Supporting Information

Computational Investigation of the Control of Thermodynamics and Microkinetics of the Reductive Amination Reaction by Solvent Coordination and a Co-Catalyst

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Contents

Selected Bond Lengths and NBO Charges for the Compounds........................................ 2

Figure S1. The selected bond lengths (in Å, black) and NBO charges (blue) of the transition state and intermediate structures for reductive amination reaction in neutral media. ...................................................................................................................................... 2

Figure S2. The selected bond lengths (in Å, black) and NBO charges (blue) of the transition state and intermediate structures for reductive amination reaction in neutral media with explicit water assistance. ........................................ 3

Figure S3. The selected bond lengths (in Å, black) and NBO charges (blue) of the transition state and intermediate structures for reductive amination reaction in low pH. ...... 4

Table S1. Relative Gibbs free energies of the transition states and intermediate structures for reductive amination reaction in neutral media calculated in the gas phase and implicit solvent (in DMF and decane). ................................................................. 5

Table S2. Relative Gibbs free energies of the transition states and intermediate structures for reductive amination reaction in neutral media with explicit water assistance calculated in the gas phase and implicit solvent (in DMF and decane). ................................................................. 5

Table S3. Relative Gibbs free energies of the transition states and intermediate structures for reductive amination reaction in the presence of an acid as a co-catalyst for Case A calculated in the gas phase and implicit solvent (in DMF and decane). ................................................................. 6

Table S4. Relative Gibbs free energies of the transition states and intermediate structures for reductive amination reaction in the presence of an acid as a co-catalyst for Case B calculated in the gas phase and implicit solvent (in DMF and decane). ................................................................. 6
Selected Bond Lengths and NBO Charges for the Compounds

Figure S1. The selected bond lengths (in Å, black) and NBO charges (blue) of the transition state and intermediate structures for reductive amination reaction in neutral media.
Figure S2. The selected bond lengths (in Å, black) and NBO charges (blue) of the transition state and intermediate structures for reductive amination reaction in neutral media with explicit water assistance.
Figure S3. The selected bond lengths (in Å, black) and NBO charges (blue) of the transition state and intermediate structures for reductive amination reaction in low pH.
|       | 1 .. 2 | TS_1  | 4   | TS_2a | TS_2b | 5a   | 5b   | 5c   | TS_3 | TS_4 | 6   | 7   | TS_5 | TS_6 | TS_7 | 8   |
|-------|--------|-------|-----|-------|-------|------|------|------|------|------|-----|-----|------|------|------|-----|
|       |        |       |     |       |       |      |      |      |      |      |     |     |      |      |      |     |
| Gas phase | 4.2    | 33.3  | 2.1 | 48.9  | 48.9  | 33.4 | 2.1  | -71.3| 0.2  | -1.2 | -28.1| -25.9| -134.9| -125.2| -46.9 | -14.7|
| DMF   | 9.1    | 32.4  | 5.6 | 41.1  | 45.1  | 26.8 | 1.3  | -53.6| 29.4 | 28.2 | 11.4 | 12.1 | -6.7  | 38.0  | -150  | -15.1|
| Decane| 7.6    | 34.1  | 3.7 | 45.7  | 47.4  | 30.7 | 1.7  | -62.2| 19.2 | 17.8 | -5.8 | -4.7 | -45.7 | -11.5 | -74.9 | -15.3|

Table S1. Relative Gibbs free energies of the transition states and intermediate structures for reductive amination reaction in neutral media calculated in the gas phase and implicit solvent (in DMF and decane).

|       | 1_w..2 | TS_0_w | 1w_2 | TS_1_w | 4_w  | TS_2a_w | TS_2b_w | TS_2c_w | 5a_w | 5b_w | 5c_w | 8   |
|-------|--------|--------|------|--------|------|---------|---------|---------|------|------|------|-----|
|       |        |        |      |        |      |         |         |         |      |      |      |     |
| Gas phase | 2.5    | 7.3    | 8.6  | 24.3   | 0.9  | 34.0    | 49.6    | 28.1    | 30.4 | -2.1 | -81.8| -21.5|
| DMF   | 7.5    | 10.6   | 8.4  | 26.2   | 4.2  | 33.1    | 45.2    | 25.8    | 27.2 | -3.1 | -53.6| -27.3|
| Decane| 9.6    | 13.7   | 13.6 | 30.2   | 7.4  | 38.6    | 53.2    | 32.1    | 34.1 | 2.5  | -62.6| -19.3|

