**Supporting information**

# Autocatalytic Decomposition of Energetic Materials: Interplay of Theory and Thermal Analysis in the Study of 5-Amino-3,4-Dinitropyrazole Thermolysis

*Nikita V. Muravyev,[a,*] Margarita V. Gorn,[b,c] Igor N. Melnikov,[a] Konstantin A. Monogarov,[a]*

*Boris L. Korsunskii,[a] Igor L. Dalinger,[d] Alla N. Pivkina,[a] Vitaly G. Kiselev[a,b,c,*]*

[a] Semenov Federal Research Center for Chemical Physics RAS, 4 Kosygina Str., 119991 Moscow, Russia

[b] Novosibirsk State University, 1 Pirogova Str., 630090 Novosibirsk, Russia

[c] Institute of Chemical Kinetics and Combustion SB RAS, 3 Institutskaya Str., 630090 Novosibirsk, Russia

[d] Zelinsky Institute of Organic Chemistry RAS, 47 Leninsky Ave., 119991 Moscow, Russia

# Contents

## S1. The Experimental Study of the 5-ADP Thermal Decomposition

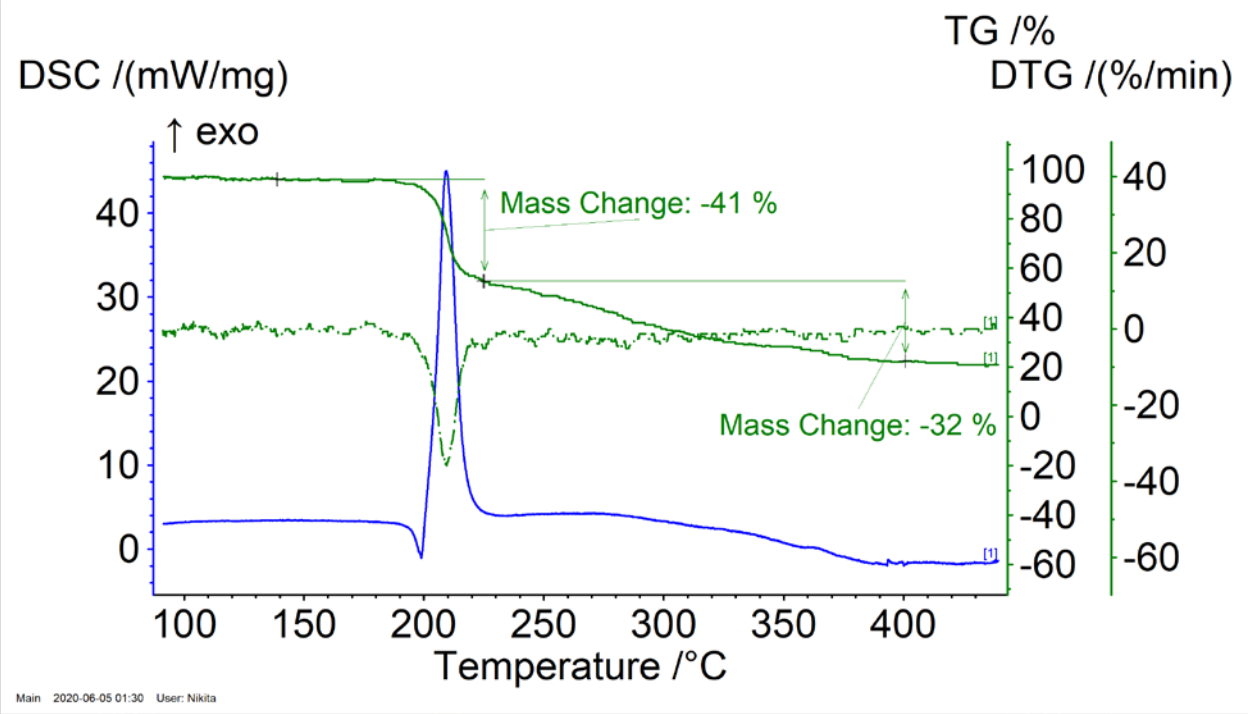


**Figure S1.** The heat flow (DSC, blue) and mass loss (TG, solid green) data along with the derivative (DTG, dashed green) for 5-ADP linearly heated at 5 K $min^{-1}$ under argon flow.

**Table S1.** The estimate of the critical mass against the sample mass used in our experiments. At the high heating rates the self-heating phenomena is possible. The methodology proposed by Farjas et al. (10.1016/j.tca.2014.05.001) is used [1].

| Heating rate, K $min^{-1}$ | Critical mass, mg | | Sample mass, mg |
|---|---|---|---|
| | Kinetic parameters by Kissinger method | Kinetic parameters from Model A | |
| 0.13 | 2520 | 53 | 0.9-1.5 |
| 1 | 172 | 3.7 | 0.6-0.7 |
| 10 | 6.8 | **0.15** | 0.15-0.23 |

https://youtu.be/Thps94lrzTI

**Video S1.** The footage of the 5-ADP sample heated at 1 K $min^{-1}$ rate in the DSC setup.

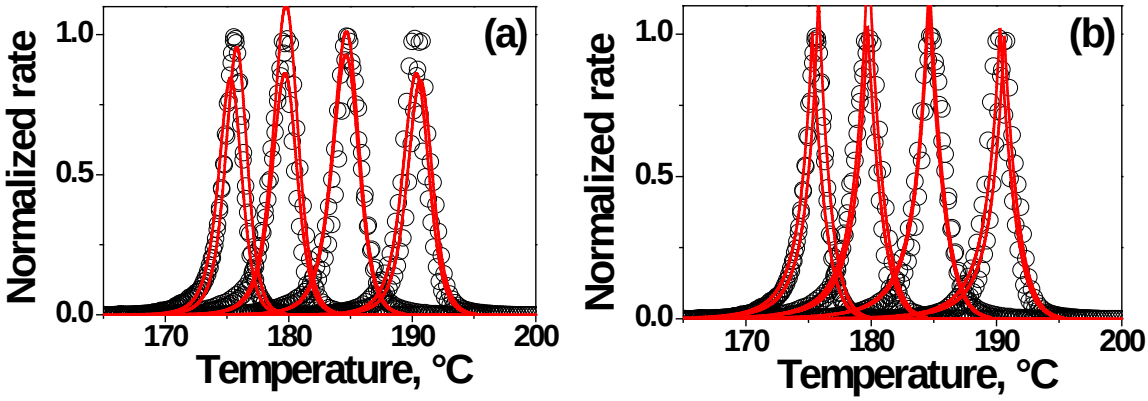


**Figure S2.** The formal kinetic fit of the low heating rate DSC data for 5-ADP. The black circles are the experimental data (rarefied for clarity) and the red curves show the fit by the extended Prout-Tompkins model (a) and the Bawn model (b). Note that the switch of the mechanism in the Bawn model results in the abrupt change of the derivative. Obviously, the residual error for the model stems from the region near the peak. That is, the model performance can be underestimated keeping in mind that the DSC setup can blur such a sharp change of the heat release. The conversion degrees dα/dt were normalized to unity for different heating rates.

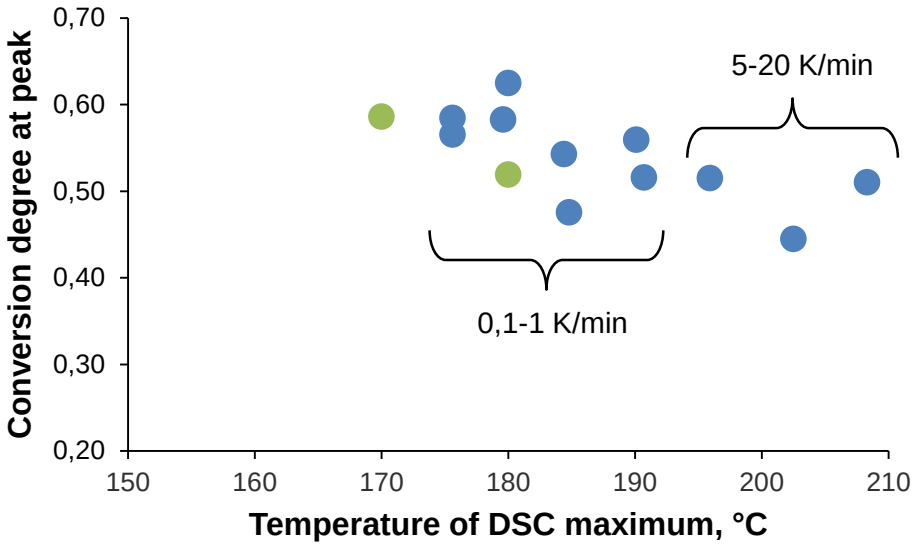


**Figure S3.** Conversion degrees at the temperatures corresponding to the maximum of the DSC peak: isothermal (green filled circles) and nonisothermal (blue) data. Note that in the experiments at high heating rates the sample mass varies from 0.15 to 0.25 mg, thus, a high sample weight uncertainty could affect the measured DSC area.

The results of isothermal pressure change studies are summarized below. The isothermal decomposition studies were carried out using the compensation manometry technique with the Bourdon-type vessels. The vessels containing a sample of 5-ADP were initially evacuated to 1 Torr. The conversion degree α for the kinetic analysis was calculated from the current pressure $P$, initial pressure $P_0$, and the final pressure $P_f$ values as $\alpha = (P - P_0) / (P_f - P_0)$. The temperatures of the isothermal runs were selected with a step of 10 K. In the long kinetic runs (viz., if the reaction was not complete in ~300 min), the final pressure values were extrapolated from the experiments at higher temperatures using the ideal gas equation of state.

Figure S4 shows the effect of m/V variation on the reaction profile. The experimental kinetics of the pressure increase at various $m/V$ along with the "model-free" isoconversional prediction based on the nonisothermal data [2,3]. As clearly seen from Figure S4a, the latter kinetics grows much faster than the experimental manometry data at the same temperature. A stronger acceleration in the non-isothermal DSC experiments (Figure 5, blue curve) is in line with the much higher $m/V$ (i.e., ~ 1 mg / 0.04 ml = 25 mg $ml^{-1}$) and a higher pressure (atmospheric in DSC vs. low pressure in manometry). All this evidence supports the autocatalytic action of the gas products during the thermal decomposition of 5-ADP.

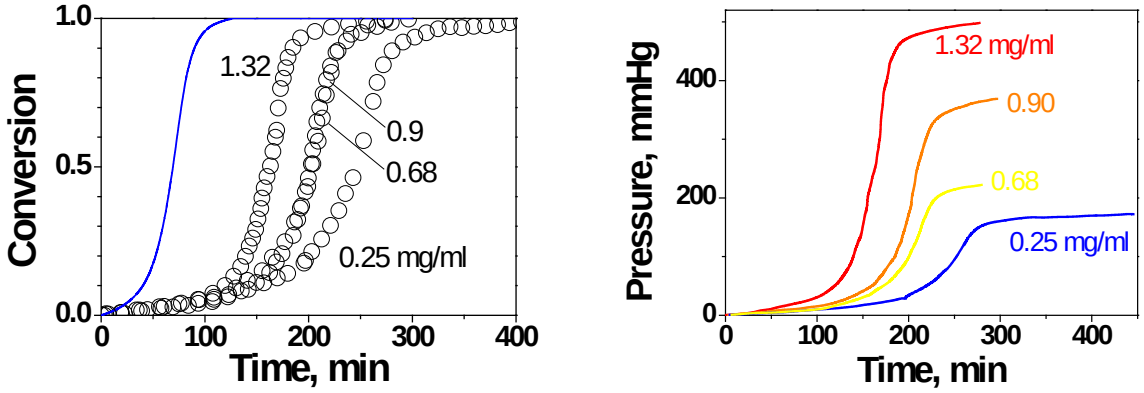


**Figure S4.** The conversion degree (a) and raw pressure (b) from the Bourdon manometry data for solid-state 5-ADP decomposition at 170°C (black circles) and the isoconversional prediction based

on the nonisothermal DSC data (blue curve). The experimental data were obtained at various *m*/*V* (indicated on the plot). The experimental points were rarefied for clarity.

Once a proper kinetic model is determined, it is instructive to compare the results of different experimental and model approaches. Indeed, very often the authors consider only the nonisothermal data and use the limited number of kinetic methods. Therefore, we compared the kinetic parameters obtained by the Kissinger method on the basis of the DSC data (Figure 2, Section 3.1) with the final results of the MD model (Table 1). While the activation energies agree well, the preexponential factors differ by the order of magnitude. This difference is caused by an oversimplified assumption of the first-order reaction model [4] in the Kissinger method. Let us discuss the reasons of Kissinger preexponential factor being incorrect for the autocatalytic reaction considered in more detail. The second derivative of the principal thermokinetic equation reads [5]:

$$\frac{d^2\alpha}{dt^2} = \left[\frac{E_a\beta}{RT_p^2} + Af'(\alpha_p)\exp\left(-\frac{E_a}{RT_p}\right)\right]\left.\frac{d\alpha}{dt}\right|_p = 0 \ , \qquad \text{(S1)}$$

where the subscript *p* denotes the position of the DSC peak, and β stands for the heating rate. Upon some rearrangement, this equation transforms to the classical Kissinger equation:

$$\ln\left(\frac{\beta}{T_{p,i}^2}\right) = \ln\left[-\frac{AR}{E_a}f'(\alpha_p)\right] - \frac{E_a}{RT_{p,i}} \ . \qquad \text{(S2)}$$

Note that in the case of the first-order reaction $f'(\alpha) = -1$ and the use of the Kissinger equation is strictly valid. In our case, assuming for simplicity the model A with both exponents equal to 1, $q = 1$ and the average $\alpha_p = 0.55$, we obtain $f'(\alpha_p) \approx 1 - 2\,\alpha_p = 0.1$. Therefore, the invalid assumption of the first-order reaction results in the difference of the preexponential factors (i.e., $A\,f'(\alpha)$) in the order of magnitude.

In this connection, it is worth emphasizing that the extrapolation of such simple kinetics outside the particular experimental temperature range often performed to assess the thermal stability of energetic materials [6,7] might lead to dubious results.

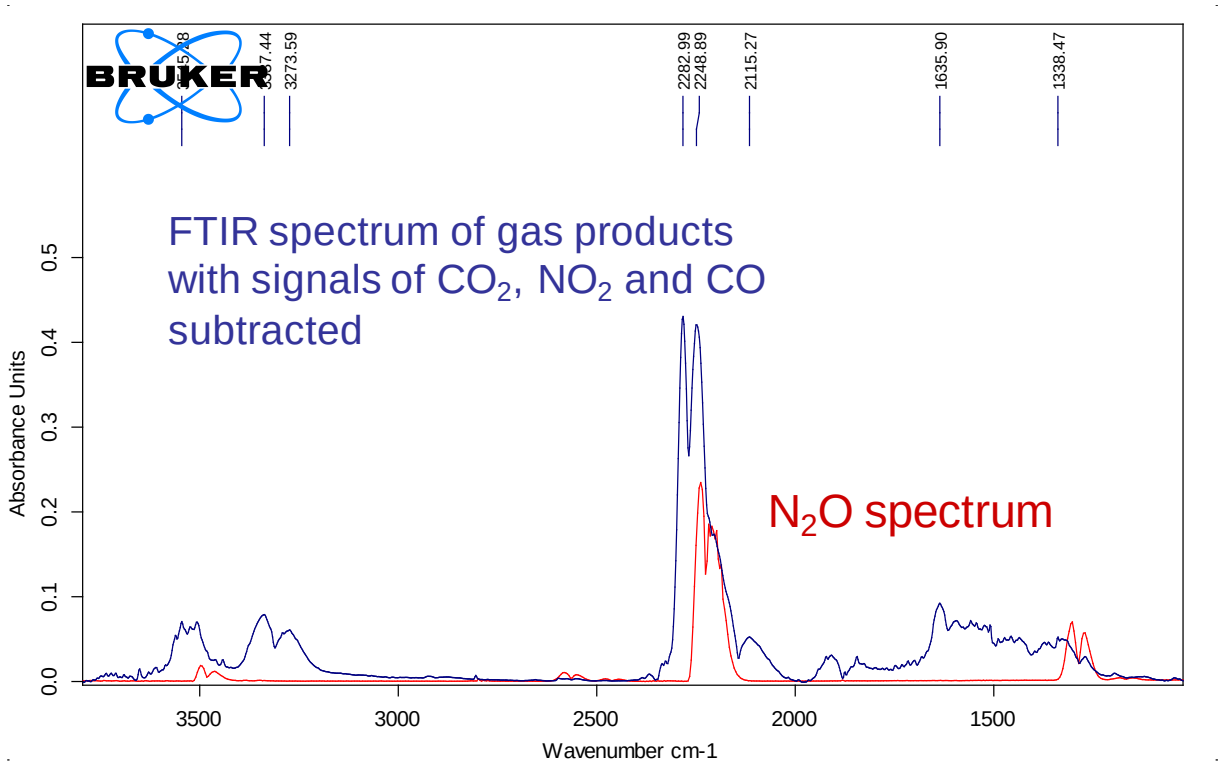


**Figure S5.** The FTIR spectrum of the non-identified decomposition products of 5-ADP in comparison with the $N_2O$ signal. The bands at 2280, 2250, and 3550 $cm^{-1}$ belong to the HNCO reaction product in accordance with the literature data [3,8,9].

