Supporting information

Too Fast and Too Furious: Thermoanalytical and Quantum Chemical Study of the Thermal Stability of 4,4'-Dinitro-3,3'-Diazenofuroxan

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1. Peak temperatures and conversion degrees of the three stages of DDF thermolysis

Table S1. The peak temperature and conversion degree at peak of the thermal decomposition of DDF obtained from the non-isothermal DSC experiments.

Heating rate, K min^{-1}	Peak I		Peak II		Peak III	
	Temperature, ^{o}C	Conversion degree	Temperature, ^{o}C	Conversion degree	Temperature, ^{o}C	Conversion degree
0.13	90.2	0.07	100.2	0.24	128.9	0.96
0.25	95.2	0.07	104.4	0.22	131.5	0.94
0.5	-		108.8	0.19	134.7	0.95
1	-		113.4	0.17	137.8	0.91
2	-		118.2	0.14	141.0	0.89
5	-		124.5	0.13	144.5	0.85

2. Details of the thermokinetic modeling of DDF decomposition

Table S2. The kinetic parameters of the thermal decomposition of DDF calculated using different kinetic schemes and the non-isothermal DSC data.

Model name	A	B	C	D
Kinetic scheme [a]	ePT + ePT	ePT → ePT	ePT + ePT + ePT	KJMAE + ePT + ePT
log (A_1/s^{-1})	16.3±0.3	16.3±0.2	12.8±0.4	13.3±0.3
E_{a1}, kJ mol^{-1}	140.2±1.9	140.2±1.3	110.7±2.6	116.4 ± 2.6
n_1	2.06±0.07	1.33±0.02	0.74±0.06	-
m_1	0.36±0.02	0.330±0.004	0.52±0.03	2.17 ± 0.10
q_1	0.999 [b]	0.999 [b]	0.999	0.999 [b]
log (A_2/s^{-1})	34.62±0.07	32.6±0.3	17.5±0.2	17.7±0.7
E_{a2}, kJ mol^{-1}	291.0±0.6	274.5±2.9	145.6±1.4	147.5 ± 1.4
n_2	0.37±0.01	0.330±0.004	3 [b]	3 [b]
m_2	0.05±0.01	-0.060±0.001	0.81±0.01	0.81 ± 0.02
q_2	-	-	0.999	0.999
log (A_3/s^{-1})	-	-	34.59±0.06	34.87±0.09
E_{a3}, kJ mol^{-1}	-	-	290.9±0.5	292.9 ± 0.6
n_3	-	-	0.361±0.004	0.38 ± 0.01
m_3	-	-	0 [b]	0 [b]
q_3	-	-	0.999	0.999
w_1 [c]	0.49±0.01	0.413±0.002	0.09 [b]	0.09 ± 0.01
w_2 [c]	-	-	0.379±0.003	0.38 ± 0.01
BIC [d]	-45812.4	-41813.1	-48027.4	-48016.2

[a] The kinetic scheme denoted as "ePT" corresponds to the extended Prout-Tompkins equation (4); "KJMAE" denotes the nucleation-growth reaction by equation (5). Connectivity between the reactions: "+" – independent parallel stages, and "→" – the consecutive stages. [b] These values were kept fixed during thermokinetic calculations. [c] The ratio of the first (w_1) and the second (w_2) reaction to the total conversion degree. [d] Bayesian informational criteria (BIC) values can be compared only for the same datasets.

3. Experimental thermochemical and phase change data for DDF

The sublimation enthalpy at a mean experimental temperature $\Delta_{sub}H_m(\langle T \rangle)$ was determined with the aid of the Langmuir equation:

$$\ln(\frac{dm}{dt}\sqrt{T}) = a - \frac{\Delta_{sub}H_m(\langle T \rangle)}{RT}. \qquad \text{(S1)}$$

Typical TGA experimental results in proper coordinates are shown in Figure S1. The vaporization enthalpies obtained were then recalculated to standard conditions using the following relationship:

$$\Delta_{sub}H^0(298\,K) = \Delta_{sub}H_m(\langle T \rangle) + \int_{298.15}^{\langle T \rangle}(c_p^{cr} - c_p^{gas})dT\,, \qquad \text{(S2)}$$

where the solid-state isobaric heat capacity c_p^{cr} values were obtained from differential scanning calorimetry (DSC) measurements.

