Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY INFORMATION

FOR

Phot0, a plausible primeval pigment on Earth and rocky exoplanets

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1. Reaction mechanism of the formation of Phot0

Figure 1 shows the full *E+ZPE* energy profile for the formation of Phot0 from **C_2H_2** and **HCN**. The lower frontier molecular orbital (FMO) interaction found between Int1Zn and **C_2H_2** and **HCN** is the HOMO (highest occupied molecular orbital) of **C_2H_2** and LUMO (lowest unoccupied molecular orbital) of **$Int1_{Zn}$** (Figure 2). This interaction yields the complex **$C2_{Zn}$**, which is 13 kcal/mol below **$Int1_{Zn}$**. Then, there is a concerted insertion of **C_2H_2** into the N-Zn bond to yield the intermediate **$Int2_{Zn}$** through the transition structure **$TS2_{Zn}$**. In this reaction there is a breaking of the Zn-N bond and the formation of two new bonds, C-N and Zn-C.

In the next step, another **HCN** molecule is needed to keep building the pigment. The latter complexes with **$Int2_{Zn}$**, forming the complex **$C3_{Zn}$**. The **HCN** moiety of **$C3_{Zn}$** reacts with the carbon that shows the highest coefficient of the HOMO in **$Int2_{Zn}$** (Figure 3), giving rise to the intermediate **Int3Zn** through the transition structure **$TS3_{Zn}$**. Although in this step the reaction is with an **HCN** unit, this new transition structure is similar to the previous (**$TS2_{Zn}$**), where the rupture of the C-Zn and the two new bond formation is a concerted process.

The formation of the next intermediate, (**$Int4_{Zn}$**), is very similar to that of the formation of **$Int2_{Zn}$**, where the unit of **C_2H_2** is inserted in the Nterminal-Zn bond. Again, the formation of **$Int5_{Zn}$** is similar to that of **$Int3_{Zn}$**. However, the complexation of the next unit of **HCN** to the metallic center is perpendicular to the ring of **$Int4_{Zn}$** (**$C5_{Zn}$**), since the angle Cterminal-Zn-Cterminal is below 180◦ and does not allow a frontal approximation of the new unit of **HCN**. The transition structure that follows to this complex (**$TS5_{Zn}$**) is similar to the previous, both from a geometrical and kinetic point of view, showing similar energy barriers. This situation is also observed in the formation of the complex **$C6_{Zn}$**. In the latter, the complexation perpendicular to the ring is with **C_2H_2**. This complex is linked to **$Int6_{Zn}$** thought the transition structure **$TS6_{Zn}$**.

The last stationary points are geometrically different than the previous, since **$Int6_{Zn}$** takes on a half-helix-like structure that does not allow anything to complex with the metal. Thus, the last unit of **HCN** complexes with the terminal carbon that, also in this case, shows the highest coefficient of the HOMO (Figure 3). In the subsequent transition structure (**$TS7_{Zn}$**) the **HCN** moiety attacks the C-Zn bond perpendicular to the ring, inserting itself in this bond and leading to the last intermediate, **$Int7_{Zn}$**. The last step is both the kinetic (2.1 kcal/mol) and thermodinamically (-66.7 kcal/mol) most favored process. It entails a molecular rearrangement where the covalent Cterminal-Zn and non-covalent Nterminal-Zn bonds break and the two new covalent bonds, Cterminal-Nterminal and Nterminal-Zn, are formed, yielding the primeval pigment **Phot0**.

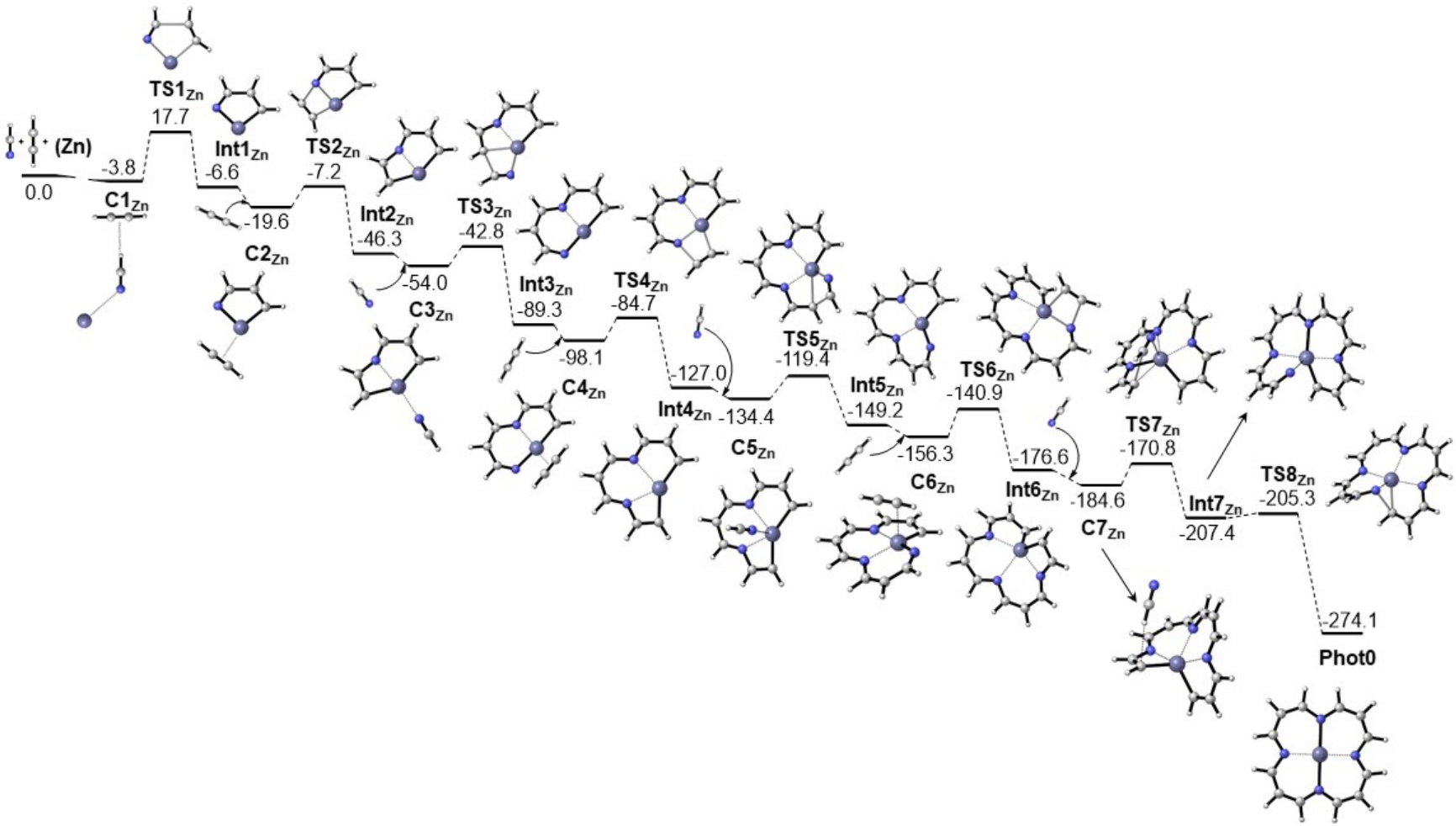


Fig. S1. Full *E*+*ZPE* energy profile leading to the primeval phosynthetic pigment **Phot0**. Energy values are given in kcal/mol.

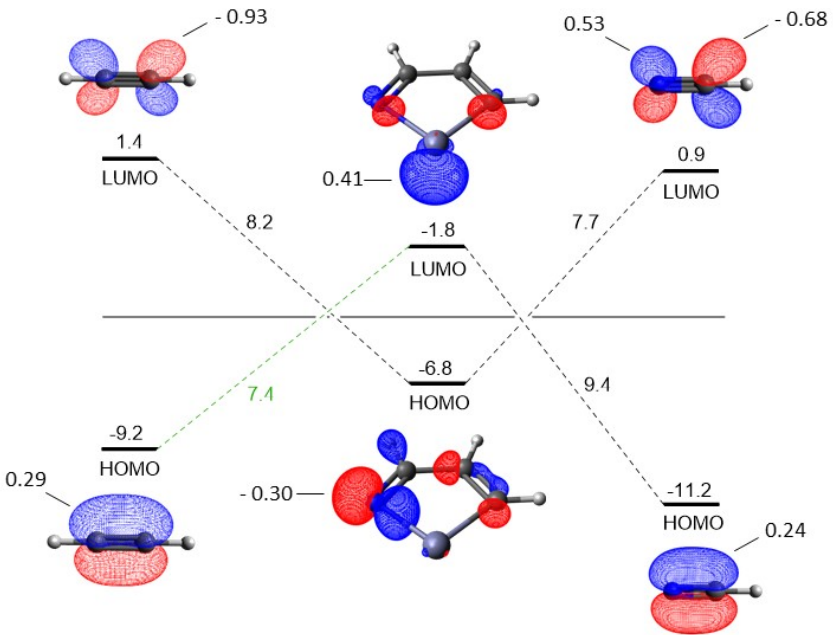
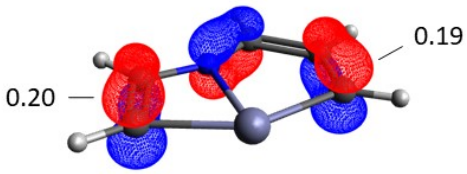
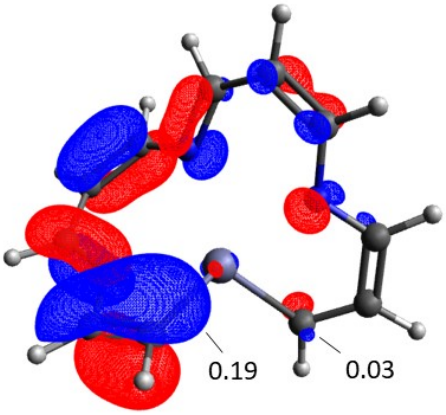


Fig. S2. Frontier molecular orbitals interactions and most relevant coefficients of the HOMO and LUMO orbitals of $\mathbf{C_2H_2}$ (left) **HCN** (right) and $\mathbf{Int1_{Zn}}$ (middle). FMO energies are given in eV and the isosurfaces are depicted for an isovalue of 0.08.



$\mathbf{Int2_{Zn}}$



$\mathbf{Int6_{Zn}}$

Fig. S3. HOMO orbitals of $\mathbf{Int1_{Zn}}$ (isovalue of 0.08) and $\mathbf{Int1_{Zn}}$ (isovalue of 0.05) and the most relevant molecular orbital coefficients.

2. [3+2] cycloaddition of Phot0 with ethylene (C2H4) and acetylene (C2H2)

Figure 4 shows the *E+ZPE* potential energy profiles for the cycloadditions and post dehydrogenation reactions of Phot0 with $\mathbf{C_2H_2}$ and $\mathbf{C_2H_4}$. Both pre-reactive complexes, $\mathbf{C_{cyc-AC}}$ and $\mathbf{C_{cyc-ET}}$, show almost identical relative energies (11.8 and 11.6 kcal/mol respectively), where the π bond of $\mathbf{C_2H_2}$ and $\mathbf{C_2H_4}$ interact with the metallic center. In the same way, both cycloadditions show similar energy barriers, 22.0 and 22.8 kcal/mol for $\mathbf{C_2H_2}$ and $\mathbf{C_2H_4}$ respectively. However, the relative energy of the intermediates $\mathbf{Int1_{cyc-AC}}$ and $\mathbf{Int1_{cyc-ET}}$ differ in 13.7 kcal/mol, being the intermediate Int1cyc−AC, the most stable. There are two geometrical parameters in $\mathbf{Int1_{cyc-ET}}$ that contribute notably to the increase in steric interaction due to the strain conformation adopted. The hydrogens of the two new sp3 carbons are closer to each other than the same carbons in $\mathbf{Int1_{cyc-AC}}$ (see Figure 5). Furthermore, the hydrogens of the two methylene groups are completely eclipsed, contributing to rise the energy of the system (Figure 5). The next transition structures correspond with the loss of molecular hydrogen from the previous intermediates to yield the new pyrrole ($\mathbf{Int2_{cyc-AC}}$) and dihydropyrrole ($\mathbf{Int2_{cyc-ET}}$) rings. The dehydrogenation of Int1cyc−AC through the transition structure $\mathbf{TS2_{cyc-AC}}$ shows an energy barrier of 27.6 kcal/mol, being the first transition structure the rate-determining step of the whole process. Likewise, the higher energy barrier for the dehydrogenation of Int2cyc−ET is 23.3 kcal/mol ($\mathbf{TS2_{cyc-ET}}$) above the reagents and is the rate-determining step of the the reaction. The lower relative energy of $\mathbf{TS2_{cyc-AC}}$ with respect to $\mathbf{TS2_{cyc-ET}}$ (8.6 kcal/mol) is ascribed to two facts: in the transition structure $\mathbf{TS2_{cyc-AC}}$ the new pyrrole ring that is being formed is already contributing to the total delocalization of the macrocycle, whereas in the more saturated intermediate $\mathbf{TS2_{cyc-ET}}$ the methylene groups hinder the delocalization in the new ring and are also in a eclipsed position as in $\mathbf{Int1_{cyc-ET}}$**.** This diedral angle turns to an alternated position in $\mathbf{Int2_{cyc-ET}}$. However, this intermediate is 43.9 kcal/mol above $\mathbf{Int2_{cyc-AC}}$, which is a much delocalized system due to the formation of the new pyrrole ring.