## S2. The Details of the Computational Study

### The kinetic parameters of 5-ADP decomposition

**Table S2.** The Arrhenius parameters (Eq. (2)) of the elementary rate constants for all channels in the temperature range 300-750 K calculated using the transition state theory (Eq. (1)).

| Reaction | $\Delta^{\neq}H^0$, kJ mol$^{-1}$ | *log (A / s$^{-1}$)* | $E_a$, kJ mol$^{-1}$ |
|---|---|---|---|
| 5-ADP (**1**) → **4**($k_4$) | 198.3 | 13.5 | 201.7 |
| **4** → **1** ($k_{-4}$) | 195.8 | 14.0 | 199.2 |
| **4** → **6** ($k_6$) | 214.2 | 13.3 | 217.1 |
| **6** → **7** ($k_{7n}$) | 80.3 | 12.7 | 83.7 |
| **7** → •**R7** + •$NO_2$ ($k_{7m}$) | (123.0)[b] | 18.0[c] | 124.7[d] |
| **6** → •**R7** + •$NO_2$ ($k_{7r}$) | (103.3)[b] | 18.0[c] | 105.4[d] |
| 5-ADP (**1**) → •**R7** + •$NO_2$ ($k_{eff,}$ TS6) | 216.7 | 12.9 | 220.1 |

[a] The reaction pathways and numeration are in accordance with Figures 8–9 and Schemes 1. [b] In the case of barrierless radical decomposition reactions, the enthalpies ($\Delta_r H^0$) of reaction at 298 K are listed in parentheses. [c] The higher estimate on the basis of experimental data [10,11]. [d] Estimated using the transition state theory expression $E_a = \Delta_r H^{0K} + RT$ ,T=525K

**The secondary reactions of 5-ADP decomposition**

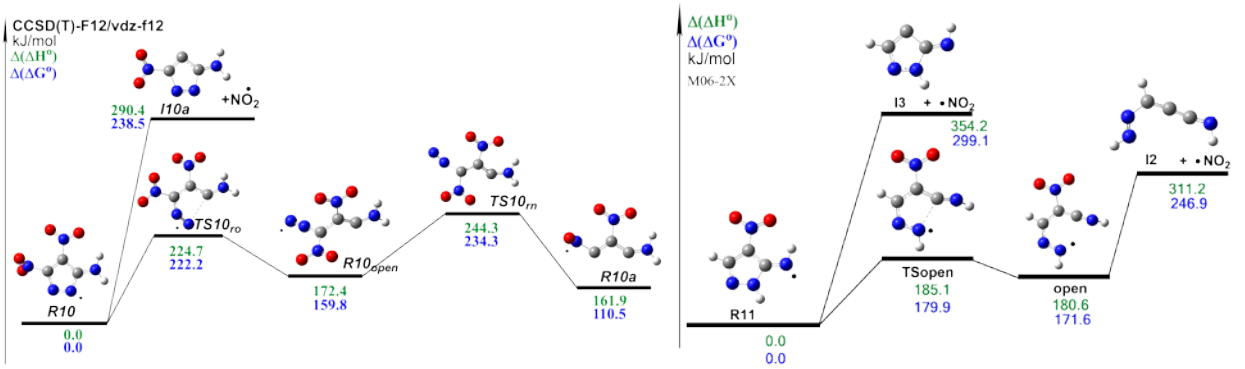


**Figure S6.** The stationary points on the PES corresponding to the most favorable reactions of thermal decomposition of •**R10** and •**R11**. The relative thermodynamical potentials are calculated from the corresponding values for •**R10** and •**R11** respectively. All values are calculated at the CCSD(T)-F12b/VDZ-F12 // M06-2X/6-311++G(2df,p) level of theory and are given in kJ·mol$^{-1}$.

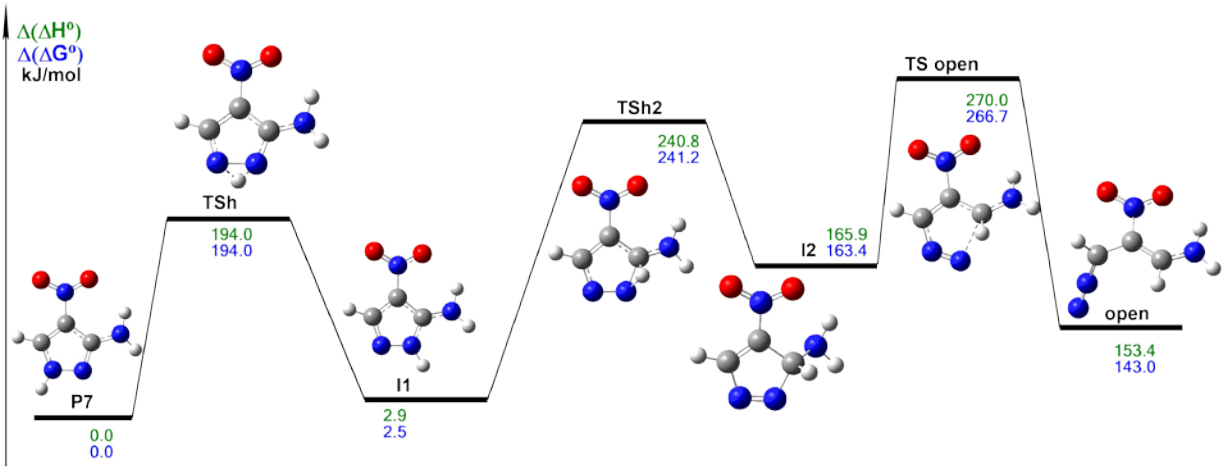


**Figure S7.** The stationary points on the PES corresponding to the most favorable reaction of thermal decomposition of **P7**. The relative thermodynamical potentials are calculated from the corresponding values for **P7**. All values are calculated at the CCSD(T)-F12b/VDZ-F12 // M06-2X/6-311++G(2df,p) level of theory and are given in kJ·mol$^{-1}$.

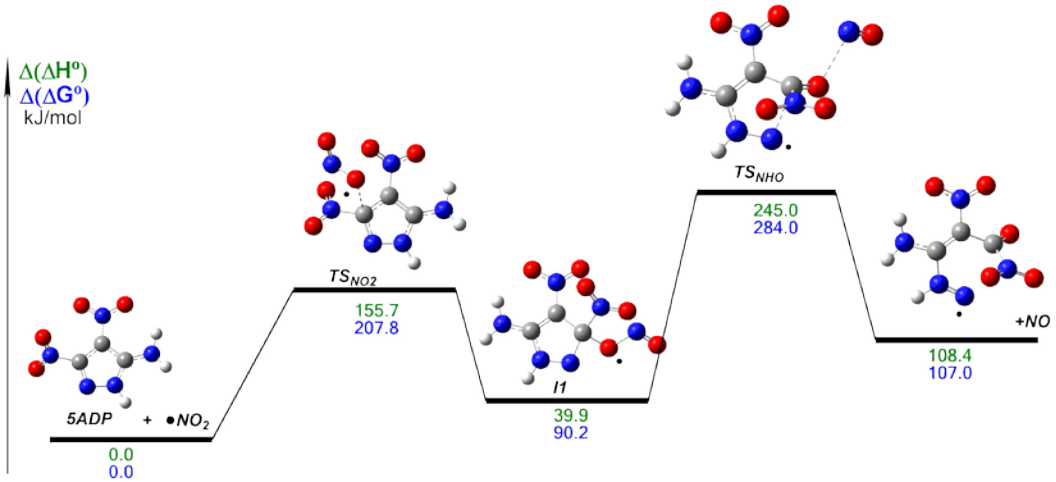


**Figure S8.** The stationary points on the PES corresponding to the addition reactions of 5-ADP with •$NO_2$ radical. The relative thermodynamical potentials are calculated from the corresponding values for the reactants. All values are calculated at the DLPNO-CCSD(T)/aug-cc-pVQZ// M06-2X/6-311++G(2df,p) level of theory and are given in kJ·mol$^{-1}$.

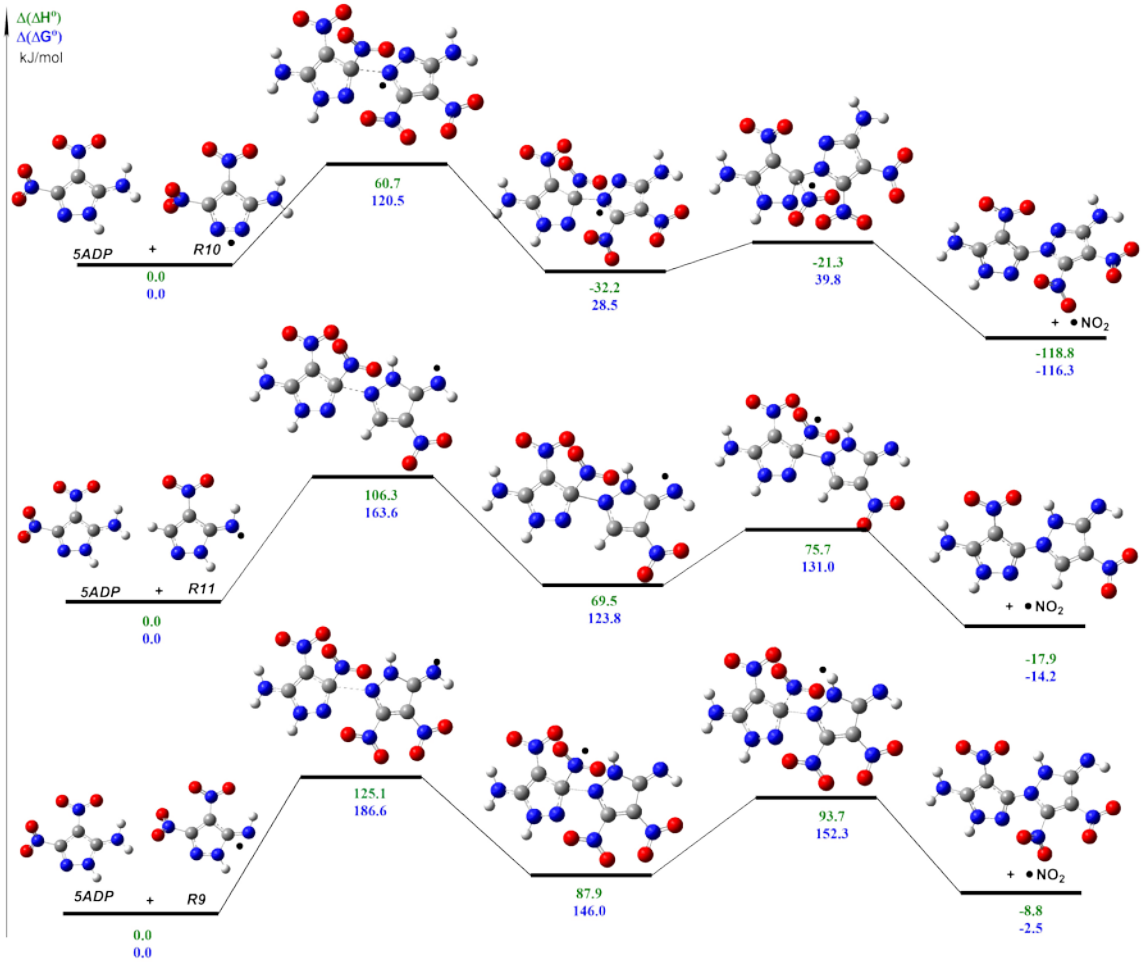


**Figure S9.** The stationary points on the PES corresponding to the secondary reactions of the addition of primary radicals **•R9**, **•R10**, and **•R11** to 5-ADP. The relative thermodynamical

potentials are calculated from the corresponding values for the reactants. All values are calculated at the DLPNO-CCSD(T)/aug-cc-pVQZ// M06-2X/6-311++G(2df,p) level of theory and are given in kJ·mol$^{-1}$.

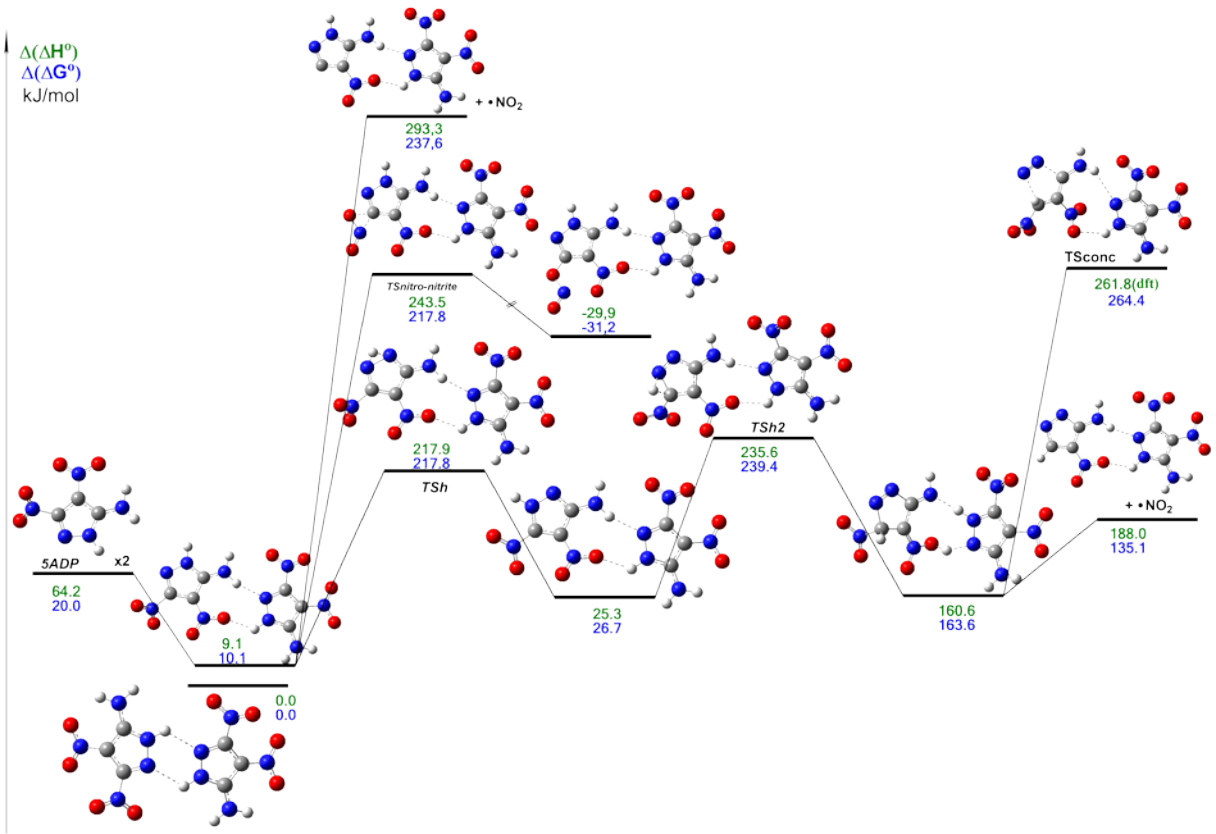


**Figure S10.** The stationary points on the PES corresponding to the decomposition reactions of 5-ADP in dimers. The relative thermodynamical potentials are calculated from the corresponding values for the most favorable dimer **D1**. All values are calculated at the DLPNO-CCSD(T)/aug-cc-pVQZ // M06-2X/6-311++G(2df,p) level of theory and are given in kJ·mol$^{-1}$.

## PCM calculations

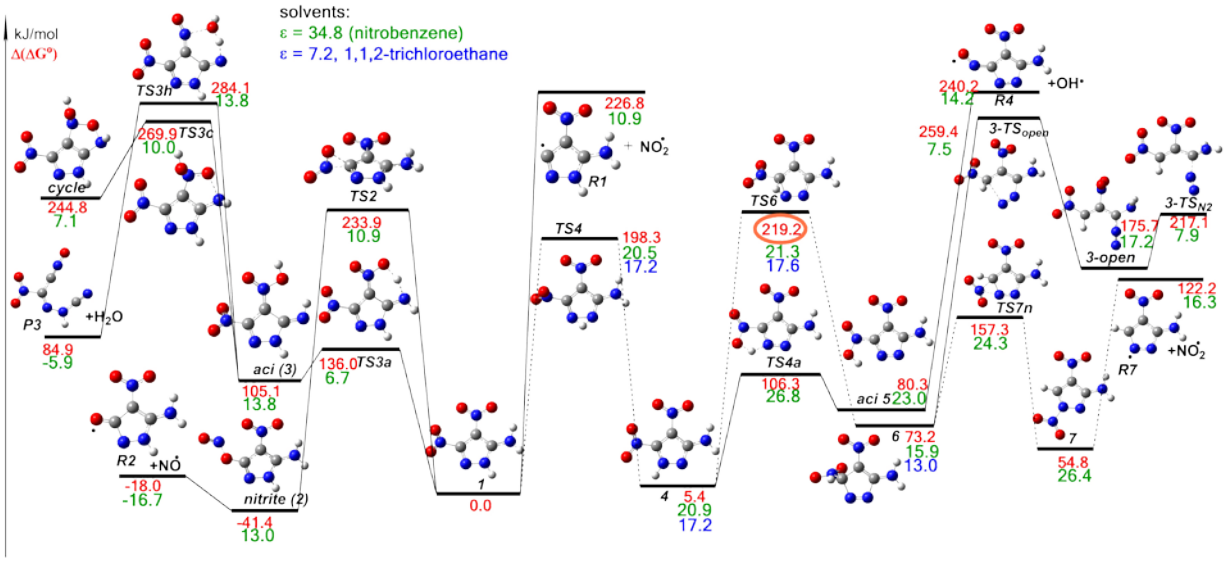


**Figure S11.** The relative Gibbs free energies at 298K and relative solvation energies in nitrobenzene ε=34.8 ( $\Delta(\Delta G^0_{solv})$ green numbers) and in 1,1,2-trichloroethanee ε=7.2 ( $\Delta(\Delta G^0_{solv})$ , blue numbers) of the stationary points on the PES corresponding to thermal decomposition of 5-ADP. The relative free energies of solvation were calculated using the PCM model at the M06-2X/6-311++G(2df,p) level of theory. All energy values are given in kJ $mol^{-1}$.

## References


[1] D. Sanchez-Rodriguez, H. Eloussifi, J. Farjas, P. Roura, M. Dammak, Thermal gradients in thermal analysis experiments: Criterions to prevent inaccuracies when determining sample temperature and kinetic parameters. *Thermochim. Acta,* 589, 37-46, **2014**.