Table S2. Relative Gibbs free energies of the transition states and intermediate structures for reductive amination reaction in neutral media with explicit water assistance calculated in the gas phase and implicit solvent (in DMF and decane).
|                | $1_{-H^+} .. 2$ | 3+2     | 3 .. 2   | TS_10   | 9       | TS_11   | 10       | TS_9    | 5b    |
|----------------|----------------|----------|----------|----------|---------|---------|----------|---------|-------|
| **Gas phase**  | -19.0          | 11.1     | 15.5     | 72.5     | 71.4    | 58.0    | 54.0     | 68.5    | 2.2   |
| **DMF**        | -10            | 11.6     | 18.1     | 66.8     | 61.6    | 48.7    | 41.1     | 64.0    | 1.7   |
| **Decane**     | -14            | 11.5     | 16.6     | 71.0     | 68.4    | 54.7    | 49.5     | 66.9    | 1.3   |

**Table S3.** Relative Gibbs free energies of the transition states and intermediate structures for reductive amination reaction following the keto-enol tautomerization in the presence of an acid calculated in the gas phase and implicit solvent (in DMF and decane).

|                | $1 + 2_{-H^+}$ | $1_{-} 2_{-H^+}$ | TS_12   | 11      | TS_13   | TS_14   | 5c       |
|----------------|----------------|------------------|---------|---------|---------|---------|----------|
| **Gas phase**  | -61.6          | -69.2            | -24.0   | -62.9   | -27.1   | -51.9   | -71.3    |
| **DMF**        | -52.8          | -44.5            | -1.7    | -42.1   | -4.1    | -33.2   | -53.6    |
| **Decane**     | -56.7          | -56.6            | -12.2   | -51.8   | -15.2   | -41.5   | -62.2    |

**Table S4.** Relative Gibbs free energies of the transition states and intermediate structures for reductive amination reaction in the presence of an acid as a co-catalyst for Case A and Case B calculated in the gas phase and implicit solvent (in DMF and decane).
Free energies and thermal corrections of the transition states and intermediate structures for reductive amination reaction

1

Zero-point correction= 0.085349 (Hartree/Particle)
Thermal correction to Energy= 0.090302
Thermal correction to Enthalpy= 0.091247
Thermal correction to Gibbs Free Energy= 0.058093
Sum of electronic and zero-point Energies= -192.560172
Sum of electronic and thermal Energies= -192.555218
Sum of electronic and thermal Enthalpies= -192.554274
Sum of electronic and thermal Free Energies= -192.587428

2

Zero-point correction= 0.151522 (Hartree/Particle)
Thermal correction to Energy= 0.158312
Thermal correction to Enthalpy= 0.159257
Thermal correction to Gibbs Free Energy= 0.121372
Sum of electronic and zero-point Energies= -213.022772
Sum of electronic and thermal Energies= -213.015982
Sum of electronic and thermal Enthalpies= -213.015038
Sum of electronic and thermal Free Energies= -213.052922

1..2

Zero-point correction= 0.237742 (Hartree/Particle)
Thermal correction to Energy= 0.251508
Thermal correction to Enthalpy= 0.252452
Thermal correction to Gibbs Free Energy= 0.192565
Sum of electronic and zero-point Energies= -405.588531
Sum of electronic and thermal Energies= -405.574764
Sum of electronic and thermal Enthalpies= -405.573820
Sum of electronic and thermal Free Energies= -405.633707

4

Zero-point correction= 0.241899 (Hartree/Particle)
Thermal correction to Energy= 0.253594
Thermal correction to Enthalpy= 0.254538
Thermal correction to Gibbs Free Energy= 0.204816
Sum of electronic and zero-point Energies= -405.599881
Sum of electronic and thermal Energies= -405.588187
Sum of electronic and thermal Enthalpies= -405.587242
Sum of electronic and thermal Free Energies = -405.636965