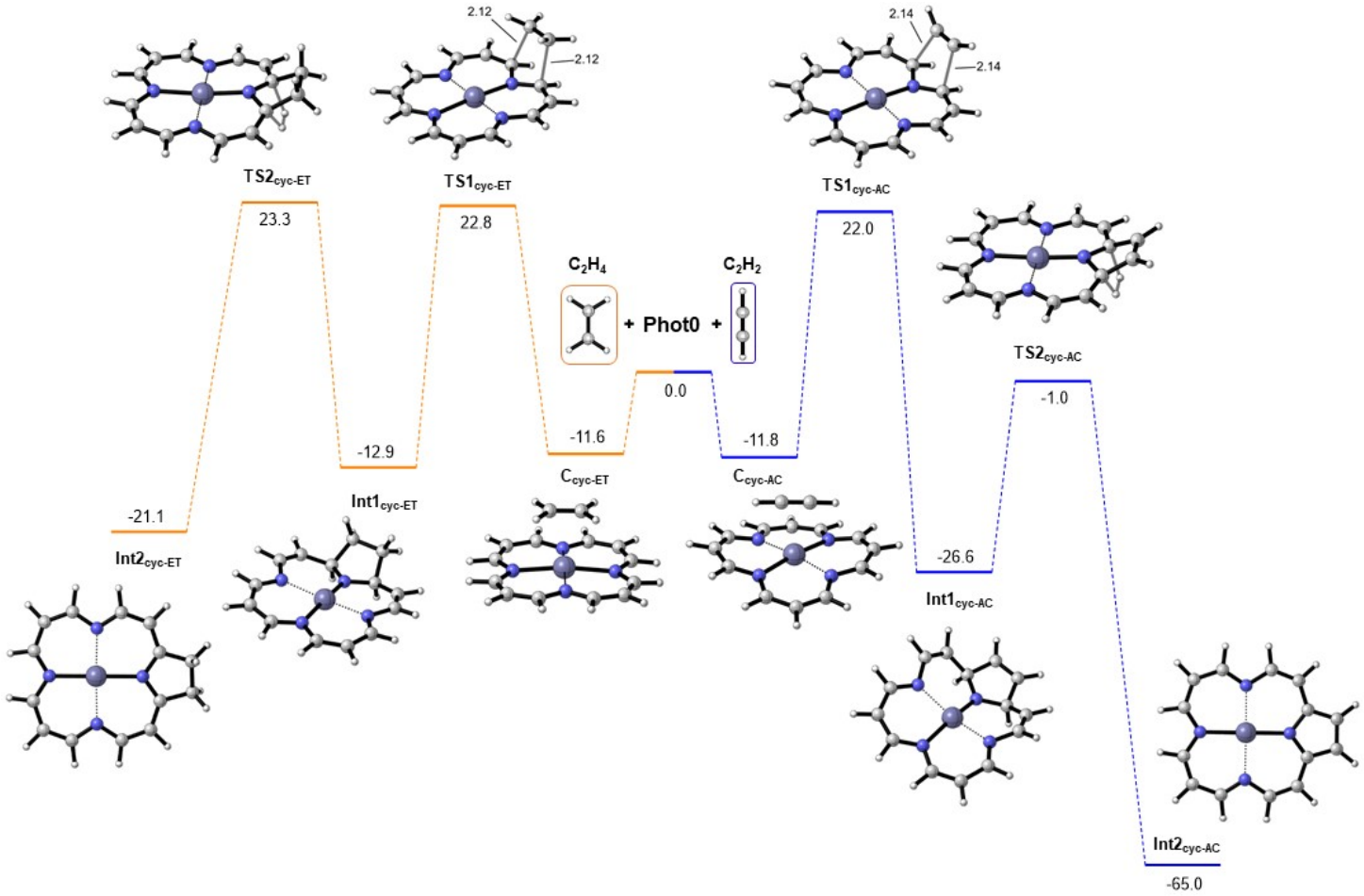


Fig. S4. *E+ZPE* energy profile leading to the first pyrrole and dihydropyrrole after the reaction of **Phot0** with C_2H_2 and C_2H_4 respectively. Energy values are given in kcal/mol.

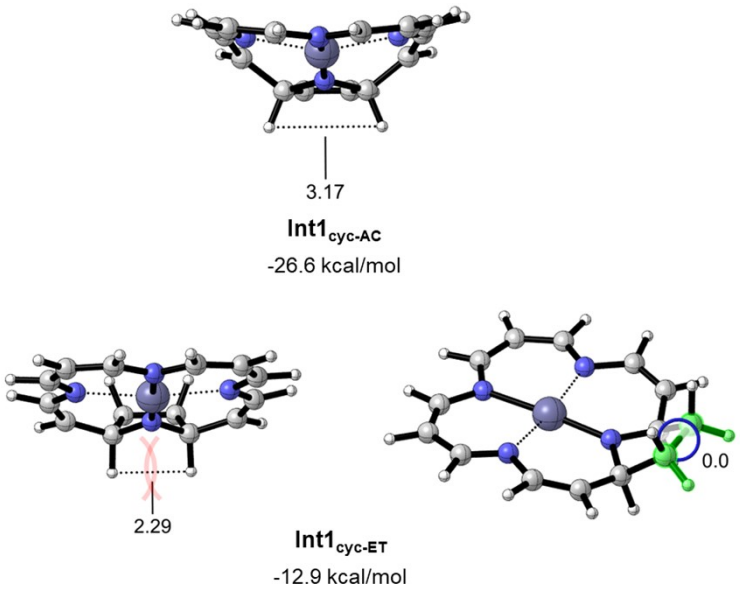


Fig. S5. Geometrical parameters that contribute to destabilize the intermediate **Int1**$_{\mathbf{cyc-ET}}$ in comparison with **Int1**$_{\mathbf{cyc-AC}}$ (also showed).

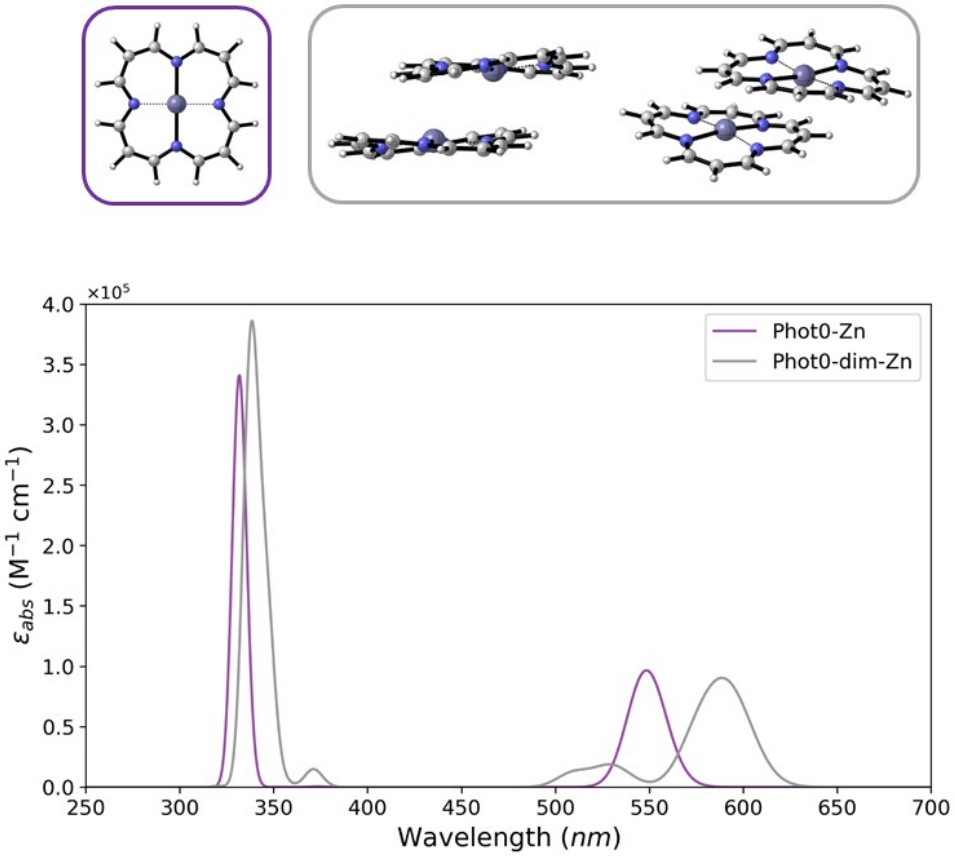


Fig. S6. Optimized geometries of Phot0-Zn and its dimmer in vacuum at CAM-B3LYP-D3(BJ)/def2-TZVP (top). Theoretical UV/Vis absorption spectra of Phot0-Zn (purple) and its dimmer (grey) in vacuum (bottom).

1. Cartesian coordinates of all optimized structures

Calculations at the (U)MN15/jun-cc-pVTZ level of theory

C_2H_2

Zero-point correction= 0.027386 (Hartree/Particle)
Thermal correction to Energy= 0.030133
Thermal correction to Enthalpy= 0.031077
Thermal correction to Gibbs Free Energy= 0.008459
Sum of electronic and zero-point Energies= -77.231575
Sum of electronic and thermal Energies= -77.228828
Sum of electronic and thermal Enthalpies= -77.227884
Sum of electronic and thermal Free Energies= -77.250502
Zero imaginary frequencies.

C	0.00000000	0.00000000	0.59823800
H	0.00000000	0.00000000	1.66132100
C	0.00000000	0.00000000	-0.59823800
H	0.00000000	0.00000000	-1.66132100

HCN

Zero-point correction= 0.016508 (Hartree/Particle)
Thermal correction to Energy= 0.019041
Thermal correction to Enthalpy= 0.019985
Thermal correction to Gibbs Free Energy= -0.002848
Sum of electronic and zero-point Energies= -93.329555
Sum of electronic and thermal Energies= -93.327021
Sum of electronic and thermal Enthalpies= -93.326077
Sum of electronic and thermal Free Energies= -93.348911
Zero imaginary frequencies.

C	0.00000000	0.00000000	-0.49698200
H	0.00000000	0.00000000	-1.56295900
N	0.00000000	0.00000000	0.64926400

C

Zero-point correction= 0.044694 (Hartree/Particle)
Thermal correction to Energy= 0.051128
Thermal correction to Enthalpy= 0.052072
Thermal correction to Gibbs Free Energy= 0.013907
Sum of electronic and zero-point Energies= -170.564248
Sum of electronic and thermal Energies= -170.557814
Sum of electronic and thermal Enthalpies= -170.556869
Sum of electronic and thermal Free Energies= -170.595035
Zero imaginary frequencies.

C	1.58663400	-0.00170600	0.00014500
H	0.51590100	-0.00271600	0.00021200
N	2.73341100	-0.00028400	-0.00011100
C	-2.07876500	0.59964900	-0.00002300
H	-2.08355400	1.66362500	-0.00002700

C	-2.08519500	-0.59753400	-0.00001600
H	-2.10226600	-1.66137600	-0.00004200

Int1

Zero-point correction= 0.046474 (Hartree/Particle)
Thermal correction to Energy= 0.051020
Thermal correction to Enthalpy= 0.051964
Thermal correction to Gibbs Free Energy= 0.020196
Sum of electronic and zero-point Energies= -170.493861
Sum of electronic and thermal Energies= -170.489315
Sum of electronic and thermal Enthalpies= -170.488371
Sum of electronic and thermal Free Energies= -170.520139
Zero imaginary frequencies.

C	-0.10199700	-0.74711300	0.00000000
H	0.83710500	-1.30689600	0.00000000
N	-1.19382400	-1.34108400	0.00000000
C	0.00000000	0.75269600	0.00000000
H	-0.94742800	1.27769700	0.00000000
C	1.14693400	1.37249000	0.00000000
H	2.19747200	1.14834200	0.00000000

Int2

Zero-point correction= 0.045854 (Hartree/Particle)
Thermal correction to Energy= 0.050578
Thermal correction to Enthalpy= 0.051522
Thermal correction to Gibbs Free Energy= 0.019034
Sum of electronic and zero-point Energies= -170.490080
Sum of electronic and thermal Energies= -170.485356
Sum of electronic and thermal Enthalpies= -170.484412
Sum of electronic and thermal Free Energies= -170.516901
Zero imaginary frequencies.

C	-0.77377000	0.37127700	0.18791000
H	-1.18896700	1.19821900	0.77509100
N	-1.49510000	-0.56735200	-0.16937700
C	0.70308500	0.50862300	-0.15180500
H	0.97291100	1.48299700	-0.54720100
C	1.57844300	-0.42646700	0.05226600
H	1.63521100	-1.43034700	0.42751800

Int1$_{Zn}$

Zero-point correction= 0.050761 (Hartree/Particle)
Thermal correction to Energy= 0.055795
Thermal correction to Enthalpy= 0.056739
Thermal correction to Gibbs Free Energy= 0.021937
Sum of electronic and zero-point Energies= -238.096342
Sum of electronic and thermal Energies= -238.091307
Sum of electronic and thermal Enthalpies= -238.090363
Sum of electronic and thermal Free Energies= -238.125165
Zero imaginary frequencies.

C	1.35927300	-0.87086200	-0.00006300
H	2.33059200	-1.38355900	0.00003600
N	0.29484300	-1.55124600	-0.00000700
C	1.50779500	0.66936400	0.00002000
H	2.54117500	1.00765600	0.00002600
C	0.47075000	1.49967900	0.00003300
H	0.57371600	2.57381500	0.00005400
Zn	-0.91787600	0.02905700	0.00000000

$C1_{Zn}$

Zero-point correction= 0.044930 (Hartree/Particle)
Thermal correction to Energy= 0.053970
Thermal correction to Enthalpy= 0.054915
Thermal correction to Gibbs Free Energy= 0.003902
Sum of electronic and zero-point Energies= -238.091876
Sum of electronic and thermal Energies= -238.082835
Sum of electronic and thermal Enthalpies= -238.081891
Sum of electronic and thermal Free Energies= -238.132904
Zero imaginary frequencies.

C	1.31533900	-0.86402500	-0.00007800
H	2.31670900	-0.48330000	-0.00036400
N	0.24142500	-1.26695800	-0.00031400
C	4.46607400	1.05309500	-0.00020300
H	4.06446300	2.03845700	-0.00071900
C	4.93071000	-0.05030900	0.00034300
H	5.35553200	-1.02583300	0.00096900
Zn	-2.58998100	0.25022700	0.00006400

$C2_{Zn}$

Zero-point correction= 0.079675 (Hartree/Particle)
Thermal correction to Energy= 0.088522
Thermal correction to Enthalpy= 0.089466
Thermal correction to Gibbs Free Energy= 0.044565
Sum of electronic and zero-point Energies= -315.348775
Sum of electronic and thermal Energies= -315.339928
Sum of electronic and thermal Enthalpies= -315.338984
Sum of electronic and thermal Free Energies= -315.383885
Zero imaginary frequencies.

C	1.47401000	-1.34280900	0.01832300
C	2.28690000	-0.28267200	0.03423300
C	1.76189400	1.15679400	0.01658200
H	1.86825700	-2.34911200	0.03259100
H	3.37150200	-0.37639000	0.06320800
H	2.56393700	1.91053100	0.04106900
C	-2.81092900	-0.38197700	0.04068300
C	-2.44076800	0.76391200	0.03139800
Zn	-0.26587100	-0.31931300	-0.03082200
N	0.54458300	1.50303600	-0.01915100
H	-2.06301300	1.76639600	0.02242200
H	-3.20327700	-1.37277100	0.05213000

$C3_{Zn}$

Zero-point correction= 0.101379 (Hartree/Particle)
Thermal correction to Energy= 0.111590
Thermal correction to Enthalpy= 0.112534
Thermal correction to Gibbs Free Energy= 0.063688
Sum of electronic and zero-point Energies= -408.733010
Sum of electronic and thermal Energies= -408.722800
Sum of electronic and thermal Enthalpies= -408.721855
Sum of electronic and thermal Free Energies= -408.770701
Zero imaginary frequencies.

