678765	-1.963263	-0.932436
O	-0.465851	2.678231	1.353110
C	-1.520257	2.083911	0.686934
H	2.231986	0.699414	2.599059
O	-1.098634	1.530944	-0.570940
H	0.204093	1.990011	1.567435
H	-0.638963	2.230372	-1.048810

C	-2.616180	3.111150	0.464722
H	-2.879555	3.530182	1.442095
H	-2.205140	3.937880	-0.130712
C	-3.852131	2.521577	-0.212378
H	-3.564384	2.102502	-1.182495
H	-4.221204	1.678887	0.387474
C	-4.967348	3.548341	-0.395617
H	-5.290635	3.956684	0.567796
H	-4.630745	4.387361	-1.013874
H	-1.917731	1.218835	1.229366
H	-5.841005	3.104773	-0.881858

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1708.0538027800

Thermal correction to Enthalpy= 0.617590

Thermal correction to Gibbs Free Energy= 0.519503

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1708.0926778100

TS9

Ru	0.070738	-0.208806	-0.835820
P	-2.066923	0.161726	-0.026083
O	-0.613093	-2.162722	-3.017802
N	0.551712	1.230261	0.636620
C	-1.547828	0.690062	1.643035
C	-0.342057	1.520001	1.606018
C	-0.006899	2.486294	2.569192
H	-0.720781	2.729495	3.347316
C	1.233909	3.090597	2.524481
H	1.503120	3.832291	3.269595
C	2.156915	2.735745	1.537560
H	3.143943	3.179555	1.525424
C	1.775752	1.786148	0.602793
C	-0.348370	-1.423668	-2.162686
C	-2.960894	1.626642	-0.846986
C	-3.108368	1.383578	-2.358330
H	-3.550548	2.273614	-2.821881
H	-2.135104	1.205715	-2.822380
H	-3.756104	0.536792	-2.590442
C	-4.333130	1.925426	-0.226816
H	-4.719656	2.860724	-0.648532
H	-5.069051	1.147072	-0.439724
H	-4.268167	2.056551	0.858288
C	-2.085433	2.878662	-0.654605
H	-2.016768	3.170489	0.397214
H	-1.074774	2.732888	-1.043583
H	-2.542139	3.712316	-1.200474
C	-3.281465	-1.257368	0.255389
C	-4.064704	-1.570394	-1.027800
H	-4.792512	-0.795723	-1.280861
H	-3.397957	-1.718120	-1.883240
H	-4.621059	-2.502839	-0.879885
C	-4.246225	-0.990652	1.423071
H	-4.888409	-1.869565	1.553336
H	-3.699943	-0.844785	2.358946
H	-4.897281	-0.130842	1.262109
C	-2.450005	-2.494127	0.624228
H	-1.737581	-2.767016	-0.157253
H	-1.894370	-2.322984	1.546282
H	-3.128247	-3.341877	0.778356
C	2.662381	1.238996	-0.453154
C	3.943986	1.727564	-0.697754
C	2.931616	-0.379571	-2.092406
C	4.732911	1.126808	-1.667995
H	4.322533	2.570469	-0.133234
C	4.221044	0.044985	-2.373427
H	2.483655	-1.211894	-2.621823
H	5.733652	1.495483	-1.865044
H	4.801366	-0.464533	-3.133161
N	2.161802	0.199758	-1.161905
H	-0.163349	0.900237	-1.919759
O	-0.164109	-1.296353	2.646007
C	0.637983	-1.863275	1.747637
C	2.131241	-1.573160	1.928046
H	2.279707	-0.490718	1.840720
H	2.384933	-1.845484	2.959253
C	3.022582	-2.322652	0.941547
H	2.598318	-2.227773	-0.066126
H	2.990952	-3.389980	1.179192

C	4.464430	-1.820482	0.940117
H	5.084561	-2.374399	0.227919
H	4.511112	-0.759025	0.669417
H	4.919043	-1.925372	1.931294
H	0.384150	-1.508370	0.651110
H	-2.327200	1.082491	2.298850
O	0.468633	-3.271348	1.687209
H	-0.972751	-0.367407	2.166100
H	-0.238219	-3.429637	2.320763

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1708.0212981800

Thermal correction to Enthalpy= 0.610277

Thermal correction to Gibbs Free Energy= 0.515919

Imaginary frequency: –1206.0462 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1708.0772133800

TS10

Ru	0.027746	-0.463343	-0.853274
P	2.062888	0.073384	0.098435
O	0.676850	0.394200	-3.660612
N	-0.343453	-1.221954	1.086720
C	1.564676	0.011188	1.851436
C	0.526039	-0.972145	2.096940
C	0.291016	-1.582517	3.348267
H	0.990322	-1.411338	4.159074
C	-0.819332	-2.380929	3.523825
H	-0.999178	-2.855975	4.483317
C	-1.725207	-2.574974	2.475259
H	-2.608315	-3.183710	2.619693
C	-1.450897	-1.967299	1.260488
C	0.406479	0.090463	-2.572844
C	3.408007	-1.262334	-0.092581
C	3.666019	-1.564712	-1.577680
H	4.381211	-2.392594	-1.656138
H	2.742126	-1.863111	-2.078815
H	4.087412	-0.715560	-2.117823
C	4.724933	-0.910127	0.614339
H	5.391116	-1.780482	0.582740
H	5.254044	-0.081332	0.139378
H	4.563897	-0.659842	1.668127
C	2.866798	-2.547257	0.562847
H	2.776733	-2.442612	1.647666
H	1.892262	-2.829826	0.157425
H	3.568837	-3.365429	0.364121
C	2.825137	1.788513	-0.170721
C	3.699159	1.800284	-1.434844
H	4.613230	1.212971	-1.327166
H	3.149484	1.434390	-2.307824
H	4.000431	2.832907	-1.645095
C	3.631866	2.266968	1.046799
H	4.021169	3.271939	0.844421
H	2.996810	2.330851	1.934701
H	4.483778	1.624266	1.275240
C	1.684181	2.796675	-0.402220
H	1.061019	2.513332	-1.253980
H	1.053286	2.906865	0.480488
H	2.128898	3.775911	-0.617350
C	-2.340951	-2.030802	0.070946
C	-3.563386	-2.698349	0.071805
C	-2.697071	-1.309040	-2.108232
C	-4.362797	-2.662521	-1.062733
H	-3.892908	-3.236217	0.952057
C	-3.927281	-1.948073	-2.171024
H	-2.316081	-0.721853	-2.933993
H	-5.316783	-3.178957	-1.074733
H	-4.523859	-1.877798	-3.072646
N	-1.915672	-1.359296	-1.023640
H	0.657513	-1.836781	-1.284584
H	0.731640	1.158947	2.045299
H	2.369200	0.001916	2.589370
O	-1.130462	1.341410	-0.005842
C	-2.305209	3.428504	0.018444
H	-1.411937	3.898156	0.446878
H	-2.744401	4.111320	-0.712256
C	-3.306972	3.132768	1.143994
H	-2.857835	2.425823	1.850011
H	-4.187582	2.637197	0.718924

C	-3.727540	4.399296	1.884746
H	-4.445975	4.174519	2.678410
H	-2.861344	4.888828	2.341963
H	-4.194845	5.116767	1.202445
C	-1.890851	2.168912	-0.717280
O	-2.239132	1.903996	-1.847861
O	-0.125109	2.001759	2.104429
H	-0.648644	1.812682	2.888529
H	-0.773053	1.693013	0.957342

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1783.2745787700

Thermal correction to Enthalpy= 0.614671

Thermal correction to Gibbs Free Energy= 0.513792

Imaginary frequency: –1230.3911 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1783.32507224

TS10’

Ru	-0.557248	-0.383643	-0.825527
P	1.433261	-1.162953	0.070816
O	0.232777	-0.299155	-3.723642
N	-1.155210	-0.471936	1.204876
C	1.172141	-0.342009	1.675766
C	-0.189498	-0.466415	2.157101
C	-0.590082	-0.443964	3.510355
H	0.163892	-0.477918	4.288602
C	-1.931601	-0.356625	3.821611
H	-2.244176	-0.337145	4.861137
C	-2.893466	-0.252435	2.809791
H	-3.937697	-0.107313	3.055227
C	-2.453035	-0.297364	1.496171
C	-0.063974	-0.308686	-2.600050
C	1.508061	-3.048400	0.317015
C	1.339674	-3.765278	-1.033478
H	1.273945	-4.845780	-0.857272
H	0.422415	-3.442724	-1.532232
H	2.175592	-3.595134	-1.713571
C	2.783994	-3.531589	1.018689
H	2.677678	-4.595160	1.262995
H	3.671628	-3.433581	0.389232
H	2.958060	-2.993283	1.956250
C	0.310992	-3.440383	1.202492
H	0.401292	-3.035254	2.214156
H	-0.635918	-3.104361	0.773337
H	0.279849	-4.533212	1.282934
C	3.110006	-0.526789	-0.542225
C	3.568186	-1.343631	-1.760579
H	3.855445	-2.363486	-1.495270
H	2.794237	-1.386836	-2.533130
H	4.449533	-0.863339	-2.200427
C	4.197629	-0.543278	0.545018
H	5.117496	-0.115092	0.129157
H	3.910375	0.072298	1.402221
H	4.435708	-1.544399	0.904063
C	2.947894	0.935235	-0.993861
H	2.137326	1.070413	-1.712475
H	2.771843	1.592451	-0.140538
H	3.882095	1.260623	-1.465856
C	-3.305365	-0.041496	0.307334
C	-4.692330	0.062611	0.372685
C	-3.337517	0.479267	-1.954042
C	-5.408819	0.392314	-0.769405
H	-5.206645	-0.115846	1.309204
C	-4.717926	0.618074	-1.953231
H	-2.753249	0.633940	-2.852941
H	-6.489730	0.475725	-0.732442
H	-5.231161	0.891076	-2.867527
N	-2.642213	0.146057	-0.859654
H	-1.053982	-1.837865	-1.157424
H	0.819132	0.984662	1.004307
H	1.939886	-0.427306	2.443591
O	0.180648	1.558874	0.227750
C	1.235359	3.623184	0.843859
H	0.505122	4.093445	1.516292
H	1.842859	2.960965	1.472948
C	2.097104	4.692263	0.177275
H	1.458493	5.296603	-0.472885
H	2.825907	4.203505	-0.480188