5a

Zero-point correction= 0.212529
(Hartree/Particle)
Thermal correction to Energy= 0.222896
Thermal correction to Enthalpy= 0.223840
Thermal correction to Gibbs Free Energy= 0.176943
Sum of electronic and zero-point Energies= -329.280828
Sum of electronic and thermal Energies= -329.270461
Sum of electronic and thermal Enthalpies= -329.269517
Sum of electronic and thermal Free Energies= -329.316414

5b

Zero-point correction= 0.212816
(Hartree/Particle)
Thermal correction to Energy= 0.223103
Thermal correction to Enthalpy= 0.224047
Thermal correction to Gibbs Free Energy= 0.177874
Sum of electronic and zero-point Energies= -329.331386
Sum of electronic and thermal Energies= -329.321099
Sum of electronic and thermal Enthalpies= -329.320155
Sum of electronic and thermal Free Energies= -329.366328

5c

Zero-point correction= 0.227197
(Hartree/Particle)
Thermal correction to Energy= 0.237652
Thermal correction to Enthalpy= 0.238597
Thermal correction to Gibbs Free Energy= 0.191530
Sum of electronic and zero-point Energies= -329.709831
Sum of electronic and thermal Energies= -329.699375
Sum of electronic and thermal Enthalpies= -329.698431
Sum of electronic and thermal Free Energies= -329.745497

6

Zero-point correction= 0.218929
(Hartree/Particle)
Thermal correction to Energy= 0.229676
Thermal correction to Enthalpy= 0.230620
Thermal correction to Gibbs Free Energy= 0.182968
Sum of electronic and zero-point Energies= -329.871368
Sum of electronic and thermal Energies= -329.860621
Sum of electronic and thermal Enthalpies= -329.859677
Sum of electronic and thermal Free Energies= -329.907330
Zero-point correction= 0.218630  
(Hartree/Particle)
Thermal correction to Energy= 0.229321
Thermal correction to Enthalpy= 0.230265
Thermal correction to Gibbs Free Energy= 0.182886
Sum of electronic and zero-point Energies= -329.868127
Sum of electronic and thermal Energies= -329.857436
Sum of electronic and thermal Enthalpies= -329.856492
Sum of electronic and thermal Free Energies= -329.903871

Zero-point correction= 0.236890  
(Hartree/Particle)
Thermal correction to Energy= 0.247539
Thermal correction to Enthalpy= 0.248484
Thermal correction to Gibbs Free Energy= 0.200831
Sum of electronic and zero-point Energies= -330.518445
Sum of electronic and thermal Energies= -330.507795
Sum of electronic and thermal Enthalpies= -330.506850
Sum of electronic and thermal Free Energies= -330.554504

Zero-point correction= 0.237190  
(Hartree/Particle)
Thermal correction to Energy= 0.248659
Thermal correction to Enthalpy= 0.249603
Thermal correction to Gibbs Free Energy= 0.199818
Sum of electronic and zero-point Energies= -405.546564
Sum of electronic and thermal Energies= -405.535095
Sum of electronic and thermal Enthalpies= -405.534151
Sum of electronic and thermal Free Energies= -405.583936

Zero-point correction= 0.235933  
(Hartree/Particle)
Thermal correction to Energy= 0.248488
Thermal correction to Enthalpy= 0.249432
Thermal correction to Gibbs Free Energy= 0.197913
Sum of electronic and zero-point Energies= -405.524475
Sum of electronic and thermal Energies= -405.511921
Sum of electronic and thermal Enthalpies= -405.510976
Sum of electronic and thermal Free Energies= -405.562496
### TS_2b

Zero-point correction= 0.235547  
(Hartree/Particle)  
Thermal correction to Energy= 0.247675  
Thermal correction to Enthalpy= 0.248620  
Thermal correction to Gibbs Free Energy= 0.198201  
Sum of electronic and zero-point Energies= -405.525038  
Sum of electronic and thermal Energies= -405.512910  
Sum of electronic and thermal Enthalpies= -405.511965  
Sum of electronic and thermal Free Energies= -405.562384