[2] S. Vyazovkin, A.K. Burnham, J.M. Criado, L.A. Perez-Maqueda, C. Popescu, N. Sbirrazzuoli, ICTAC Kinetics Committee recommendations for performing kinetic computations on thermal analysis data. *Thermochim. Acta,* 520, 1-19, **2011**.

[3] H.E. Kissinger, Reaction Kinetics in Differential Thermal Analysis. *Analytical Chemistry*, 29, 1702–1706, **1957**.

[4] T.B. Brill, Multiphase Chemistry Considerations at the Surface of Burning Nitramine Monopropellants. *J. Propul. Power,* 11, 740-751, **1995**.

[5] H.J. Werner, P.J. Knowles, G. Knizia, F.R. Manby, M. Schutz, Molpro: a general-purpose quantum chemistry program package. *Wires Comput. Mol. Sci.*, 2, 242-253, **2012**.

[6] N.V. Muravyev, A.A. Bragin, K.A. Monogarov, A.S. Nikiforova, A.A. Korlyukov, I.V. Fomenkov, N.I. Shishov, A.N. Pivkina, 5-Amino-3,4-dinitropyrazole as a Promising Energetic Material. *Propell. Explos. Pyrot.*, 41, 999-1005, **2016**.

[7] V.P. Sinditskii, S.P. Smirnov, V.Y. Egorshev, A.N. Chernyi, T.K. Shkineva, N.V. Palysaeva, K.Y. Suponitsky, I.L. Dalinger, Thermal decomposition peculiarities and combustion behavior of nitropyrazoles. *Thermochim. Acta,* 651, 83-99, **2017**.

[8] F.I. Dubovitskii, G.B. Manelis, A.G. Merzhanov, Formal Kinetic Model of Thermal Decomposition of Explosives in Liquid State. *Trans. Acad. Nauk SSSR Dokl.*, 121, 668–670, **1958**.

[9] A. E698-05, Standard Test Method for Arrhenius Kinetic Constants for Thermally Unstable Materials. ASTM International: West Conshohocken, PA, 2005.

[10] G.M. Nazin, G.B. Manelis, Thermal-Decomposition of Aliphatic Nitrocompounds. *Russ. Chem. Rev.*, 63, 327-337, **1994**.

[11] T.B. Brill, K.J. James, Kinetics and Mechanisms of Thermal-Decomposition of Nitroaromatic Explosives. *Chem. Rev.*, 93, 2667-2692, **1993**.

## Raw computational data

**5ADP**

Zero-point correction= 0.094738 (Hartree/Particle)
Thermal correction to Energy= 0.104892 (Hartree/Particle)
Thermal correction to Enthalpy= 0.105836 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.058109 (Hartree/Particle)

Electronic energy:
M06-2X=-690.529603
CCSD(T)-F12=-689.72417047
T1=0.01798398
DLPNO-CCSD(T)=-689.755655011197

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.497718 | 0.124637 | 0.007307 |
| 2 | 7 | 0 | -0.527228 | -1.881736 | 0.026791 |
| 3 | 7 | 0 | 0.823388 | -2.021604 | 0.043944 |
| 4 | 7 | 0 | 2.830380 | -0.729897 | -0.018388 |
| 5 | 7 | 0 | -2.079388 | -0.082818 | 0.069651 |
| 6 | 6 | 0 | -0.712133 | -0.600552 | 0.001069 |
| 7 | 6 | 0 | 1.491292 | -0.851699 | 0.030066 |
| 8 | 8 | 0 | -2.310492 | 0.666365 | 0.985543 |
| 9 | 8 | 0 | -2.850358 | -0.466437 | -0.772236 |
| 10 | 1 | 0 | 1.210480 | -2.951337 | 0.051392 |
| 11 | 7 | 0 | 0.727195 | 1.516852 | -0.103784 |
| 12 | 8 | 0 | -0.214453 | 2.237261 | -0.329166 |
| 13 | 8 | 0 | 1.887399 | 1.891021 | 0.024014 |
| 14 | 1 | 0 | 3.417748 | -1.515767 | 0.201462 |
| 15 | 1 | 0 | 3.193306 | 0.201532 | 0.123759 |

**4**

Zero-point correction= 0.095173 (Hartree/Particle)
Thermal correction to Energy= 0.10495 (Hartree/Particle)
Thermal correction to Enthalpy= 0.105894 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.059206 (Hartree/Particle)

Electronic energy:
M06-2X=-690.527349
CCSD(T)-F12=-689.72325773
T1=0.01759091

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.522215 | 0.094229 | 0.007617 |
| 2 | 7 | 0 | -0.625027 | -1.752599 | -0.028602 |
| 3 | 7 | 0 | 0.650719 | -2.154814 | -0.004253 |
| 4 | 7 | 0 | 2.729799 | -1.059915 | -0.036288 |
| 5 | 7 | 0 | -2.089022 | 0.127492 | 0.079692 |
| 6 | 6 | 0 | -0.756702 | -0.432456 | -0.017362 |
| 7 | 6 | 0 | 1.375024 | -1.039552 | 0.014202 |
| 8 | 8 | 0 | -2.197736 | 1.247888 | 0.495636 |
| 9 | 8 | 0 | -2.990656 | -0.623025 | -0.238712 |
| 10 | 1 | 0 | -1.386548 | -2.417126 | -0.027157 |
| 11 | 7 | 0 | 0.954013 | 1.454117 | -0.081876 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 8 | 0 | 0.187905 | 2.278257 | -0.513273 |
| 13 | 8 | 0 | 2.103471 | 1.669103 | 0.267179 |
| 14 | 1 | 0 | 3.166321 | -1.954655 | 0.116605 |
| 15 | 1 | 0 | 3.209767 | -0.239292 | 0.296457 |

**TS6**

Zero-point correction= 0.089191 (Hartree/Particle)
Thermal correction to Energy= 0.098979 (Hartree/Particle)
Thermal correction to Enthalpy= 0.099923 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.053122 (Hartree/Particle)

Electronic energy:
M06-2X=-690.4389965
CCSD(T)-F12=-689.63572594
T1=0.01910346

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.526023 | 0.106869 | 0.039373 |
| 2 | 7 | 0 | -0.531788 | -1.903580 | 0.037242 |
| 3 | 7 | 0 | 0.763472 | -2.133575 | -0.007485 |
| 4 | 7 | 0 | 2.764412 | -0.911810 | -0.143329 |
| 5 | 7 | 0 | -2.063373 | 0.013107 | -0.137035 |
| 6 | 6 | 0 | -0.718369 | -0.512008 | 0.152659 |
| 7 | 6 | 0 | 1.434708 | -0.952667 | -0.062162 |
| 8 | 8 | 0 | -2.960714 | -0.398673 | 0.555091 |
| 9 | 8 | 0 | -2.137506 | 0.774135 | -1.063289 |
| 10 | 1 | 0 | -0.897311 | -1.335509 | 1.153420 |
| 11 | 7 | 0 | 0.829123 | 1.489446 | 0.154981 |
| 12 | 8 | 0 | -0.060049 | 2.240093 | 0.480873 |
| 13 | 8 | 0 | 1.983991 | 1.810626 | -0.075830 |
| 14 | 1 | 0 | 3.276251 | -1.776959 | -0.182876 |
| 15 | 1 | 0 | 3.228192 | -0.025279 | -0.255142 |

**6**

Zero-point correction= 0.093807 (Hartree/Particle)
Thermal correction to Energy= 0.103708 (Hartree/Particle)
Thermal correction to Enthalpy= 0.104652 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.057243 (Hartree/Particle)

Electronic energy:
M06-2X=-690.4955817
CCSD(T)-F12=-689.69544105
T1=0.0191454

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.525693 | 0.109235 | -0.281036 |
| 2 | 7 | 0 | 0.774115 | -1.780584 | -0.564291 |
| 3 | 7 | 0 | -0.344883 | -2.151733 | -0.200012 |
| 4 | 7 | 0 | -2.453930 | -1.241573 | 0.413416 |
| 5 | 7 | 0 | 1.928440 | 0.125445 | 0.294914 |
| 6 | 6 | 0 | 0.825530 | -0.297356 | -0.674867 |
| 7 | 6 | 0 | -1.219205 | -1.014805 | 0.008855 |
| 8 | 8 | 0 | 3.012491 | 0.304317 | -0.189942 |
| 9 | 8 | 0 | 1.622992 | 0.205548 | 1.455560 |
| 10 | 1 | 0 | 1.181550 | -0.010613 | -1.663450 |
| 11 | 7 | 0 | -1.003423 | 1.425060 | -0.183615 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 8 | 0 | -0.234925 | 2.326130 | -0.449593 |
| 13 | 8 | 0 | -2.168782 | 1.568503 | 0.166740 |
| 14 | 1 | 0 | -2.758267 | -2.188507 | 0.572396 |
| 15 | 1 | 0 | -3.063525 | -0.455612 | 0.588326 |

**R7**

Zero-point correction= 0.078941 (Hartree/Particle)
Thermal correction to Energy= 0.08594 (Hartree/Particle)
Thermal correction to Enthalpy= 0.086884 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.046569 (Hartree/Particle)

Electronic energy:
M06-2X=-485.3875862
CCSD(T)-F12=-484.79593582
T1=0.02084069
DLPNO-CCSD(T)=-484.816966593164

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.118152 | -0.333274 | -0.000374 |
| 2 | 7 | 0 | 1.918563 | -1.263765 | 0.000292 |
| 3 | 7 | 0 | 2.125433 | 0.016905 | 0.000046 |
| 4 | 7 | 0 | 0.804028 | 1.967946 | -0.000006 |
| 5 | 6 | 0 | 0.559406 | -1.520083 | -0.000241 |
| 6 | 6 | 0 | 0.901746 | 0.652794 | -0.000060 |
| 7 | 1 | 0 | 0.175016 | -2.527347 | -0.000362 |
| 8 | 7 | 0 | -1.517415 | -0.089471 | -0.000049 |
| 9 | 8 | 0 | -2.267944 | -1.035541 | 0.000240 |
| 10 | 8 | 0 | -1.867534 | 1.084635 | 0.000023 |
| 11 | 1 | 0 | 1.648739 | 2.520617 | 0.000324 |
| 12 | 1 | 0 | -0.112199 | 2.396048 | -0.000007 |

**$NO_2$**

Zero-point correction= 0.009192 (Hartree/Particle)
Thermal correction to Energy= 0.012114 (Hartree/Particle)
Thermal correction to Enthalpy= 0.013058 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= -0.014772 (Hartree/Particle)

Electronic energy:
M06-2X=-205.0652724
CCSD(T)-F12=-204.85534916
T1=0.02412041
DLPNO-CCSD(T)=-204.864844294672

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 0.000000 | 0.313924 | 0.000000 |
| 2 | 8 | 0 | 1.090165 | -0.136679 | 0.000000 |
| 3 | 8 | 0 | -1.090165 | -0.138005 | 0.000000 |

**TS7n**

Zero-point correction= 0.091854 (Hartree/Particle)
Thermal correction to Energy= 0.101416 (Hartree/Particle)
Thermal correction to Enthalpy= 0.10236 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.056249 (Hartree/Particle)

Electronic energy:
M06-2X=-690.4595501
CCSD(T)-F12=-689.66246794
T1=0.02311431

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.702915 | -0.162643 | -0.350513 |
| 2 | 7 | 0 | -1.270667 | 0.575406 | -1.124267 |
| 3 | 7 | 0 | -0.656947 | 1.624209 | -0.663968 |
| 4 | 7 | 0 | 1.413142 | 2.102815 | 0.334004 |
| 5 | 7 | 0 | -2.098173 | -0.355501 | 0.431994 |
| 6 | 6 | 0 | -0.474586 | -0.571991 | -0.907976 |
| 7 | 6 | 0 | 0.559085 | 1.237596 | -0.177533 |
| 8 | 8 | 0 | -2.970301 | -1.098954 | 0.157145 |
| 9 | 8 | 0 | -1.777902 | 0.206685 | 1.413608 |
| 10 | 1 | 0 | -0.781752 | -1.541080 | -1.268656 |
| 11 | 7 | 0 | 1.815557 | -0.956674 | 0.038772 |
| 12 | 8 | 0 | 1.761272 | -2.149522 | -0.149632 |
| 13 | 8 | 0 | 2.760544 | -0.365409 | 0.540002 |
| 14 | 1 | 0 | 1.140682 | 3.069943 | 0.409521 |
| 15 | 1 | 0 | 2.307293 | 1.779179 | 0.670538 |

**7**
Zero-point correction= 0.094166 (Hartree/Particle)
Thermal correction to Energy= 0.104021 (Hartree/Particle)
Thermal correction to Enthalpy= 0.104966 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.058064 (Hartree/Particle)

Electronic energy:
M06-2X=-690.5100425
CCSD(T)-F12=-689.7032395
T1=0.01897925

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.940384 | -0.203596 | -0.010788 |
| 2 | 7 | 0 | 1.181714 | 0.010236 | -0.004380 |
| 3 | 7 | 0 | 0.746828 | 1.288537 | -0.003528 |
| 4 | 7 | 0 | -1.388042 | 2.250208 | -0.053206 |
| 5 | 7 | 0 | 2.572763 | -0.266589 | 0.005704 |
| 6 | 6 | 0 | 0.218458 | -0.927059 | -0.007284 |
| 7 | 6 | 0 | -0.567784 | 1.181116 | -0.010865 |
| 8 | 8 | 0 | 2.845567 | -1.437980 | 0.007221 |
| 9 | 8 | 0 | 3.294277 | 0.678680 | 0.011398 |
| 10 | 1 | 0 | 0.414645 | -1.985221 | -0.004508 |
| 11 | 7 | 0 | -2.257990 | -0.749057 | 0.003053 |
| 12 | 8 | 0 | -2.374094 | -1.952782 | -0.021496 |
| 13 | 8 | 0 | -3.179121 | 0.048122 | 0.043232 |
| 14 | 1 | 0 | -0.987376 | 3.158892 | 0.107624 |
| 15 | 1 | 0 | -2.368956 | 2.101910 | 0.114167 |

**TS4**
Zero-point correction= 0.088771 (Hartree/Particle)
Thermal correction to Energy= 0.098779 (Hartree/Particle)
Thermal correction to Enthalpy= 0.099723 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.052023 (Hartree/Particle)

Electronic energy:
M06-2X=-690.4458478
CCSD(T)-F12=-689.64255779
T1=0.0186749

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.502184 | 0.116769 | -0.021003 |
| 2 | 7 | 0 | -0.438381 | -1.911896 | -0.095272 |
| 3 | 7 | 0 | 1.011273 | -2.065070 | -0.066596 |
| 4 | 7 | 0 | 2.861955 | -0.625616 | 0.105774 |
| 5 | 7 | 0 | -2.046927 | -0.130073 | 0.078764 |
| 6 | 6 | 0 | -0.667733 | -0.616841 | -0.026470 |
| 7 | 6 | 0 | 1.540640 | -0.831492 | 0.015996 |
| 8 | 8 | 0 | -2.331674 | 0.404741 | 1.120644 |
| 9 | 8 | 0 | -2.762751 | -0.328892 | -0.866591 |
| 10 | 1 | 0 | 0.171423 | -2.464792 | 0.798442 |
| 11 | 7 | 0 | 0.645228 | 1.534570 | -0.099366 |
| 12 | 8 | 0 | -0.351047 | 2.190803 | -0.281570 |
| 13 | 8 | 0 | 1.777365 | 1.973260 | 0.016485 |
| 14 | 1 | 0 | 3.485443 | -1.398799 | -0.052450 |
| 15 | 1 | 0 | 3.205403 | 0.320281 | 0.067996 |

**TS4a**

Zero-point correction= 0.089718 (Hartree/Particle)
Thermal correction to Energy= 0.099373 (Hartree/Particle)
Thermal correction to Enthalpy= 0.100317 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.053842 (Hartree/Particle)

Electronic energy:
M06-2X=-6.0
CCSD(T)-F12=-689.67946047
T1=0.01832319

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.597435 | 0.110944 | 0.006213 |
| 2 | 7 | 0 | 0.833947 | -1.580684 | -0.003810 |
| 3 | 7 | 0 | -0.350315 | -2.143615 | -0.002856 |
| 4 | 7 | 0 | -2.577647 | -1.381279 | 0.030200 |
| 5 | 7 | 0 | 2.060875 | 0.273221 | 0.000405 |
| 6 | 6 | 0 | 0.755607 | -0.258273 | 0.001730 |
| 7 | 6 | 0 | -1.258638 | -1.129818 | 0.004810 |
| 8 | 8 | 0 | 2.346570 | 1.420147 | 0.004323 |
| 9 | 8 | 0 | 2.946069 | -0.666048 | -0.006221 |
| 10 | 1 | 0 | 2.146680 | -1.586111 | -0.007772 |
| 11 | 7 | 0 | -1.196825 | 1.389706 | -0.000955 |
| 12 | 8 | 0 | -0.476062 | 2.362831 | 0.004805 |
| 13 | 8 | 0 | -2.419718 | 1.419775 | -0.014142 |
| 14 | 1 | 0 | -2.886637 | -2.331582 | -0.079191 |
| 15 | 1 | 0 | -3.222363 | -0.614504 | -0.060561 |

**Aci(5)**

Zero-point correction= 0.093594 (Hartree/Particle)
Thermal correction to Energy= 0.103524 (Hartree/Particle)
Thermal correction to Enthalpy= 0.104469 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.056898 (Hartree/Particle)