C	2.821280	5.572772	1.192244
H	3.435717	6.327774	0.693569
H	2.109203	6.096081	1.839832
H	3.479385	4.978866	1.836156
C	0.441791	2.797437	-0.158381
O	0.043752	3.244461	-1.212805

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1706.8380217700

Thermal correction to Enthalpy= 0.588255

Thermal correction to Gibbs Free Energy= 0.491362

Imaginary frequency: –1129.9498 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1706.8804647900

6

Ru	0.013525	-0.195041	-0.761109
P	2.068242	0.314845	0.084301
O	0.163175	1.558180	-3.199456
N	-0.055368	-1.531351	0.874737
C	1.813675	-0.317306	1.825103
C	0.851971	-1.474926	1.861280
C	0.834728	-2.417497	2.886270
H	1.580712	-2.375153	3.671838
C	-0.153855	-3.392884	2.888582
H	-0.182174	-4.140249	3.674480
C	-1.124044	-3.393238	1.893727
H	-1.917226	-4.130121	1.906925
C	-1.055960	-2.428598	0.892793
C	0.081125	0.903217	-2.245757
C	3.525022	-0.718399	-0.552399
C	3.631267	-0.548021	-2.077293
H	4.417723	-1.210829	-2.457248
H	2.689549	-0.814558	-2.562540
H	3.890911	0.471992	-2.368082
C	4.874183	-0.393567	0.102991
H	5.620068	-1.117739	-0.244610
H	5.241173	0.600251	-0.162556
H	4.833878	-0.468424	1.194836
C	3.200923	-2.195937	-0.259926
H	3.223179	-2.418994	0.811867
H	2.224450	-2.478121	-0.660974
H	3.961383	-2.823676	-0.738134
C	2.596225	2.111392	0.356171
C	3.252147	2.656519	-0.922667
H	4.243544	2.233113	-1.102223
H	2.628981	2.475799	-1.803937
H	3.373030	3.741076	-0.822625
C	3.533942	2.314687	1.557688
H	3.775351	3.380914	1.637312
H	3.057473	2.024396	2.498845
H	4.475761	1.772570	1.468865
C	1.312663	2.924310	0.606125
H	0.658394	2.918093	-0.267720
H	0.723243	2.539168	1.441203
H	1.595874	3.960926	0.824257
C	-2.065758	-2.253740	-0.181146
C	-3.205962	-3.045373	-0.288822
C	-2.754815	-0.936769	-1.963350
C	-4.138071	-2.762021	-1.278463
H	-3.373976	-3.867606	0.395904
C	-3.914368	-1.683404	-2.123314
H	-2.545057	-0.063810	-2.566987
H	-5.032100	-3.368594	-1.376129
H	-4.624746	-1.409983	-2.894242
N	-1.841735	-1.227322	-1.030911
H	0.696814	-1.309660	-1.684773
H	1.324162	0.509685	2.353722
H	2.742916	-0.549068	2.353639
O	-1.064068	1.043601	0.712933
C	-2.693831	2.618292	1.382540
H	-2.826108	1.984608	2.267420
H	-1.972580	3.393812	1.677497
C	-4.011512	3.260053	0.964099
H	-4.719978	2.472272	0.683051
H	-3.843676	3.846072	0.055720
C	-4.614034	4.135120	2.061460
H	-5.560255	4.583504	1.742603
H	-4.809369	3.554776	2.970604

H	-3.934029	4.950598	2.333161
C	-2.026331	1.782991	0.286926
O	-2.408142	1.877389	-0.884624

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1706.8843166200

Thermal correction to Enthalpy= 0.592998

Thermal correction to Gibbs Free Energy= 0.494436

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1706.9392011100

TS8[e]

Ru	0.248425	0.188661	-0.902575
P	2.356220	0.223817	0.053334
O	0.530449	2.690413	-2.540992
N	0.165281	-1.683593	0.058597
C	2.002625	-0.959307	1.406989
C	1.103452	-2.023889	0.969346
C	1.066782	-3.314771	1.528325
H	1.816454	-3.596763	2.258399
C	0.073817	-4.194704	1.149413
H	0.042792	-5.193996	1.571380
C	-0.911907	-3.796067	0.240687
H	-1.710465	-4.473960	-0.032185
C	-0.842053	-2.512395	-0.274527
C	0.408440	1.738677	-1.882649
C	3.714693	-0.604341	-0.993461
C	3.880799	0.123117	-2.338017
H	4.601971	-0.425723	-2.955610
H	2.931351	0.161887	-2.878229
H	4.253198	1.142129	-2.228428
C	5.063167	-0.696619	-0.262348
H	5.758480	-1.287709	-0.870093
H	5.527468	0.276403	-0.093505
H	4.962770	-1.201862	0.703810
C	3.269987	-2.047694	-1.298152
H	3.247500	-2.666130	-0.396874
H	2.286044	-2.082030	-1.771460
H	3.993789	-2.496945	-1.988024
C	3.049902	1.783727	0.876629
C	3.895921	2.607991	-0.106629
H	4.837573	2.129366	-0.382048
H	3.338932	2.838315	-1.020506
H	4.145170	3.561918	0.371767
C	3.860476	1.439398	2.136765
H	4.259799	2.366444	2.564656
H	3.219860	0.976324	2.891709
H	4.706124	0.777358	1.937458
C	1.866061	2.667466	1.303226
H	1.295163	3.006178	0.434779
H	1.203671	2.132375	1.988185
H	2.265244	3.555116	1.809758
C	-1.877372	-1.895790	-1.140339
C	-3.064011	-2.541090	-1.481153
C	-2.562680	0.020932	-2.253323
C	-4.021750	-1.866549	-2.224561
H	-3.248644	-3.555242	-1.150149
C	-3.769352	-0.558096	-2.617405
H	-2.314438	1.036836	-2.537446
H	-4.953675	-2.355350	-2.487177
H	-4.488164	0.011410	-3.194395
N	-1.637945	-0.622759	-1.531371
H	0.891181	-0.499450	-2.154260
O	0.314028	0.459527	2.857126
C	-0.934830	0.543439	2.425734
C	-1.737922	-0.761486	2.548925
H	-1.151364	-1.583143	2.133011
H	-1.801818	-0.962094	3.625725
C	-3.139074	-0.763032	1.945970
H	-3.078670	-0.480807	0.889817
H	-3.750668	0.007916	2.432234
C	-3.834293	-2.116352	2.079620
H	-4.830027	-2.105091	1.624507
H	-3.246947	-2.902140	1.589964
H	-3.947401	-2.402702	3.130767
H	-1.503532	1.338694	2.951733
H	2.864277	-1.320291	1.971849
O	-1.006641	1.010281	0.979710
H	1.200424	-0.292678	2.154626

C	-1.463829	2.346300	0.834006
H	-1.146591	2.944141	1.699953
H	-0.966858	2.773358	-0.041268
C	-2.972730	2.444106	0.649299
H	-3.479659	2.090149	1.554735
H	-3.272001	1.764432	-0.159290
C	-3.425091	3.867540	0.326924
H	-2.912850	4.215119	-0.579887
H	-3.108669	4.541571	1.133218
C	-4.936300	3.976379	0.133991
H	-5.238785	5.001337	-0.099625
H	-5.273268	3.332127	-0.685722
H	-5.470345	3.666230	1.038373

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1865.2463336800

Thermal correction to Enthalpy= 0.732226

Thermal correction to Gibbs Free Energy= 0.626089

Imaginary frequency: –937.9484 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1865.2932258100

TS9[e]