C	2.50493300	-0.47867500	-0.00003800
H	3.59753700	-0.42068200	0.00017200
N	1.72148500	0.51088300	-0.00023200
C	1.82115700	-1.80482200	0.00000500
H	2.46633700	-2.68034500	0.00002400
C	0.47307700	-1.88571200	0.00008400
H	0.07221300	-2.89683000	0.00013900
Zn	-0.36917300	0.03801100	0.00004000
C	1.45657100	1.86887500	-0.00005700
H	2.26100300	2.60425800	-0.00004000
C	0.12055300	2.10867400	0.00013000
H	-0.20025100	3.14900300	0.00034600
C	-3.88175700	-0.27339400	-0.00007600
H	-4.94607300	-0.35020500	-0.00009100
N	-2.74188100	-0.19019600	-0.00006100

$C4_{Zn}$

Zero-point correction= 0.135843 (Hartree/Particle)
Thermal correction to Energy= 0.148364
Thermal correction to Enthalpy= 0.149309
Thermal correction to Gibbs Free Energy= 0.096069
Sum of electronic and zero-point Energies= -486.035005
Sum of electronic and thermal Energies= -486.022484
Sum of electronic and thermal Enthalpies= -486.021540
Sum of electronic and thermal Free Energies= -486.074779
Zero imaginary frequencies.

C	-1.05640700	-1.98964300	0.43296700
H	-1.06057700	-3.02771100	0.77540000
N	0.03287700	-1.31419600	0.40637700
C	-2.29379600	-1.36893000	-0.05474000
H	-3.20597400	-1.94278300	0.08279800
C	-2.24101700	-0.17426100	-0.68135400
H	-3.19186600	0.22052300	-1.02907900
Zn	-0.28933900	0.53343000	-0.59519000
C	1.29524800	-1.79776100	0.69540400
H	1.36790600	-2.76139500	1.19725300
C	2.39461400	-1.11465900	0.33587600
H	3.34626500	-1.56788900	0.59046500
C	2.50519200	0.19991300	-0.37286300

H	3.56657100	0.49856000	-0.44518000
N	1.61718600	0.96029200	-0.85991500
C	0.02928100	2.51028300	1.12092300
H	1.00981000	2.81543400	0.83064900
C	-1.07452200	2.13816300	1.41419300
H	-2.05394700	1.82107100	1.68573800

$C5_{Zn}$

Zero-point correction= 0.157804 (Hartree/Particle)
Thermal correction to Energy= 0.172380
Thermal correction to Enthalpy= 0.173324
Thermal correction to Gibbs Free Energy= 0.115204
Sum of electronic and zero-point Energies= -579.422267
Sum of electronic and thermal Energies= -579.407692
Sum of electronic and thermal Enthalpies= -579.406747
Sum of electronic and thermal Free Energies= -579.464868
Zero imaginary frequencies.

C	2.24510900	1.14448300	-0.30309600
H	2.84812600	2.05449200	-0.20498700
N	0.96029000	1.22019700	-0.25128600
C	2.91110500	-0.13299700	-0.49597500
H	3.99550300	-0.09785100	-0.56689900
C	2.18143300	-1.26807600	-0.57379700
H	2.76743500	-2.17387600	-0.72313200
Zn	0.10792400	-1.01935100	-0.33703500
C	0.33858400	2.43631700	-0.07137400
H	0.98517000	3.30440400	0.06974400
C	-1.00118000	2.61684000	-0.07813600
H	-1.36222800	3.62788300	0.05613400
C	-2.00678600	1.58648600	-0.28656700
H	-3.05123400	1.90158000	-0.36114200
N	-1.67737800	0.35754800	-0.39190500
C	-2.48965700	-0.75389600	-0.62067300
C	-1.78786800	-1.90269500	-0.70164000
H	-2.34693200	-2.81538000	-0.89417300
H	-3.56756100	-0.60418200	-0.71463000
C	-0.12265700	-0.46297000	3.10307700
N	0.02370400	-0.71614600	1.99819200
H	-0.26079700	-0.22868600	4.13421500

$C6_{Zn}$

Zero-point correction= 0.191362 (Hartree/Particle)
Thermal correction to Energy= 0.207907
Thermal correction to Enthalpy= 0.208851
Thermal correction to Gibbs Free Energy= 0.146738
Sum of electronic and zero-point Energies= -656.688844
Sum of electronic and thermal Energies= -656.672299
Sum of electronic and thermal Enthalpies= -656.671355
Sum of electronic and thermal Free Energies= -656.733468
Zero imaginary frequencies.

C	2.85096200	-0.03224500	-0.47423700
H	3.82368500	0.46554800	-0.42111100
N	1.78044800	0.65512200	-0.21178100
C	2.77571200	-1.42036800	-0.84656100
H	3.71634500	-1.91899000	-1.06182200
C	1.54931500	-1.99259300	-0.90814100
H	1.53865200	-3.04585300	-1.18294500
Zn	-0.03677900	-0.73690000	-0.25089300
C	1.88944300	1.98078700	0.09818400
H	2.89036700	2.38350200	0.25767100
C	0.82211900	2.80495100	0.18498700
H	1.01068800	3.84371900	0.41658800
C	-0.55610100	2.46972800	-0.07527900
H	-1.23911600	3.32432500	-0.07465800
N	-1.06407900	1.30430700	-0.30348200
C	-2.44423500	1.28888700	-0.55086300
C	-3.24438300	0.21418600	-0.51142000
H	-2.88168900	2.26315300	-0.76556700
C	-2.91476100	-1.18943200	-0.15538700
N	-1.77083600	-1.68590100	0.02226900
H	-4.29173800	0.41228000	-0.71663700
H	-3.82806700	-1.80152000	-0.03439700
C	-0.03821200	-1.27616700	2.37034500
C	0.52697200	-0.22408700	2.48965400
H	1.01839700	0.71267800	2.60804200
H	-0.57388900	-2.18842200	2.22488900

$C7_{Zn}$

Zero-point correction= 0.213218 (Hartree/Particle)
Thermal correction to Energy= 0.231738
Thermal correction to Enthalpy= 0.232682
Thermal correction to Gibbs Free Energy= 0.165521
Sum of electronic and zero-point Energies= -750.063386
Sum of electronic and thermal Energies= -750.044866
Sum of electronic and thermal Enthalpies= -750.043921
Sum of electronic and thermal Free Energies= -750.111082
Zero imaginary frequencies.

C	3.17696400	0.51813300	0.06268400
H	4.00059400	1.21950300	0.22266600
N	1.95784900	0.92079600	0.24781700
C	3.44852700	-0.81601600	-0.41120000
H	4.49491500	-1.08635400	-0.52186200
C	2.39651800	-1.61691800	-0.72190900
H	2.66902400	-2.61234100	-1.06926400
Zn	0.60177200	-0.78398500	0.04012700
C	1.67735100	2.23060300	0.53049600
H	2.43439200	2.81723000	1.04963600
C	0.52967000	2.82269100	0.13437900
H	0.39018200	3.86711300	0.37273800
C	-0.49117500	2.23179400	-0.69919100
H	-1.21634400	2.94444000	-1.10082500

N	-0.63513200	0.98302000	-0.99857700
C	-1.69375100	0.69926600	-1.87690000
C	-2.50426200	-0.37424400	-1.84953900
H	-1.88532200	1.46125100	-2.62855400
C	-2.48398400	-1.40627200	-0.82364300
N	-1.42869000	-1.57370200	-0.13027600
H	-3.30167800	-0.40297800	-2.57944200
H	-3.40266000	-1.95921200	-0.61644100
C	-1.26833700	-2.28739400	1.06966300
C	-0.17275600	-1.88804300	1.74316700
H	-0.00025700	-2.33288500	2.72100200
H	-2.03418200	-3.01265300	1.34876700
C	-2.23289700	0.99658300	1.84817500
N	-2.87573500	1.93202200	1.67721600
H	-1.62106300	0.12039600	1.98743200

Int2$_{Zn}$

Zero-point correction= 0.084281 (Hartree/Particle)
Thermal correction to Energy= 0.091254
Thermal correction to Enthalpy= 0.092199
Thermal correction to Gibbs Free Energy= 0.052512
Sum of electronic and zero-point Energies= -315.391220
Sum of electronic and thermal Energies= -315.384246
Sum of electronic and thermal Enthalpies= -315.383302
Sum of electronic and thermal Free Energies= -315.422988
Zero imaginary frequencies.

C	-1.06702000	1.57133200	0.00000600
H	-1.36177100	2.62377900	0.00019300
N	0.12219000	1.14528100	-0.00008000
C	-2.10723100	0.49990800	0.00004500
H	-3.14203900	0.83269300	0.00007700
C	-1.77098400	-0.80736700	0.00001000
H	-2.59144500	-1.51678000	-0.00000100
Zn	0.29874800	-0.93967000	-0.00003900
C	1.50184700	1.29456800	0.00006500
H	1.96836900	2.27831100	0.00013100
C	2.12632900	0.09048100	0.00006600
H	3.21146600	0.06160200	0.00017700

Int3$_{Zn}$

Zero-point correction= 0.107197 (Hartree/Particle)
Thermal correction to Energy= 0.115903
Thermal correction to Enthalpy= 0.116848
Thermal correction to Gibbs Free Energy= 0.073045
Sum of electronic and zero-point Energies= -408.789403
Sum of electronic and thermal Energies= -408.780696
Sum of electronic and thermal Enthalpies= -408.779752
Sum of electronic and thermal Free Energies= -408.823555
Zero imaginary frequencies.

C	1.33442800	1.60291100	0.00010100

H	1.49388400	2.68407800	0.00019800
N	0.15332000	1.11019000	-0.00007700
C	2.48644800	0.68429600	-0.00000300
H	3.46845700	1.14760600	-0.00001500
C	2.28829000	-0.64835700	-0.00001500
H	3.17785000	-1.26913400	-0.00003800
Zn	0.25701000	-1.00507300	-0.00000600
C	-1.04660000	1.79498800	-0.00007200
H	-1.01717000	2.88326600	-0.00006500
C	-2.20919600	1.12219400	-0.00001000
H	-3.11209300	1.72246700	0.00005100
C	-2.45718900	-0.35956600	0.00012900
H	-3.54381800	-0.55447900	-0.00026500
N	-1.66110600	-1.34453500	0.00000800

Int4$_{Zn}$

Zero-point correction= 0.140081 (Hartree/Particle)
Thermal correction to Energy= 0.151063
Thermal correction to Enthalpy= 0.152007
Thermal correction to Gibbs Free Energy= 0.102354
Sum of electronic and zero-point Energies= -486.080959
Sum of electronic and thermal Energies= -486.069978
Sum of electronic and thermal Enthalpies= -486.069034
Sum of electronic and thermal Free Energies= -486.118686
Zero imaginary frequencies.

C	-2.24060300	1.06074000	-0.00010400
H	-2.84892300	1.97125500	0.00007900
N	-0.95647700	1.14620400	-0.00020100
C	-2.89994900	-0.23818500	0.00003900
H	-3.98636600	-0.22191900	0.00008000
C	-2.16212600	-1.36690100	0.00012900
H	-2.73131000	-2.29386500	0.00019300
Zn	-0.09471300	-1.09280600	0.00001000
C	-0.33863200	2.37919400	-0.00010100
H	-0.98907900	3.25480500	-0.00014000
C	0.99990400	2.56015200	-0.00000300
H	1.35989800	3.57998000	0.00001700
C	2.00787100	1.51266400	0.00003300
H	3.05779700	1.81468500	-0.00005600
N	1.67657700	0.27916800	0.00013800
C	2.49998300	-0.84901000	0.00005900
C	1.80042600	-2.00100100	-0.00004300
H	2.35516400	-2.93464600	-0.00015500
H	3.58225700	-0.70963700	0.00005400

Int5$_{Zn}$

Zero-point correction= 0.162812 (Hartree/Particle)
Thermal correction to Energy= 0.175320
Thermal correction to Enthalpy= 0.176264
Thermal correction to Gibbs Free Energy= 0.123767

Sum of electronic and zero-point Energies= -579.445988
Sum of electronic and thermal Energies= -579.433480
Sum of electronic and thermal Enthalpies= -579.432536
Sum of electronic and thermal Free Energies= -579.485033
Zero imaginary frequencies.

C	2.82916300	-0.03779600	0.03728600
H	3.77356100	0.51196800	0.07083200
N	1.72513700	0.59317000	0.29399600
C	2.82019700	-1.42449100	-0.36393200
H	3.78842300	-1.90094300	-0.48653900
C	1.62595100	-2.00528200	-0.62972200
H	1.67175500	-3.04618000	-0.94200600
Zn	0.02332300	-0.80376200	0.02210100
C	1.74492400	1.95371400	0.46538600
H	2.69306100	2.41059700	0.74613100
C	0.66716300	2.73738300	0.25367900
H	0.78700600	3.80164200	0.39764800
C	-0.64703700	2.30801400	-0.16313200
H	-1.38449300	3.10809200	-0.27147900
N	-1.03776200	1.09965300	-0.38192500
C	-2.39358800	0.92135600	-0.71374400
C	-3.13429700	-0.11984700	-0.31372700
H	-2.84682300	1.72768100	-1.28550300
C	-2.72785700	-1.23636200	0.58642700
N	-1.55983800	-1.57805800	0.91580900
H	-4.17484700	-0.10712500	-0.62106000
H	-3.60780900	-1.77634100	0.98265800

Int6$_{Zn}$

Zero-point correction= 0.195471 (Hartree/Particle)
Thermal correction to Energy= 0.210121
Thermal correction to Enthalpy= 0.211065
Thermal correction to Gibbs Free Energy= 0.153882
Sum of electronic and zero-point Energies= -656.721237
Sum of electronic and thermal Energies= -656.706587
Sum of electronic and thermal Enthalpies= -656.705643
Sum of electronic and thermal Free Energies= -656.762826
Zero imaginary frequencies.