Electronic energy:
M06-2X=-690.4972093
CCSD(T)-F12=-689.69235966
T1=0.01847837

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.579466 | 0.097453 | 0.000208 |
| 2 | 7 | 0 | -0.795284 | -1.702359 | -0.000179 |
| 3 | 7 | 0 | 0.404826 | -2.160524 | -0.000053 |
| 4 | 7 | 0 | 2.604841 | -1.321175 | -0.000010 |
| 5 | 7 | 0 | -1.988468 | 0.258134 | 0.000179 |
| 6 | 6 | 0 | -0.774832 | -0.344827 | -0.000040 |
| 7 | 6 | 0 | 1.291544 | -1.091799 | 0.000109 |
| 8 | 8 | 0 | -2.224882 | 1.421044 | 0.000758 |
| 9 | 8 | 0 | -3.060156 | -0.570159 | -0.000315 |
| 10 | 1 | 0 | -2.675063 | -1.475852 | -0.000641 |
| 11 | 7 | 0 | 1.156214 | 1.386943 | -0.000131 |
| 12 | 8 | 0 | 0.434109 | 2.357026 | -0.000786 |
| 13 | 8 | 0 | 2.382194 | 1.429448 | 0.000281 |
| 14 | 1 | 0 | 2.930148 | -2.272847 | 0.000305 |
| 15 | 1 | 0 | 3.242816 | -0.542268 | 0.000520 |

**TS3a**

Zero-point correction= 0.092527 (Hartree/Particle)
Thermal correction to Energy= 0.102234 (Hartree/Particle)
Thermal correction to Enthalpy= 0.103178 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.056611 (Hartree/Particle)

Electronic energy:
M06-2X=-690.474469
CCSD(T)-F12=-689.67090477
T1=0.0183511

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.516719 | 0.098328 | 0.042647 |
| 2 | 7 | 0 | 0.637065 | -1.841763 | -0.022565 |
| 3 | 7 | 0 | -0.683022 | -2.114197 | 0.004386 |
| 4 | 7 | 0 | -2.777139 | -0.915337 | 0.045850 |
| 5 | 7 | 0 | 2.082102 | 0.030208 | 0.086038 |
| 6 | 6 | 0 | 0.757368 | -0.566361 | -0.032432 |
| 7 | 6 | 0 | -1.512289 | -0.990727 | 0.063298 |
| 8 | 8 | 0 | 2.982489 | -0.484542 | -0.526459 |
| 9 | 8 | 0 | 2.152261 | 0.985244 | 0.823212 |
| 10 | 1 | 0 | -0.972542 | -3.073824 | 0.095325 |
| 11 | 7 | 0 | -0.758827 | 1.381597 | -0.125239 |
| 12 | 8 | 0 | 0.014563 | 2.242933 | -0.467385 |
| 13 | 8 | 0 | -2.043883 | 1.763070 | 0.196694 |
| 14 | 1 | 0 | -3.210544 | -1.834566 | -0.024328 |
| 15 | 1 | 0 | -2.531771 | 1.823737 | -0.639862 |

**Aci(3)**

Zero-point correction= 0.09363 (Hartree/Particle)
Thermal correction to Energy= 0.103645 (Hartree/Particle)
Thermal correction to Enthalpy= 0.104589 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.057488 (Hartree/Particle)

Electronic energy:
M06-2X=-690.4823567
CCSD(T)-F12=-689.67818391
T1=0.01825178

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.532013 | 0.092272 | 0.034953 |
| 2 | 7 | 0 | 0.614901 | -1.848785 | -0.071371 |
| 3 | 7 | 0 | -0.707401 | -2.117679 | -0.060071 |
| 4 | 7 | 0 | -2.789891 | -0.914332 | 0.164432 |
| 5 | 7 | 0 | 2.070782 | 0.007045 | 0.097966 |
| 6 | 6 | 0 | 0.740751 | -0.575216 | -0.040737 |
| 7 | 6 | 0 | -1.531057 | -0.991977 | 0.072971 |
| 8 | 8 | 0 | 2.958005 | -0.467623 | -0.564514 |
| 9 | 8 | 0 | 2.160989 | 0.904741 | 0.901862 |
| 10 | 1 | 0 | -0.995250 | -3.074011 | 0.065987 |
| 11 | 7 | 0 | -0.750227 | 1.377251 | -0.128675 |
| 12 | 8 | 0 | 0.065977 | 2.243843 | -0.381763 |
| 13 | 8 | 0 | -2.047554 | 1.759310 | -0.004142 |
| 14 | 1 | 0 | -3.230977 | -1.831439 | 0.113524 |
| 15 | 1 | 0 | -2.006350 | 2.708297 | -0.210139 |

**TS5**

Zero-point correction= 0.092431 (Hartree/Particle)
Thermal correction to Energy= 0.101873 (Hartree/Particle)
Thermal correction to Enthalpy= 0.102817 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.056797 (Hartree/Particle)

Electronic energy:
M06-2X=-690.4268694
CCSD(T)-F12=-689.62757413
T1=0.01990799

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.333803 | 0.307541 | 0.555764 |
| 2 | 7 | 0 | 0.475813 | -1.473206 | -0.625216 |
| 3 | 7 | 0 | -0.904842 | -1.509205 | -0.669658 |
| 4 | 7 | 0 | -2.473588 | -1.005754 | 1.031207 |
| 5 | 7 | 0 | 2.218333 | -0.079430 | 0.193348 |
| 6 | 6 | 0 | 0.809026 | -0.429582 | 0.023324 |
| 7 | 6 | 0 | -1.482156 | -0.578667 | 0.186254 |
| 8 | 8 | 0 | 2.417268 | 0.964504 | 0.770331 |
| 9 | 8 | 0 | 3.046960 | -0.830895 | -0.251720 |
| 10 | 1 | 0 | -1.305014 | -2.410480 | -0.878271 |
| 11 | 7 | 0 | -0.836659 | 1.348877 | -0.175295 |
| 12 | 8 | 0 | -0.439274 | 2.424408 | -0.470999 |
| 13 | 8 | 0 | -2.020324 | 0.874555 | -0.577200 |
| 14 | 1 | 0 | -3.220332 | -1.532894 | 0.596880 |
| 15 | 1 | 0 | -2.823495 | -0.281921 | 1.645350 |

**P5**

Zero-point correction= 0.093756 (Hartree/Particle)
Thermal correction to Energy= 0.103326 (Hartree/Particle)
Thermal correction to Enthalpy= 0.104271 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.058 (Hartree/Particle)

Electronic energy:
M06-2X=-690.430249
CCSD(T)-F12=-689.63201693
T1=0.01878456

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.311398 | 0.350429 | 0.507257 |
| 2 | 7 | 0 | 0.505210 | -1.359092 | -0.731475 |
| 3 | 7 | 0 | -0.864209 | -1.389888 | -0.832085 |
| 4 | 7 | 0 | -2.229932 | -1.233963 | 1.123876 |
| 5 | 7 | 0 | 2.252440 | -0.030449 | 0.196104 |
| 6 | 6 | 0 | 0.849381 | -0.350344 | -0.034024 |
| 7 | 6 | 0 | -1.473460 | -0.547634 | 0.169183 |
| 8 | 8 | 0 | 2.446903 | 0.969314 | 0.850734 |
| 9 | 8 | 0 | 3.086123 | -0.759629 | -0.275284 |
| 10 | 1 | 0 | -1.214391 | -2.327287 | -0.973995 |
| 11 | 7 | 0 | -0.935063 | 1.342105 | -0.153347 |
| 12 | 8 | 0 | -0.720147 | 2.436901 | -0.540086 |
| 13 | 8 | 0 | -2.151296 | 0.685718 | -0.372286 |
| 14 | 1 | 0 | -3.022434 | -1.725574 | 0.725044 |
| 15 | 1 | 0 | -2.542097 | -0.621266 | 1.868325 |

**R1**

Zero-point correction= 0.079295 (Hartree/Particle)
Thermal correction to Energy= 0.086656 (Hartree/Particle)
Thermal correction to Enthalpy= 0.0876 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.046724 (Hartree/Particle)

Electronic energy:
M06-2X=-485.3522819
CCSD(T)-F12=-484.75624338
T1=0.02008739

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.136081 | -0.353865 | -0.017317 |
| 2 | 7 | 0 | 1.856653 | -1.388448 | 0.008317 |
| 3 | 7 | 0 | 2.014083 | -0.016677 | 0.011512 |
| 4 | 7 | 0 | 0.716948 | 1.987124 | -0.057304 |
| 5 | 6 | 0 | 0.593190 | -1.558523 | -0.004763 |
| 6 | 6 | 0 | 0.841890 | 0.643576 | -0.007777 |
| 7 | 1 | 0 | 2.942657 | 0.370766 | -0.023883 |
| 8 | 7 | 0 | -1.529936 | -0.145403 | -0.000282 |
| 9 | 8 | 0 | -2.259354 | -1.109832 | 0.008867 |
| 10 | 8 | 0 | -1.913899 | 1.021343 | 0.006982 |
| 11 | 1 | 0 | 1.470914 | 2.563407 | 0.277375 |
| 12 | 1 | 0 | -0.225778 | 2.330439 | 0.063167 |

**TS2**

Zero-point correction= 0.091089 (Hartree/Particle)
Thermal correction to Energy= 0.101236 (Hartree/Particle)
Thermal correction to Enthalpy= 0.10218 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.055153 (Hartree/Particle)

Electronic energy:
M06-2X=-690.4368047
CCSD(T)-F12=-689.63209433

T1=0.02057944

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.523897 | 0.140780 | 0.043262 |
| 2 | 7 | 0 | -0.539904 | -1.862560 | 0.100861 |
| 3 | 7 | 0 | 0.830649 | -2.012613 | -0.023282 |
| 4 | 7 | 0 | 2.829169 | -0.725516 | -0.205954 |
| 5 | 7 | 0 | -2.121847 | 0.049927 | -0.234765 |
| 6 | 6 | 0 | -0.699810 | -0.574644 | 0.137242 |
| 7 | 6 | 0 | 1.499325 | -0.853925 | -0.055879 |
| 8 | 8 | 0 | -1.986935 | -0.034593 | 1.043641 |
| 9 | 8 | 0 | -3.153883 | 0.017004 | -0.793452 |
| 10 | 1 | 0 | 1.200117 | -2.942583 | -0.123224 |
| 11 | 7 | 0 | 0.733042 | 1.522563 | 0.013274 |
| 12 | 8 | 0 | -0.240132 | 2.248259 | 0.045848 |
| 13 | 8 | 0 | 1.894784 | 1.914883 | -0.051319 |
| 14 | 1 | 0 | 3.436180 | -1.507885 | -0.032407 |
| 15 | 1 | 0 | 3.194785 | 0.210177 | -0.100800 |

**Nitrite (2)**

Zero-point correction= 0.092583 (Hartree/Particle)
Thermal correction to Energy= 0.103068 (Hartree/Particle)
Thermal correction to Enthalpy= 0.104012 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.056015 (Hartree/Particle)

Electronic energy:
M06-2X=-690.5444771
CCSD(T)-F12=-689.7378384
T1=0.01907895

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.521510 | 0.132205 | -0.072728 |
| 2 | 7 | 0 | -0.170464 | -2.089961 | -0.182779 |
| 3 | 7 | 0 | -1.489795 | -1.802485 | 0.022747 |
| 4 | 7 | 0 | -2.973334 | 0.035605 | 0.357505 |
| 5 | 7 | 0 | 2.417741 | -0.132592 | 0.601301 |
| 6 | 6 | 0 | 0.411265 | -0.928515 | -0.250976 |
| 7 | 6 | 0 | -1.755484 | -0.490397 | 0.105030 |
| 8 | 8 | 0 | 1.727798 | -0.832448 | -0.506081 |
| 9 | 8 | 0 | 3.512629 | 0.027495 | 0.327961 |
| 10 | 1 | 0 | -2.136061 | -2.565435 | 0.135586 |
| 11 | 7 | 0 | -0.319016 | 1.525047 | -0.130784 |
| 12 | 8 | 0 | 0.804871 | 1.942081 | -0.314896 |
| 13 | 8 | 0 | -1.306794 | 2.239690 | 0.004646 |
| 14 | 1 | 0 | -3.794051 | -0.514864 | 0.168345 |
| 15 | 1 | 0 | -3.039468 | 1.036693 | 0.239143 |

**R2**

Zero-point correction= 0.08299 (Hartree/Particle)
Thermal correction to Energy= 0.091565 (Hartree/Particle)
Thermal correction to Enthalpy= 0.092509 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.048491 (Hartree/Particle)

Electronic energy:
M06-2X=-560.6261461
CCSD(T)-F12=-559.95638752

T1=0.02632646

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.141636 | -0.105466 | -0.000067 |
| 2 | 7 | 0 | 2.137980 | -0.510133 | 0.000090 |
| 3 | 7 | 0 | 1.866650 | 0.781725 | 0.000028 |
| 4 | 7 | 0 | 0.081955 | 2.350713 | -0.000234 |
| 5 | 6 | 0 | 0.868067 | -1.162631 | 0.000005 |
| 6 | 6 | 0 | 0.521083 | 1.095599 | -0.000028 |
| 7 | 8 | 0 | 0.770896 | -2.363343 | -0.000024 |
| 8 | 1 | 0 | 2.627587 | 1.445131 | -0.000058 |
| 9 | 7 | 0 | -1.547461 | -0.222997 | 0.000005 |
| 10 | 8 | 0 | -2.042660 | -1.321439 | -0.000031 |
| 11 | 8 | 0 | -2.187557 | 0.831801 | 0.000108 |
| 12 | 1 | 0 | 0.708533 | 3.136306 | 0.000638 |
| 13 | 1 | 0 | -0.920502 | 2.482248 | 0.000311 |

**TS3c**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.381690 | -0.039916 | -0.338752 |
| 2 | 7 | 0 | 0.898359 | 1.718105 | 0.223683 |
| 3 | 7 | 0 | -0.404639 | 2.062175 | 0.235414 |
| 4 | 7 | 0 | -2.555409 | 0.851155 | -0.180084 |
| 5 | 7 | 0 | 2.146728 | -0.307059 | -0.130545 |
| 6 | 6 | 0 | 0.907741 | 0.447632 | -0.069519 |
| 7 | 6 | 0 | -1.229427 | 1.049795 | -0.129867 |
| 8 | 8 | 0 | 3.176391 | 0.262551 | 0.119165 |
| 9 | 8 | 0 | 2.018999 | -1.475713 | -0.428965 |
| 10 | 1 | 0 | -0.642245 | 3.032636 | 0.364333 |
| 11 | 7 | 0 | -1.107446 | -1.210301 | -0.217836 |
| 12 | 8 | 0 | -0.872000 | -1.809493 | 1.026822 |
| 13 | 8 | 0 | -2.324817 | -0.972505 | -0.489565 |
| 14 | 1 | 0 | -3.034620 | 1.142622 | 0.676416 |
| 15 | 1 | 0 | -0.934618 | -2.757566 | 0.853988 |

**P3c**

Zero-point correction= 0.095324 (Hartree/Particle)
Thermal correction to Energy= 0.104489 (Hartree/Particle)
Thermal correction to Enthalpy= 0.105433 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.0601 (Hartree/Particle)

Electronic energy:
M06-2X=-690.4401254
CCSD(T)-F12=-689.63290435
T1=0.01636465

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.337221 | -0.064531 | 0.191513 |
| 2 | 7 | 0 | -1.038519 | 1.672075 | -0.191656 |
| 3 | 7 | 0 | 0.240710 | 2.080345 | -0.202125 |
| 4 | 7 | 0 | 2.454688 | 0.811070 | 0.121491 |
| 5 | 7 | 0 | -2.188513 | -0.426264 | 0.097050 |
| 6 | 6 | 0 | -0.979533 | 0.376702 | 0.034704 |

| | | | | | |
|---|---|---|---|---|---|
| 7 | 6 | 0 | 1.078573 | 1.053834 | 0.013079 |
| 8 | 8 | 0 | -3.249608 | 0.125956 | -0.035126 |
| 9 | 8 | 0 | -2.005492 | -1.610643 | 0.278129 |
| 10 | 1 | 0 | 0.441151 | 3.057947 | -0.341849 |
| 11 | 7 | 0 | 1.198700 | -1.191270 | 0.330739 |
| 12 | 8 | 0 | 1.309365 | -1.731444 | -0.962624 |
| 13 | 8 | 0 | 2.432262 | -0.530384 | 0.647444 |
| 14 | 1 | 0 | 2.893792 | 0.762547 | -0.800266 |
| 15 | 1 | 0 | 1.485819 | -2.666092 | -0.804748 |

**TS3h**

Zero-point correction= 0.086037 (Hartree/Particle)
Thermal correction to Energy= 0.09617 (Hartree/Particle)
Thermal correction to Enthalpy= 0.097114 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.049669 (Hartree/Particle)

Electronic energy:
M06-2X=-690.4063375
CCSD(T)-F12=-689.60758887
T1=0.02949418

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.410786 | -0.059671 | -0.008443 |
| 2 | 7 | 0 | -0.995769 | 1.726566 | 0.010599 |
| 3 | 7 | 0 | 0.211031 | 2.220503 | 0.025970 |
| 4 | 7 | 0 | 2.484394 | 1.401550 | 0.000412 |
| 5 | 7 | 0 | -2.158617 | -0.354320 | -0.008345 |
| 6 | 6 | 0 | -0.952605 | 0.439121 | 0.000781 |
| 7 | 6 | 0 | 1.277768 | 1.263752 | 0.002092 |
| 8 | 8 | 0 | -3.217616 | 0.215212 | -0.006765 |
| 9 | 8 | 0 | -1.978697 | -1.556316 | -0.016509 |
| 10 | 1 | 0 | 0.350366 | 3.218718 | -0.005765 |
| 11 | 7 | 0 | 0.823576 | -1.235466 | 0.016457 |
| 12 | 8 | 0 | 0.727204 | -2.388876 | 0.033627 |
| 13 | 8 | 0 | 2.808199 | -1.028371 | -0.126693 |
| 14 | 1 | 0 | 2.879246 | 0.086867 | -0.058620 |
| 15 | 1 | 0 | 3.089663 | -1.409813 | 0.712879 |

**P3**

Zero-point correction= 0.063234 (Hartree/Particle)
Thermal correction to Energy= 0.073286 (Hartree/Particle)
Thermal correction to Enthalpy= 0.074231 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.02563 (Hartree/Particle)