Ru	-0.189217	-0.177563	0.941307
P	-2.235734	0.337074	-0.037452
O	-0.029708	2.111748	2.885503
N	-0.316857	-1.801219	-0.402128
C	-1.863560	-0.458190	-1.644295
C	-1.155126	-1.726951	-1.459721
C	-1.202837	-2.805604	-2.359363
H	-1.875714	-2.759028	-3.207491
C	-0.378655	-3.896205	-2.160960
H	-0.408355	-4.731667	-2.852823
C	0.518882	-3.917027	-1.090531
H	1.199021	-4.749142	-0.962531
C	0.531407	-2.829789	-0.230205
C	-0.083650	1.236719	2.123625
C	-3.700156	-0.612507	0.729660
C	-3.893323	-0.208289	2.201233
H	-4.666499	-0.845073	2.647521
H	-2.969928	-0.347522	2.769583
H	-4.214719	0.826742	2.320085
C	-5.009157	-0.420252	-0.050838
H	-5.774739	-1.084369	0.367318
H	-5.396336	0.598377	0.010617
H	-4.889761	-0.682098	-1.107300
C	-3.375610	-2.117920	0.702678
H	-3.321736	-2.506841	-0.317745
H	-2.436781	-2.343125	1.213456
H	-4.180044	-2.655951	1.217343
C	-2.789253	2.095723	-0.465411
C	-3.589310	2.737146	0.677928
H	-4.584068	2.305558	0.807983
H	-3.051899	2.675921	1.629649
H	-3.724063	3.799986	0.447494
C	-3.592785	2.136588	-1.776512
H	-3.911541	3.169351	-1.959048
H	-2.971685	1.831683	-2.622735
H	-4.489012	1.513942	-1.757902
C	-1.521692	2.934550	-0.671729
H	-0.971266	3.059101	0.264107
H	-0.864272	2.477954	-1.416614
H	-1.813772	3.932088	-1.022660
C	1.510205	-2.634695	0.867493
C	2.473988	-3.581746	1.202134
C	2.371137	-1.155680	2.436051
C	3.414398	-3.286789	2.178996
H	2.497815	-4.538240	0.695411
C	3.366518	-2.048066	2.805475
H	2.287355	-0.179213	2.897452
H	4.175395	-4.013335	2.442179
H	4.082838	-1.769006	3.568866
N	1.463128	-1.433371	1.492189
H	-0.978676	-0.918412	2.069155
O	0.177955	1.004609	-2.488135
C	1.252882	0.682474	-1.776384
C	1.786843	2.861335	-0.968042
H	1.252189	2.579332	-0.043818
H	1.083983	3.429690	-1.592100

C	2.994557	3.713968	-0.620087
H	3.688166	3.115818	-0.015656
H	3.526209	3.976658	-1.542836
H	0.955236	0.430955	-0.656282
H	-2.688327	-0.526218	-2.356342
H	-0.905150	0.286400	-2.119817
C	3.288908	-0.886251	-1.519049
H	3.048678	-0.901138	-0.449561
H	4.030221	-0.091970	-1.643178
C	3.885269	-2.231303	-1.928839
H	3.159129	-3.041395	-1.790137
H	4.171155	-2.229558	-2.986186
O	2.219121	1.701972	-1.626986
C	2.601574	4.981483	0.138273
H	1.892869	5.561312	-0.466978
H	2.064473	4.703166	1.054510
C	2.038043	-0.522401	-2.315428
H	2.304378	-0.270467	-3.348275
H	1.356068	-1.376689	-2.376917
H	4.776621	-2.473315	-1.340665
C	3.802118	5.855611	0.495000
H	4.337079	6.173403	-0.406368
H	3.496576	6.754705	1.038471
H	4.511912	5.308201	1.124635

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1865.2295494500

Thermal correction to Enthalpy= 0.730427

Thermal correction to Gibbs Free Energy= 0.622470

Imaginary frequency: –1169.0417 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1865.2840079500

TS18

Ru	0.316170	-0.807966	-0.227986
P	-1.791267	0.114787	-0.104050
O	-0.531954	-3.617782	-0.869668
N	0.905869	1.211018	0.015111
C	-1.333198	1.712295	0.713151
C	0.003749	2.178778	0.267639
C	0.386130	3.519943	0.222720
H	-0.347427	4.291033	0.428639
C	1.700209	3.843342	-0.073392
H	2.011719	4.881398	-0.119701
C	2.627173	2.827003	-0.297494
H	3.659057	3.069570	-0.518527
C	2.196221	1.509710	-0.239582
C	-0.201149	-2.536024	-0.600872
C	-2.548656	0.630345	-1.769984
C	-2.651274	-0.597298	-2.690674
H	-3.039540	-0.281492	-3.666299
H	-1.669478	-1.051129	-2.842907
H	-3.325247	-1.362391	-2.300507
C	-3.920431	1.311108	-1.652829
H	-4.219134	1.674132	-2.643157
H	-4.704092	0.633698	-1.308228
H	-3.891539	2.177650	-0.984419
C	-1.595204	1.643606	-2.432102
H	-1.586894	2.601682	-1.904291
H	-0.572891	1.263310	-2.490294
H	-1.944575	1.835265	-3.453180
C	-3.141958	-0.595014	1.019115
C	-3.944450	-1.674779	0.276084
H	-4.589434	-1.266526	-0.505152
H	-3.287390	-2.426959	-0.172521
H	-4.590718	-2.190041	0.995802
C	-4.081623	0.481025	1.588661
H	-4.830445	-0.007146	2.223235
H	-3.535463	1.189147	2.217927
H	-4.618195	1.039675	0.821363
C	-2.444408	-1.272331	2.211484
H	-1.860459	-2.137131	1.878338
H	-1.789998	-0.575889	2.750060
H	-3.212040	-1.638716	2.903890
C	3.075262	0.329646	-0.412037
C	4.461499	0.421166	-0.520563
C	3.186250	-1.986223	-0.506490
C	5.216641	-0.737370	-0.631321
H	4.949190	1.387966	-0.503386

C	4.568231	-1.966283	-0.620644
H	2.632301	-2.916621	-0.484047
H	6.296591	-0.679912	-0.714725
H	5.115990	-2.898175	-0.693902
N	2.452549	-0.871411	-0.412957
H	0.232594	-0.542438	-1.790825
H	-2.095077	2.493858	0.665900
O	0.821488	-1.217460	1.931469
H	-1.120685	1.402504	1.786333
C	1.293703	-0.064043	2.944865
H	1.655767	-0.709218	3.754390
C	0.291351	0.907521	3.292517
H	0.516945	1.937533	3.010816
H	-0.124120	0.826267	4.296944
H	2.146159	0.313652	2.372902
H	0.006441	-1.517915	2.342642

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1554.1493194200

Thermal correction to Enthalpy= 0.546802

Thermal correction to Gibbs Free Energy= 0.459320

Imaginary frequency: –271.4531 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1554.19464652

TS19

Ru	0.125522	-0.505298	-0.682859
P	-2.004187	0.122164	-0.059332
O	-0.639360	-3.055487	-2.074500
N	0.621773	1.380833	0.133738
C	-1.542797	1.442018	1.137522
C	-0.312423	2.141996	0.740976
C	0.003448	3.450664	1.123956
H	-0.751079	4.059026	1.609463
C	1.277016	3.938664	0.898243
H	1.534736	4.951027	1.191247
C	2.238777	3.120985	0.301674
H	3.239962	3.494659	0.128252
C	1.872468	1.837830	-0.073034
C	-0.340708	-2.078776	-1.517439
C	-3.002797	1.017724	-1.406125
C	-3.140257	0.115386	-2.643665
H	-3.674260	0.663089	-3.429463
H	-2.157613	-0.165982	-3.029173
H	-3.701338	-0.798526	-2.440095
C	-4.390123	1.482375	-0.938622
H	-4.844290	2.091855	-1.728725
H	-5.071137	0.652827	-0.738781
H	-4.329608	2.105279	-0.040346
C	-2.217153	2.276685	-1.819616
H	-2.199598	3.024747	-1.021986
H	-1.188444	2.040567	-2.101805
H	-2.712023	2.729201	-2.686785
C	-3.127888	-1.048059	0.911977
C	-3.945632	-1.928316	-0.046298
H	-4.715222	-1.374809	-0.589224
H	-3.302936	-2.436574	-0.772261
H	-4.454082	-2.702624	0.539442
C	-4.054093	-0.307396	1.890386
H	-4.660434	-1.046243	2.427459
H	-3.475224	0.243635	2.636967
H	-4.739855	0.385395	1.400459
C	-2.221893	-1.976401	1.738346
H	-1.556096	-2.565583	1.105478
H	-1.593885	-1.412235	2.429083
H	-2.861751	-2.658210	2.312638
C	2.781835	0.866058	-0.725095
C	4.143029	1.103432	-0.908284
C	2.971635	-1.197702	-1.767227
C	4.926867	0.150182	-1.541283
H	4.589410	2.022259	-0.549065
C	4.328097	-1.020975	-1.990511
H	2.458503	-2.094598	-2.093435
H	5.988378	0.321570	-1.683559
H	4.895489	-1.791310	-2.498915
N	2.213903	-0.291363	-1.135960
H	-0.161039	0.205034	-2.064675
C	1.827921	-2.438183	1.208772
H	-2.347402	2.108553	1.454722

O	0.785348	-1.500940	1.288150
H	-1.088139	0.824558	2.050913
C	3.084084	-1.751857	1.786773
H	3.702869	-2.463647	2.342434
H	3.708558	-1.332695	0.990882
C	2.508256	-0.644938	2.686441
H	2.972536	-0.628027	3.677193
C	1.006127	-0.880103	2.827426
H	0.801928	-1.817033	3.361001
H	1.576853	-3.327595	1.810715
C	0.147225	0.193316	3.209163
H	0.623253	1.175074	3.276781
H	-0.528637	-0.015046	4.037624
H	2.653996	0.346782	2.243512
H	1.963686	-2.776267	0.177435

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1670.85252275

Thermal correction to Enthalpy= 0.613088

Thermal correction to Gibbs Free Energy= 0.521935

Imaginary frequency: –564.4115 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1670.89121095