C	2.95158800	-0.34973700	-0.29670300
H	3.98608300	-0.01200100	-0.18519600
N	2.00089400	0.33201800	0.26676100
C	2.65351700	-1.49559700	-1.11547200
H	3.50454600	-2.02883900	-1.53033200
C	1.34848800	-1.79843500	-1.34508800
H	1.19007800	-2.67863700	-1.96723200
Zn	0.10452100	-0.75472500	0.03006700
C	2.26824800	1.52776500	0.87616400
H	3.26210100	1.67702700	1.29748900
C	1.37565000	2.54164900	0.90386600
H	1.68084800	3.46926200	1.36677200
C	0.09451000	2.56497800	0.23721900

H	-0.34632600	3.56187500	0.13568900
N	-0.55768800	1.56028700	-0.24356900
C	-1.74810300	1.87841600	-0.91684500
C	-2.86978300	1.13693300	-0.96918000
H	-1.75267400	2.84582600	-1.41479700
C	-3.08389600	-0.10932800	-0.24737600
N	-2.07567300	-0.78672500	0.13364400
H	-3.70990100	1.56402400	-1.50066900
H	-4.10323000	-0.38643100	0.03044900
C	-2.02318100	-1.83779000	1.06039100
C	-0.77015900	-2.05890500	1.49981900
H	-0.64035200	-2.80340600	2.28207200
H	-2.96079600	-2.30569700	1.36510900

Int7$_{Zn}$

Zero-point correction= 0.215815 (Hartree/Particle)
Thermal correction to Energy= 0.232250
Thermal correction to Enthalpy= 0.233194
Thermal correction to Gibbs Free Energy= 0.172374
Sum of electronic and zero-point Energies= -750.099775
Sum of electronic and thermal Energies= -750.083340
Sum of electronic and thermal Enthalpies= -750.082396
Sum of electronic and thermal Free Energies= -750.143216
Zero imaginary frequencies.

C	2.33115800	-1.91391800	-0.49888100
H	3.29255600	-2.40384200	-0.33638300
N	2.13867700	-0.70580800	-0.02794900
C	1.29909300	-2.55891500	-1.27182800
H	1.54699600	-3.53942100	-1.67151100
C	0.11194300	-1.92997400	-1.47612900
H	-0.61090400	-2.48152000	-2.07406000
Zn	0.03195100	-0.20325500	-0.27922600
C	3.07713900	0.00720200	0.60808800
H	4.02745100	-0.46821300	0.84714500
C	2.90190400	1.36185300	0.89721800
H	3.74028200	1.85976100	1.36608800
C	1.82866100	2.18076200	0.60028800
H	1.94956200	3.23947700	0.82210500
N	0.62220000	1.82940600	0.05736100
C	-0.17909600	2.83127200	-0.28115000
C	-1.51346400	2.76042100	-0.69802400
H	0.24547700	3.83485400	-0.21453100
C	-2.35758600	1.66580400	-0.60109400
N	-2.01296000	0.46102000	-0.15600700
H	-1.95989400	3.68873600	-1.02306400
H	-3.40758300	1.82407000	-0.85690200
C	-3.01151400	-0.44774500	0.03575100
C	-2.91223400	-1.55102800	0.81384300
H	-3.75879900	-2.21421000	0.90467600
H	-3.96903300	-0.23814800	-0.44220700
C	-1.74609400	-1.83928200	1.63772700

H	-1.86008800	-2.62091000	2.39903500
N	-0.62992100	-1.26771900	1.56395900

Phot0-Zn

Zero-point correction= 0.223846 (Hartree/Particle)
Thermal correction to Energy= 0.238629
Thermal correction to Enthalpy= 0.239573
Thermal correction to Gibbs Free Energy= 0.180673
Sum of electronic and zero-point Energies= -750.206124
Sum of electronic and thermal Energies= -750.191341
Sum of electronic and thermal Enthalpies= -750.190397
Sum of electronic and thermal Free Energies= -750.249297
Zero imaginary frequencies.

C	2.82147500	1.29362100	-0.02146400
C	3.43566000	0.05951300	-0.03479500
C	1.19515200	2.86456600	0.02280000
N	1.49954600	1.55239800	0.00027900
C	2.86457700	-1.19515200	-0.02234200
N	1.55240000	-1.49954500	-0.00034500
C	1.29362100	-2.82146500	0.02189600
C	0.05951100	-3.43564600	0.03536700
C	-1.19515300	-2.86456700	0.02271700
C	-2.82147300	-1.29362000	-0.02157500
N	-1.49954600	-1.55239800	0.00020600
N	-1.55239900	1.49954500	-0.00037200
C	-2.86457600	1.19515200	-0.02241600
C	-1.29362100	2.82146500	0.02189900
C	-3.43565800	-0.05951200	-0.03490700
C	-0.05951300	3.43564500	0.03541900
H	0.07826500	-4.51689800	0.05327900
H	-4.51691900	-0.07826600	-0.05231400
H	-0.07826600	4.51689700	0.05334800
H	4.51692200	0.07826600	-0.05216700
H	2.16479400	-3.47313300	0.02693900
H	3.54599500	-2.04327900	-0.02762700
H	3.47314800	2.16479400	-0.02600200
H	2.04328000	3.54597800	0.02858900
H	-2.16479500	3.47313200	0.02692400
H	-3.54599300	2.04328000	-0.02770900
H	-3.47314600	-2.16479300	-0.02614700
H	-2.04328100	-3.54597900	0.02846800
Zn	-0.00000100	0.00000000	-0.00065200

$C_{cyc\text{-}AC}$

Zero-point correction= 0.252132 (Hartree/Particle)
Thermal correction to Energy= 0.270542
Thermal correction to Enthalpy= 0.271486
Thermal correction to Gibbs Free Energy= 0.206902
Sum of electronic and zero-point Energies= -827.456580
Sum of electronic and thermal Energies= -827.438170

Sum of electronic and thermal Enthalpies= -827.437226
Sum of electronic and thermal Free Energies= -827.501811
Zero imaginary frequencies.

C	-2.81411900	-1.24656300	-0.00804600
C	-1.25124000	-2.81025100	-0.53705700
N	-1.52366300	-1.52167600	-0.26866000
C	-2.81088500	1.25346300	-0.00757300
N	-1.51978500	1.52538500	-0.26853100
C	-1.24433000	2.81326700	-0.53707600
C	1.25126500	2.81033100	-0.53713500
C	2.81398200	1.24658000	-0.00786200
N	1.52355300	1.52171900	-0.26868100
N	1.51975800	-1.52536700	-0.26832900
C	2.81087300	-1.25341000	-0.00767800
C	1.24434800	-2.81329300	-0.53702200
C	-0.60034300	0.00052300	2.43455300
C	0.60033600	-0.00042400	2.43436200
H	-1.66840500	0.00150300	2.41393600
H	1.66839100	-0.00127500	2.41347200
H	2.10268000	-3.47945700	-0.60709800
H	3.47979600	-2.11089400	0.04304300
C	-0.00410200	-3.38544700	-0.69033200
C	-3.38357100	0.00416600	0.15548800
C	0.00415800	3.38549100	-0.69040400
C	3.38354500	-0.00411700	0.15550600
H	-0.00545800	-4.44591800	-0.90351900
H	-2.11102000	-3.47462000	-0.60695900
H	-3.48526400	-2.10232200	0.04260700
H	-4.44579700	0.00550800	0.36090400
H	-3.47977400	2.11094800	0.04369600
H	-2.10253800	3.47966100	-0.60703700
H	0.00539700	4.44597100	-0.90353700
H	2.11109600	3.47461900	-0.60705600
H	3.48507700	2.10236900	0.04305500
H	4.44578500	-0.00542200	0.36081800
Zn	0.00005000	-0.00010000	-0.12284200

$C_{cyc\text{-}ET}$

Zero-point correction= 0.276641 (Hartree/Particle)
Thermal correction to Energy= 0.295575
Thermal correction to Enthalpy= 0.296519
Thermal correction to Gibbs Free Energy= 0.229222
Sum of electronic and zero-point Energies= -828.680217
Sum of electronic and thermal Energies= -828.661283
Sum of electronic and thermal Enthalpies= -828.660339
Sum of electronic and thermal Free Energies= -828.727636
Zero imaginary frequencies.

C	-2.90095600	1.12950300	-0.34420900
C	-2.89861200	-1.13498800	-0.34815300
N	-2.17461400	-0.00200200	-0.33953700
C	-1.13509700	2.89480000	-0.24846600

N	-0.00210800	2.16994000	-0.26255400
C	1.12938300	2.89713500	-0.25253000
C	2.89863600	1.13525900	-0.34821700
C	2.90099300	-1.12920500	-0.34428800
N	2.17461400	0.00227800	-0.33960200
N	0.00220300	-2.16970400	-0.26275100
C	1.13520500	-2.89455900	-0.24844300
C	-1.12933000	-2.89692000	-0.25289900
C	-0.66609400	-0.00032200	2.39672000
C	0.66599100	-0.00027000	2.39661900
H	-1.23329800	0.92352800	2.38655200
H	1.23301500	0.92366600	2.38633600
H	-0.99828200	-3.97739100	-0.22569400
H	1.00625200	-3.97522400	-0.21968000
C	-2.42957800	-2.43287500	-0.29199200
C	-2.43449300	2.42820200	-0.28540300
C	2.42965900	2.43313300	-0.29178200
C	2.43459000	-2.42792500	-0.28539100
H	-3.19282000	-3.19954700	-0.28954000
H	-3.97919800	-1.00767700	-0.38656300
H	-3.98131700	1.00006400	-0.38189500
H	-3.19930700	3.19329000	-0.27973100
H	-1.00612600	3.97547300	-0.21998800
H	0.99826700	3.97757800	-0.22503600
H	3.19290700	3.19979800	-0.28926200
H	3.97921800	1.00792200	-0.38677800
H	3.98135100	-0.99973900	-0.38197400
H	3.19942000	-3.19299300	-0.27958700
Zn	-0.00008500	-0.00032600	-0.16859900
H	-1.23314700	-0.92424600	2.38637600
H	1.23317400	-0.92411500	2.38614800

Int1$_{cyc\text{-}AC}$

Zero-point correction= 0.257857 (Hartree/Particle)
Thermal correction to Energy= 0.273984
Thermal correction to Enthalpy= 0.274928
Thermal correction to Gibbs Free Energy= 0.214744
Sum of electronic and zero-point Energies= -827.480039
Sum of electronic and thermal Energies= -827.463912
Sum of electronic and thermal Enthalpies= -827.462968
Sum of electronic and thermal Free Energies= -827.523151
Zero imaginary frequencies.

C	1.47024900	-2.84026800	-0.28796200
C	-0.79229800	-2.74150400	-0.67688400
N	0.40372600	-2.10260700	-0.30678000
C	3.18539600	-1.13666000	0.30319400
N	2.44751700	-0.00000100	0.24510700
C	3.18539700	1.13665800	0.30319400
C	1.47025200	2.84026700	-0.28795800
C	-0.79229500	2.74150500	-0.67687800
N	0.40372800	2.10260700	-0.30677700

N	-1.56919900	0.00000200	0.43447800
C	-2.41576300	1.17228100	0.51920300
C	-2.41576100	-1.17227900	0.51920500
C	-3.79725000	-0.66076300	0.18393300
C	-3.79724000	0.66076400	0.18389000
H	-4.64616300	-1.31119300	0.02213500
H	-4.64614600	1.31119600	0.02206100
H	-2.47588700	-1.58558100	1.55106900
H	-2.47590300	1.58558600	1.55106600
C	-2.01645400	-2.34032800	-0.33736300
C	2.77678000	-2.41683100	0.07202000
C	2.77678300	2.41682900	0.07202200
C	-2.01645200	2.34032900	-0.33736200
H	-2.83140200	-2.97741000	-0.66455200
H	-0.66827900	-3.65883400	-1.24904900
H	1.36106900	-3.89409000	-0.55586000
H	3.53342800	-3.18567300	0.12413300
H	4.24573200	-0.99784700	0.51663600
H	4.24573400	0.99784300	0.51663600
H	3.53343100	3.18567100	0.12413500
H	1.36107200	3.89409000	-0.55585500
H	-0.66827600	3.65883600	-1.24904300
H	-2.83140000	2.97740700	-0.66456000
Zn	0.34115000	-0.00000100	0.09117700

Int1$_{cyc\text{-}ET}$

Zero-point correction= 0.282783 (Hartree/Particle)
Thermal correction to Energy= 0.299345
Thermal correction to Enthalpy= 0.300289
Thermal correction to Gibbs Free Energy= 0.238440
Sum of electronic and zero-point Energies= -828.682187
Sum of electronic and thermal Energies= -828.665624
Sum of electronic and thermal Enthalpies= -828.664680
Sum of electronic and thermal Free Energies= -828.726529
Zero imaginary frequencies.

C	1.53323900	-2.89363200	-0.11398900
C	-0.73837200	-2.92122400	-0.08783100
N	0.45169800	-2.17705700	-0.05515700
C	3.27441200	-1.12804000	-0.01200200
N	2.51864300	0.00000100	0.01091300
C	3.27441200	1.12804200	-0.01200500
C	1.53323700	2.89363300	-0.11399100
C	-0.73837300	2.92122400	-0.08782800
N	0.45169700	2.17705700	-0.05515700
N	-1.56847800	0.00000000	0.28690600
C	-2.47212600	1.11184300	0.42774300
C	-2.47212500	-1.11184400	0.42774200
C	-3.68475300	-0.76499100	-0.47587500
C	-3.68475200	0.76499100	-0.47587500
H	-4.61002700	-1.20113100	-0.09749000
H	-4.61002600	1.20113300	-0.09749400

H	-2.87479700	-1.14445800	1.46442600
H	-2.87479900	1.14445500	1.46442700
C	-1.97322300	-2.47595000	0.13105300
C	2.86807800	-2.42504400	-0.07108900
C	2.86807700	2.42504600	-0.07109300
C	-1.97322400	2.47595000	0.13105600
H	-2.75304700	-3.22969000	0.09140600
H	-0.59954500	-3.98250000	-0.28708300
H	1.41244000	-3.97647900	-0.19339100
H	3.64269800	-3.17695800	-0.09836400
H	4.35211700	-0.96681900	0.00170300
H	4.35211700	0.96682200	0.00169900
H	3.64269700	3.17696100	-0.09837000
H	1.41243800	3.97648000	-0.19339300
H	-0.59954600	3.98250100	-0.28707800
H	-2.75304800	3.22969000	0.09141200
Zn	0.37386400	-0.00000100	0.07673800
H	-3.50877100	1.16060400	-1.47658900
H	-3.50877500	-1.16060500	-1.47658800

Int2$_{cyc\text{-}AC}$

Zero-point correction= 0.237509 (Hartree/Particle)
Thermal correction to Energy= 0.252882
Thermal correction to Enthalpy= 0.253826
Thermal correction to Gibbs Free Energy= 0.195176
Sum of electronic and zero-point Energies= -826.382166
Sum of electronic and thermal Energies= -826.366794
Sum of electronic and thermal Enthalpies= -826.365850
Sum of electronic and thermal Free Energies= -826.424499
Zero imaginary frequencies.