Electronic energy:
M06-2X=-614.0449674
CCSD(T)-F12=-613.30586829
T1=0.01930893

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.267994 | 0.837934 | -0.000037 |
| 2 | 7 | 0 | 0.360976 | -1.512729 | 0.000170 |
| 3 | 7 | 0 | -0.871891 | -2.018421 | -0.000824 |
| 4 | 7 | 0 | -3.050487 | -0.806726 | 0.000810 |
| 5 | 7 | 0 | 2.069631 | 0.071469 | 0.000067 |
| 6 | 6 | 0 | 0.601751 | -0.272197 | 0.000443 |

| | | | | | |
|---|---|---|---|---|---|
| 7 | 6 | 0 | -2.033372 | -1.340839 | -0.000431 |
| 8 | 8 | 0 | 2.854108 | -0.834228 | 0.000202 |
| 9 | 8 | 0 | 2.315213 | 1.252681 | -0.000169 |
| 10 | 1 | 0 | -0.901987 | -3.026669 | 0.000143 |
| 11 | 7 | 0 | -0.942274 | 1.775390 | -0.000085 |
| 12 | 8 | 0 | -1.652073 | 2.720847 | -0.000153 |

**R4**

Zero-point correction= 0.076205 (Hartree/Particle)
Thermal correction to Energy= 0.085122 (Hartree/Particle)
Thermal correction to Enthalpy= 0.086067 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.040961 (Hartree/Particle)

Electronic energy:
M06-2X=-614.6842701
CCSD(T)-F12=-613.94910901
T1=0.02651916

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.224182 | 0.132299 | -0.000570 |
| 2 | 7 | 0 | 0.218014 | -2.120116 | 0.000436 |
| 3 | 7 | 0 | -1.036949 | -1.987278 | 0.000117 |
| 4 | 7 | 0 | -2.654954 | -0.262603 | -0.000034 |
| 5 | 7 | 0 | 2.113332 | -0.820952 | -0.000155 |
| 6 | 6 | 0 | 0.819136 | -0.854597 | 0.000049 |
| 7 | 6 | 0 | -1.377390 | -0.609940 | 0.000007 |
| 8 | 8 | 0 | 2.938520 | 0.034129 | -0.000653 |
| 9 | 7 | 0 | -0.144226 | 1.535350 | 0.000081 |
| 10 | 8 | 0 | 0.953740 | 2.050671 | 0.001434 |
| 11 | 8 | 0 | -1.206302 | 2.146838 | -0.000918 |
| 12 | 1 | 0 | -3.356083 | -0.985435 | 0.000795 |
| 13 | 1 | 0 | -2.903484 | 0.714957 | 0.000272 |

**TS8o**

Zero-point correction= 0.088679 (Hartree/Particle)
Thermal correction to Energy= 0.099295 (Hartree/Particle)
Thermal correction to Enthalpy= 0.100239 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.05173 (Hartree/Particle)

Electronic energy:
M06-2X=-690.4156099
CCSD(T)-F12=-689.61901424
T1=0.02136273

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.373631 | 0.007495 | -0.184767 |
| 2 | 7 | 0 | -0.609686 | -2.572708 | 0.243327 |
| 3 | 7 | 0 | -1.537717 | -1.935486 | 0.069894 |
| 4 | 7 | 0 | -2.855557 | 0.093414 | -0.132891 |
| 5 | 7 | 0 | 2.032843 | -0.289778 | 0.091053 |
| 6 | 6 | 0 | 0.756284 | -0.784830 | -0.334645 |
| 7 | 6 | 0 | -1.641409 | -0.497150 | -0.024105 |
| 8 | 8 | 0 | 3.008841 | -0.908514 | -0.280175 |
| 9 | 8 | 0 | 2.053493 | 0.691456 | 0.811616 |
| 10 | 1 | 0 | 0.840899 | -1.577844 | -1.062473 |
| 11 | 7 | 0 | -0.294304 | 1.489971 | -0.089619 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 8 | 0 | 0.179185 | 2.049955 | -1.045041 |
| 13 | 8 | 0 | -0.751937 | 2.002192 | 0.898507 |
| 14 | 1 | 0 | -3.430544 | 0.139802 | 0.697423 |
| 15 | 1 | 0 | -2.923534 | 0.906357 | -0.725458 |

**8**

Zero-point correction= 0.091035 (Hartree/Particle)
Thermal correction to Energy= 0.102227 (Hartree/Particle)
Thermal correction to Enthalpy= 0.103171 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.052625 (Hartree/Particle)

Electronic energy:
M06-2X=-690.4570058
CCSD(T)-F12=-689.65168174
T1=0.01873453

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.221685 | -0.000193 | -0.000110 |
| 2 | 7 | 0 | 2.522036 | -2.378245 | 0.000155 |
| 3 | 7 | 0 | 2.138520 | -1.332196 | 0.000093 |
| 4 | 7 | 0 | 2.581199 | 0.941621 | -0.000246 |
| 5 | 7 | 0 | -2.105009 | -0.761761 | -0.000247 |
| 6 | 6 | 0 | -0.684191 | -0.985407 | -0.000550 |
| 7 | 6 | 0 | 1.649795 | -0.100279 | 0.000056 |
| 8 | 8 | 0 | -2.794159 | -1.760726 | 0.000479 |
| 9 | 8 | 0 | -2.519027 | 0.378336 | -0.000697 |
| 10 | 1 | 0 | -0.422237 | -2.031699 | -0.000680 |
| 11 | 7 | 0 | -0.169404 | 1.432347 | 0.000239 |
| 12 | 8 | 0 | -0.257049 | 1.953972 | 1.079684 |
| 13 | 8 | 0 | -0.256263 | 1.954729 | -1.078860 |
| 14 | 1 | 0 | 2.569277 | 1.512047 | -0.836223 |
| 15 | 1 | 0 | 2.569818 | 1.512079 | 0.835714 |

**TS8m**

Zero-point correction= 0.088336 (Hartree/Particle)
Thermal correction to Energy= 0.099552 (Hartree/Particle)
Thermal correction to Enthalpy= 0.100497 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.050121 (Hartree/Particle)

Electronic energy:
M06-2X=-690.4356897
CCSD(T)-F12=-689.63345389
T1=0.01953798

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.228255 | -0.110686 | 0.000184 |
| 2 | 7 | 0 | -2.878853 | 2.127456 | 0.426476 |
| 3 | 7 | 0 | -2.209942 | 1.324739 | 0.087058 |
| 4 | 7 | 0 | -2.363550 | -1.076986 | -0.576385 |
| 5 | 7 | 0 | 1.972778 | 0.961532 | -0.084331 |
| 6 | 6 | 0 | 0.540786 | 0.967893 | -0.207764 |
| 7 | 6 | 0 | -1.639827 | -0.219603 | 0.140502 |
| 8 | 8 | 0 | 2.521798 | 2.029052 | -0.272496 |
| 9 | 8 | 0 | 2.537175 | -0.078616 | 0.182938 |
| 10 | 1 | 0 | 0.150738 | 1.932790 | -0.484203 |
| 11 | 7 | 0 | 0.359802 | -1.472360 | 0.160025 |

| | | | | | |
|---|---|---|---|---|---|
| 12 | 8 | 0 | 0.507622 | -1.881678 | 1.275762 |
| 13 | 8 | 0 | 0.551637 | -2.062199 | -0.874777 |
| 14 | 1 | 0 | -2.096264 | -1.375641 | -1.506195 |
| 15 | 1 | 0 | -3.198197 | -1.485913 | -0.188449 |

**TS9**

Zero-point correction= 0.074141 (Hartree/Particle)
Thermal correction to Energy= 0.080412 (Hartree/Particle)
Thermal correction to Enthalpy= 0.081356 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.042492 (Hartree/Particle)

Electronic energy:
M06-2X=-485.3589909
CCSD(T)-F12=-484.76679143
T1=0.02308385

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.046165 | -0.391068 | -0.000026 |
| 2 | 7 | 0 | 2.092450 | -1.010843 | -0.000064 |
| 3 | 7 | 0 | 2.127285 | 0.299081 | 0.000024 |
| 4 | 7 | 0 | 0.352518 | 1.962304 | 0.000132 |
| 5 | 6 | 0 | 0.814256 | -1.477075 | -0.000097 |
| 6 | 6 | 0 | 0.820233 | 0.760598 | 0.000053 |
| 7 | 1 | 0 | 0.599873 | -2.533333 | -0.000169 |
| 8 | 7 | 0 | -1.403614 | -0.273103 | -0.000021 |
| 9 | 8 | 0 | -2.164685 | -1.198952 | -0.000084 |
| 10 | 8 | 0 | -1.878690 | 0.945756 | 0.000059 |
| 11 | 1 | 0 | 1.035597 | 2.713184 | 0.000184 |
| 12 | 1 | 0 | -0.998893 | 1.648912 | 0.000108 |

**9**

Zero-point correction= 0.076657 (Hartree/Particle)
Thermal correction to Energy= 0.083405 (Hartree/Particle)
Thermal correction to Enthalpy= 0.084349 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.04463 (Hartree/Particle)

Electronic energy:
M06-2X=-485.3595516
CCSD(T)-F12=-484.76891431
T1=0.02331932

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.061400 | -0.371918 | 0.012558 |
| 2 | 7 | 0 | 2.059352 | -1.060183 | -0.004176 |
| 3 | 7 | 0 | 2.141588 | 0.244095 | -0.004759 |
| 4 | 7 | 0 | 0.454809 | 1.982093 | -0.000423 |
| 5 | 6 | 0 | 0.769662 | -1.485740 | 0.003891 |
| 6 | 6 | 0 | 0.845319 | 0.763299 | 0.003353 |
| 7 | 1 | 0 | 0.519717 | -2.534058 | 0.006052 |
| 8 | 7 | 0 | -1.403743 | -0.257024 | 0.000926 |
| 9 | 8 | 0 | -2.182219 | -1.171671 | -0.007553 |
| 10 | 8 | 0 | -1.906925 | 0.977983 | 0.000703 |
| 11 | 1 | 0 | -1.111212 | 1.632314 | -0.000340 |
| 12 | 1 | 0 | 1.219121 | 2.654528 | -0.010689 |

**TS11**

Zero-point correction= 0.071101 (Hartree/Particle)
Thermal correction to Energy= 0.079577 (Hartree/Particle)
Thermal correction to Enthalpy= 0.080522 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.036759 (Hartree/Particle)

Electronic energy:
M06-2X=-485.2586325
CCSD(T)-F12=-484.69013644
T1=0.07720086

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.004329 | -0.059018 | 0.104418 |
| 2 | 7 | 0 | 2.404221 | -0.202942 | 0.384164 |
| 3 | 7 | 0 | 3.118576 | 0.030294 | -0.506031 |
| 4 | 7 | 0 | -0.794684 | 2.240218 | -0.025559 |
| 5 | 6 | 0 | 1.103844 | -0.828017 | 0.214810 |
| 6 | 6 | 0 | 0.088781 | 1.390020 | 0.096275 |
| 7 | 1 | 0 | 1.083895 | -1.906961 | 0.241041 |
| 8 | 7 | 0 | -1.235128 | -0.688982 | -0.041801 |
| 9 | 8 | 0 | -1.353276 | -1.908943 | -0.116753 |
| 10 | 8 | 0 | -2.393148 | 0.037430 | -0.044183 |
| 11 | 1 | 0 | -2.143054 | 0.982693 | -0.105616 |
| 12 | 1 | 0 | -0.550118 | 3.228342 | -0.016370 |

**11**

Zero-point correction= 0.073918 (Hartree/Particle)
Thermal correction to Energy= 0.082449 (Hartree/Particle)
Thermal correction to Enthalpy= 0.083393 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.03962 (Hartree/Particle)

Electronic energy:
M06-2X=-485.3031753
CCSD(T)-F12=-484.71003413
T1=0.02181928

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.045451 | -0.044237 | 0.000494 |
| 2 | 7 | 0 | 2.312113 | -0.288910 | -0.000110 |
| 3 | 7 | 0 | 3.319577 | 0.208201 | -0.001353 |
| 4 | 7 | 0 | -0.896793 | 2.232814 | 0.000087 |
| 5 | 6 | 0 | 1.148222 | -0.862447 | 0.001429 |
| 6 | 6 | 0 | 0.003327 | 1.381124 | 0.000829 |
| 7 | 1 | 0 | 1.119475 | -1.938510 | 0.003329 |
| 8 | 7 | 0 | -1.208728 | -0.694108 | -0.000292 |
| 9 | 8 | 0 | -1.323704 | -1.909473 | -0.000294 |
| 10 | 8 | 0 | -2.378422 | -0.002326 | -0.000762 |
| 11 | 1 | 0 | -2.156315 | 0.957646 | -0.000296 |
| 12 | 1 | 0 | -0.665930 | 3.222637 | 0.000577 |

**TS10**

Zero-point correction= 0.075139 (Hartree/Particle)
Thermal correction to Energy= 0.082718 (Hartree/Particle)
Thermal correction to Enthalpy= 0.083662 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.041698 (Hartree/Particle)

Electronic energy:
M06-2X=-485.2996447
CCSD(T)-F12=-484.70718705
T1=0.02494505

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.000182 | -0.111434 | 0.000003 |
| 2 | 7 | 0 | -2.169371 | -0.797345 | -0.000007 |
| 3 | 7 | 0 | -2.811702 | 0.140078 | -0.000092 |
| 4 | 7 | 0 | 0.271929 | 2.247595 | 0.000046 |
| 5 | 6 | 0 | -0.895136 | -1.194106 | 0.000185 |
| 6 | 6 | 0 | -0.517124 | 1.207754 | -0.000064 |
| 7 | 1 | 0 | -0.650070 | -2.240619 | 0.000310 |
| 8 | 7 | 0 | 1.391957 | -0.494827 | -0.000035 |
| 9 | 8 | 0 | 1.675331 | -1.676519 | -0.000097 |
| 10 | 8 | 0 | 2.223848 | 0.403438 | 0.000017 |
| 11 | 1 | 0 | -0.137510 | 3.169500 | -0.000064 |
| 12 | 1 | 0 | 1.286912 | 2.173978 | 0.000255 |

**10**

Zero-point correction= 0.075737 (Hartree/Particle)
Thermal correction to Energy= 0.08406 (Hartree/Particle)
Thermal correction to Enthalpy= 0.085004 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.041407 (Hartree/Particle)

Electronic energy:
M06-2X=-485.0
CCSD(T)-F12=-484.71657167
T1=0.02014594

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.052588 | 0.010144 | 0.000044 |
| 2 | 7 | 0 | -2.279841 | -0.287553 | -0.000065 |
| 3 | 7 | 0 | -3.316512 | 0.130376 | -0.000229 |
| 4 | 7 | 0 | 0.920764 | 2.201695 | -0.000044 |
| 5 | 6 | 0 | -1.068692 | -0.820039 | 0.000061 |
| 6 | 6 | 0 | -0.137718 | 1.434164 | -0.000110 |
| 7 | 1 | 0 | -1.039787 | -1.899409 | 0.000158 |
| 8 | 7 | 0 | 1.303661 | -0.726369 | 0.000138 |
| 9 | 8 | 0 | 1.273584 | -1.942948 | -0.000000 |
| 10 | 8 | 0 | 2.339467 | -0.073645 | 0.000163 |
| 11 | 1 | 0 | 0.783648 | 3.201335 | -0.000183 |
| 12 | 1 | 0 | 1.878165 | 1.858168 | 0.000144 |

**TS12**

Zero-point correction= 0.071934 (Hartree/Particle)
Thermal correction to Energy= 0.080733 (Hartree/Particle)
Thermal correction to Enthalpy= 0.081677 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.036403 (Hartree/Particle)

Electronic energy:
M06-2X=-485.2782829
CCSD(T)-F12=-484.69185573
T1=0.02086728

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.021344 | -0.074125 | -0.059460 |
| 2 | 7 | 0 | -2.562924 | -0.719736 | 0.124611 |
| 3 | 7 | 0 | -3.099330 | 0.242859 | -0.041397 |
| 4 | 7 | 0 | 0.591262 | 2.211319 | 0.075975 |
| 5 | 6 | 0 | -0.875704 | -1.003613 | -0.365048 |
| 6 | 6 | 0 | -0.335967 | 1.310763 | 0.201338 |
| 7 | 1 | 0 | -0.729676 | -2.052992 | -0.568025 |
| 8 | 7 | 0 | 1.434473 | -0.599163 | 0.018098 |
| 9 | 8 | 0 | 1.611424 | -1.729844 | 0.392478 |
| 10 | 8 | 0 | 2.316317 | 0.169203 | -0.318325 |
| 11 | 1 | 0 | 0.358336 | 3.169808 | 0.295506 |
| 12 | 1 | 0 | 1.547005 | 2.023199 | -0.222701 |

**12**

Zero-point correction= 0.064443 (Hartree/Particle)
Thermal correction to Energy= 0.071158 (Hartree/Particle)
Thermal correction to Enthalpy= 0.072102 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.031862 (Hartree/Particle)

Electronic energy:
M06-2X=-375.7755
CCSD(T)-F12=-375.3186001
T1=0.02109463

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.054449 | 0.747297 | 0.000020 |
| 2 | 7 | 0 | -2.150693 | -0.358208 | 0.000088 |
| 3 | 6 | 0 | 0.592020 | 1.892986 | -0.000010 |
| 4 | 6 | 0 | -1.516333 | 0.777521 | 0.000140 |
| 5 | 1 | 0 | 1.617206 | 2.227446 | -0.000083 |
| 6 | 7 | 0 | 0.830650 | -0.487499 | -0.000062 |
| 7 | 8 | 0 | 2.025029 | -0.334351 | -0.000083 |
| 8 | 8 | 0 | 0.270534 | -1.566092 | -0.000060 |
| 9 | 1 | 0 | -3.160591 | -0.335938 | 0.000247 |
| 10 | 1 | 0 | -1.708250 | -1.274836 | -0.000102 |

**$N_2$**

Zero-point correction= 0.005723 (Hartree/Particle)
Thermal correction to Energy= 0.008083 (Hartree/Particle)
Thermal correction to Enthalpy= 0.009027 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= -0.012693 (Hartree/Particle)