TS20

Ru	0.309239	-0.813705	-0.217717
P	-1.802128	0.142266	-0.097736
O	-0.551306	-3.668908	-0.623334
N	0.908468	1.203831	-0.049489
C	-1.289165	1.662356	0.751372
C	0.001460	2.146992	0.302225
C	0.418492	3.493657	0.344444
H	-0.300575	4.262402	0.602354
C	1.734290	3.807992	0.082784
H	2.060816	4.842468	0.118068
C	2.663866	2.799875	-0.201762
H	3.705936	3.044870	-0.359747
C	2.208139	1.494721	-0.249439
C	-0.216374	-2.572211	-0.444353
C	-2.529449	0.640345	-1.782843
C	-2.654557	-0.586216	-2.701473
H	-2.995180	-0.258718	-3.690992
H	-1.689078	-1.083806	-2.822341
H	-3.372641	-1.321092	-2.334616
C	-3.880398	1.361028	-1.671703
H	-4.163700	1.743178	-2.659411
H	-4.685086	0.702495	-1.337517
H	-3.825927	2.217400	-0.991707
C	-1.536087	1.620004	-2.434995
H	-1.472563	2.561387	-1.882525
H	-0.532773	1.193518	-2.511205
H	-1.884830	1.849952	-3.448297
C	-3.147992	-0.620394	0.993335
C	-3.944812	-1.679815	0.216503
H	-4.579302	-1.247444	-0.560166
H	-3.287236	-2.424379	-0.243332
H	-4.602701	-2.208642	0.915303
C	-4.094867	0.443161	1.573954
H	-4.839592	-0.053532	2.206651
H	-3.550192	1.152780	2.202552
H	-4.634785	1.002235	0.808600
C	-2.469096	-1.331105	2.177543
H	-1.812075	-2.138770	1.844764
H	-1.891889	-0.641748	2.795612
H	-3.247591	-1.773081	2.810055
C	3.072574	0.303171	-0.442128
C	4.449247	0.385677	-0.631772
C	3.176883	-2.016233	-0.471982
C	5.197791	-0.777848	-0.738843
H	4.934895	1.351751	-0.687113
C	4.552003	-2.004052	-0.650075
H	2.625034	-2.945585	-0.401841
H	6.271565	-0.725133	-0.882611
H	5.094662	-2.939284	-0.716401
N	2.448753	-0.897101	-0.377533
H	0.260035	-0.732085	-1.773570
H	-2.040794	2.438981	0.894734
O	-0.004482	0.815487	2.882653
H	-0.724735	1.154045	2.002149

C	0.748751	-0.191343	2.590171
O	1.811688	-0.507508	3.074614
H	0.293765	-0.893391	1.800064

Optimization results in gas phase at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1588.91053551

Thermal correction to Enthalpy= 0.497595

Thermal correction to Gibbs Free Energy= 0.411534

Imaginary frequency: –1183.9299 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1588.95589983

The following structures are optimized in water and then do the single-point corrections：

6

Ru	-0.020815	-0.315789	-0.775631
P	2.042324	0.266274	0.098437
O	0.316148	1.083689	-3.402555
N	-0.147485	-1.464141	1.008236
C	1.768909	-0.234042	1.868113
C	0.755057	-1.338617	1.994553
C	0.691252	-2.164012	3.114926
H	1.434415	-2.065791	3.897584
C	-0.334645	-3.092947	3.209310
H	-0.401331	-3.747366	4.071457
C	-1.293894	-3.171470	2.204263
H	-2.110657	-3.877231	2.285393
C	-1.174177	-2.332822	1.103409
C	0.163354	0.565219	-2.364247
C	3.486861	-0.824217	-0.456782
C	3.603366	-0.791806	-1.988800
H	4.440862	-1.430919	-2.291586
H	2.697565	-1.174744	-2.465636
H	3.797555	0.211686	-2.374147
C	4.831147	-0.428307	0.168427
H	5.573130	-1.190824	-0.094754
H	5.200419	0.528477	-0.207102
H	4.779708	-0.382841	1.260561
C	3.180797	-2.269233	-0.022248
H	3.210257	-2.387851	1.065239
H	2.210940	-2.615719	-0.387677
H	3.950890	-2.925733	-0.442677
C	2.564261	2.079904	0.210691
C	3.187540	2.520561	-1.122086
H	4.169461	2.072889	-1.292530
H	2.540832	2.278974	-1.972256
H	3.320519	3.608319	-1.104899
C	3.529396	2.373793	1.369705
H	3.735937	3.450329	1.380723
H	3.092694	2.117044	2.339129
H	4.484630	1.858620	1.274741
C	1.293401	2.916487	0.435920
H	0.602111	2.839554	-0.406715
H	0.759404	2.626313	1.344924
H	1.587238	3.967063	0.541046
C	-2.140320	-2.288610	-0.022927
C	-3.288117	-3.074346	-0.064602
C	-2.696985	-1.301271	-2.052392
C	-4.157338	-2.954841	-1.141619
H	-3.508953	-3.770894	0.734295
C	-3.859160	-2.051396	-2.153390
H	-2.419175	-0.588771	-2.820148
H	-5.055788	-3.560218	-1.185304
H	-4.508518	-1.921965	-3.010729
N	-1.853252	-1.414687	-1.017634
H	0.724699	-1.523815	-1.485684
H	1.355094	0.643560	2.379124
H	2.699774	-0.491374	2.380048
O	-1.237749	1.064512	0.529278
C	-2.591097	2.869554	1.230683
H	-3.030624	2.192768	1.972935
H	-1.753099	3.366417	1.738294
C	-3.616203	3.901593	0.774853
H	-4.431914	3.393947	0.247261
H	-3.151805	4.577965	0.049019
C	-4.179730	4.705686	1.943354
H	-4.914224	5.441914	1.602738
H	-4.673010	4.051536	2.670835
H	-3.384552	5.245181	2.469935

C	-1.986682	2.015957	0.120410
O	-2.223437	2.283177	-1.077169

Optimization results in water at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1706.9187324800

Thermal correction to Enthalpy= 0.592590

Thermal correction to Gibbs Free Energy= 0.494796

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1706.9457683700

3

Ru	0.343748	-0.749577	-0.046399
P	-1.737708	0.265514	-0.032800
O	-0.589522	-3.603142	-0.077939
N	1.003023	1.249236	-0.073157
C	-1.272616	1.980909	-0.074713
C	0.078058	2.281934	-0.069889
C	0.605646	3.623909	-0.055777
H	-0.092830	4.454304	-0.056307
C	1.951619	3.839294	-0.035962
H	2.335432	4.855221	-0.021660
C	2.865144	2.753900	-0.029029
H	3.931217	2.934650	-0.004291
C	2.339238	1.482739	-0.048368
C	-0.230128	-2.487530	-0.046287
C	-2.929995	-0.031748	-1.461565
C	-3.093117	-1.534585	-1.730255
H	-3.803504	-1.675984	-2.553759
H	-2.143053	-1.987065	-2.028699
H	-3.476608	-2.080378	-0.865470
C	-4.302128	0.608943	-1.216783
H	-4.897786	0.545336	-2.135342
H	-4.858425	0.095252	-0.428377
H	-4.216160	1.667278	-0.949200
C	-2.301325	0.612142	-2.708089
H	-2.238505	1.699463	-2.613795
H	-1.293938	0.226353	-2.897294
H	-2.921962	0.378422	-3.581182
C	-2.561477	-0.020462	1.644714
C	-3.257222	-1.383828	1.719918
H	-4.158632	-1.418216	1.101614
H	-2.594220	-2.199280	1.413642
H	-3.562387	-1.574949	2.755963
C	-3.542000	1.089713	2.042654
H	-3.869132	0.924035	3.076489
H	-3.068352	2.074751	1.995590
H	-4.434981	1.106995	1.414858
C	-1.387444	-0.004135	2.641996
H	-0.669211	-0.809246	2.435685
H	-0.853858	0.951904	2.614767
H	-1.768223	-0.147274	3.660361
C	3.171871	0.251862	-0.033488
C	4.564965	0.274726	-0.038085
C	3.187128	-2.076328	0.014481
C	5.271801	-0.919463	-0.013040
H	5.096856	1.217438	-0.062104
C	4.571635	-2.120041	0.016218
H	2.597368	-2.985220	0.032800
H	6.356263	-0.909972	-0.016552
H	5.080710	-3.075983	0.037643
N	2.497010	-0.924783	-0.011274
H	0.307142	-0.828655	-1.601808
H	-2.004496	2.781777	-0.087392

Optimization results in water at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1399.1985694800

Thermal correction to Enthalpy= 0.461326

Thermal correction to Gibbs Free Energy= 0.381590

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1399.2338248300

TS11

Ru	-0.057725	-0.414424	-0.839041
P	2.013153	0.215491	0.005210
O	0.262221	0.912381	-3.503936
N	-0.127393	-1.520496	0.972119