### TS_3

Zero-point correction= 0.212840  
(Hartree/Particle)  
Thermal correction to Energy= 0.223670  
Thermal correction to Enthalpy= 0.224615  
Thermal correction to Gibbs Free Energy= 0.177393  
Sum of electronic and zero-point Energies= -329.826768  
Sum of electronic and thermal Energies= -329.815938  
Sum of electronic and thermal Enthalpies= -329.814994  
Sum of electronic and thermal Free Energies= -329.862215

### TS_4

Zero-point correction= 0.213594  
(Hartree/Particle)  
Thermal correction to Energy= 0.224274  
Thermal correction to Enthalpy= 0.225218  
Thermal correction to Gibbs Free Energy= 0.178328  
Sum of electronic and zero-point Energies= -329.829301  
Sum of electronic and thermal Energies= -329.818620  
Sum of electronic and thermal Enthalpies= -329.817676  
Sum of electronic and thermal Free Energies= -329.864567

### TS_5

Zero-point correction= 0.222958  
(Hartree/Particle)  
Thermal correction to Energy= 0.235123  
Thermal correction to Enthalpy= 0.236067  
Thermal correction to Gibbs Free Energy= 0.185221  
Sum of electronic and zero-point Energies= -330.302066  
Sum of electronic and thermal Energies= -330.289901  
Sum of electronic and thermal Enthalpies= -330.288957  
Sum of electronic and thermal Free Energies= -330.339803
### TS_6

Zero-point correction= 0.222299
(Hartree/Particle)
Thermal correction to Energy= 0.234377
Thermal correction to Enthalpy= 0.235322
Thermal correction to Gibbs Free Energy= 0.184221
Sum of electronic and zero-point Energies= -330.286258
Sum of electronic and thermal Energies= -330.274179
Sum of electronic and thermal Enthalpies= -330.273235
Sum of electronic and thermal Free Energies= -330.324335

### TS_7

Zero-point correction= 0.222964
(Hartree/Particle)
Thermal correction to Energy= 0.235039
Thermal correction to Enthalpy= 0.235984
Thermal correction to Gibbs Free Energy= 0.184901
Sum of electronic and zero-point Energies= -330.305654
Sum of electronic and thermal Energies= -330.293578
Sum of electronic and thermal Enthalpies= -330.292634
Sum of electronic and thermal Free Energies= -330.343717

### 1_w

Zero-point correction= 0.134452
(Hartree/Particle)
Thermal correction to Energy= 0.146576
Thermal correction to Enthalpy= 0.147520
Thermal correction to Gibbs Free Energy= 0.094394
Sum of electronic and zero-point Energies= -345.077930
Sum of electronic and thermal Energies= -345.065807
Sum of electronic and thermal Enthalpies= -345.064863
Sum of electronic and thermal Free Energies= -345.117989

### 1w..2

Zero-point correction= 0.288043
(Hartree/Particle)
Thermal correction to Energy= 0.308158
Thermal correction to Enthalpy= 0.309103
Thermal correction to Gibbs Free Energy= 0.236771
Sum of electronic and zero-point Energies= -558.115591
Sum of electronic and thermal Energies= -558.095475
Sum of electronic and thermal Enthalpies= -558.094531
Sum of electronic and thermal Free Energies= -558.166862
1w_2

Zero-point correction= 0.292837
(Hartree/Particle)
Thermal correction to Energy= 0.310149
Thermal correction to Enthalpy= 0.311093
Thermal correction to Gibbs Free Energy= 0.247712
Sum of electronic and zero-point Energies= -558.112066
Sum of electronic and thermal Energies= -558.094755
Sum of electronic and thermal Enthalpies= -558.093811
Sum of electronic and thermal Free Energies= -558.157192