Electronic energy:
M06-2X=-109.5298731
CCSD(T)-F12=-109.40200366
T1=0.01413166

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 0.000000 | 0.000000 | 0.542938 |
| 2 | 7 | 0 | 0.000000 | 0.000000 | -0.542938 |

**D3**

Zero-point correction= 0.175196 (Hartree/Particle)

Thermal correction to Energy= 0.19421 (Hartree/Particle)
Thermal correction to Enthalpy= 0.195155 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.121947 (Hartree/Particle)

Electronic energy:
M06-2X=-1175.9377462
DLPNO-CCSD(T)=-1174.594435694725

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.886006 | 0.512759 | 0.067919 |
| 2 | 7 | 0 | -1.996929 | -1.557411 | 0.010432 |
| 3 | 7 | 0 | -1.025653 | -0.616566 | 0.116613 |
| 4 | 7 | 0 | -0.723925 | 1.733385 | 0.254044 |
| 5 | 7 | 0 | -4.371417 | -1.602251 | -0.033741 |
| 6 | 6 | 0 | -3.100272 | -0.880184 | -0.021372 |
| 7 | 6 | 0 | -1.497729 | 0.642918 | 0.151459 |
| 8 | 8 | 0 | -5.156579 | -1.303780 | 0.832095 |
| 9 | 8 | 0 | -4.515614 | -2.444723 | -0.884002 |
| 10 | 1 | 0 | -0.045725 | -0.885835 | 0.160385 |
| 11 | 7 | 0 | -3.791362 | 1.584735 | -0.074681 |
| 12 | 8 | 0 | -4.937120 | 1.339927 | -0.372624 |
| 13 | 8 | 0 | -3.338099 | 2.713207 | 0.096584 |
| 14 | 1 | 0 | 0.274259 | 1.657464 | 0.113556 |
| 15 | 1 | 0 | -1.194538 | 2.623709 | 0.209760 |
| 16 | 6 | 0 | 4.182077 | -0.417048 | 0.025938 |
| 17 | 7 | 0 | 1.960618 | -0.541081 | 0.140115 |
| 18 | 7 | 0 | 2.222934 | 0.723003 | -0.014960 |
| 19 | 7 | 0 | 4.160760 | 2.044709 | -0.253150 |
| 20 | 6 | 0 | 3.132490 | -1.271837 | 0.169676 |
| 21 | 6 | 0 | 3.588486 | 0.870439 | -0.093320 |
| 22 | 1 | 0 | 3.129365 | -2.343254 | 0.290243 |
| 23 | 7 | 0 | 5.580159 | -0.700292 | -0.004795 |
| 24 | 8 | 0 | 5.932131 | -1.846285 | 0.109526 |
| 25 | 8 | 0 | 6.322189 | 0.261340 | -0.147277 |
| 26 | 1 | 0 | 3.589603 | 2.874867 | -0.323936 |
| 27 | 1 | 0 | 5.171197 | 2.095652 | -0.305372 |

**TSD34**
Zero-point correction= 0.168829 (Hartree/Particle)
Thermal correction to Energy= 0.187152 (Hartree/Particle)
Thermal correction to Enthalpy= 0.188096 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.118171 (Hartree/Particle)

Electronic energy:
M06-2X=-1175.91
DLPNO-CCSD(T)=-1174.566127284007

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.743802 | 0.518324 | 0.006722 |
| 2 | 7 | 0 | -1.730899 | -1.489764 | 0.001051 |
| 3 | 7 | 0 | -0.797901 | -0.554008 | 0.007567 |
| 4 | 7 | 0 | -0.605004 | 1.793504 | 0.000923 |
| 5 | 7 | 0 | -4.127686 | -1.644365 | 0.065744 |
| 6 | 6 | 0 | -2.899523 | -0.857267 | 0.002706 |
| 7 | 6 | 0 | -1.341309 | 0.695930 | 0.008003 |

| | | | | | |
|---|---|---|---|---|---|
| 8 | 8 | 0 | -4.877558 | -1.384160 | 0.972891 |
| 9 | 8 | 0 | -4.265767 | -2.491144 | -0.779481 |
| 10 | 1 | 0 | 0.379542 | -0.736608 | 0.013320 |
| 11 | 7 | 0 | -3.704169 | 1.562386 | -0.083272 |
| 12 | 8 | 0 | -4.855285 | 1.265106 | -0.277211 |
| 13 | 8 | 0 | -3.271057 | 2.702012 | 0.028950 |
| 14 | 1 | 0 | 0.426614 | 1.697774 | -0.004879 |
| 15 | 1 | 0 | -1.090944 | 2.680891 | 0.021962 |
| 16 | 6 | 0 | 3.923213 | -0.403112 | 0.008738 |
| 17 | 7 | 0 | 1.731889 | -0.531827 | 0.013671 |
| 18 | 7 | 0 | 2.019731 | 0.781883 | 0.000854 |
| 19 | 7 | 0 | 3.994542 | 2.073643 | -0.014740 |
| 20 | 6 | 0 | 2.848333 | -1.267770 | 0.018317 |
| 21 | 6 | 0 | 3.358575 | 0.898034 | -0.002639 |
| 22 | 1 | 0 | 2.835776 | -2.345415 | 0.027975 |
| 23 | 7 | 0 | 5.302423 | -0.724341 | 0.009666 |
| 24 | 8 | 0 | 5.620538 | -1.891738 | 0.020729 |
| 25 | 8 | 0 | 6.089101 | 0.214854 | -0.000894 |
| 26 | 1 | 0 | 3.472217 | 2.932962 | -0.022773 |
| 27 | 1 | 0 | 5.003610 | 2.076349 | -0.016828 |

**D4**

Zero-point correction= 0.175267 (Hartree/Particle)
Thermal correction to Energy= 0.193902 (Hartree/Particle)
Thermal correction to Enthalpy= 0.194846 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.123836 (Hartree/Particle)

Electronic energy:
M06-2X=-1175.94121
DLPNO-CCSD(T)=-1174.599407596143

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.822277 | 0.505527 | 0.011706 |
| 2 | 7 | 0 | -1.950455 | -1.570377 | -0.043362 |
| 3 | 7 | 0 | -0.935568 | -0.759283 | -0.040956 |
| 4 | 7 | 0 | -0.578457 | 1.564927 | -0.009447 |
| 5 | 7 | 0 | -4.378969 | -1.517549 | 0.040097 |
| 6 | 6 | 0 | -3.094982 | -0.830687 | -0.007222 |
| 7 | 6 | 0 | -1.398155 | 0.542785 | -0.010798 |
| 8 | 8 | 0 | -5.069374 | -1.294854 | 1.001964 |
| 9 | 8 | 0 | -4.615403 | -2.257346 | -0.880441 |
| 10 | 1 | 0 | 1.019833 | -1.160398 | -0.025650 |
| 11 | 7 | 0 | -3.694927 | 1.632264 | -0.016915 |
| 12 | 8 | 0 | -4.873829 | 1.434167 | -0.157655 |
| 13 | 8 | 0 | -3.160667 | 2.726385 | 0.093061 |
| 14 | 1 | 0 | 0.447189 | 1.382918 | -0.035159 |
| 15 | 1 | 0 | -0.978805 | 2.494658 | 0.032949 |
| 16 | 6 | 0 | 4.087788 | -0.394993 | 0.033086 |
| 17 | 7 | 0 | 1.966161 | -0.776824 | -0.016183 |
| 18 | 7 | 0 | 2.080567 | 0.576662 | -0.080152 |
| 19 | 7 | 0 | 3.894295 | 2.087009 | -0.053118 |
| 20 | 6 | 0 | 3.132835 | -1.393651 | 0.053127 |
| 21 | 6 | 0 | 3.381930 | 0.831046 | -0.051437 |
| 22 | 1 | 0 | 3.242477 | -2.463625 | 0.107996 |
| 23 | 7 | 0 | 5.493030 | -0.578867 | 0.057886 |
| 24 | 8 | 0 | 5.919491 | -1.710313 | 0.139314 |
| 25 | 8 | 0 | 6.185412 | 0.425563 | -0.009267 |
| 26 | 1 | 0 | 3.306040 | 2.829755 | -0.391293 |

| | | | | | |
|---|---|---|---|---|---|
| 27 | 1 | 0 | 4.885668 | 2.161973 | -0.220381 |

**P7**

Zero-point correction= 0.0924 (Hartree/Particle)
Thermal correction to Energy= 0.099684 (Hartree/Particle)
Thermal correction to Enthalpy= 0.100628 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.060484 (Hartree/Particle)

Electronic energy:
M06-2X=-486.0480804
DLPNO-CCSD(T)=-485.479812894889

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -2.626633 | -1.797312 | 0.029490 |
| 2 | 6 | 0 | 0.121868 | -0.292915 | -0.012617 |
| 3 | 7 | 0 | -1.838444 | -1.171527 | 0.015871 |
| 4 | 7 | 0 | -2.072934 | 0.163596 | 0.009153 |
| 5 | 7 | 0 | -0.692746 | 2.066872 | -0.078753 |
| 6 | 6 | 0 | -0.551387 | -1.496613 | 0.003206 |
| 7 | 6 | 0 | -0.874539 | 0.721104 | -0.011705 |
| 8 | 1 | 0 | -0.181170 | -2.507533 | 0.009512 |
| 9 | 7 | 0 | 1.528605 | -0.127432 | 0.000238 |
| 10 | 8 | 0 | 2.223132 | -1.122774 | -0.025128 |
| 11 | 8 | 0 | 1.954088 | 1.016531 | 0.042099 |
| 12 | 1 | 0 | -1.483217 | 2.637489 | 0.172469 |
| 13 | 1 | 0 | 0.226235 | 2.407278 | 0.153889 |

**R10**

Zero-point correction= 0.081652 (Hartree/Particle)
Thermal correction to Energy= 0.09137 (Hartree/Particle)
Thermal correction to Enthalpy= 0.092314 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.044452 (Hartree/Particle)

Electronic energy:
M06-2X=-689.8680278
DLPNO-CCSD(T)=-689.09233145728

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.489425 | 0.118643 | 0.002250 |
| 2 | 7 | 0 | 0.448754 | -1.932962 | 0.055541 |
| 3 | 7 | 0 | -0.830597 | -2.135056 | 0.063029 |
| 4 | 7 | 0 | -2.780910 | -0.816831 | 0.017713 |
| 5 | 7 | 0 | 2.051786 | -0.096224 | 0.052604 |
| 6 | 6 | 0 | 0.680351 | -0.583190 | 0.024974 |
| 7 | 6 | 0 | -1.468164 | -0.910411 | 0.028250 |
| 8 | 8 | 0 | 2.755065 | -0.450787 | -0.858383 |
| 9 | 8 | 0 | 2.354481 | 0.596675 | 0.990794 |
| 10 | 7 | 0 | -0.739296 | 1.517276 | -0.091909 |
| 11 | 8 | 0 | 0.198194 | 2.255447 | -0.247738 |
| 12 | 8 | 0 | -1.912694 | 1.856392 | -0.016636 |
| 13 | 1 | 0 | -3.331564 | -1.663921 | 0.037306 |
| 14 | 1 | 0 | -3.213530 | 0.098432 | 0.006708 |

**D5**

Zero-point correction= 0.174817 (Hartree/Particle)

Thermal correction to Energy=  0.193662 (Hartree/Particle)
Thermal correction to Enthalpy=  0.194606 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=  0.123365 (Hartree/Particle)

Electronic energy:
M06-2X=-1175.9454724
DLPNO-CCSD(T)=-1174.602273344896

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.962347 | -0.381818 | -0.000860 |
| 2 | 7 | 0 | -0.839593 | 0.329796 | -0.141553 |
| 3 | 7 | 0 | -0.878624 | -1.018923 | -0.126571 |
| 4 | 7 | 0 | -2.429049 | -2.810415 | 0.042909 |
| 5 | 7 | 0 | -2.346735 | 2.144460 | -0.175223 |
| 6 | 6 | 0 | -2.078103 | 0.712789 | -0.064047 |
| 7 | 6 | 0 | -2.128169 | -1.505421 | -0.040948 |
| 8 | 8 | 0 | -3.328368 | 2.462917 | -0.793648 |
| 9 | 8 | 0 | -1.532074 | 2.884631 | 0.326128 |
| 10 | 1 | 0 | 0.041873 | -1.479777 | -0.157673 |
| 11 | 7 | 0 | -4.362323 | -0.432635 | 0.225666 |
| 12 | 8 | 0 | -4.932783 | 0.574794 | 0.562501 |
| 13 | 8 | 0 | -4.891727 | -1.528776 | 0.084139 |
| 14 | 1 | 0 | -1.716282 | -3.506555 | -0.091238 |
| 15 | 1 | 0 | -3.401022 | -3.063404 | -0.046729 |
| 16 | 6 | 0 | 3.987640 | -0.332430 | 0.004918 |
| 17 | 7 | 0 | 2.782678 | -2.203818 | -0.181883 |
| 18 | 7 | 0 | 1.918297 | -1.230787 | -0.139685 |
| 19 | 7 | 0 | 1.976709 | 1.122617 | 0.042780 |
| 20 | 6 | 0 | 4.057776 | -1.690579 | -0.097023 |
| 21 | 6 | 0 | 2.595247 | -0.033646 | -0.023518 |
| 22 | 1 | 0 | 4.925362 | -2.329909 | -0.114876 |
| 23 | 7 | 0 | 5.046936 | 0.613079 | 0.115145 |
| 24 | 8 | 0 | 6.181462 | 0.200456 | 0.122355 |
| 25 | 8 | 0 | 4.722759 | 1.789047 | 0.195624 |
| 26 | 1 | 0 | 0.952721 | 1.144146 | -0.000969 |
| 27 | 1 | 0 | 2.532856 | 1.963973 | 0.132463 |

**TSD56**
Zero-point correction=  0.170556 (Hartree/Particle)
Thermal correction to Energy=  0.188123 (Hartree/Particle)
Thermal correction to Enthalpy=  0.189067 (Hartree/Particle)
Thermal correction to Gibbs Free Energy=  0.121632 (Hartree/Particle)

Electronic energy:
M06-2X=-1175.9301385
DLPNO-CCSD(T)=-1174.585972803608

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.876436 | 0.351792 | 0.007094 |
| 2 | 7 | 0 | -0.739163 | -0.229359 | 0.102190 |
| 3 | 7 | 0 | -0.786397 | 1.122077 | 0.105588 |
| 4 | 7 | 0 | -2.445385 | 2.803184 | -0.031081 |
| 5 | 7 | 0 | -2.109528 | -2.145447 | 0.140348 |
| 6 | 6 | 0 | -1.956188 | -0.703345 | 0.039857 |

| | | | | | |
|---|---|---|---|---|---|
| 7 | 6 | 0 | -2.067047 | 1.503224 | 0.049260 |
| 8 | 8 | 0 | -3.141768 | -2.570518 | 0.586360 |
| 9 | 8 | 0 | -1.147218 | -2.808207 | -0.197709 |
| 10 | 1 | 0 | 0.745290 | 1.486969 | 0.104537 |
| 11 | 7 | 0 | -4.284122 | 0.352252 | -0.183040 |
| 12 | 8 | 0 | -4.822620 | -0.654189 | -0.576409 |
| 13 | 8 | 0 | -4.860287 | 1.409246 | 0.045159 |
| 14 | 1 | 0 | -1.754650 | 3.497293 | 0.200752 |
| 15 | 1 | 0 | -3.407841 | 3.001628 | 0.193728 |
| 16 | 6 | 0 | 3.815329 | 0.335253 | -0.015635 |
| 17 | 7 | 0 | 2.713314 | 2.274866 | 0.089725 |
| 18 | 7 | 0 | 1.830215 | 1.314168 | 0.081859 |
| 19 | 7 | 0 | 1.709032 | -1.025623 | -0.000531 |
| 20 | 6 | 0 | 3.944804 | 1.694578 | 0.032059 |
| 21 | 6 | 0 | 2.413195 | 0.065105 | 0.017130 |
| 22 | 1 | 0 | 4.841151 | 2.292762 | 0.028282 |
| 23 | 7 | 0 | 4.847564 | -0.653960 | -0.081947 |
| 24 | 8 | 0 | 5.989897 | -0.268486 | -0.100763 |
| 25 | 8 | 0 | 4.481431 | -1.814977 | -0.114059 |
| 26 | 1 | 0 | 0.577958 | -0.880270 | 0.047783 |
| 27 | 1 | 0 | 2.211952 | -1.906093 | -0.056077 |

**D6**

Zero-point correction= 0.175022 (Hartree/Particle)
Thermal correction to Energy= 0.193535 (Hartree/Particle)
Thermal correction to Enthalpy= 0.194479 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.123785 (Hartree/Particle)

Electronic energy:
M06-2X=-117.0
DLPNO-CCSD(T)=-1174.600016905343

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.976621 | -0.375079 | -0.009495 |
| 2 | 7 | 0 | -0.890312 | 0.265885 | 0.003397 |
| 3 | 7 | 0 | -0.844648 | -1.077207 | -0.024536 |
| 4 | 7 | 0 | -2.445557 | -2.805099 | 0.016341 |
| 5 | 7 | 0 | -2.337130 | 2.156632 | -0.079200 |
| 6 | 6 | 0 | -2.128236 | 0.721348 | 0.008675 |
| 7 | 6 | 0 | -2.109476 | -1.494864 | -0.029439 |
| 8 | 8 | 0 | -3.360184 | 2.537676 | -0.579736 |
| 9 | 8 | 0 | -1.422924 | 2.841007 | 0.327893 |
| 10 | 1 | 0 | 1.059895 | -1.557705 | -0.010176 |
| 11 | 7 | 0 | -4.398304 | -0.432359 | 0.102765 |
| 12 | 8 | 0 | -4.986912 | 0.537649 | 0.509093 |
| 13 | 8 | 0 | -4.914447 | -1.496466 | -0.202770 |
| 14 | 1 | 0 | -1.713845 | -3.474907 | -0.154034 |
| 15 | 1 | 0 | -3.383148 | -3.044081 | -0.265045 |
| 16 | 6 | 0 | 3.990913 | -0.289747 | 0.003892 |
| 17 | 7 | 0 | 2.979274 | -2.280105 | 0.005295 |
| 18 | 7 | 0 | 2.063318 | -1.339973 | -0.005896 |
| 19 | 7 | 0 | 1.811669 | 0.989687 | -0.018117 |
| 20 | 6 | 0 | 4.172719 | -1.651149 | 0.011210 |
| 21 | 6 | 0 | 2.576444 | -0.054113 | -0.007812 |
| 22 | 1 | 0 | 5.094286 | -2.209286 | 0.020388 |
| 23 | 7 | 0 | 5.004214 | 0.716549 | 0.005371 |
| 24 | 8 | 0 | 6.156316 | 0.349103 | 0.016284 |
| 25 | 8 | 0 | 4.629589 | 1.875244 | -0.004858 |

| | | | | | |
|---|---|---|---|---|---|
| 26 | 1 | 0 | 0.008038 | 0.793401 | -0.004531 |
| 27 | 1 | 0 | 2.371140 | 1.842426 | -0.013964 |