C	1.761884	-0.244966	1.755763
C	0.837149	-1.376389	1.906225
C	0.826392	-2.219343	3.030951
H	1.610104	-2.123790	3.773867
C	-0.187981	-3.145312	3.179496
H	-0.205233	-3.800207	4.044457
C	-1.205275	-3.234544	2.225201
H	-2.010944	-3.946704	2.348347
C	-1.141164	-2.398348	1.122670
C	0.109941	0.420916	-2.449833
C	3.472182	-0.860555	-0.570702
C	3.589871	-0.853079	-2.102383
H	4.416654	-1.509714	-2.399046
H	2.677437	-1.231052	-2.571820
H	3.797429	0.138877	-2.507430
C	4.810076	-0.447463	0.060043
H	5.568715	-1.192443	-0.207785
H	5.169147	0.521093	-0.293158
H	4.751284	-0.419069	1.152750
C	3.193456	-2.306648	-0.121203
H	3.215423	-2.407244	0.967715
H	2.231275	-2.675175	-0.485421
H	3.977366	-2.954899	-0.529832
C	2.524462	2.040393	0.001111
C	3.244110	2.404158	-1.305984
H	4.232706	1.950135	-1.395332
H	2.651189	2.122794	-2.182942
H	3.381808	3.491351	-1.337029
C	3.394632	2.396846	1.216452
H	3.669729	3.456785	1.156657
H	2.840366	2.251644	2.148029
H	4.318319	1.818329	1.269167
C	1.252733	2.903321	0.069033
H	0.607532	2.744604	-0.799327
H	0.682983	2.703304	0.977926
H	1.553356	3.958183	0.078192
C	-2.152347	-2.372081	0.035272
C	-3.313502	-3.139772	0.064488
C	-2.777260	-1.443114	-2.002106
C	-4.223120	-3.043157	-0.980419
H	-3.512612	-3.803161	0.896783
C	-3.952556	-2.178277	-2.033559
H	-2.520496	-0.759497	-2.802778
H	-5.131495	-3.635210	-0.967953
H	-4.633542	-2.067049	-2.868757
N	-1.894170	-1.534831	-0.997986
H	0.697143	-1.638197	-1.512189
H	1.069861	0.673690	2.317160
H	2.685588	-0.376219	2.325190
O	-1.315208	1.018559	0.381489
C	-2.643407	2.867967	1.014219
H	-3.323626	2.234342	1.597977
H	-1.842026	3.152918	1.707675
C	-3.377686	4.101935	0.503654
H	-4.186294	3.792132	-0.167666
H	-2.691730	4.708738	-0.098356
C	-3.945221	4.945499	1.642066
H	-4.472349	5.825594	1.260805
H	-4.652538	4.367788	2.247563
H	-3.148392	5.294998	2.308013
C	-2.019136	1.988255	-0.065330
O	-2.214578	2.240220	-1.273168
O	0.145184	1.510070	2.922751
H	-0.470936	1.434607	2.181409

Optimization results in water at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1782.8119113600

Thermal correction to Enthalpy= 0.601868

Thermal correction to Gibbs Free Energy= 0.502456

Imaginary frequency: –1006.3477 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1782.8587257600

TS11'

Ru	-0.171393	-0.269106	-0.892502
P	1.917593	0.390343	-0.103827
O	-0.079757	1.240515	-3.476067
N	-0.108262	-1.483534	0.854582
C	1.896359	-0.279854	1.595462

C	0.852894	-1.307320	1.788563
C	0.828059	-2.105346	2.945736
H	1.633884	-2.002041	3.663060
C	-0.199785	-3.008065	3.138999
H	-0.227494	-3.622723	4.032763
C	-1.210193	-3.129043	2.183265
H	-2.032227	-3.815299	2.340784
C	-1.129661	-2.348085	1.040806
C	-0.139923	0.681836	-2.445342
C	3.361240	-0.492578	-0.970421
C	3.287506	-0.290557	-2.491719
H	4.123792	-0.821715	-2.962202
H	2.359933	-0.692367	-2.907020
H	3.361943	0.760562	-2.779680
C	4.743180	-0.051304	-0.468219
H	5.503102	-0.698108	-0.924180
H	4.982837	0.975845	-0.752636
H	4.825324	-0.157490	0.616848
C	3.225086	-1.996973	-0.670443
H	3.354482	-2.208440	0.393980
H	2.259564	-2.396781	-0.990158
H	4.009193	-2.536213	-1.215036
C	2.314821	2.228850	0.111152
C	2.723538	2.854125	-1.229609
H	3.708392	2.519569	-1.564448
H	1.995206	2.635433	-2.017326
H	2.769399	3.943609	-1.113842
C	3.401064	2.503240	1.164781
H	3.524658	3.588733	1.260880
H	3.124365	2.118085	2.149933
H	4.371284	2.085850	0.897399
C	1.025409	2.925533	0.576579
H	0.248604	2.885598	-0.190777
H	0.625898	2.485522	1.494790
H	1.249876	3.979527	0.778782
C	-2.157530	-2.345451	-0.031715
C	-3.275878	-3.175255	-0.011548
C	-2.866286	-1.386210	-2.027094
C	-4.209351	-3.090302	-1.036066
H	-3.421170	-3.882579	0.795144
C	-4.004239	-2.177001	-2.062972
H	-2.657448	-0.665948	-2.809475
H	-5.084344	-3.730804	-1.029014
H	-4.705776	-2.072918	-2.881940
N	-1.961259	-1.465261	-1.041607
H	0.591002	-1.389406	-1.715376
H	3.066123	-0.729157	2.111362
O	-1.406131	0.959568	0.564085
C	-2.794710	2.650883	1.460745
H	-3.104109	1.912686	2.209623
H	-1.961089	3.205572	1.913462
C	-3.941884	3.601449	1.136750
H	-4.753426	3.040883	0.658465
H	-3.602206	4.340142	0.402879
C	-4.470131	4.313117	2.379574
H	-5.284262	5.000135	2.128557
H	-4.853474	3.595102	3.113057
H	-3.679663	4.894652	2.866925
C	-2.217067	1.899187	0.265398
O	-2.529024	2.242044	-0.896219
O	4.091999	-1.118840	2.752615
H	4.368613	-1.891589	2.249639
H	1.701461	0.537598	2.300140

Optimization results in water at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1782.8010750300

Thermal correction to Enthalpy= 0.600660

Thermal correction to Gibbs Free Energy= 0.499256

Imaginary frequency: –1301.0498 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1782.8487211500

13

Ru	0.098205	-0.316883	-0.781456
P	2.141809	0.205259	0.227468
O	0.587596	1.218548	-3.309198
N	-0.127277	-1.491206	0.961673
C	1.891783	-0.539744	1.821860
C	0.793740	-1.377038	1.984179

C	0.540861	-2.154029	3.169308
H	1.264948	-2.119697	3.976986
C	-0.596090	-2.904298	3.277213
H	-0.777588	-3.481101	4.179655
C	-1.549005	-2.936170	2.232165
H	-2.457660	-3.514280	2.332128
C	-1.263684	-2.208242	1.094930
C	0.368903	0.641704	-2.308351
C	3.652028	-0.676384	-0.541586
C	3.742125	-0.413054	-2.052307
H	4.610469	-0.946461	-2.458608
H	2.852458	-0.779346	-2.572114
H	3.865534	0.645178	-2.291569
C	4.980290	-0.298320	0.129368
H	5.770677	-0.956865	-0.251264
H	5.285158	0.728342	-0.084786
H	4.937498	-0.431650	1.215421
C	3.457151	-2.187492	-0.328472
H	3.473664	-2.448425	0.733460
H	2.515643	-2.544655	-0.753435
H	4.275634	-2.723393	-0.824058
C	2.584582	2.028632	0.530972
C	3.192668	2.677809	-0.719789
H	4.198736	2.312096	-0.937333
H	2.566522	2.516714	-1.603841
H	3.266963	3.760332	-0.559606
C	3.520395	2.218935	1.734829
H	3.686476	3.292309	1.888411
H	3.071857	1.820620	2.649837
H	4.497124	1.753424	1.602160
C	1.278044	2.771983	0.851937
H	0.602952	2.792726	-0.007107
H	0.747236	2.316363	1.692422
H	1.517695	3.807187	1.123190
C	-2.173379	-2.134334	-0.079739
C	-3.390680	-2.810834	-0.144102
C	-2.538677	-1.227525	-2.191784
C	-4.191286	-2.677926	-1.269924
H	-3.713700	-3.436738	0.678351
C	-3.759682	-1.870406	-2.316034
H	-2.155248	-0.591143	-2.980986
H	-5.139725	-3.200635	-1.328199
H	-4.350569	-1.736743	-3.214182
N	-1.760984	-1.353340	-1.106743
H	0.872401	-1.504516	-1.498915
O	-1.239918	1.017752	0.471405
C	-2.816017	2.652767	1.124382
H	-3.056089	1.963329	1.941473
H	-2.089167	3.366838	1.536750
C	-4.067146	3.389447	0.658679
H	-4.774704	2.666864	0.234661
H	-3.802743	4.076132	-0.152413
C	-4.738325	4.162532	1.790268
H	-5.635890	4.681098	1.439101
H	-5.036194	3.492846	2.604670
H	-4.060203	4.913630	2.210642
C	-2.083429	1.869480	0.038232
O	-2.313719	2.116216	-1.167573
H	2.656819	-0.519709	2.592177

Optimization results in water at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1706.4015378800

Thermal correction to Enthalpy= 0.577993

Thermal correction to Gibbs Free Energy= 0.481202

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1706.4342346500

TS12

Ru	-0.236521	0.215122	-0.771415
P	-2.254901	-0.376106	0.228906
O	-0.345893	-1.790057	-2.998264
N	-0.235680	1.667588	0.753652
C	-2.247499	0.718532	1.630089
C	-1.233073	1.660288	1.713169
C	-1.138364	2.655825	2.750580
H	-1.914677	2.689402	3.508070
C	-0.089546	3.528492	2.780898
H	-0.028669	4.270836	3.571530
C	0.927423	3.481569	1.795364