C	1.45380800	-2.89611100	-0.00013200
C	-0.81504600	-2.92282600	-0.00016700
N	0.35233300	-2.17947500	-0.00010300
C	3.20379500	-1.13060300	0.00015100
N	2.45717500	0.00003800	0.00009800
C	3.20377700	1.13069800	0.00018700
C	1.45373600	2.89615300	-0.00008100
C	-0.81510400	2.92283000	-0.00016600
N	0.35228200	2.17949400	-0.00008600
N	-1.69450200	0.00000900	-0.00009000
C	-2.51776000	1.09419700	0.00006400
C	-2.51772800	-1.09420800	0.00006900
C	-3.86366200	-0.69185900	0.00027300
C	-3.86368300	0.69180900	0.00023300
H	-4.71056800	-1.35944000	0.00040200
H	-4.71060800	1.35936500	0.00033100
C	-2.07705700	-2.44282400	-0.00005400
C	2.77624600	-2.42705800	0.00002500
C	2.77619300	2.42713500	0.00008700
C	-2.07711100	2.44281900	-0.00006400
H	-2.86699100	-3.18346800	-0.00006300

H	-0.67586100	-4.00125400	-0.00027900
H	1.33255700	-3.97996400	-0.00025600
H	3.54702400	-3.18413700	0.00005500
H	4.28185600	-0.97774700	0.00029400
H	4.28184100	0.97785900	0.00033800
H	3.54694600	3.18424000	0.00014600
H	1.33246600	3.98000400	-0.00018600
H	-0.67593200	4.00126100	-0.00028300
H	-2.86705300	3.18345600	-0.00009300
Zn	0.33302900	-0.00005100	-0.00005600

Int2$_{cyc\text{-}ET}$

Zero-point correction= 0.258929 (Hartree/Particle)
Thermal correction to Energy= 0.275061
Thermal correction to Enthalpy= 0.276005
Thermal correction to Gibbs Free Energy= 0.215696
Sum of electronic and zero-point Energies= -827.536190
Sum of electronic and thermal Energies= -827.520058
Sum of electronic and thermal Enthalpies= -827.519114
Sum of electronic and thermal Free Energies= -827.579423
Zero imaginary frequencies.

C	-1.51932900	-2.89217600	0.14994900
C	0.73539900	-2.87283000	-0.10072900
N	-0.39180300	-2.15564400	0.01814800
C	-3.28523700	-1.12812300	0.13104800
N	-2.56262300	-0.00000300	0.00000100
C	-3.28524100	1.12811600	-0.13103000
C	-1.51933800	2.89217300	-0.14994300
C	0.73539100	2.87283100	0.10072900
N	-0.39181000	2.15564400	-0.01815500
N	1.69246400	0.00000200	-0.00000400
C	2.47316000	1.09887100	0.14419700
C	2.47316400	-1.09886500	-0.14419300
C	3.92468800	-0.70957300	-0.27733300
C	3.92468300	0.70958100	0.27735200
H	4.59079600	-1.39463800	0.24206300
H	4.20040600	0.71681500	1.33610100
C	2.03376300	-2.40234900	-0.20075900
C	-2.81216700	-2.42562500	0.21426700
C	-2.81217600	2.42561900	-0.21425000
C	2.03375500	2.40235300	0.20076300
H	2.80049400	-3.15816600	-0.31204000
H	0.60900500	-3.95417700	-0.11087900
H	-1.37913900	-3.97031200	0.19007200
H	-3.57385700	-3.18695200	0.31766400
H	-4.36492900	-0.99691100	0.15805900
H	-4.36493300	0.99690200	-0.15802500
H	-3.57386800	3.18694400	-0.31763300
H	-1.37915200	3.97031000	-0.19005800
H	0.60899300	3.95417800	0.11088600
H	2.80048300	3.15817200	0.31205400

Zn	-0.42640700	-0.00000100	-0.00001600
H	4.20042100	-0.71680600	-1.33607900
H	4.59079600	1.39464800	-0.24203600

TS1

Zero-point correction= 0.043295 (Hartree/Particle)
Thermal correction to Energy= 0.048162
Thermal correction to Enthalpy= 0.049106
Thermal correction to Gibbs Free Energy= 0.016290
Sum of electronic and zero-point Energies= -170.490951
Sum of electronic and thermal Energies= -170.486084
Sum of electronic and thermal Enthalpies= -170.485140
Sum of electronic and thermal Free Energies= -170.517956
One imaginary frequency (806.72i).

C	-0.79035600	-0.08747300	0.42103800
H	-0.81363700	-0.35601000	1.47446800
N	-1.64557600	-0.12889800	-0.42819600
C	0.70903900	0.51817800	0.00899400
H	0.64090200	1.59234700	-0.07297200
C	1.68339000	-0.27522700	-0.13432700
H	2.07932900	-1.26692400	-0.17835300

TS2

Zero-point correction= 0.045047 (Hartree/Particle)
Thermal correction to Energy= 0.049111
Thermal correction to Enthalpy= 0.050055
Thermal correction to Gibbs Free Energy= 0.019204
Sum of electronic and zero-point Energies= -170.490348
Sum of electronic and thermal Energies= -170.486284
Sum of electronic and thermal Enthalpies= -170.485340
Sum of electronic and thermal Free Energies= -170.516191
One imaginary frequency (89.18i).

C	0.74209900	0.11099600	0.39604100
H	0.89313400	0.26707600	1.46809200
N	1.62173400	-0.30359800	-0.35348200
C	-0.67077900	0.48965300	-0.12868800
H	-0.72022900	1.49205600	-0.53910200
C	-1.66899700	-0.32043800	-0.05057500
H	-1.93898000	-1.31522000	0.24471300

$TS1_{Zn}$

Zero-point correction= 0.045455 (Hartree/Particle)
Thermal correction to Energy= 0.051736
Thermal correction to Enthalpy= 0.052680
Thermal correction to Gibbs Free Energy= 0.015062
Sum of electronic and zero-point Energies= -238.057739
Sum of electronic and thermal Energies= -238.051458
Sum of electronic and thermal Enthalpies= -238.050514
Sum of electronic and thermal Free Energies= -238.088132

One imaginary frequency (400.98i).

C	1.51618400	-1.18562100	-0.00001500
H	2.58088900	-1.30900800	-0.00000900
N	0.45670300	-1.69463400	-0.00003500
C	1.66678000	1.07826200	0.00003800
H	2.73674800	1.09417300	0.00004700
C	0.58215000	1.67328000	0.00004300
H	0.02321100	2.58472800	0.00005900
Zn	-1.03761500	0.00323400	-0.00000800

$TS2_{Zn}$

Zero-point correction= 0.079329 (Hartree/Particle)
Thermal correction to Energy= 0.086884
Thermal correction to Enthalpy= 0.087828
Thermal correction to Gibbs Free Energy= 0.047198
Sum of electronic and zero-point Energies= -315.329015
Sum of electronic and thermal Energies= -315.321460
Sum of electronic and thermal Enthalpies= -315.320516
Sum of electronic and thermal Free Energies= -315.361146
One imaginary frequency (336.29i).

C	-0.95394600	1.51535600	0.00594500
H	-1.10431200	2.51100300	0.44678000
N	0.10030800	1.19715500	-0.61754600
C	-2.07362200	0.52637500	0.28743100
H	-3.04342600	0.96824900	0.50517400
C	-1.83528100	-0.78745800	0.33328200
H	-2.62661000	-1.47934800	0.58897200
Zn	0.13257900	-0.77319000	-0.20805300
C	2.13003500	0.96474500	0.25319100
H	2.25409600	2.01624400	0.14912700
C	2.22886400	-0.24870700	0.45922700
H	2.86442700	-1.02238100	0.83990100

$TS3_{Zn}$

Zero-point correction= 0.102374 (Hartree/Particle)
Thermal correction to Energy= 0.111666
Thermal correction to Enthalpy= 0.112610
Thermal correction to Gibbs Free Energy= 0.067662
Sum of electronic and zero-point Energies= -408.715279
Sum of electronic and thermal Energies= -408.705987
Sum of electronic and thermal Enthalpies= -408.705043
Sum of electronic and thermal Free Energies= -408.749990
One imaginary frequency (300.45i).

C	1.94720900	1.01798100	0.31839100
H	2.57023600	1.90058700	0.16192400
N	0.68115800	1.08878900	0.43912600
C	2.53322900	-0.33291600	0.18974000
H	3.60160400	-0.43215100	0.35716900
C	1.74888500	-1.34052000	-0.24392800
H	2.22724100	-2.30317500	-0.39288800

Zn	-0.20767100	-0.66098400	-0.24148000
C	-0.26008500	2.04232400	0.01383700
H	-0.03710100	3.10391800	0.11052000
C	-1.31197300	1.45590200	-0.58317300
H	-2.04395700	2.10796700	-1.06149400
C	-2.52165900	-0.19467100	0.32814300
H	-3.36103600	0.47050900	0.23626600
N	-2.04408600	-1.21832100	0.66013600

$TS4_{Zn}$

Zero-point correction= 0.135524 (Hartree/Particle)
Thermal correction to Energy= 0.146839
Thermal correction to Enthalpy= 0.147783
Thermal correction to Gibbs Free Energy= 0.098379
Sum of electronic and zero-point Energies= -486.013656
Sum of electronic and thermal Energies= -486.002341
Sum of electronic and thermal Enthalpies= -486.001397
Sum of electronic and thermal Free Energies= -486.050801
One imaginary frequency (378.33i).

C	2.41286800	0.48845000	0.21594300
H	3.23548300	1.20835100	0.24761500
N	1.19636800	0.89187800	0.29025500
C	2.69455300	-0.93477500	0.02673600
H	3.73713000	-1.23254400	0.09728800
C	1.68593900	-1.77832900	-0.27638700
H	1.96534200	-2.81928600	-0.41457800
Zn	-0.13027800	-0.76832900	-0.20992000
C	0.82995500	2.22421200	0.32029100
H	1.60681800	2.95343500	0.54645500
C	-0.42863300	2.62055600	0.06522600
H	-0.63049100	3.68356800	0.12167200
C	-1.59175000	1.76093500	-0.25694100
H	-2.54942500	2.29321700	-0.13305300
N	-1.58652600	0.55058400	-0.63239400
C	-2.80385600	-0.96201500	0.28291500
H	-3.69293500	-0.46279700	-0.02545500
C	-1.99849600	-1.75730500	0.77237700
H	-1.83596400	-2.64167400	1.35166000

$TS4_{Zn}$

Zero-point correction= 0.158575 (Hartree/Particle)
Thermal correction to Energy= 0.171498
Thermal correction to Enthalpy= 0.172442
Thermal correction to Gibbs Free Energy= 0.119520
Sum of electronic and zero-point Energies= -579.398412
Sum of electronic and thermal Energies= -579.385489
Sum of electronic and thermal Enthalpies= -579.384545
Sum of electronic and thermal Free Energies= -579.437467
One imaginary frequency (335.16i).

C	2.67600900	-0.32631700	0.01331300

H	3.69579600	0.04855500	0.14219600
N	1.67501400	0.47054100	0.18936100
C	2.46326000	-1.70135400	-0.40034400
H	3.35418400	-2.31169900	-0.51540100
C	1.20442500	-2.13428700	-0.63854200
H	1.11722100	-3.16930400	-0.95925600
Zn	-0.22129700	-0.70179900	-0.12750100
C	1.85936400	1.80470500	0.46146900
H	2.85961500	2.12541800	0.75209700
C	0.87797400	2.72453800	0.33367800
H	1.13056900	3.75661600	0.53215000
C	-0.47133800	2.46998600	-0.13178100
H	-1.08262800	3.33965600	-0.38369000
N	-0.96202200	1.29495700	-0.28252100
C	-2.23470400	1.00376100	-0.78050900
C	-2.51663600	-0.31227300	-0.81475600
H	-3.48875200	-0.60837200	-1.20799900
H	-2.86589100	1.83998000	-1.08765400
C	-2.29900600	-1.23170600	1.04070900
H	-3.34773100	-1.48710300	1.01707400
N	-1.29721500	-1.23151300	1.66974100

$TS6_{Zn}$

Zero-point correction= 0.190897 (Hartree/Particle)
Thermal correction to Energy= 0.206216
Thermal correction to Enthalpy= 0.207160
Thermal correction to Gibbs Free Energy= 0.148620
Sum of electronic and zero-point Energies= -656.664239
Sum of electronic and thermal Energies= -656.648920
Sum of electronic and thermal Enthalpies= -656.647976
Sum of electronic and thermal Free Energies= -656.706516
One imaginary frequency (425.66i).

C	2.93458900	-0.13317700	-0.20645900
H	3.93611400	0.25470100	0.00180900
N	1.90233600	0.58080100	0.13013400
C	2.77971400	-1.39847400	-0.87368200
H	3.69270500	-1.93986500	-1.10555000
C	1.52391900	-1.80916100	-1.18401900
H	1.46450900	-2.77989600	-1.67400200
Zn	0.03320200	-0.60925200	-0.26526300
C	2.08306300	1.83069000	0.64974300
H	3.08578200	2.09863000	0.98431000
C	1.09870800	2.75461200	0.70872500
H	1.35099300	3.72839000	1.10389900
C	-0.25129600	2.61245100	0.22569100
H	-0.83829700	3.53591200	0.23458600
N	-0.83244300	1.53873200	-0.19540900
C	-2.16192400	1.69879500	-0.61476700
C	-3.10489400	0.74529200	-0.62738500
H	-2.43719800	2.71181600	-0.90398900
C	-2.95749300	-0.64807400	-0.16884300

N	-1.86904100	-1.28669900	-0.15770000
H	-4.09597100	1.05836100	-0.93636600
H	-3.89468400	-1.10041800	0.19528100
C	-1.19690900	-2.30831700	1.52558600
H	-2.03414500	-2.96875300	1.53840100
C	-0.13420500	-1.75721100	1.82783300
H	0.68854400	-1.67569200	2.50578500

$TS7_{Zn}$

Zero-point correction= 0.213065 (Hartree/Particle)
Thermal correction to Energy= 0.230348
Thermal correction to Enthalpy= 0.231292
Thermal correction to Gibbs Free Energy= 0.168301
Sum of electronic and zero-point Energies= -750.041533
Sum of electronic and thermal Energies= -750.024250
Sum of electronic and thermal Enthalpies= -750.023306
Sum of electronic and thermal Free Energies= -750.086297
One imaginary frequency (242.23i).