4_w

Zero-point correction= 0.291361
(Hartree/Particle)
Thermal correction to Energy= 0.309871
Thermal correction to Enthalpy= 0.310815
Thermal correction to Gibbs Free Energy= 0.244154
Sum of electronic and zero-point Energies= -558.122304
Sum of electronic and thermal Energies= -558.103795
Sum of electronic and thermal Enthalpies= -558.102850
Sum of electronic and thermal Free Energies= -558.169512

5a_w

Zero-point correction= 0.260838
(Hartree/Particle)
Thermal correction to Energy= 0.278627
Thermal correction to Enthalpy= 0.279571
Thermal correction to Gibbs Free Energy= 0.213730
Sum of electronic and zero-point Energies= -481.804653
Sum of electronic and thermal Energies= -481.786863
Sum of electronic and thermal Enthalpies= -481.785919
Sum of electronic and thermal Free Energies= -481.851760

5b_w

Zero-point correction= 0.263056
(Hartree/Particle)
Thermal correction to Energy= 0.279499
Thermal correction to Enthalpy= 0.280444
Thermal correction to Gibbs Free Energy= 0.218939
Sum of electronic and zero-point Energies= -481.859412
Sum of electronic and thermal Energies= -481.842968
Sum of electronic and thermal Enthalpies= -481.842024
Sum of electronic and thermal Free Energies= -481.903528
\textbf{5c\_w}

\begin{itemize}
\item \textbf{Zero-point correction=} 0.276565 \\
\text{(Hartree/Particle)}
\item \textbf{Thermal correction to Energy=} 0.293813
\item \textbf{Thermal correction to Enthalpy=} 0.294757
\item \textbf{Thermal correction to Gibbs Free Energy=} 0.229173
\item \textbf{Sum of electronic and zero-point Energies=} -482.245461
\item \textbf{Sum of electronic and thermal Energies=} -482.228214
\item \textbf{Sum of electronic and thermal Enthalpies=} -482.227269
\item \textbf{Sum of electronic and thermal Free Energies=} -482.292853
\end{itemize}

\textbf{TS\_0\_w}

\begin{itemize}
\item \textbf{Zero-point correction=} 0.290158 \\
\text{(Hartree/Particle)}
\item \textbf{Thermal correction to Energy=} 0.308202
\item \textbf{Thermal correction to Enthalpy=} 0.309146
\item \textbf{Thermal correction to Gibbs Free Energy=} 0.243226
\item \textbf{Sum of electronic and zero-point Energies=} -558.112346
\item \textbf{Sum of electronic and thermal Energies=} -558.094302
\item \textbf{Sum of electronic and thermal Enthalpies=} -558.093357
\item \textbf{Sum of electronic and thermal Free Energies=} -558.159278
\end{itemize}

\textbf{TS\_1\_w}

\begin{itemize}
\item \textbf{Zero-point correction=} 0.287629 \\
\text{(Hartree/Particle)}
\item \textbf{Thermal correction to Energy=} 0.305228
\item \textbf{Thermal correction to Enthalpy=} 0.306172
\item \textbf{Thermal correction to Gibbs Free Energy=} 0.241545
\item \textbf{Sum of electronic and zero-point Energies=} -558.086110
\item \textbf{Sum of electronic and thermal Energies=} -558.068511
\item \textbf{Sum of electronic and thermal Enthalpies=} -558.067567
\item \textbf{Sum of electronic and thermal Free Energies=} -558.132194
\end{itemize}

\textbf{TS\_2a\_w}

\begin{itemize}
\item \textbf{Zero-point correction=} 0.282535 \\
\text{(Hartree/Particle)}
\item \textbf{Thermal correction to Energy=} 0.302110
\item \textbf{Thermal correction to Enthalpy=} 0.303054
\item \textbf{Thermal correction to Gibbs Free Energy=} 0.232475
\item \textbf{Sum of electronic and zero-point Energies=} -558.066631
\item \textbf{Sum of electronic and thermal Energies=} -558.047056
\item \textbf{Sum of electronic and thermal Enthalpies=} -558.046112
\item \textbf{Sum of electronic and thermal Free Energies=} -558.116691
\end{itemize}
TS_2b_w
Zero-point correction= 0.284207
(Hartree/Particle)
Thermal correction to Energy= 0.303455
Thermal correction to Enthalpy= 0.304399
Thermal correction to Gibbs Free Energy= 0.236576
Sum of electronic and zero-point Energies= -558.044193
Sum of electronic and thermal Energies= -558.024945
Sum of electronic and thermal Enthalpies= -558.024001
Sum of electronic and thermal Free Energies= -558.091824