H	1.762563	4.167889	1.833190
C	0.805450	2.531557	0.805325
C	-0.284240	-1.022235	-2.112525
C	-3.813899	0.031146	-0.777125
C	-3.725821	-0.566643	-2.188978
H	-4.642482	-0.324540	-2.740689
H	-2.881693	-0.146595	-2.742949
H	-3.621935	-1.653819	-2.182898
C	-5.106179	-0.435389	-0.093514
H	-5.965851	-0.027796	-0.639283
H	-5.208686	-1.523085	-0.091606
H	-5.171370	-0.076405	0.938866
C	-3.885376	1.561820	-0.906543
H	-4.042047	2.040133	0.064290
H	-2.976284	1.980056	-1.348825
H	-4.727871	1.824210	-1.557496
C	-2.363098	-2.138529	0.914302
C	-2.710325	-3.155862	-0.179302
H	-3.744219	-3.065976	-0.522075
H	-2.046947	-3.060644	-1.045312
H	-2.586153	-4.168923	0.222558
C	-3.346559	-2.266339	2.086709
H	-3.296750	-3.288545	2.481309
H	-3.084867	-1.584165	2.900987
H	-4.381657	-2.076016	1.800142
C	-0.958011	-2.467611	1.442921
H	-0.226776	-2.528828	0.631784
H	-0.611831	-1.718927	2.162707
H	-0.982498	-3.438479	1.952555
C	1.798130	2.357493	-0.288463
C	2.942763	3.142655	-0.411605
C	2.406604	1.131529	-2.172512
C	3.834424	2.898106	-1.446969
H	3.140484	3.937612	0.296557
C	3.565510	1.871298	-2.344533
H	2.149565	0.323580	-2.847704
H	4.729082	3.502572	-1.548676
H	4.234488	1.642374	-3.165285
N	1.539493	1.366838	-1.176401
H	-1.071672	1.136707	-1.707945
O	1.887262	-0.802213	1.171335
C	3.853318	-2.132602	1.371786
H	4.267949	-1.266283	1.898978
H	3.508611	-2.824722	2.152691
C	4.925892	-2.806829	0.522087
H	5.260449	-2.111578	-0.257433
H	4.486336	-3.664264	0.001947
C	6.123890	-3.264319	1.349565
H	6.881613	-3.743637	0.721719
H	6.599266	-2.419561	1.860501
H	5.819527	-3.985809	2.116125
C	2.607014	-1.677642	0.605551
O	2.359434	-2.212881	-0.508003
H	-3.058229	0.741828	2.351377

Optimization results in water at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1706.3933063800

Thermal correction to Enthalpy= 0.576383

Thermal correction to Gibbs Free Energy= 0.478658

Imaginary frequency: –74.9656 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1706.4287592500

TS13

Ru	0.171074	0.041857	0.718635
P	2.229675	-0.467504	-0.191951
O	0.231024	-2.024520	2.886668
N	0.249966	1.642690	-0.684352
C	2.172309	0.581180	-1.727265
C	1.252492	1.760281	-1.571429
C	1.366660	2.905917	-2.355484
H	2.188193	2.996875	-3.056336
C	0.413344	3.905795	-2.229252
H	0.485759	4.807167	-2.827743
C	-0.647752	3.745670	-1.342773
H	-1.401521	4.517124	-1.250705
C	-0.706475	2.588342	-0.577922
C	0.188499	-1.242999	2.018507
C	3.724932	0.195392	0.749558

C	3.695239	-0.319762	2.197289
H	4.575342	0.064854	2.725278
H	2.804799	0.030861	2.726143
H	3.722941	-1.410007	2.256058
C	5.063038	-0.172171	0.095156
H	5.863934	0.371735	0.608996
H	5.285539	-1.238257	0.180428
H	5.096429	0.111551	-0.961277
C	3.613480	1.731032	0.775158
H	3.753405	2.171099	-0.216898
H	2.654300	2.070323	1.175505
H	4.405060	2.124500	1.422616
C	2.509203	-2.213932	-0.843221
C	2.951932	-3.136932	0.300861
H	3.965392	-2.914263	0.643280
H	2.272042	-3.080600	1.156901
H	2.945330	-4.171443	-0.060908
C	3.516266	-2.294245	-1.999815
H	3.565530	-3.333791	-2.344109
H	3.211447	-1.683445	-2.854392
H	4.523662	-1.996820	-1.707246
C	1.141933	-2.701476	-1.353537
H	0.405354	-2.753925	-0.546985
H	0.740885	-2.059641	-2.144247
H	1.262129	-3.707480	-1.771886
C	-1.791806	2.276304	0.385359
C	-2.946687	3.043767	0.492922
C	-2.569312	0.806282	2.009069
C	-3.935491	2.663953	1.392281
H	-3.084272	3.921767	-0.125655
C	-3.744850	1.526386	2.165229
H	-2.374470	-0.084426	2.594193
H	-4.843022	3.250329	1.482075
H	-4.488644	1.191711	2.878060
N	-1.613620	1.166497	1.141743
H	0.950916	0.925346	1.731948
O	-1.752436	-0.848459	-1.284297
C	-3.926444	-1.799032	-1.480145
H	-4.273446	-0.809590	-1.801055
H	-3.700320	-2.349051	-2.403467
C	-5.022345	-2.517246	-0.700152
H	-5.243074	-1.954997	0.214961
H	-4.654325	-3.497528	-0.378713
C	-6.299195	-2.687724	-1.518680
H	-7.077749	-3.197052	-0.942142
H	-6.699019	-1.717773	-1.835169
H	-6.111666	-3.278827	-2.422052
C	-2.601479	-1.614505	-0.733335
O	-2.425654	-2.231565	0.348057
H	3.166178	0.891231	-2.059961
H	1.751743	-0.046313	-2.521607

Optimization results in water at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1706.9083652200

Thermal correction to Enthalpy= 0.590066

Thermal correction to Gibbs Free Energy= 0.495217

Imaginary frequency: –259.4545 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1706.9383708300

14

Ru	-0.360453	-0.780500	-0.021052
P	1.734601	0.174575	-0.079668
O	0.547225	-3.548505	0.689103
N	-1.000723	1.234148	-0.281275
C	1.308042	1.881457	-0.686961
C	-0.121219	2.244817	-0.400250
C	-0.553448	3.566386	-0.324949
H	0.166442	4.372114	-0.407505
C	-1.905086	3.823591	-0.150556
H	-2.261947	4.845423	-0.084615
C	-2.808489	2.767829	-0.067398
H	-3.864508	2.965520	0.063190
C	-2.322551	1.469567	-0.137164
C	0.194693	-2.479398	0.379403
C	2.593799	0.460986	1.566375
C	2.673360	-0.866668	2.335311
H	3.178845	-0.690192	3.291556
H	1.676683	-1.263233	2.548641

H	3.239398	-1.630312	1.796559
C	3.996003	1.060676	1.409168
H	4.374369	1.334470	2.400640
H	4.699369	0.346806	0.973613
H	3.989913	1.966955	0.795337
C	1.724194	1.441544	2.373678
H	1.712316	2.443794	1.935189
H	0.692570	1.090393	2.472280
H	2.145676	1.529243	3.381193
C	2.872946	-0.504980	-1.413824
C	3.570437	-1.776517	-0.911486
H	4.318620	-1.556658	-0.145538
H	2.860196	-2.504132	-0.506901
H	4.088200	-2.249858	-1.753453
C	3.924249	0.492717	-1.919872
H	4.475368	0.025621	-2.744258
H	3.476045	1.411463	-2.308260
H	4.648520	0.762026	-1.149982
C	1.938466	-0.883435	-2.579352
H	1.211223	-1.645894	-2.277794
H	1.390679	-0.019515	-2.970496
H	2.539655	-1.292338	-3.399196
C	-3.170992	0.254563	-0.055999
C	-4.560269	0.306354	-0.035319
C	-3.217892	-2.067532	0.045957
C	-5.286155	-0.876817	0.031830
H	-5.076998	1.256789	-0.075955
C	-4.604550	-2.085456	0.072898
H	-2.644603	-2.986297	0.078139
H	-6.369879	-0.849294	0.049270
H	-5.128047	-3.032288	0.124462
N	-2.510534	-0.929881	-0.017827
H	-0.387019	-0.542227	1.510458
H	1.421338	1.875096	-1.776725
H	1.996267	2.639942	-0.306578

Optimization results in water at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1399.7224057700