C	2.76880400	-1.02995500	-0.73796900
H	3.86200800	-1.05837800	-0.71004300
N	2.14298000	-0.05479100	-0.15173300
C	2.03523300	-2.04164100	-1.44925900
H	2.61440200	-2.83542900	-1.91191100
C	0.68349400	-1.91342500	-1.50748600
H	0.15476900	-2.70258500	-2.03923500
Zn	-0.06878900	-0.46187900	-0.16193100
C	2.80645600	0.94674000	0.47741700
H	3.84878800	0.78635100	0.75450600
C	2.22575100	2.14599900	0.72910900
H	2.82602900	2.90705300	1.20645500
C	0.91916600	2.56341700	0.31319500
H	0.74197000	3.63808200	0.41586700
N	-0.05513800	1.85064900	-0.17017600
C	-1.17209700	2.58277900	-0.56182400
C	-2.41748300	2.11370100	-0.77146900
H	-1.00697700	3.65047300	-0.69817700
C	-2.91250000	0.77485300	-0.53788500
N	-2.16576400	-0.19375900	-0.15801200
H	-3.15295800	2.84159200	-1.08658300
H	-3.98557200	0.60843900	-0.65323400
C	-2.65135500	-1.46989400	0.16838700
C	-1.73872900	-2.33285600	0.64497500
H	-2.14203800	-3.31057700	0.92983600
H	-3.72332900	-1.62299700	0.00731000
C	-0.30301800	-1.46514100	2.29737800
H	-0.63192100	-2.32655500	2.84029900
N	0.24880300	-0.45446500	2.11069600

$TS8_{Zn}$

Zero-point correction= 0.218143 (Hartree/Particle)

Thermal correction to Energy= 0.233236
Thermal correction to Enthalpy= 0.234181
Thermal correction to Gibbs Free Energy= 0.176847
Sum of electronic and zero-point Energies= -750.096440
Sum of electronic and thermal Energies= -750.081347
Sum of electronic and thermal Enthalpies= -750.080402
Sum of electronic and thermal Free Energies= -750.137736
One imaginary frequency (112.78i).

C	2.04570900	-2.14377800	-0.52711300
H	2.95344300	-2.72734800	-0.36726200
N	2.02623100	-0.86852800	-0.12740900
C	0.91341500	-2.71087600	-1.11245400
H	0.96331000	-3.76295900	-1.37617800
C	-0.22321600	-1.92389900	-1.26672900
H	-1.12542300	-2.47878900	-1.52830200
Zn	-0.02375400	-0.17043200	-0.10708500
C	3.09049400	-0.28117800	0.38965100
H	3.98838000	-0.87755100	0.56528500
C	3.12907900	1.07818800	0.67501600
H	4.05991300	1.47983500	1.04812300
C	2.11051700	2.00510800	0.45324000
H	2.39020900	3.04852500	0.61074800
N	0.85041400	1.79343500	0.07336100
C	0.12745700	2.92369000	-0.18165600
C	-1.19870200	3.02384300	-0.47659700
H	0.69017500	3.85691400	-0.15404300
C	-2.18366500	1.99258300	-0.46148100
N	-1.95131100	0.75759100	-0.15366000
H	-1.56294100	4.01903200	-0.68885500
H	-3.21277400	2.29130900	-0.67793300
C	-3.02296800	-0.12290700	-0.06357000
C	-2.99065100	-1.29479100	0.59593800
H	-3.92237300	-1.84939600	0.62468000
H	-3.95695400	0.21605500	-0.51010000
C	-1.86464100	-1.87549400	1.36012300
H	-2.20311900	-2.61502700	2.10819800
N	-0.63193200	-1.61258200	1.24370300

$TS1_{cyc\text{-}AC}$

Zero-point correction= 0.253349 (Hartree/Particle)
Thermal correction to Energy= 0.270406
Thermal correction to Enthalpy= 0.271350
Thermal correction to Gibbs Free Energy= 0.208864
Sum of electronic and zero-point Energies= -827.402647
Sum of electronic and thermal Energies= -827.385591
Sum of electronic and thermal Enthalpies= -827.384647
Sum of electronic and thermal Free Energies= -827.447133
One imaginary frequency (628.87i).

C	1.46110500	2.88810800	0.07380400
C	-0.78841900	2.91777600	-0.18946600
N	0.37040400	2.17086200	-0.07839600

C	3.20064200	1.12686400	0.20880300
N	2.45429900	0.00002200	0.11712200
C	3.20067200	-1.12680500	0.20873800
C	1.46117200	-2.88808500	0.07375200
C	-0.78836600	-2.91779600	-0.18939200
N	0.37045000	-2.17085800	-0.07838800
N	-1.69831600	-0.00002500	-0.57487500
C	-2.48834200	-1.10395300	-0.54800700
C	-2.48835500	1.10389300	-0.54806500
C	-3.53130700	0.62135800	1.26305900
C	-3.53128600	-0.62136900	1.26307800
H	-3.78724400	1.56118900	1.70621400
H	-3.78719600	-1.56118800	1.70627300
H	-3.45791600	1.00094300	-1.03317600
H	-3.45790200	-1.00104100	-1.03313000
C	-2.02943000	2.44458200	-0.42096700
C	2.77783400	2.42402400	0.19593100
C	2.77789600	-2.42397500	0.19583000
C	-2.02939100	-2.44463100	-0.42086900
H	-2.80721600	3.19519000	-0.49189200
H	-0.65736700	3.99340200	-0.09928700
H	1.33243700	3.97066700	0.09977600
H	3.54269600	3.18052000	0.29470300
H	4.27276800	0.97059700	0.31752500
H	4.27279800	-0.97051600	0.31743900
H	3.54277900	-3.18045700	0.29455000
H	1.33252700	-3.97064600	0.09971800
H	-0.65729100	-3.99341600	-0.09918600
H	-2.80716700	-3.19525400	-0.49174400
Zn	0.31396300	0.00000200	-0.14278000

$TS1_{cyc\text{-}ET}$

Zero-point correction= 0.277981 (Hartree/Particle)
Thermal correction to Energy= 0.295227
Thermal correction to Enthalpy= 0.296171
Thermal correction to Gibbs Free Energy= 0.233111
Sum of electronic and zero-point Energies= -828.625332
Sum of electronic and thermal Energies= -828.608086
Sum of electronic and thermal Enthalpies= -828.607142
Sum of electronic and thermal Free Energies= -828.670202
One imaginary frequency (637.89i).

C	1.50216400	2.88949100	0.07813300
C	-0.74512900	2.92062500	-0.21322600
N	0.41438700	2.17300200	-0.08648000
C	3.24101900	1.12760600	0.22589600
N	2.49571500	0.00021300	0.12498300
C	3.24128900	-1.12705000	0.22564100
C	1.50275900	-2.88928700	0.07802500
C	-0.74460400	-2.92083900	-0.21277800
N	0.41480600	-2.17302400	-0.08640700
N	-1.63956600	-0.00020100	-0.58477500

C	-2.44009200	-1.10418500	-0.57770100
C	-2.44047500	1.10361400	-0.57739000
C	-3.50367500	0.69877100	1.20977900
C	-3.50420900	-0.69878700	1.21018100
H	-4.41723600	1.23727400	0.99046800
H	-4.41786500	-1.23693600	0.99045600
H	-3.37884200	0.99885600	-1.12087300
H	-3.37865500	-0.99960400	-1.12084900
C	-1.98205200	2.44758700	-0.46138600
C	2.81891800	2.42443100	0.21186400
C	2.81945100	-2.42394600	0.21150400
C	-1.98160800	-2.44800800	-0.46108300
H	-2.75921300	3.19731200	-0.54655200
H	-0.61376600	3.99642200	-0.12541400
H	1.37396500	3.97221500	0.10538800
H	3.58291100	3.18058300	0.31943000
H	4.31202100	0.97099400	0.34504300
H	4.31226700	-0.97022100	0.34469600
H	3.58361900	-3.17995100	0.31887900
H	1.37478200	-3.97203500	0.10535600
H	-0.61311000	-3.99658900	-0.12459400
H	-2.75869000	-3.19783500	-0.54605300
Zn	0.36418800	-0.00000500	-0.16306600
H	-2.81359000	1.23251800	1.85023900
H	-2.81417400	-1.23292300	1.85034300

$TS2_{cyc\text{-}AC}$

Zero-point correction= 0.251293 (Hartree/Particle)
Thermal correction to Energy= 0.266912
Thermal correction to Enthalpy= 0.267856
Thermal correction to Gibbs Free Energy= 0.208785
Sum of electronic and zero-point Energies= -827.439228
Sum of electronic and thermal Energies= -827.423609
Sum of electronic and thermal Enthalpies= -827.422665
Sum of electronic and thermal Free Energies= -827.481736
One imaginary frequency (1757.16i).

C	1.47539200	-2.90272400	0.02112700
C	-0.79572700	-2.92727100	0.14340800
N	0.38695100	-2.18692300	0.06551000
C	3.22057800	-1.13239000	-0.10920400
N	2.47382300	0.00000100	-0.07570700
C	3.22057800	1.13239400	-0.10920300
C	1.47539000	2.90272400	0.02112700
C	-0.79572800	2.92727000	0.14340800
N	0.38695000	2.18692100	0.06551100
N	-1.59615100	0.00000000	-0.05760200
C	-2.48301500	1.06127300	0.13319600
C	-2.48301500	-1.06127300	0.13319700
C	-3.77018800	-0.67187000	-0.46201300
C	-3.77018800	0.67187000	-0.46201300
H	-4.57786200	-1.35077400	-0.68793100

H	-4.57786200	1.35077400	-0.68793200
H	-2.88037400	-0.58329600	1.40390900
H	-2.88037400	0.58329700	1.40390900
C	-2.04461200	-2.44696400	0.16098800
C	2.80310800	-2.42873900	-0.06732200
C	2.80310600	2.42874100	-0.06732100
C	-2.04461200	2.44696400	0.16098800
H	-2.83791000	-3.18254800	0.21740500
H	-0.65570000	-4.00560800	0.18131700
H	1.35999900	-3.98805300	0.05155000
H	3.57546200	-3.18298100	-0.10216500
H	4.29697500	-0.97745100	-0.17262000
H	4.29697500	0.97745500	-0.17261900
H	3.57546000	3.18298400	-0.10216400
H	1.35999500	3.98805300	0.05155100
H	-0.65570000	4.00560700	0.18131700
H	-2.83791000	3.18254800	0.21740400
Zn	0.36704700	-0.00000100	0.01303000

$TS2_{cyc\text{-}ET}$

Zero-point correction= 0.273969 (Hartree/Particle)
Thermal correction to Energy= 0.290119
Thermal correction to Enthalpy= 0.291063
Thermal correction to Gibbs Free Energy= 0.231059
Sum of electronic and zero-point Energies= -828.624611
Sum of electronic and thermal Energies= -828.608461
Sum of electronic and thermal Enthalpies= -828.607517
Sum of electronic and thermal Free Energies= -828.667521
One imaginary frequency (1693.14i).

C	-1.54171200	-2.89438800	-0.07346700
C	0.72249200	-2.90561200	-0.27733900
N	-0.44583000	-2.17599900	-0.12644000
C	-3.27689500	-1.13174100	0.19284200
N	-2.53366700	0.00015800	0.13809700
C	-3.27658700	1.13218500	0.19438900
C	-1.54121900	2.89460200	-0.07216900
C	0.72274100	2.90532600	-0.27892200
N	-0.44555600	2.17598600	-0.12649900
N	1.58379800	-0.00007200	0.08261700
C	2.42917200	1.07179300	-0.11645300
C	2.42906800	-1.07215100	-0.11555400
C	3.77999400	-0.76872500	0.53546400
C	3.78040100	0.76880500	0.53424900
H	4.60616900	-1.21291500	-0.01774600
H	4.60628900	1.21154900	-0.02055300
H	2.93557200	-0.50910100	-1.41120400
H	2.93564600	0.50749200	-1.41182000
C	1.98162000	-2.42321900	-0.24644500
C	-2.85635100	-2.42680000	0.09583600
C	-2.85579300	2.42722800	0.09826200
C	1.98182800	2.42279200	-0.24852100

H	2.77119500	-3.15824900	-0.35171700
H	0.58477100	-3.97708000	-0.40475900
H	-1.42604900	-3.97608700	-0.15699100
H	-3.62572100	-3.18366600	0.14614000
H	-4.34885200	-0.98039600	0.31168700
H	-4.34851100	0.98098800	0.31371800
H	-3.62493700	3.18424100	0.14979100
H	-1.42542000	3.97629500	-0.15559400
H	0.58506500	3.97670800	-0.40711600
H	2.77143500	3.15761300	-0.35498800
Zn	-0.41957700	-0.00001000	-0.01472400
H	3.80262000	-1.16124100	1.55367300
H	3.80426400	1.16306400	1.55174700

Calculations at the CAM-B3LYP-D3(BJ)/def2-TZVP level of theory

BChl *a*

Electronic energy -1997.98813863 Eh
Zero point energy 0.61866578 Eh
Total thermal energy -1997.33010088 Eh
Total Enthalpy -1997.32915667 Eh
Final entropy term 0.10472697 Eh
Final Gibbs free energy -1997.43388364 Eh
Zero imaginary frequencies.