TS_2c_w
Zero-point correction= 0.289165
(Hartree/Particle)
Thermal correction to Energy= 0.306285
Thermal correction to Enthalpy= 0.307229
Thermal correction to Gibbs Free Energy= 0.245228
Sum of electronic and zero-point Energies= -558.082204
Sum of electronic and thermal Energies= -558.065084
Sum of electronic and thermal Enthalpies= -558.064140
Sum of electronic and thermal Free Energies= -558.126141

1_H+
Zero-point correction= 0.098501
(Hartree/Particle)
Thermal correction to Energy= 0.103597
Thermal correction to Enthalpy= 0.104541
Thermal correction to Gibbs Free Energy= 0.071127
Sum of electronic and zero-point Energies= -192.852571
Sum of electronic and thermal Energies= -192.847475
Sum of electronic and thermal Enthalpies= -192.846530
Sum of electronic and thermal Free Energies= -192.879945

3
Zero-point correction= 0.085485
(Hartree/Particle)
Thermal correction to Energy= 0.090659
Thermal correction to Enthalpy= 0.091603
Thermal correction to Gibbs Free Energy= 0.057792
Sum of electronic and zero-point Energies= -192.541993
Sum of electronic and thermal Energies= -192.536819
Sum of electronic and thermal Enthalpies= -192.535875
Sum of electronic and thermal Free Energies= -192.569686
3.2

Zero-point correction= 0.238010
(Hartree/Particle)
Thermal correction to Energy= 0.252007
Thermal correction to Enthalpy= 0.252951
Thermal correction to Gibbs Free Energy= 0.193581
Sum of electronic and zero-point Energies= -405.571272
Sum of electronic and thermal Energies= -405.557276
Sum of electronic and thermal Enthalpies= -405.556332
Sum of electronic and thermal Free Energies= -405.615701

9

Zero-point correction= 0.241288
(Hartree/Particle)
Thermal correction to Energy= 0.252716
Thermal correction to Enthalpy= 0.253660
Thermal correction to Gibbs Free Energy= 0.204910
Sum of electronic and zero-point Energies= -405.490156
Sum of electronic and thermal Energies= -405.478729
Sum of electronic and thermal Enthalpies= -405.477785
Sum of electronic and thermal Free Energies= -405.526534

10

Zero-point correction= 0.212675
(Hartree/Particle)
Thermal correction to Energy= 0.223006
Thermal correction to Enthalpy= 0.223950
Thermal correction to Gibbs Free Energy= 0.177513
Sum of electronic and zero-point Energies= -329.248498
Sum of electronic and thermal Energies= -329.238166
Sum of electronic and thermal Enthalpies= -329.237222
Sum of electronic and thermal Free Energies= -329.283659

TS_8

Zero-point correction= 0.250819
(Hartree/Particle)
Thermal correction to Energy= 0.263702
Thermal correction to Enthalpy= 0.264646
Thermal correction to Gibbs Free Energy= 0.209943
Sum of electronic and zero-point Energies= -405.897342
Sum of electronic and thermal Energies= -405.884460
Sum of electronic and thermal Enthalpies= -405.883516
Sum of electronic and thermal Free Energies= -405.938219
**TS_9**

Zero-point correction= 0.239328  
(Hartree/Particle)  
Thermal correction to Energy= 0.251114  
Thermal correction to Enthalpy= 0.252058  
Thermal correction to Gibbs Free Energy= 0.202321  
Sum of electronic and zero-point Energies= -405.494122  
Sum of electronic and thermal Energies= -405.482336  
Sum of electronic and thermal Enthalpies= -405.481392  
Sum of electronic and thermal Free Energies= -405.531128