**I1**

Zero-point correction= 0.095092 (Hartree/Particle)
Thermal correction to Energy= 0.104925 (Hartree/Particle)
Thermal correction to Enthalpy= 0.105869 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.059006 (Hartree/Particle)

Electronic energy:
M06-2X=-690.5273388
DLPNO-CCSD(T)=-689.754403314186

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.522589 | 0.094718 | 0.008981 |
| 2 | 7 | 0 | -0.625479 | -1.751599 | -0.027677 |
| 3 | 7 | 0 | 0.649898 | -2.154645 | -0.002676 |
| 4 | 7 | 0 | 2.729304 | -1.060441 | -0.033348 |
| 5 | 7 | 0 | -2.089977 | 0.127695 | 0.079368 |
| 6 | 6 | 0 | -0.756846 | -0.431395 | -0.016439 |
| 7 | 6 | 0 | 1.375019 | -1.039732 | 0.015937 |
| 8 | 8 | 0 | -2.201601 | 1.244295 | 0.504270 |
| 9 | 8 | 0 | -2.989421 | -0.620898 | -0.249374 |
| 10 | 7 | 0 | 0.955305 | 1.453808 | -0.082918 |
| 11 | 8 | 0 | 0.187236 | 2.279626 | -0.507792 |
| 12 | 8 | 0 | 2.107793 | 1.667370 | 0.257440 |
| 13 | 1 | 0 | 3.167309 | -1.954825 | 0.116640 |
| 14 | 1 | 0 | 3.210179 | -0.237729 | 0.293108 |
| 15 | 1 | 0 | -1.387479 | -2.415857 | -0.026216 |

**R11**

Zero-point correction= 0.079044 (Hartree/Particle)
Thermal correction to Energy= 0.085934 (Hartree/Particle)
Thermal correction to Enthalpy= 0.086878 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.046537 (Hartree/Particle)

Electronic energy:
M06-2X=-485.39097
DLPNO-CCSD(T)=-484.82314530704

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 1 | 0 | -2.965751 | 0.445218 | 0.000797 |
| 2 | 6 | 0 | 0.124677 | -0.267041 | 0.000164 |
| 3 | 7 | 0 | -1.874022 | -1.264258 | 0.000087 |
| 4 | 7 | 0 | -2.039387 | 0.041888 | -0.000391 |
| 5 | 7 | 0 | -0.870594 | 2.065736 | -0.000073 |
| 6 | 6 | 0 | -0.546438 | -1.469878 | 0.000150 |
| 7 | 6 | 0 | -0.861918 | 0.773890 | 0.000041 |
| 8 | 1 | 0 | -0.140498 | -2.467871 | 0.000135 |

| | | | | | |
|---|---|---|---|---|---|
| 9 | 7 | 0 | 1.538450 | -0.077087 | 0.000037 |
| 10 | 8 | 0 | 2.235349 | -1.067526 | -0.000216 |
| 11 | 8 | 0 | 1.944133 | 1.071115 | 0.000098 |
| 12 | 1 | 0 | 0.091346 | 2.408164 | 0.000269 |

**C1**

Zero-point correction= 0.105308 (Hartree/Particle)
Thermal correction to Energy= 0.119993 (Hartree/Particle)
Thermal correction to Enthalpy= 0.120937 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.059607 (Hartree/Particle)

Electronic energy:
M06-2X=-895.6021084
DLPNO-CCSD(T)=-894.626142269155

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.802507 | 0.418242 | 0.832440 |
| 2 | 7 | 0 | -0.868622 | -0.882364 | 1.175808 |
| 3 | 1 | 0 | -1.667803 | -1.374085 | 1.544940 |
| 4 | 6 | 0 | 0.458641 | 0.574942 | 0.264855 |
| 5 | 6 | 0 | 1.036676 | -0.710339 | 0.328142 |
| 6 | 7 | 0 | 0.248158 | -1.586026 | 0.865863 |
| 7 | 7 | 0 | 2.323696 | -1.151415 | -0.210179 |
| 8 | 8 | 0 | 3.048928 | -1.757356 | 0.536594 |
| 9 | 8 | 0 | 2.526167 | -0.883938 | -1.368119 |
| 10 | 7 | 0 | -1.812415 | 1.302279 | 0.987732 |
| 11 | 7 | 0 | -3.252114 | -0.638730 | -1.094050 |
| 12 | 8 | 0 | -3.615073 | -0.944572 | -0.007988 |
| 13 | 8 | 0 | -2.203150 | -0.498190 | -1.605231 |
| 14 | 7 | 0 | 1.028636 | 1.811381 | -0.123729 |
| 15 | 8 | 0 | 2.206880 | 1.843243 | -0.381894 |
| 16 | 8 | 0 | 0.274048 | 2.777215 | -0.148846 |
| 17 | 1 | 0 | -2.494415 | 1.137312 | 1.710639 |
| 18 | 1 | 0 | -1.568409 | 2.262601 | 0.785552 |

**$TS_{C13}$**

Zero-point correction= 0.100234 (Hartree/Particle)
Thermal correction to Energy= 0.113592 (Hartree/Particle)
Thermal correction to Enthalpy= 0.114536 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.056531 (Hartree/Particle)

Electronic energy:
M06-2X=-895.56077
DLPNO-CCSD(T)=-894.579593591966

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.694407 | -0.146225 | 0.722542 |
| 2 | 7 | 0 | -0.481979 | -1.493127 | 0.736591 |
| 3 | 1 | 0 | -1.158540 | -2.206311 | 0.973983 |
| 4 | 6 | 0 | 0.535673 | 0.389032 | 0.293847 |
| 5 | 6 | 0 | 1.360073 | -0.715945 | 0.101623 |
| 6 | 7 | 0 | 0.741405 | -1.847277 | 0.359948 |
| 7 | 7 | 0 | 2.779447 | -0.754585 | -0.250686 |
| 8 | 8 | 0 | 3.096149 | -1.515067 | -1.127518 |
| 9 | 8 | 0 | 3.496667 | -0.031628 | 0.393574 |
| 10 | 7 | 0 | -1.849169 | 0.398996 | 1.076845 |

| | | | | | |
|---|---|---|---|---|---|
| 11 | 7 | 0 | -3.806506 | -0.477106 | -0.979096 |
| 12 | 8 | 0 | -3.741557 | -0.900917 | 0.216553 |
| 13 | 8 | 0 | -3.101540 | 0.430641 | -1.294213 |
| 14 | 7 | 0 | 0.774554 | 1.770441 | 0.011794 |
| 15 | 8 | 0 | 1.753697 | 2.047804 | -0.631745 |
| 16 | 8 | 0 | -0.057070 | 2.556435 | 0.431569 |
| 17 | 1 | 0 | -2.866287 | -0.241927 | 0.795451 |
| 18 | 1 | 0 | -1.858239 | 1.407528 | 0.928974 |

**C3**

Zero-point correction= 0.104021 (Hartree/Particle)
Thermal correction to Energy= 0.118247 (Hartree/Particle)
Thermal correction to Enthalpy= 0.119191 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.058118 (Hartree/Particle)

Electronic energy:
M06-2X=-895.5803891
DLPNO-CCSD(T)=-894.61002005671

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.509619 | 0.415162 | 0.005173 |
| 2 | 7 | 0 | 0.704151 | -0.957883 | -0.006988 |
| 3 | 1 | 0 | 1.613336 | -1.414688 | -0.015516 |
| 4 | 6 | 0 | -0.919848 | 0.529636 | 0.002491 |
| 5 | 6 | 0 | -1.390962 | -0.762304 | -0.014275 |
| 6 | 7 | 0 | -0.404849 | -1.657431 | -0.017099 |
| 7 | 7 | 0 | -2.769547 | -1.247945 | -0.083636 |
| 8 | 8 | 0 | -3.105332 | -2.019162 | 0.776755 |
| 9 | 8 | 0 | -3.424586 | -0.841745 | -1.008735 |
| 10 | 7 | 0 | 1.497426 | 1.251376 | 0.019502 |
| 11 | 7 | 0 | 4.900588 | -0.788128 | -0.023985 |
| 12 | 8 | 0 | 3.535052 | -0.663374 | -0.016476 |
| 13 | 8 | 0 | 5.458102 | 0.238308 | -0.011545 |
| 14 | 7 | 0 | -1.656071 | 1.753798 | 0.096747 |
| 15 | 8 | 0 | -2.831470 | 1.674813 | 0.352479 |
| 16 | 8 | 0 | -1.023665 | 2.779071 | -0.074164 |
| 17 | 1 | 0 | 3.281639 | 0.290146 | -0.001597 |
| 18 | 1 | 0 | 1.145480 | 2.209774 | 0.018470 |

**R9**

Zero-point correction= 0.081528 (Hartree/Particle)
Thermal correction to Energy= 0.091083 (Hartree/Particle)
Thermal correction to Enthalpy= 0.092028 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.044344 (Hartree/Particle)

Electronic energy:
M06-2X=-689.8686995
DLPNO-CCSD(T)=-689.096427027502

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.568594 | -0.877791 | 0.019258 |
| 2 | 7 | 0 | -0.841557 | -2.057191 | 0.036962 |
| 3 | 1 | 0 | -1.243184 | -2.985178 | 0.057435 |
| 4 | 6 | 0 | -0.538027 | 0.117425 | 0.005126 |
| 5 | 6 | 0 | 0.650537 | -0.580757 | 0.019044 |
| 6 | 7 | 0 | 0.462521 | -1.895762 | 0.036405 |

| | | | | | |
|---|---|---|---|---|---|
| 7 | 7 | 0 | 2.022990 | -0.076350 | 0.079028 |
| 8 | 8 | 0 | 2.777744 | -0.481110 | -0.766580 |
| 9 | 8 | 0 | 2.267168 | 0.679107 | 0.984644 |
| 10 | 7 | 0 | -2.862246 | -0.884716 | 0.013601 |
| 11 | 7 | 0 | -0.747570 | 1.528752 | -0.106039 |
| 12 | 8 | 0 | 0.205845 | 2.209197 | -0.394787 |
| 13 | 8 | 0 | -1.881923 | 1.924428 | 0.083734 |
| 14 | 1 | 0 | -3.209948 | 0.075808 | 0.006207 |

**C2**

Zero-point correction= 0.104799 (Hartree/Particle)
Thermal correction to Energy= 0.119814 (Hartree/Particle)
Thermal correction to Enthalpy= 0.120758 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.057419 (Hartree/Particle)

Electronic energy:
M06-2X=-895.6017906
DLPNO-CCSD(T)=-894.627025718412

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.677432 | 1.592475 | 0.028243 |
| 2 | 7 | 0 | 0.642144 | 1.326271 | 0.027356 |
| 3 | 1 | 0 | 1.415467 | 1.975824 | 0.030090 |
| 4 | 6 | 0 | -1.295358 | 0.342224 | 0.009339 |
| 5 | 6 | 0 | -0.229002 | -0.579506 | -0.008930 |
| 6 | 7 | 0 | 0.929555 | 0.000295 | 0.005785 |
| 7 | 7 | 0 | -0.285972 | -2.039799 | 0.061952 |
| 8 | 8 | 0 | 0.356675 | -2.649811 | -0.754387 |
| 9 | 8 | 0 | -0.954109 | -2.496365 | 0.955173 |
| 10 | 7 | 0 | -1.212129 | 2.825584 | -0.009892 |
| 11 | 7 | 0 | 3.784640 | 0.281871 | -0.281396 |
| 12 | 8 | 0 | 3.570512 | 1.392720 | 0.085188 |
| 13 | 8 | 0 | 4.324771 | -0.647496 | 0.183094 |
| 14 | 7 | 0 | -2.690456 | 0.125667 | -0.094408 |
| 15 | 8 | 0 | -3.081776 | -0.990860 | -0.331818 |
| 16 | 8 | 0 | -3.407177 | 1.109325 | 0.050544 |
| 17 | 1 | 0 | -2.208007 | 2.882918 | 0.144983 |
| 18 | 1 | 0 | -0.642354 | 3.630778 | 0.184886 |

**TSC24**

Zero-point correction= 0.100189 (Hartree/Particle)
Thermal correction to Energy= 0.113514 (Hartree/Particle)
Thermal correction to Enthalpy= 0.114458 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.058149 (Hartree/Particle)

Electronic energy:
M06-2X=-895.0
DLPNO-CCSD(T)=-894.573530100022

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 0.082012 | -0.243031 | -0.361180 |
| 2 | 7 | 0 | 0.748015 | 0.896084 | -0.671509 |
| 3 | 1 | 0 | 1.990291 | 1.007557 | -0.619760 |
| 4 | 6 | 0 | -1.212907 | 0.080162 | -0.056571 |
| 5 | 6 | 0 | -1.233129 | 1.503901 | -0.143957 |
| 6 | 7 | 0 | -0.012061 | 1.952348 | -0.515961 |

| | | | | | |
|---|---|---|---|---|---|
| 7 | 7 | 0 | 3.277857 | 0.552739 | 0.855085 |
| 8 | 8 | 0 | 2.316151 | 0.059677 | 1.364951 |
| 9 | 8 | 0 | 3.171589 | 1.096586 | -0.272239 |
| 10 | 7 | 0 | -2.361023 | -0.744145 | 0.166918 |
| 11 | 8 | 0 | -3.342440 | -0.167817 | 0.614791 |
| 12 | 8 | 0 | -2.302408 | -1.909463 | -0.119492 |
| 13 | 7 | 0 | -2.255747 | 2.329544 | 0.038795 |
| 14 | 1 | 0 | -3.148112 | 1.956378 | 0.328543 |
| 15 | 1 | 0 | -2.112240 | 3.320610 | -0.079069 |
| 16 | 7 | 0 | 0.802405 | -1.504744 | -0.355429 |
| 17 | 8 | 0 | 1.740342 | -1.574024 | -1.116180 |
| 18 | 8 | 0 | 0.424025 | -2.342899 | 0.417575 |

**C4**

Zero-point correction= 0.104539 (Hartree/Particle)
Thermal correction to Energy= 0.118744 (Hartree/Particle)
Thermal correction to Enthalpy= 0.119688 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.060167 (Hartree/Particle)

Electronic energy:
M06-2X=-895.5788467
DLPNO-CCSD(T)=-894.603847644235

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -0.029779 | -0.121342 | -0.329423 |
| 2 | 7 | 0 | 0.594610 | 1.080672 | -0.545607 |
| 3 | 1 | 0 | 2.577758 | 1.073041 | -0.530844 |
| 4 | 6 | 0 | -1.349476 | 0.070076 | -0.040099 |
| 5 | 6 | 0 | -1.475180 | 1.487597 | -0.071054 |
| 6 | 7 | 0 | -0.252497 | 2.042706 | -0.389075 |
| 7 | 7 | 0 | 3.726350 | 0.361609 | 0.800138 |
| 8 | 8 | 0 | 2.742177 | -0.132474 | 1.227750 |
| 9 | 8 | 0 | 3.539014 | 1.090671 | -0.309558 |
| 10 | 7 | 0 | -2.433180 | -0.844216 | 0.157186 |
| 11 | 8 | 0 | -3.471565 | -0.344667 | 0.570116 |
| 12 | 8 | 0 | -2.269144 | -2.001809 | -0.112427 |
| 13 | 7 | 0 | -2.532113 | 2.240300 | 0.144228 |
| 14 | 1 | 0 | -3.408049 | 1.803792 | 0.405314 |
| 15 | 1 | 0 | -2.439060 | 3.244683 | 0.075908 |
| 16 | 7 | 0 | 0.762521 | -1.339919 | -0.395799 |
| 17 | 8 | 0 | 1.599795 | -1.368051 | -1.265166 |
| 18 | 8 | 0 | 0.526738 | -2.184616 | 0.426233 |

**D1**

Zero-point correction= 0.190647 (Hartree/Particle)
Thermal correction to Energy= 0.212622 (Hartree/Particle)
Thermal correction to Enthalpy= 0.213566 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.134976 (Hartree/Particle)