6	16.463371000	95.862082000	26.415658000
6	9.133419000	92.011325000	30.624364000
6	14.348721000	93.510307000	35.813373000
6	17.828703000	98.449595000	30.552917000
7	14.175109000	95.831369000	28.880111000
6	8.567353000	90.954533000	29.707662000
6	14.780425000	92.423916000	34.839835000
6	17.283463000	98.072737000	29.114045000
7	12.086455000	94.224745000	30.222249000
8	8.696697000	92.118815000	31.749385000
8	18.776557000	99.169180000	30.732533000
6	16.964192000	99.332628000	28.352208000
7	15.184243000	96.369624000	31.580547000
6	17.888369000	101.051783000	27.061753000
6	16.090486000	97.178934000	29.376876000
6	12.309718000	94.680868000	27.835793000
6	11.265394000	93.432258000	32.374511000
6	14.994135000	96.040926000	33.983821000
6	12.982171000	97.270928000	26.121641000
6	9.827094000	92.895636000	27.581725000
6	10.821018000	94.689734000	35.232595000
6	17.498986000	98.014171000	34.019042000
6	15.243883000	96.610620000	28.484363000
6	11.696858000	94.090051000	28.924871000
6	12.181326000	94.038277000	33.233941000
6	15.622811000	96.626786000	32.862176000

8	15.894471000	99.878696000	28.331269000
6	15.314658000	96.694321000	26.979062000
6	10.525043000	93.236044000	28.854263000
6	12.050994000	93.934146000	34.735924000
6	16.746139000	97.493502000	32.843436000
8	18.040054000	99.789621000	27.709137000
6	13.935094000	96.161572000	26.559773000
6	10.229178000	92.877368000	30.137524000
6	13.373287000	94.540246000	35.230850000
6	16.975516000	97.749538000	31.491443000
6	13.439707000	95.495159000	27.825113000
6	11.214457000	93.520858000	30.999012000
6	13.921258000	95.204803000	33.984371000
6	16.002022000	97.046099000	30.775491000
7	13.210941000	94.797734000	32.876151000
12	13.662085000	95.298397000	30.883333000
1	17.428738000	96.224213000	26.766486000
1	16.367355000	94.817491000	26.716399000
1	15.232947000	94.040071000	36.174784000
1	13.881193000	93.056517000	36.691601000
1	7.760124000	91.381977000	29.110832000
1	9.312170000	90.547095000	29.027381000
1	8.144254000	90.164683000	30.323078000
1	15.475561000	91.733745000	35.317238000
1	13.932741000	91.838438000	34.481823000
1	15.282391000	92.851489000	33.971266000
1	18.099840000	97.563261000	28.601223000
1	18.853486000	101.273060000	26.617401000
1	17.115948000	100.998543000	26.296382000
1	17.617656000	101.816828000	27.786825000
1	11.862536000	94.498349000	26.869557000
1	10.481279000	92.854479000	32.837110000
1	15.423663000	96.269703000	34.951174000
1	10.214331000	91.969228000	27.151831000
1	9.966895000	93.679262000	26.840493000
1	8.757700000	92.770388000	27.724574000
1	10.749964000	94.626948000	36.319068000
1	10.880521000	95.743617000	34.956095000
1	9.905441000	94.280639000	34.806529000
1	16.877918000	98.671601000	34.631008000
1	17.848783000	97.205166000	34.663069000
1	18.365045000	98.584461000	33.690468000
1	15.434149000	97.731711000	26.664295000
1	11.958930000	92.886751000	35.030419000
1	14.025038000	95.428585000	25.755184000
1	13.179092000	95.289332000	36.000757000
1	16.465532000	95.903417000	25.325453000
1	13.353434000	97.754891000	25.217792000
1	11.985222000	96.881918000	25.914903000
1	12.896805000	98.030291000	26.900134000

Phot0-Zn

Electronic energy	-2462.91401460 Eh
Zero point energy	0.22576989 Eh
Total thermal energy	-2462.67361664 Eh
Total Enthalpy	-2462.67267243 Eh
Final entropy term	0.05577018 Eh
Final Gibbs free energy	-2462.72844261 Eh

Zero imaginary frequencies.

6	2.797961000	1.284342000	-0.111885000
6	3.410310000	0.058996000	-0.174745000
6	1.186588000	2.840643000	0.108338000
7	1.483961000	1.536060000	-0.001238000
6	2.840654000	-1.186582000	-0.107725000
7	1.536078000	-1.483930000	0.001988000
6	1.284337000	-2.797943000	0.112478000
6	0.058990000	-3.410289000	0.175336000
6	-1.186591000	-2.840645000	0.108265000
6	-2.797955000	-1.284340000	-0.111997000
7	-1.483959000	-1.536059000	-0.001301000
7	-1.536080000	1.483930000	0.001967000
6	-2.840652000	1.186584000	-0.107797000
6	-1.284342000	2.797940000	0.112487000
6	-3.410304000	-0.058994000	-0.174856000
6	-0.058996000	3.410287000	0.175385000
1	0.077497000	-4.487906000	0.262988000
1	-4.487906000	-0.077498000	-0.262695000
1	-0.077505000	4.487902000	0.263054000
1	4.487916000	0.077500000	-0.262539000
1	2.155923000	-3.446824000	0.140304000
1	3.519590000	-2.035026000	-0.132741000
1	3.446823000	2.155934000	-0.139896000
1	2.035018000	3.519605000	0.133166000
1	-2.155927000	3.446822000	0.140302000
1	-3.519588000	2.035028000	-0.132824000
1	-3.446815000	-2.155933000	-0.140050000
1	-2.035023000	-3.519605000	0.133056000
30	0.000003000	0.000000000	0.000472000

Phot0-Mg

Electronic energy	-883.55302558 Eh
Zero point energy	0.22601153 Eh
Total thermal energy	-883.31297706 Eh
Total Enthalpy	-883.31203285 Eh
Final entropy term	0.05354542 Eh
Final Gibbs free energy	-883.36557827 Eh

Zero imaginary frequencies.

6	2.795069000	1.290735000	-0.200014000
6	3.395467000	0.058599000	-0.312165000

6	1.193208000	2.838132000	0.194251000
7	1.490972000	1.543273000	-0.002193000
6	2.838292000	-1.193211000	-0.193905000
7	1.543322000	-1.490946000	0.001819000
6	1.290744000	-2.794926000	0.200368000
6	0.058596000	-3.395260000	0.312687000
6	-1.193209000	-2.838133000	0.194174000
6	-2.795059000	-1.290739000	-0.200152000
7	-1.490972000	-1.543274000	-0.002262000
7	-1.543314000	1.490940000	0.001800000
6	-2.838283000	1.193207000	-0.193946000
6	-1.290744000	2.794920000	0.200358000
6	-3.395453000	-0.058599000	-0.312269000
6	-0.058601000	3.395258000	0.312719000
1	0.076874000	-4.465038000	0.471434000
1	-4.465345000	-0.076889000	-0.470242000
1	-0.076884000	4.465036000	0.471468000
1	4.465364000	0.076895000	-0.470099000
1	2.158366000	-3.448557000	0.252277000
1	3.522347000	-2.037372000	-0.239775000
1	3.448766000	2.158355000	-0.251128000
1	2.037380000	3.522119000	0.240886000
1	-2.158368000	3.448550000	0.252240000
1	-3.522337000	2.037368000	-0.239793000
1	-3.448748000	-2.158360000	-0.251343000
1	-2.037381000	-3.522125000	0.240764000
12	0.000007000	-0.000002000	-0.001098000

Phot0-Dimer

Electronic energy	-4925.86691362 Eh
Zero point energy	0.45254038 Eh
Total thermal energy	-4925.38346777 Eh
Total Enthalpy	-4925.38252356 Eh
Final entropy term	0.08819458 Eh
Final Gibbs free energy	-4925.47071814 Eh

Zero imaginary frequencies.

6	3.328298000	1.308617000	0.471930000
6	3.936945000	0.074519000	0.561409000
6	1.716013000	2.852443000	0.191080000
7	2.019468000	1.557016000	0.330420000
6	3.370799000	-1.178722000	0.452730000
7	2.071432000	-1.468817000	0.317510000
6	1.807770000	-2.773494000	0.176588000
6	0.573255000	-3.377309000	0.132225000
6	-0.671303000	-2.813906000	0.264853000
6	-2.259384000	-1.263263000	0.660379000
7	-0.963272000	-1.517676000	0.444067000
7	-1.013527000	1.509013000	0.425147000
6	-2.302229000	1.214418000	0.638200000
6	-0.763143000	2.812349000	0.239680000

6	-2.860370000	-0.032885000	0.780504000
6	0.463843000	3.416827000	0.125793000
1	0.586520000	-4.451377000	0.005905000
1	-3.927232000	-0.049866000	0.956519000
1	0.444388000	4.490568000	-0.001931000
1	5.015669000	0.093112000	0.648035000
1	2.672265000	-3.429977000	0.116890000
1	4.052656000	-2.023804000	0.488946000
1	3.980874000	2.176014000	0.517557000
1	2.559511000	3.536761000	0.145701000
1	-1.632570000	3.465611000	0.211396000
1	-2.984462000	2.060479000	0.685037000
1	-2.912693000	-2.130945000	0.722237000
1	-1.518723000	-3.495747000	0.251742000
30	0.536347000	0.019579000	0.531670000
6	6.557940000	1.431301000	3.083749000
6	7.161923000	0.202089000	2.967652000
6	4.967647000	2.977237000	3.489664000
7	5.262461000	1.682269000	3.308919000
6	6.608367000	-1.045801000	3.122366000
7	5.321153000	-1.342494000	3.342364000
6	5.075096000	-2.644643000	3.540141000
6	3.849660000	-3.252350000	3.655942000
6	2.596037000	-2.692955000	3.580935000
6	0.980538000	-1.155480000	3.284410000
7	2.288929000	-1.398886000	3.434739000
7	2.228735000	1.623723000	3.449922000
6	0.930152000	1.331261000	3.314958000
6	2.489346000	2.928627000	3.596901000
6	0.367959000	0.077029000	3.197875000
6	3.722041000	3.535999000	3.634197000
1	3.872455000	-4.324995000	3.792098000
1	-0.710663000	0.055102000	3.110638000
1	3.706293000	4.609675000	3.763619000
1	8.227655000	0.220982000	2.785064000
1	5.946531000	-3.294897000	3.575109000
1	7.292882000	-1.890215000	3.079954000
1	7.207881000	2.300868000	3.013640000
1	5.812612000	3.662240000	3.495729000
1	1.623216000	3.582135000	3.665088000
1	0.245660000	2.174489000	3.285873000
1	0.331288000	-2.025093000	3.233241000
1	1.754436000	-3.379653000	3.626038000
30	3.767517000	0.140890000	3.230063000

C-Zn-4W

Zero-point correction= 0.096011 (Hartree/Particle)
Thermal correction to Energy= 0.110312
Thermal correction to Enthalpy= 0.111257
Thermal correction to Gibbs Free Energy= 0.051879

Sum of electronic and zero-point Energies= -373.001668
Sum of electronic and thermal Energies= -372.987367
Sum of electronic and thermal Enthalpies= -372.986423
Sum of electronic and thermal Free Energies= -373.045800
Zero imaginary frequencies.

Zn -0.99858000 0.59629200 1.18582300
O 1.12639300 -0.21429000 0.38133500
H 1.04965600 -1.03654700 -0.14390100
H 1.41750700 0.49482300 -0.21379000
O 1.21829000 2.39086200 -0.91333500
H 0.26924200 2.53569400 -0.81421400
H 1.64711600 3.07279400 -0.38602800
O -2.28661800 -2.19055300 -0.61033500
H -2.82522000 -1.87015600 -1.34144400
H -2.32379800 -1.49961400 0.06901000
O 0.49016700 -2.55424700 -1.02991000
H -0.48167800 -2.53763200 -0.94295000
H 0.78149500 -3.42748600 -0.75348100

P-Zn-4W

Zero-point correction= 0.094272 (Hartree/Particle)
Thermal correction to Energy= 0.105081
Thermal correction to Enthalpy= 0.106025
Thermal correction to Gibbs Free Energy= 0.058997
Sum of electronic and zero-point Energies= -373.034835
Sum of electronic and thermal Energies= -373.024026
Sum of electronic and thermal Enthalpies= -373.023082
Sum of electronic and thermal Free Energies= -373.070110
Zero imaginary frequencies.

Zn -0.84778000 -0.23063400 -0.42888800
O 0.39496700 1.29070200 -0.62047200
H 1.90722600 0.72976500 -0.33153200
H 0.31940000 1.89612100 -1.36093700
O -1.08148900 0.82840200 1.49836000
H -0.42618500 1.43722600 1.09291800
H -0.64718500 0.37459900 2.22919300
O 0.63693500 -1.45163700 0.55810200
H 0.71183700 -2.37580500 0.30104000
H -2.00479200 -1.06146800 -1.19644400
O 2.65099600 0.12184000 -0.04041900
H 1.52284300 -1.01329400 0.43275500
H 3.23897600 0.61740500 0.53507100

$C1_{Zn}$-2W

Zero-point correction= 0.094027 (Hartree/Particle)
Thermal correction to Energy= 0.109325

Thermal correction to Enthalpy= 0.110269
Thermal correction to Gibbs Free Energy= 0.048055
Sum of electronic and zero-point Energies= -390.841142
Sum of electronic and thermal Energies= -390.825844
Sum of electronic and thermal Enthalpies= -390.824900
Sum of electronic and thermal Free Energies= -390.887113
Zero imaginary frequencies.

C 0.08344000 -1.82165000 -1.22011000
H -0.94030000 -1.77090900 -0.90591400
N 1.18152000 -1.86647400 -1.54720200
C -2.52993200 -0.69216700 0.68121800
H -1.67061000 -0.60729400 1.31420600
C -3.47362100 -0.81562900 -0.04820500
H -4.31917400 -0.91148100 -0.68619200
Zn 0.00040400 1.65308400 -0.28234800
O 2.87543100 -0.51791300 0.49176800
H 3.23397300 0.33985500 0.24371700
H 2.64917400 -0.97322800 -0.33392300
H 1.29430900 -0.67293500 1.46677600
O 0.42346300 -0.81870800 1.88390500
H 0.59938600 -1.26157400 2.71939300

Int1$_{Zn}$-2W

Zero-point correction= 0.101238 (Hartree/Particle)
Thermal correction to Energy= 0.111074
Thermal correction to Enthalpy= 0.112018
Thermal correction to Gibbs Free Energy= 0.065969
Sum of electronic and zero-point Energies= -390.882861
Sum of electronic and thermal Energies= -390.873025
Sum of electronic and thermal Enthalpies= -390.872081
Sum of electronic and thermal Free Energies= -390.918130
Zero imaginary frequencies.

C -1.28233900 1.57412300 -0.00439700
H -1.65299300 2.60969700 -0.02856500
N -0.04451700 1.31741800 0.03480200
C -2.38101400 0.52111200 -0.02809700
H -3.39841300 0.90852500 -0.04873500
C -2.10305600 -0.78786600 -0.02920300
H -2.91029900 -1.50805700 -0.04796800
Zn -0.08266800 -0.70258700 0.02443700
O 2.57790500 1.28322300 -0.10522700
H 3.08822300 1.79973400 0.52390800
H 1.60804300 1.57414800 -0.04388000
H 2.35343700 -0.27795200 -0.00111000
O 1.90817000 -1.19081100 0.04294600
H 2.41351700 -1.83391800 -0.46195400

$C2_{Zn}$-2W

Zero-point correction= 0.130154 (Hartree/Particle)
Thermal correction to Energy= 0.143716
Thermal correction to Enthalpy= 0.144660
Thermal correction to Gibbs Free Energy= 0.090087
Sum of electronic and zero-point Energies= -468.129687
Sum of electronic and thermal Energies= -468.116125
Sum of electronic and thermal Enthalpies= -468.115180
Sum of electronic and thermal Free Energies= -468.169754
Zero imaginary frequencies.