**TS_10**

Zero-point correction= 0.239770  
(Hartree/Particle)  
Thermal correction to Energy= 0.251137  
Thermal correction to Enthalpy= 0.252081  
Thermal correction to Gibbs Free Energy= 0.202996  
Sum of electronic and zero-point Energies= -405.488090  
Sum of electronic and thermal Energies= -405.476723  
Sum of electronic and thermal Enthalpies= -405.475779  
Sum of electronic and thermal Free Energies= -405.524863

**TS_11**

Zero-point correction= 0.234270  
(Hartree/Particle)  
Thermal correction to Energy= 0.246693  
Thermal correction to Enthalpy= 0.247637  
Thermal correction to Gibbs Free Energy= 0.196589  
Sum of electronic and zero-point Energies= -405.510237  
Sum of electronic and thermal Energies= -405.497815  
Sum of electronic and thermal Enthalpies= -405.496871  
Sum of electronic and thermal Free Energies= -405.547918

**2_H+**

Zero-point correction= 0.166872  
(Hartree/Particle)  
Thermal correction to Energy= 0.173773  
Thermal correction to Enthalpy= 0.174717  
Thermal correction to Gibbs Free Energy= 0.136558  
Sum of electronic and zero-point Energies= -213.383006  
Sum of electronic and thermal Energies= -213.376106  
Sum of electronic and thermal Enthalpies= -213.375161  
Sum of electronic and thermal Free Energies= -213.413320

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516
1.. 2_H+

Zero-point correction= 0.253744
(Hartree/Particle)
Thermal correction to Energy= 0.267427
Thermal correction to Enthalpy= 0.268372
Thermal correction to Gibbs Free Energy= 0.209590
Sum of electronic and zero-point Energies= -405.968589
Sum of electronic and thermal Energies= -405.954905
Sum of electronic and thermal Enthalpies= -405.953961
Sum of electronic and thermal Free Energies= -406.012743

1_H+..2

Zero-point correction= 0.257920
(Hartree/Particle)
Thermal correction to Energy= 0.269274
Thermal correction to Enthalpy= 0.270219
Thermal correction to Gibbs Free Energy= 0.221868
Sum of electronic and zero-point Energies= -405.953070
Sum of electronic and thermal Energies= -405.941715
Sum of electronic and thermal Enthalpies= -405.940771
Sum of electronic and thermal Free Energies= -405.989122

11

Zero-point correction= 0.256815
(Hartree/Particle)
Thermal correction to Energy= 0.268761
Thermal correction to Enthalpy= 0.269705
Thermal correction to Gibbs Free Energy= 0.219508
Sum of electronic and zero-point Energies= -405.965383
Sum of electronic and thermal Energies= -405.953438
Sum of electronic and thermal Enthalpies= -405.952494
Sum of electronic and thermal Free Energies= -406.002691

TS_12

Zero-point correction= 0.252168
(Hartree/Particle)
Thermal correction to Energy= 0.264896
Thermal correction to Enthalpy= 0.265841
Thermal correction to Gibbs Free Energy= 0.210936
Sum of electronic and zero-point Energies= -405.899577
Sum of electronic and thermal Energies= -405.886848
Sum of electronic and thermal Enthalpies= -405.885904
Sum of electronic and thermal Free Energies= -405.940809
TS_13

Zero-point correction= 0.250629
(Hartree/Particle)
Thermal correction to Energy= 0.262062
Thermal correction to Enthalpy= 0.263006
Thermal correction to Gibbs Free Energy= 0.214254
Sum of electronic and zero-point Energies= -405.909339
Sum of electronic and thermal Energies= -405.897906
Sum of electronic and thermal Enthalpies= -405.896962
Sum of electronic and thermal Free Energies= -405.945714

TS_14

Zero-point correction= 0.256992
(Hartree/Particle)
Thermal correction to Energy= 0.267829
Thermal correction to Enthalpy= 0.268773
Thermal correction to Gibbs Free Energy= 0.221719
Sum of electronic and zero-point Energies= -405.949928
Sum of electronic and thermal Energies= -405.939091
Sum of electronic and thermal Enthalpies= -405.938146
Sum of electronic and thermal Free Energies= -405.985200