Electronic energy:
M06-2X=-1381.0855063
DLPNO-CCSD(T)=-1379.537685098463

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.432283 | -0.431948 | -0.056550 |
| 2 | 7 | 0 | 1.381889 | 0.328803 | 0.456905 |

| | | | | | |
|---|---|---|---|---|---|
| 3 | 7 | 0 | 1.365973 | -1.013400 | 0.333329 |
| 4 | 7 | 0 | 2.805312 | -2.839699 | -0.152317 |
| 5 | 7 | 0 | 2.930481 | 2.094145 | 0.388009 |
| 6 | 6 | 0 | 2.608682 | 0.678522 | 0.223140 |
| 7 | 6 | 0 | 2.568959 | -1.531004 | 0.020461 |
| 8 | 8 | 0 | 4.012115 | 2.358706 | 0.839263 |
| 9 | 8 | 0 | 2.055795 | 2.880078 | 0.093828 |
| 10 | 1 | 0 | 0.463639 | -1.468938 | 0.440533 |
| 11 | 7 | 0 | 4.767347 | -0.499886 | -0.531981 |
| 12 | 8 | 0 | 5.316207 | 0.520612 | -0.866288 |
| 13 | 8 | 0 | 5.261246 | -1.619485 | -0.596023 |
| 14 | 1 | 0 | 2.042692 | -3.477568 | -0.306887 |
| 15 | 1 | 0 | 3.738109 | -3.099578 | -0.435912 |
| 16 | 6 | 0 | -3.430431 | 0.432677 | -0.057169 |
| 17 | 7 | 0 | -1.382106 | -0.335574 | 0.453686 |
| 18 | 7 | 0 | -1.361779 | 1.006723 | 0.330870 |
| 19 | 7 | 0 | -2.795179 | 2.838416 | -0.151783 |
| 20 | 7 | 0 | -2.937789 | -2.095133 | 0.386004 |
| 21 | 6 | 0 | -2.610408 | -0.680828 | 0.221031 |
| 22 | 6 | 0 | -2.563220 | 1.528641 | 0.019575 |
| 23 | 8 | 0 | -4.019539 | -2.355064 | 0.839855 |
| 24 | 8 | 0 | -2.067380 | -2.884782 | 0.089409 |
| 25 | 1 | 0 | -0.457658 | 1.458872 | 0.438099 |
| 26 | 7 | 0 | -4.765610 | 0.505344 | -0.531457 |
| 27 | 8 | 0 | -5.318144 | -0.513153 | -0.865922 |
| 28 | 8 | 0 | -5.255834 | 1.626617 | -0.594562 |
| 29 | 1 | 0 | -2.030322 | 3.473069 | -0.308736 |
| 30 | 1 | 0 | -3.727139 | 3.101368 | -0.435357 |

**$TS_{D12}$**

Zero-point correction= 0.18201 (Hartree/Particle)
Thermal correction to Energy= 0.203692 (Hartree/Particle)
Thermal correction to Enthalpy= 0.204637 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.128 (Hartree/Particle)

Electronic energy:
M06-2X=-1381.0504806
DLPNO-CCSD(T)=-1379.502150006411

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.324120 | -0.458261 | -0.003465 |
| 2 | 7 | 0 | 1.304610 | 0.438757 | 0.123617 |
| 3 | 7 | 0 | 1.149020 | -0.912827 | 0.100162 |
| 4 | 7 | 0 | 2.537279 | -2.815095 | -0.083367 |
| 5 | 7 | 0 | 2.956262 | 2.124046 | 0.182687 |
| 6 | 6 | 0 | 2.577415 | 0.722916 | 0.059666 |
| 7 | 6 | 0 | 2.355871 | -1.483746 | 0.020292 |
| 8 | 8 | 0 | 4.015966 | 2.369104 | 0.692784 |
| 9 | 8 | 0 | 2.135858 | 2.931893 | -0.202989 |
| 10 | 1 | 0 | -0.283533 | -1.046829 | 0.101284 |
| 11 | 7 | 0 | 4.715154 | -0.657547 | -0.213257 |
| 12 | 8 | 0 | 5.389564 | 0.276392 | -0.573250 |
| 13 | 8 | 0 | 5.129674 | -1.795587 | -0.035234 |
| 14 | 1 | 0 | 1.747296 | -3.422963 | 0.050054 |
| 15 | 1 | 0 | 3.467502 | -3.170273 | 0.068726 |
| 16 | 6 | 0 | -3.298614 | 0.461328 | -0.009392 |
| 17 | 7 | 0 | -1.310839 | -0.487045 | 0.082188 |
| 18 | 7 | 0 | -1.124619 | 0.854970 | 0.058748 |

| | | | | | |
|---|---|---|---|---|---|
| 19 | 7 | 0 | -2.449139 | 2.798999 | -0.051147 |
| 20 | 7 | 0 | -3.021722 | -2.131105 | 0.169855 |
| 21 | 6 | 0 | -2.593998 | -0.739982 | 0.044914 |
| 22 | 6 | 0 | -2.308396 | 1.471919 | 0.000786 |
| 23 | 8 | 0 | -4.046526 | -2.332960 | 0.760442 |
| 24 | 8 | 0 | -2.266024 | -2.952479 | -0.296536 |
| 25 | 1 | 0 | 0.059649 | 1.028605 | 0.097756 |
| 26 | 7 | 0 | -4.690697 | 0.691998 | -0.207772 |
| 27 | 8 | 0 | -5.388974 | -0.235991 | -0.527470 |
| 28 | 8 | 0 | -5.065073 | 1.845991 | -0.061336 |
| 29 | 1 | 0 | -1.642288 | 3.395515 | -0.124671 |
| 30 | 1 | 0 | -3.379879 | 3.183946 | -0.053270 |

**D2**

Zero-point correction= 0.190562 (Hartree/Particle)
Thermal correction to Energy= 0.21239 (Hartree/Particle)
Thermal correction to Enthalpy= 0.213334 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.134639 (Hartree/Particle)

Electronic energy:
M06-2X=-1381.0713139
DLPNO-CCSD(T)=-1379.526391249561

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | 3.793411 | -0.365722 | 0.002120 |
| 2 | 7 | 0 | 1.613098 | -0.325372 | -0.046354 |
| 3 | 7 | 0 | 1.927777 | -1.623357 | -0.073510 |
| 4 | 7 | 0 | 3.936699 | -2.846863 | -0.144904 |
| 5 | 7 | 0 | 2.464936 | 1.879629 | 0.163593 |
| 6 | 6 | 0 | 2.676631 | 0.459156 | 0.002324 |
| 7 | 6 | 0 | 3.260269 | -1.676948 | -0.050161 |
| 8 | 8 | 0 | 3.353198 | 2.542090 | 0.617480 |
| 9 | 8 | 0 | 1.354891 | 2.281222 | -0.150505 |
| 10 | 1 | 0 | -1.449312 | -1.996609 | 0.023037 |
| 11 | 7 | 0 | 5.178575 | -0.032622 | -0.073589 |
| 12 | 8 | 0 | 5.489993 | 1.079315 | -0.422288 |
| 13 | 8 | 0 | 5.958681 | -0.930899 | 0.201006 |
| 14 | 1 | 0 | 3.397496 | -3.689495 | -0.031720 |
| 15 | 1 | 0 | 4.894267 | -2.849005 | 0.167631 |
| 16 | 6 | 0 | -3.392393 | 0.497230 | -0.011601 |
| 17 | 7 | 0 | -1.901366 | -1.091107 | 0.000484 |
| 18 | 7 | 0 | -1.189526 | 0.048281 | -0.022754 |
| 19 | 7 | 0 | -1.719590 | 2.332718 | -0.110395 |
| 20 | 7 | 0 | -4.090549 | -2.017779 | 0.156020 |
| 21 | 6 | 0 | -3.206653 | -0.872481 | 0.015029 |
| 22 | 6 | 0 | -2.079020 | 1.043206 | -0.034631 |
| 23 | 8 | 0 | -5.177586 | -1.829001 | 0.624523 |
| 24 | 8 | 0 | -3.610930 | -3.080995 | -0.180902 |
| 25 | 1 | 0 | 0.619053 | -0.036290 | -0.035736 |
| 26 | 7 | 0 | -4.601134 | 1.248827 | -0.137771 |
| 27 | 8 | 0 | -5.597974 | 0.681056 | -0.506608 |
| 28 | 8 | 0 | -4.514126 | 2.438905 | 0.116028 |
| 29 | 1 | 0 | -0.739120 | 2.569405 | -0.094182 |
| 30 | 1 | 0 | -2.417457 | 3.035313 | 0.066874 |

**$TS_{D57}$**

Zero-point correction= 0.173559 (Hartree/Particle)
Thermal correction to Energy= 0.191568 (Hartree/Particle)

Thermal correction to Enthalpy= 0.192512 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.125716 (Hartree/Particle)

Electronic energy:
M06-2X=-1175.9001819
DLPNO-CCSD(T)=-1174.554142717034

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.841159 | -1.130909 | 1.260419 |
| 2 | 7 | 0 | -1.045790 | -0.435934 | 2.122105 |
| 3 | 1 | 0 | -0.823661 | -0.684553 | 3.073823 |
| 4 | 6 | 0 | -2.049707 | -0.288260 | 0.184349 |
| 5 | 6 | 0 | -1.222694 | 0.848471 | 0.439636 |
| 6 | 7 | 0 | -0.759434 | 0.814553 | 1.704304 |
| 7 | 7 | 0 | -2.563425 | -0.703280 | -1.059043 |
| 8 | 8 | 0 | -2.387656 | 0.009860 | -2.016818 |
| 9 | 8 | 0 | -3.148154 | -1.784404 | -1.082210 |
| 10 | 7 | 0 | -1.514486 | 2.216642 | -0.072261 |
| 11 | 8 | 0 | -2.658028 | 2.428058 | -0.374629 |
| 12 | 8 | 0 | -0.601536 | 3.002790 | -0.085804 |
| 13 | 7 | 0 | -2.284786 | -2.370608 | 1.487875 |
| 14 | 1 | 0 | -2.777846 | -2.805515 | 0.718749 |
| 15 | 1 | 0 | -1.857576 | -2.947657 | 2.191924 |
| 16 | 6 | 0 | 2.514610 | 0.089548 | -0.180287 |
| 17 | 7 | 0 | 0.386788 | 0.479052 | -0.536639 |
| 18 | 7 | 0 | 0.532887 | -0.828963 | -0.741196 |
| 19 | 7 | 0 | 2.347940 | -2.317935 | -0.786809 |
| 20 | 6 | 0 | 1.553823 | 1.055269 | -0.115804 |
| 21 | 6 | 0 | 1.829158 | -1.106381 | -0.569516 |
| 22 | 1 | 0 | 1.608052 | 2.090555 | 0.173934 |
| 23 | 7 | 0 | 3.907540 | 0.224782 | 0.075308 |
| 24 | 8 | 0 | 4.330006 | 1.309623 | 0.398929 |
| 25 | 8 | 0 | 4.589133 | -0.784031 | -0.050084 |
| 26 | 1 | 0 | 1.755874 | -3.036622 | -1.169670 |
| 27 | 1 | 0 | 3.350231 | -2.425953 | -0.772125 |

**D7**

Zero-point correction= 0.176041 (Hartree/Particle)
Thermal correction to Energy= 0.194175 (Hartree/Particle)
Thermal correction to Enthalpy= 0.195119 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.128013 (Hartree/Particle)

Electronic energy:
M06-2X=-1175.9410146
DLPNO-CCSD(T)=-1174.593519532289

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.745648 | 0.120016 | 1.213811 |
| 2 | 7 | 0 | -2.207002 | 1.315403 | 1.645343 |
| 3 | 1 | 0 | -2.529005 | 1.868037 | 2.426333 |
| 4 | 6 | 0 | -1.915001 | -0.352267 | 0.238137 |
| 5 | 6 | 0 | -0.845418 | 0.641163 | 0.040806 |
| 6 | 7 | 0 | -1.075973 | 1.673192 | 1.038734 |
| 7 | 7 | 0 | -2.252385 | -1.378388 | -0.655882 |
| 8 | 8 | 0 | -1.632663 | -1.456034 | -1.692032 |
| 9 | 8 | 0 | -3.184931 | -2.113749 | -0.334750 |

| | | | | | |
|---|---|---|---|---|---|
| 10 | 7 | 0 | -1.051870 | 1.387841 | -1.362883 |
| 11 | 8 | 0 | -0.077894 | 1.629848 | -2.013802 |
| 12 | 8 | 0 | -2.191642 | 1.683902 | -1.603311 |
| 13 | 7 | 0 | -3.868422 | -0.385892 | 1.717933 |
| 14 | 1 | 0 | -4.210950 | -1.230043 | 1.275689 |
| 15 | 1 | 0 | -4.489645 | 0.175985 | 2.274716 |
| 16 | 6 | 0 | 2.640738 | 0.031041 | 0.229666 |
| 17 | 7 | 0 | 0.496071 | 0.171901 | 0.116394 |
| 18 | 7 | 0 | 0.751453 | -1.167976 | 0.068344 |
| 19 | 7 | 0 | 2.703510 | -2.466909 | 0.170238 |
| 20 | 6 | 0 | 1.600033 | 0.922338 | 0.214423 |
| 21 | 6 | 0 | 2.062349 | -1.269988 | 0.135703 |
| 22 | 1 | 0 | 1.587509 | 1.998238 | 0.255940 |
| 23 | 7 | 0 | 4.019444 | 0.364513 | 0.306396 |
| 24 | 8 | 0 | 4.319599 | 1.532788 | 0.425150 |
| 25 | 8 | 0 | 4.815724 | -0.558419 | 0.244115 |
| 26 | 1 | 0 | 2.178325 | -3.260703 | -0.159727 |
| 27 | 1 | 0 | 3.692122 | -2.447810 | -0.023489 |

**$TS_{D78}$**

Zero-point correction= 0.174198 (Hartree/Particle)
Thermal correction to Energy= 0.192199 (Hartree/Particle)
Thermal correction to Enthalpy= 0.193143 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.126622 (Hartree/Particle)

Electronic energy:
M06-2X=-1175.9367
DLPNO-CCSD(T)=-1174.587674013932

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -2.918719 | -0.221630 | -1.046825 |
| 2 | 7 | 0 | -2.379944 | -1.412856 | -1.458971 |
| 3 | 1 | 0 | -2.814739 | -2.093440 | -2.064053 |
| 4 | 6 | 0 | -1.919133 | 0.431624 | -0.361528 |
| 5 | 6 | 0 | -0.814034 | -0.501778 | -0.289638 |
| 6 | 7 | 0 | -1.097495 | -1.577756 | -1.125328 |
| 7 | 7 | 0 | -2.185209 | 1.482820 | 0.541474 |
| 8 | 8 | 0 | -1.442856 | 1.629176 | 1.482994 |
| 9 | 8 | 0 | -3.191930 | 2.153816 | 0.326318 |
| 10 | 7 | 0 | -1.059543 | -1.310226 | 1.378368 |
| 11 | 8 | 0 | -0.072793 | -1.599354 | 1.977269 |
| 12 | 8 | 0 | -2.204804 | -1.528475 | 1.644779 |
| 13 | 7 | 0 | -4.178447 | 0.137187 | -1.301405 |
| 14 | 1 | 0 | -4.482153 | 1.001749 | -0.871042 |
| 15 | 1 | 0 | -4.866737 | -0.555576 | -1.544326 |
| 16 | 6 | 0 | 2.680015 | -0.069722 | -0.241041 |
| 17 | 7 | 0 | 0.527831 | -0.103885 | -0.264959 |
| 18 | 7 | 0 | 0.846019 | 1.224932 | -0.264593 |
| 19 | 7 | 0 | 2.863523 | 2.421478 | -0.294771 |
| 20 | 6 | 0 | 1.598512 | -0.909843 | -0.254341 |
| 21 | 6 | 0 | 2.161558 | 1.260769 | -0.247773 |
| 22 | 1 | 0 | 1.533613 | -1.984453 | -0.247974 |
| 23 | 7 | 0 | 4.042178 | -0.470176 | -0.204958 |
| 24 | 8 | 0 | 4.291135 | -1.655738 | -0.243415 |
| 25 | 8 | 0 | 4.877657 | 0.417028 | -0.134562 |
| 26 | 1 | 0 | 2.360029 | 3.257222 | -0.044889 |
| 27 | 1 | 0 | 3.837123 | 2.365731 | -0.041894 |

**D8**

Zero-point correction= 0.163869 (Hartree/Particle)
Thermal correction to Energy= 0.178959 (Hartree/Particle)
Thermal correction to Enthalpy= 0.179903 (Hartree/Particle)
Thermal correction to Gibbs Free Energy= 0.120509 (Hartree/Particle)

Electronic energy:
M06-2X=-970.8992419
DLPNO-CCSD(T)=-969.755318419666

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.240129 | -0.753633 | -0.168865 |
| 2 | 7 | 0 | -2.691895 | -1.938890 | -0.487630 |
| 3 | 1 | 0 | -3.171772 | -2.782124 | -0.756597 |
| 4 | 6 | 0 | -2.157506 | 0.101340 | 0.026120 |
| 5 | 6 | 0 | -1.011088 | -0.691766 | -0.233185 |
| 6 | 7 | 0 | -1.333123 | -1.912901 | -0.553655 |
| 7 | 7 | 0 | -2.262390 | 1.404622 | 0.570947 |
| 8 | 8 | 0 | -1.267215 | 1.940095 | 0.994348 |
| 9 | 8 | 0 | -3.387885 | 1.894403 | 0.604999 |
| 10 | 7 | 0 | -4.568123 | -0.519927 | -0.102849 |
| 11 | 1 | 0 | -4.822567 | 0.392893 | 0.248480 |
| 12 | 1 | 0 | -5.190628 | -1.286477 | 0.092006 |
| 13 | 6 | 0 | 2.468543 | -0.266558 | 0.045536 |
| 14 | 7 | 0 | 0.330223 | -0.308407 | -0.203667 |
| 15 | 7 | 0 | 0.722128 | 0.837350 | -0.830747 |
| 16 | 7 | 0 | 2.797606 | 1.865891 | -1.214552 |
| 17 | 6 | 0 | 1.342735 | -1.002170 | 0.324320 |
| 18 | 6 | 0 | 2.030646 | 0.879343 | -0.681191 |
| 19 | 1 | 0 | 1.210006 | -1.932128 | 0.850145 |
| 20 | 7 | 0 | 3.789171 | -0.584194 | 0.452304 |
| 21 | 8 | 0 | 3.968484 | -1.620013 | 1.058223 |
| 22 | 8 | 0 | 4.666332 | 0.215794 | 0.166326 |
| 23 | 1 | 0 | 2.317501 | 2.717115 | -1.458060 |
| 24 | 1 | 0 | 3.735346 | 1.944348 | -0.854608 |