C -1.59690700 1.45367600 0.68535000
H -2.06038600 2.32956300 1.16562200
N -0.33987100 1.34073900 0.58884100
C -2.58577900 0.43310300 0.16214000
H -3.63543000 0.65866400 0.34833300
C -2.18225300 -0.66445800 -0.49510700
H -2.93324600 -1.36132300 -0.84796200
Zn -0.16446500 -0.42424400 -0.40230200
O 2.20053800 1.72449100 0.32039900
H 2.62783300 2.58309300 0.36860800
H 1.21129900 1.82421500 0.56364100
H 1.98467900 0.69188100 -0.99442000
O 1.59408400 -0.05343800 -1.53425600
H 1.53686500 0.23603700 -2.45026700
C 0.85384200 -2.23706000 1.14021400
C 1.49127500 -1.23825600 1.34176400
H 2.04325100 -0.33466500 1.49887200
H 0.30015100 -3.13578600 0.99944800

$Int2_{Zn}$-2W

Zero-point correction= 0.134231 (Hartree/Particle)
Thermal correction to Energy= 0.146768
Thermal correction to Enthalpy= 0.147713
Thermal correction to Gibbs Free Energy= 0.095310
Sum of electronic and zero-point Energies= -468.152923
Sum of electronic and thermal Energies= -468.140386
Sum of electronic and thermal Enthalpies= -468.139442
Sum of electronic and thermal Free Energies= -468.191844
Zero imaginary frequencies.

C -2.01598500 0.68872400 -0.57104400
H -2.83158200 1.37139700 -0.31451100
N -0.79184800 1.05116300 -0.52343600
C -2.29512900 -0.74872400 -0.70028500
H -3.23837300 -1.05764600 -1.14213500
C -1.43716000 -1.59002200 -0.07662600
H -1.72902800 -2.63911500 -0.09684700
Zn 0.22541800 -0.52248100 0.65550100

C -0.25547100 2.04925300 0.36366000
C 0.55705000 1.48490600 1.26641900
H 1.84736900 -2.25970600 -0.65518300
O 2.00490900 -1.44768700 -0.16122700
H 2.22402000 -0.73784200 -0.81303700
H 0.96767900 2.11322700 2.05082200
H -0.57364000 3.08470300 0.26334000
O 1.95686900 0.80843600 -1.63425900
H 0.98547300 0.80774700 -1.70265000
H 2.11440900 1.44269800 -0.91964400

TS-Zn-4W

Zero-point correction= 0.090701 (Hartree/Particle)
Thermal correction to Energy= 0.100951
Thermal correction to Enthalpy= 0.101895
Thermal correction to Gibbs Free Energy= 0.055138
Sum of electronic and zero-point Energies= -372.953674
Sum of electronic and thermal Energies= -372.943423
Sum of electronic and thermal Enthalpies= -372.942479
Sum of electronic and thermal Free Energies= -372.989236
One imaginary frequency (1101.39i)

Zn -0.55055200 -0.68173000 -0.17730900
O -0.43066500 1.41205400 -0.47142600
H 1.02843300 1.51317800 -0.07385500
H -0.55503200 1.84831900 -1.32036200
O -2.51327200 0.26539100 0.52092500
H -1.96190400 1.05938500 0.29547000
H -2.78956500 0.32257700 1.44088600
O 2.43325700 -1.05615500 0.27400200
H 2.87675900 -1.34022900 -0.53947600
H 1.23756100 -1.29836700 0.13121900
O 2.02457200 1.42341600 0.19667200
H 2.37835900 -0.01242700 0.27793400
H 2.19081800 2.00182600 0.94607500

$TS1_{Zn}$-2W

Zero-point correction= 0.093996 (Hartree/Particle)
Thermal correction to Energy= 0.106934
Thermal correction to Enthalpy= 0.107878
Thermal correction to Gibbs Free Energy= 0.053777
Sum of electronic and zero-point Energies= -390.801235
Sum of electronic and thermal Energies= -390.788297
Sum of electronic and thermal Enthalpies= -390.787353
Sum of electronic and thermal Free Energies= -390.841454
One imaginary frequency (367.55i)

C -0.58927100 2.01338200 -0.04934300

H -1.08067100 2.86339600 -0.47306100
N 0.32064400 1.48359700 0.45832900
C -2.52705100 0.69951700 -0.49956300
H -3.04417100 1.54733900 -0.89252200
C -2.41815500 -0.48473200 -0.17807200
H -2.82019400 -1.46811200 -0.06655900
Zn -0.17101600 -0.83384500 0.51933200
O 3.04498400 0.55197800 0.16087300
H 3.37086200 0.05347600 0.91633300
H 2.26660500 1.04653600 0.47341900
H 2.01272600 -0.33166300 -1.14101300
O 1.19934100 -0.67188600 -1.56454100
H 1.43306500 -1.49052500 -2.01365200

$TS2_{Zn}$-2W

Zero-point correction= 0.129984 (Hartree/Particle)
Thermal correction to Energy= 0.142595
Thermal correction to Enthalpy= 0.143539
Thermal correction to Gibbs Free Energy= 0.091836
Sum of electronic and zero-point Energies= -468.101593
Sum of electronic and thermal Energies= -468.088982
Sum of electronic and thermal Enthalpies= -468.088038
Sum of electronic and thermal Free Energies= -468.139740
One imaginary frequency (403.58i)

C -1.49109900 1.28833500 -0.77810700
H -1.91096800 2.30915200 -0.91169700
N -0.22792400 1.07757400 -0.72902800
C -2.50518600 0.20462500 -0.55231900
H -3.53302600 0.43026500 -0.87154100
C -2.15324300 -0.93721900 0.08714800
H -2.94574800 -1.66769300 0.28904600
Zn -0.14611800 -0.68255500 0.35045200
O 2.36988600 0.48871200 -1.36185800
H 2.86928000 1.01496200 -0.71846300
H 1.44936500 0.87020100 -1.31092300
H 2.03653200 -0.95350400 -0.73461900
O 1.56898300 -1.71034300 -0.24577200
H 1.51063600 -2.45659300 -0.86067400
C 0.89120300 0.86933000 1.75811400
C 0.75593000 1.87209000 1.02583900
H 0.74669200 2.86639300 0.61395400
H 1.25967900 0.51052000 2.71152000

Int2 (binding)

Zero-point correction= 0.079002 (Hartree/Particle)
Thermal correction to Energy= 0.085725
Thermal correction to Enthalpy= 0.086669
Thermal correction to Gibbs Free Energy= 0.048809

Sum of electronic and zero-point Energies= -247.742943
Sum of electronic and thermal Energies= -247.736220
Sum of electronic and thermal Enthalpies= -247.735276
Sum of electronic and thermal Free Energies= -247.773137
Zero imaginary frequencies.

C 0.50644500 -0.68260400 0.00007400
H 0.24581800 -1.74718500 0.00009100
N -0.40232000 0.21282500 -0.00000900
C 1.93722100 -0.36015300 -0.00002200
H 2.61741100 -1.21242000 -0.00001500
C 2.42519300 0.85775700 -0.00007900
H 3.38615500 1.33669300 -0.00013400
C -1.72566700 -0.23093800 -0.00001400
H -1.88725900 -1.31730500 0.00016000
C -2.76224500 0.57628700 0.00001600
H -3.83156400 0.48834100 0.00011300

Int3 (binding)

Zero-point correction= 0.101396 (Hartree/Particle)
Thermal correction to Energy= 0.109292
Thermal correction to Enthalpy= 0.110236
Thermal correction to Gibbs Free Energy= 0.068454
Sum of electronic and zero-point Energies= -341.121620
Sum of electronic and thermal Energies= -341.113725
Sum of electronic and thermal Enthalpies= -341.112780
Sum of electronic and thermal Free Energies= -341.154562
Zero imaginary frequencies.

C 1.45480600 -0.86159400 -0.00009700
H 1.57793600 -1.95104600 -0.00012700
N 0.28903000 -0.33723700 0.00002200
C 2.68066400 -0.06183200 0.00000900
H 3.61748200 -0.61906300 -0.00001400
C 2.69856200 1.25093400 0.00009900
H 3.42017200 2.04580900 0.00016700
C -0.79404500 -1.19293400 0.00004600
H -0.59565200 -2.26664700 0.00006300
C -2.06398400 -0.76187400 0.00003900
H -2.85588000 -1.49801400 0.00006600
C -2.49478300 0.64606000 0.00001200
H -3.58285700 0.80020300 0.00032100
N -1.78453300 1.67669400 -0.00018300

Int4 (binding)

Zero-point correction= 0.133854 (Hartree/Particle)
Thermal correction to Energy= 0.144007
Thermal correction to Enthalpy= 0.144951
Thermal correction to Gibbs Free Energy= 0.097437

Sum of electronic and zero-point Energies= -418.373763
Sum of electronic and thermal Energies= -418.363611
Sum of electronic and thermal Enthalpies= -418.362667
Sum of electronic and thermal Free Energies= -418.410181
Zero imaginary frequencies.

C 2.50397500 -0.35578300 0.00013400
H 3.13259500 -1.25508900 0.00051100
N 1.22846600 -0.44998800 -0.00015700
C 3.20079300 0.93109900 -0.00000800
H 4.29010000 0.88725700 0.00021800
C 2.59335200 2.09519800 -0.00037500
H 2.85428700 3.13669100 -0.00054400
C 0.70259500 -1.72484300 -0.00001900
H 1.41639200 -2.55327400 0.00010200
C -0.61026700 -2.02763100 -0.00007500
H -0.85130000 -3.08335000 -0.00006200
C -1.76610200 -1.14593000 -0.00019500
H -2.73427400 -1.66467900 -0.00067600
N -1.73653900 0.13286200 0.00025500
C -2.97140000 0.77873300 0.00001700
C -3.11288600 2.08584700 0.00048100
H -3.92316600 2.78944300 0.00048400
H -3.86848900 0.14274000 -0.00048300

Int5 (binding)

Zero-point correction= 0.157520 (Hartree/Particle)
Thermal correction to Energy= 0.170154
Thermal correction to Enthalpy= 0.171098
Thermal correction to Gibbs Free Energy= 0.117614
Sum of electronic and zero-point Energies= -511.761677
Sum of electronic and thermal Energies= -511.749043
Sum of electronic and thermal Enthalpies= -511.748099
Sum of electronic and thermal Free Energies= -511.801583
Zero imaginary frequencies.

C -1.47849500 -0.66557100 -0.47830200
H -0.84374600 -0.46561900 -1.33861400
N -2.16314500 0.25405800 0.07309900
C -1.52692000 -2.05660000 -0.00184200
H -0.82817300 -2.73834800 -0.48382300
C -2.34095200 -2.48226300 0.93249300
H -2.57181200 -3.40293300 1.43528500
C -2.11760400 1.57655700 -0.25319300
H -3.09510200 2.00866400 -0.44637900
C -1.06374700 2.42887800 -0.19838100
H -1.29452900 3.47849100 -0.32383400
C 0.30147200 2.13710700 0.15483600
H 0.88547500 2.99917600 0.50253700
N 0.87366800 0.98506300 0.08522900

C 2.17457200 0.90774900 0.53095200
C 2.93983900 -0.18687200 0.39187400
H 2.59372700 1.78375400 1.03053800
C 2.51598400 -1.42852600 -0.26692200
N 1.52078800 -1.60633200 -1.00630900
H 3.94284400 -0.17703500 0.79422800
H 3.16724000 -2.29842700 -0.10316300

Int6 (binding)

Zero-point correction= 0.197702 (Hartree/Particle)
Thermal correction to Energy= 0.210362
Thermal correction to Enthalpy= 0.211306
Thermal correction to Gibbs Free Energy= 0.158847
Sum of electronic and zero-point Energies= -589.179537
Sum of electronic and thermal Energies= -589.166878
Sum of electronic and thermal Enthalpies= -589.165934
Sum of electronic and thermal Free Energies= -589.218392
Zero imaginary frequencies.

C 0.49488000 1.75552300 -0.65337800
H -0.16497200 2.06266800 -1.47374500
N 0.05156400 1.79936000 0.53685700
C 1.87515900 1.48475000 -1.06481400
H 2.13951300 2.03201300 -1.96431300
C 2.85631500 0.75549500 -0.51853000
H 3.82641900 0.86634200 -0.99677400
C -1.22498900 2.28853800 0.76124100
H -1.22259700 3.24536800 1.27519900
C -2.41724700 1.75482500 0.43221900
H -3.29766300 2.34698200 0.64596500
C -2.62944700 0.44236900 -0.15285300
H -3.56220200 0.27685300 -0.70865700
N -1.77878100 -0.49431000 0.00992000
C -2.01056400 -1.75327900 -0.49742000
C -1.07939400 -2.71831400 -0.39500200
H -2.99051200 -1.97281000 -0.92708200
C 0.21532700 -2.46718000 0.22747700
N 0.89116900 -1.40303200 0.01856800
H -1.32484100 -3.73068300 -0.68761600
H 0.58064200 -3.22812300 0.93047200
C 2.02281100 -1.20404700 0.79447000
C 2.87890300 -0.19496800 0.58844900
H 3.76052700 -0.16086000 1.21793000
H 2.21748800 -1.91413700 1.60004900

Int7 (binding)

Zero-point correction= 0.219586 (Hartree/Particle)
Thermal correction to Energy= 0.234427

Thermal correction to Enthalpy= 0.235371
Thermal correction to Gibbs Free Energy= 0.176357
Sum of electronic and zero-point Energies= -682.524272
Sum of electronic and thermal Energies= -682.509431
Sum of electronic and thermal Enthalpies= -682.508487
Sum of electronic and thermal Free Energies= -682.567501
Zero imaginary frequencies.

C -2.52506900 -1.77513500 0.00001000
H -3.07004300 -2.73062700 0.00003200
N -1.23840900 -1.79861000 -0.00001900
C -3.38384400 -0.61395500 0.00004400
H -4.44214400 -0.84087500 0.00006800
C -3.06335800 0.69785800 0.00005300
H -3.89807900 1.40708000 0.00009900
C -0.69785500 -3.06331900 -0.00003500
H -1.40709000 -3.89802800 -0.00005000
C 0.61395400 -3.38382300 -0.00005200
H 0.84086300 -4.44212400 -0.00008600
C 1.77514400 -2.52506100 -0.00005800
H 2.73063000 -3.07004700 -0.00016300
N 1.79863100 -1.23840200 0.00006200
C 3.06334400 -0.69785500 0.00006700
C 3.38384900 0.61395300 0.00006000
H 3.89805000 -1.40709500 0.00009700
C 2.52508000 1.77513900 0.00001600
N 1.23842100 1.79861500 -0.00000200
H 4.44215000 0.84086500 0.00007300
H 3.07005900 2.73062900 -0.00002400
C 0.69785800 3.06332200 -0.00007000
C -0.61395300 3.38381900 -0.00005800
H -0.84086400 4.44212000 -0.00010200
H 1.40708900 3.89803500 -0.00014700
C -1.77514400 2.52505800 0.00000500
H -2.73062700 3.07004600 0.00007800
N -1.79864700 1.23839900 -0.00000900