Thermal correction to Enthalpy= 0.474909

Thermal correction to Gibbs Free Energy= 0.395427

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1399.7379347600

TS14

Ru	0.390544	-0.844735	-0.062311
P	-1.706799	0.113248	0.068516
O	-0.506991	-3.707051	-0.051912
N	1.001766	1.181262	-0.136989
C	-1.291425	1.791556	-0.523847
C	0.085590	2.172734	-0.191510
C	0.512093	3.504102	-0.053079
H	-0.220104	4.302721	-0.083865
C	1.855916	3.772851	0.114258
H	2.195943	4.797435	0.222322
C	2.788397	2.730346	0.140341
H	3.841732	2.943561	0.266110
C	2.321561	1.434029	0.014182
C	-0.153069	-2.592716	-0.031572
C	-3.170287	-0.457226	-0.976155
C	-3.966866	-1.562439	-0.269810
H	-4.703166	-1.963265	-0.975911
H	-3.323622	-2.391711	0.042196
H	-4.515924	-1.195460	0.599942
C	-4.092779	0.724560	-1.312853
H	-4.958707	0.349897	-1.870959
H	-4.466454	1.235685	-0.422404
H	-3.580813	1.457042	-1.942994
C	-2.632835	-1.043021	-2.292496
H	-2.034977	-0.313647	-2.843131
H	-2.031951	-1.939894	-2.118295
H	-3.487626	-1.324930	-2.919122
C	-2.183957	0.285706	1.892808
C	-2.312329	-1.095545	2.556478
H	-3.169806	-1.664089	2.195861
H	-1.411025	-1.698125	2.400314
H	-2.441131	-0.956959	3.636479
C	-3.458876	1.107811	2.112710
H	-3.598754	1.273301	3.187760
H	-3.392864	2.089331	1.632315

H	-4.351500	0.599830	1.739557
C	-1.009865	1.011674	2.576510
H	-0.061398	0.480870	2.430066
H	-0.890425	2.037627	2.217578
H	-1.204369	1.056497	3.654032
C	3.185011	0.225915	0.030583
C	4.571047	0.286389	0.133522
C	3.260420	-2.097489	-0.074944
C	5.308216	-0.891004	0.131175
H	5.076252	1.240619	0.214000
C	4.643263	-2.105563	0.021370
H	2.698068	-3.019489	-0.161108
H	6.388908	-0.855568	0.211948
H	5.177536	-3.047770	0.011740
N	2.541218	-0.964832	-0.068894
H	0.261026	-0.930101	-1.608633
H	-0.341242	0.741869	-3.072043
O	-0.769345	1.603662	-3.124918
H	-2.020902	2.564844	-0.274494
H	-1.160209	1.695597	-1.785510

Optimization results in water at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1475.6157893900

Thermal correction to Enthalpy= 0.484080

Thermal correction to Gibbs Free Energy= 0.400444

Imaginary frequency: –947.1762 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1475.6509272100

TS14'

Ru	0.392474	-0.845950	0.020522
P	-1.709682	0.120768	-0.041284
O	-0.497196	-3.667385	-0.459874
N	1.014354	1.177123	0.110816
C	-1.253795	1.762088	0.622265
C	0.096478	2.163620	0.215138
C	0.513627	3.497774	0.075563
H	-0.219484	4.293786	0.137985
C	1.852008	3.772479	-0.127202
H	2.184996	4.799308	-0.236555
C	2.789288	2.734938	-0.177663
H	3.839888	2.953986	-0.316202
C	2.329409	1.435257	-0.054787
C	-0.150014	-2.573023	-0.232825
C	-2.427586	0.435313	-1.764376
C	-2.542940	-0.876692	-2.555838
H	-2.876832	-0.646628	-3.574593
H	-1.578175	-1.387933	-2.626111
H	-3.265917	-1.570081	-2.123212
C	-3.787794	1.145412	-1.715962
H	-4.083579	1.412175	-2.737416
H	-4.578130	0.515417	-1.302235
H	-3.740779	2.071304	-1.133621
C	-1.446619	1.358137	-2.509626
H	-1.387507	2.349242	-2.050998
H	-0.438210	0.937421	-2.557882
H	-1.805351	1.488553	-3.537007
C	-3.024846	-0.577185	1.120835
C	-3.839361	-1.684028	0.436966
H	-4.496693	-1.304769	-0.347986
H	-3.192593	-2.456697	0.008420
H	-4.474219	-2.164524	1.190374
C	-3.955542	0.521377	1.654314
H	-4.699108	0.066249	2.319373
H	-3.398403	1.261402	2.235927
H	-4.495111	1.041676	0.860313
C	-2.295630	-1.214428	2.316963
H	-1.649324	-2.040796	2.004401
H	-1.696929	-0.479594	2.859089
H	-3.044469	-1.618664	3.008959
C	3.194638	0.228873	-0.067900
C	4.581134	0.292413	-0.161202
C	3.275283	-2.092253	0.055883
C	5.322162	-0.882525	-0.141277
H	5.083329	1.247944	-0.245924
C	4.659407	-2.097576	-0.026673
H	2.714617	-3.016082	0.135027
H	6.403415	-0.844691	-0.213178
H	5.195662	-3.038492	-0.005147

N	2.552560	-0.962344	0.037870
H	0.436867	-0.759811	-1.526681
H	-2.000793	2.545231	0.476375
O	-0.461615	1.416119	3.125583
H	-0.001385	0.579370	2.999065
H	-0.993183	1.582822	1.873708

Optimization results in water at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1475.6138757200

Thermal correction to Enthalpy= 0.485491

Thermal correction to Gibbs Free Energy= 0.408684

Imaginary frequency: –615.2531 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1475.6476754100

TS15

Ru	0.389165	-0.782590	-0.203262
P	-1.753068	0.123575	-0.160928
O	-0.419377	-3.613391	-0.749175
N	0.926486	1.257306	0.058030
C	-1.372836	1.740017	0.604113
C	-0.015515	2.199488	0.279725
C	0.363268	3.552384	0.302746
H	-0.393007	4.312358	0.463498
C	1.690150	3.893238	0.124126
H	1.991273	4.935553	0.134912
C	2.650900	2.897382	-0.066459
H	3.692206	3.159443	-0.200969
C	2.228895	1.577636	-0.092097
C	-0.098571	-2.507239	-0.528235
C	-2.450172	0.564363	-1.880333
C	-2.508902	-0.674519	-2.787693
H	-2.862095	-0.371828	-3.780975
H	-1.521221	-1.127667	-2.908304
H	-3.192791	-1.439911	-2.416566
C	-3.835197	1.225674	-1.819108
H	-4.106036	1.565946	-2.825780
H	-4.619698	0.543306	-1.486976
H	-3.837829	2.104170	-1.166074
C	-1.498857	1.587456	-2.528702
H	-1.501290	2.541396	-1.993718
H	-0.470727	1.221183	-2.583411
H	-1.841400	1.780197	-3.552041
C	-3.132087	-0.645964	0.888044
C	-3.893338	-1.718143	0.094170
H	-4.513427	-1.305651	-0.703655
H	-3.210986	-2.456407	-0.340877
H	-4.560459	-2.251874	0.781217
C	-4.100006	0.414031	1.437218
H	-4.881573	-0.089213	2.019439
H	-3.578595	1.102366	2.108457
H	-4.593649	0.996410	0.658110
C	-2.487998	-1.350176	2.091875
H	-1.808130	-2.146998	1.782255
H	-1.932084	-0.649022	2.714671
H	-3.287604	-1.793477	2.698826
C	3.135804	0.418259	-0.281188
C	4.522416	0.542707	-0.327780
C	3.298469	-1.884473	-0.536344
C	5.304849	-0.593390	-0.486106
H	4.991156	1.514144	-0.231285
C	4.683018	-1.831327	-0.593080
H	2.768894	-2.827046	-0.612655
H	6.385400	-0.509738	-0.521561
H	5.251606	-2.745415	-0.714978
N	2.538462	-0.791588	-0.386444
H	0.330490	-0.502778	-1.756208
H	-2.128326	2.509205	0.422518
Cl	0.968329	-1.190632	2.326451
O	-0.991279	1.463765	3.220469
H	-0.458173	0.663648	3.120142
H	-1.275876	1.581322	1.858970

Optimization results in water at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1935.9746370800

Thermal correction to Enthalpy= 0.487309

Thermal correction to Gibbs Free Energy= 0.399893

Imaginary frequency: –907.2955 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1936.0160632100

TS15'

Ru	0.534659	-0.831285	-0.092290
P	-1.685618	-0.120163	-0.031582
O	0.010840	-3.740117	-0.558073
N	0.872246	1.257788	0.162074
C	-1.513113	1.573694	0.629379
C	-0.137211	2.091914	0.498941
C	0.149079	3.450771	0.718068
H	-0.671653	4.124679	0.934620
C	1.451186	3.904482	0.632290
H	1.678693	4.950779	0.808309
C	2.478543	3.015095	0.313314
H	3.503278	3.359975	0.262551
C	2.148834	1.689939	0.072348
C	0.218443	-2.600787	-0.364022
C	-2.426997	0.106542	-1.772609
C	-2.312807	-1.190137	-2.589628
H	-2.732997	-1.019882	-3.588361
H	-1.271772	-1.499719	-2.712607
H	-2.863206	-2.019374	-2.138952
C	-3.892820	0.564979	-1.764696
H	-4.187391	0.806760	-2.793531
H	-4.571727	-0.215330	-1.413098
H	-4.028366	1.465741	-1.160155
C	-1.613366	1.203688	-2.483872
H	-1.728171	2.173299	-1.992698
H	-0.548553	0.963429	-2.534265
H	-1.983237	1.304666	-3.511162
C	-2.963415	-0.941184	1.098394
C	-3.474461	-2.247739	0.474677
H	-4.114643	-2.070802	-0.392970
H	-2.651742	-2.904001	0.172320
H	-4.073305	-2.787050	1.218407
C	-4.155755	-0.033923	1.447335
H	-4.768201	-0.542752	2.201671
H	-3.837466	0.921232	1.873441
H	-4.798532	0.175077	0.593038
C	-2.245252	-1.289547	2.410247
H	-1.410334	-1.973607	2.248982
H	-1.846385	-0.400639	2.907378
H	-2.964401	-1.762787	3.089939
C	3.145537	0.639646	-0.254891
C	4.497225	0.914861	-0.450888
C	3.521920	-1.625173	-0.603975
C	5.374042	-0.126028	-0.725327
H	4.865834	1.931431	-0.394417
C	4.880035	-1.422661	-0.796935
H	3.090115	-2.617919	-0.659561
H	6.428108	0.076068	-0.880570
H	5.526054	-2.267491	-1.003566
N	2.669674	-0.623901	-0.346793
H	0.418775	-0.616786	-1.651358
H	-3.059766	3.579707	-1.035134
Cl	1.188774	-1.013157	2.453903
O	-3.166961	3.474132	-0.084346
H	-1.785820	1.575017	1.691618
H	-2.385439	2.513032	0.181768

Optimization results in water at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1935.9653755400

Thermal correction to Enthalpy= 0.486050

Thermal correction to Gibbs Free Energy= 0.397046

Imaginary frequency: –1291.7587 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1936.0053062000

15

Ru	0.325080	-0.705702	-0.130577
P	-1.805761	0.266319	-0.046565
O	-0.566646	-3.550621	-0.425016
N	0.923277	1.317477	0.038482
C	-1.364960	1.945238	0.335110
C	-0.021958	2.297300	0.274816
C	0.466783	3.640279	0.444361

H	-0.250814	4.434661	0.623193
C	1.806263	3.904919	0.383956
H	2.161649	4.923175	0.514480
C	2.741382	2.870432	0.150408
H	3.800689	3.085776	0.106532
C	2.243513	1.593058	-0.014608
C	-0.215495	-2.435032	-0.304640
C	-2.686346	0.307172	-1.745711
C	-2.740220	-1.094873	-2.372101
H	-3.260987	-1.039640	-3.336249
H	-1.735481	-1.484851	-2.556404
H	-3.275632	-1.815945	-1.749911
C	-4.103249	0.895247	-1.688899
H	-4.470049	1.035998	-2.713153
H	-4.813030	0.239012	-1.180600
H	-4.116858	1.873902	-1.198332
C	-1.865972	1.219789	-2.673166
H	-1.878978	2.257140	-2.326688
H	-0.824235	0.898684	-2.752490
H	-2.303718	1.189464	-3.678349
C	-3.064470	-0.270853	1.271006
C	-3.753526	-1.585563	0.882247
H	-4.446184	-1.466729	0.045536
H	-3.025237	-2.360671	0.620565
H	-4.334485	-1.952621	1.737238
C	-4.115183	0.805575	1.587188
H	-4.728510	0.460330	2.428696
H	-3.641285	1.743919	1.890815
H	-4.790366	1.014921	0.758214
C	-2.273335	-0.514828	2.562728
H	-1.548653	-1.323009	2.454256
H	-1.720812	0.378513	2.869861
H	-2.974818	-0.772692	3.366059
C	3.103998	0.407571	-0.266926
C	4.493637	0.482312	-0.351277
C	3.182029	-1.888671	-0.618135
C	5.232119	-0.671470	-0.572139
H	4.997690	1.434030	-0.241273
C	4.564955	-1.883642	-0.707235
H	2.618080	-2.809354	-0.714152
H	6.313654	-0.622697	-0.636878
H	5.097411	-2.811638	-0.878374
N	2.463864	-0.776565	-0.407653
H	0.166465	-0.517961	-1.689722
Cl	1.113006	-1.011073	2.397670
H	-2.110317	2.727429	0.443027

Optimization results in water at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1859.5649366400

Thermal correction to Enthalpy= 0.463386

Thermal correction to Gibbs Free Energy= 0.379056

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1859.5900382400

TS16

Ru	0.302014	-0.565393	-0.340480
P	-1.848633	0.293211	-0.036898
O	-0.449286	-3.401242	-0.967315
N	0.841490	1.426422	0.102329
C	-1.471434	1.997950	0.301709
C	-0.140453	2.376206	0.337259
C	0.308285	3.720202	0.604500
H	-0.436642	4.482641	0.808048
C	1.637629	4.025147	0.586233
H	1.960855	5.043785	0.780538
C	2.608889	3.031109	0.307405
H	3.660344	3.283040	0.274149
C	2.156709	1.751339	0.074927
C	-0.159880	-2.290361	-0.725939
C	-2.966827	0.256141	-1.570829
C	-2.983977	-1.150652	-2.187341
H	-3.683428	-1.165140	-3.032229
H	-1.996657	-1.428333	-2.566068
H	-3.306129	-1.917752	-1.478643
C	-4.405985	0.703014	-1.283043
H	-4.937204	0.825697	-2.234730
H	-4.957011	-0.036732	-0.697162
H	-4.440498	1.662944	-0.758107
C	-2.371941	1.228733	-2.602196

H	-2.431901	2.265316	-2.259037
H	-1.324114	1.003173	-2.821946
H	-2.937988	1.143876	-3.537629
C	-2.788000	-0.330949	1.486067
C	-3.318460	-1.752304	1.266150
H	-4.134382	-1.778885	0.538339
H	-2.528731	-2.431073	0.926234
H	-3.710227	-2.145139	2.212532
C	-3.927848	0.593789	1.940092
H	-4.275916	0.264539	2.926940
H	-3.587932	1.629078	2.041251
H	-4.788509	0.576570	1.271561
C	-1.744667	-0.356711	2.614826
H	-0.907632	-1.027488	2.396213
H	-1.338172	0.644420	2.798301
H	-2.224878	-0.696914	3.540729
C	3.056066	0.612710	-0.244364
C	4.446237	0.711604	-0.223688
C	3.198028	-1.621032	-0.874158
C	5.217351	-0.395472	-0.547740
H	4.924739	1.643759	0.049465
C	4.582894	-1.585374	-0.886259
H	2.659232	-2.528625	-1.119046
H	6.299740	-0.327910	-0.535019
H	5.142513	-2.475135	-1.148965
N	2.447129	-0.554462	-0.562673
H	0.098225	-0.190957	-1.837422
Cl	1.462665	-2.154375	2.308259
H	-2.243857	2.740425	0.475182

Optimization results in water at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1859.5592280100

Thermal correction to Enthalpy= 0.462360

Thermal correction to Gibbs Free Energy= 0.378537

Imaginary frequency: –93.3015 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1859.5866343100

TS17

Ru	0.270678	-0.644121	-0.331103
P	-1.866505	0.147257	0.053775
O	-0.536059	-3.262446	-1.550729
N	0.814257	1.315687	0.293125
C	-1.470122	1.669014	1.047254
C	-0.096841	2.197123	0.740467
C	0.259134	3.524956	0.962666
H	-0.486923	4.229440	1.310960
C	1.570801	3.916424	0.738234
H	1.867843	4.946763	0.899769
C	2.512034	2.983008	0.313374
H	3.538081	3.284149	0.145206
C	2.101634	1.673826	0.100688
C	-0.219375	-2.260918	-1.039733
C	-2.768297	0.812922	-1.462854
C	-2.840825	-0.281735	-2.538861
H	-3.360978	0.120885	-3.415589
H	-1.842764	-0.597539	-2.855384
H	-3.390686	-1.164017	-2.203554
C	-4.179148	1.327439	-1.148997
H	-4.577990	1.819404	-2.043442
H	-4.864873	0.518844	-0.885611
H	-4.176606	2.064209	-0.339811
C	-1.943182	1.988410	-2.018056
H	-1.949381	2.851633	-1.345744
H	-0.905229	1.708930	-2.218898
H	-2.393146	2.307657	-2.964727
C	-2.995111	-0.854874	1.178186
C	-3.696389	-1.953870	0.367511
H	-4.457158	-1.550917	-0.305566
H	-2.985804	-2.543073	-0.221145
H	-4.197945	-2.636536	1.062775
C	-4.035116	-0.013510	1.932123
H	-4.608315	-0.678076	2.588952
H	-3.569105	0.746974	2.565115
H	-4.743146	0.479810	1.265604
C	-2.069417	-1.530616	2.204159
H	-1.366954	-2.214425	1.717869
H	-1.493395	-0.805552	2.788205
H	-2.680423	-2.111527	2.904464

C	2.998190	0.575135	-0.336226
C	4.376631	0.724523	-0.443223
C	3.148565	-1.648866	-0.988999
C	5.150865	-0.359253	-0.839008
H	4.848616	1.671341	-0.213661
C	4.527400	-1.567910	-1.117765
H	2.619922	-2.572217	-1.194119
H	6.226816	-0.256217	-0.924558
H	5.089515	-2.440557	-1.427725
N	2.397550	-0.607881	-0.607646
H	0.118925	-0.102257	-1.773860
H	-1.470818	1.369905	2.101679
H	-2.228938	2.447892	0.938143
Cl	1.961520	-1.714406	2.735789

Optimization results in water at the level of ωB97X-D/BS1 (Energies are in Hartree)

E(RwB97XD) = –1860.0712876600

Thermal correction to Enthalpy= 0.476990

Thermal correction to Gibbs Free Energy= 0.393527

Imaginary frequency: –53.8584 cm^{-1}

Single-point correction results in water at the level of ωB97X-D/BS2 (Energies are in Hartree)

E(RwB97XD) = –1860.0951888000