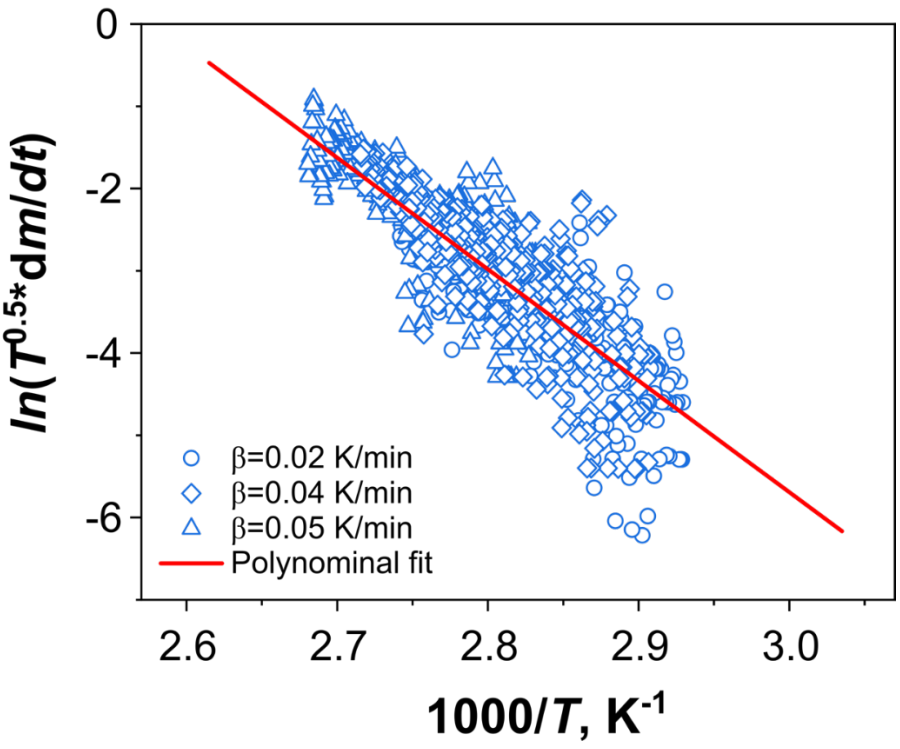

Figure S1. Logarithm of the TGA mass loss rate at various heating rates against reciprocal temperature obtained under reduced pressure 0.2 Pa.

4. PCM estimations of the solvation free energies for various decomposition channels of DDF

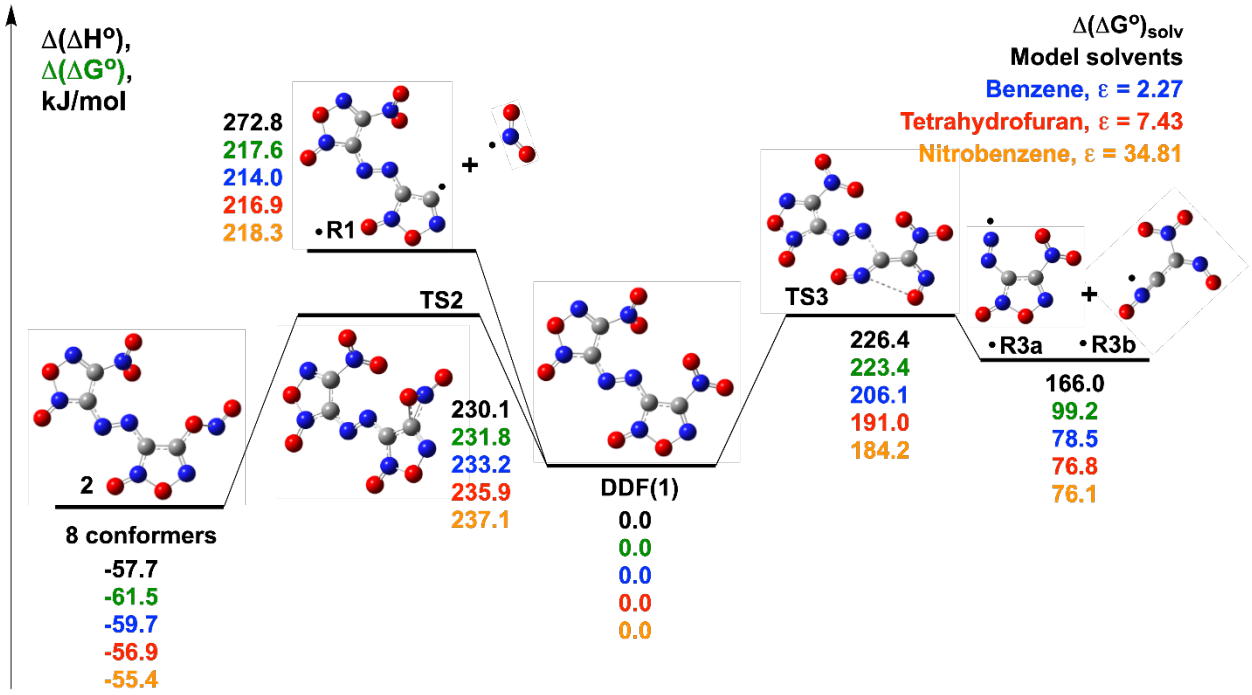

Figure S2. The stationary points on the PES for the three decomposition channels of BCHMX at 298 K in the three model solvents with the dielectric constants of ε = 2.3, 7.4, and 34.8 (cf. Figure 6 in the manuscript). All solvation Gibbs free energy values are calculated at the M06-2X/6-311++G(2df,p) level of theory and are given in kJ mol^{-1}.

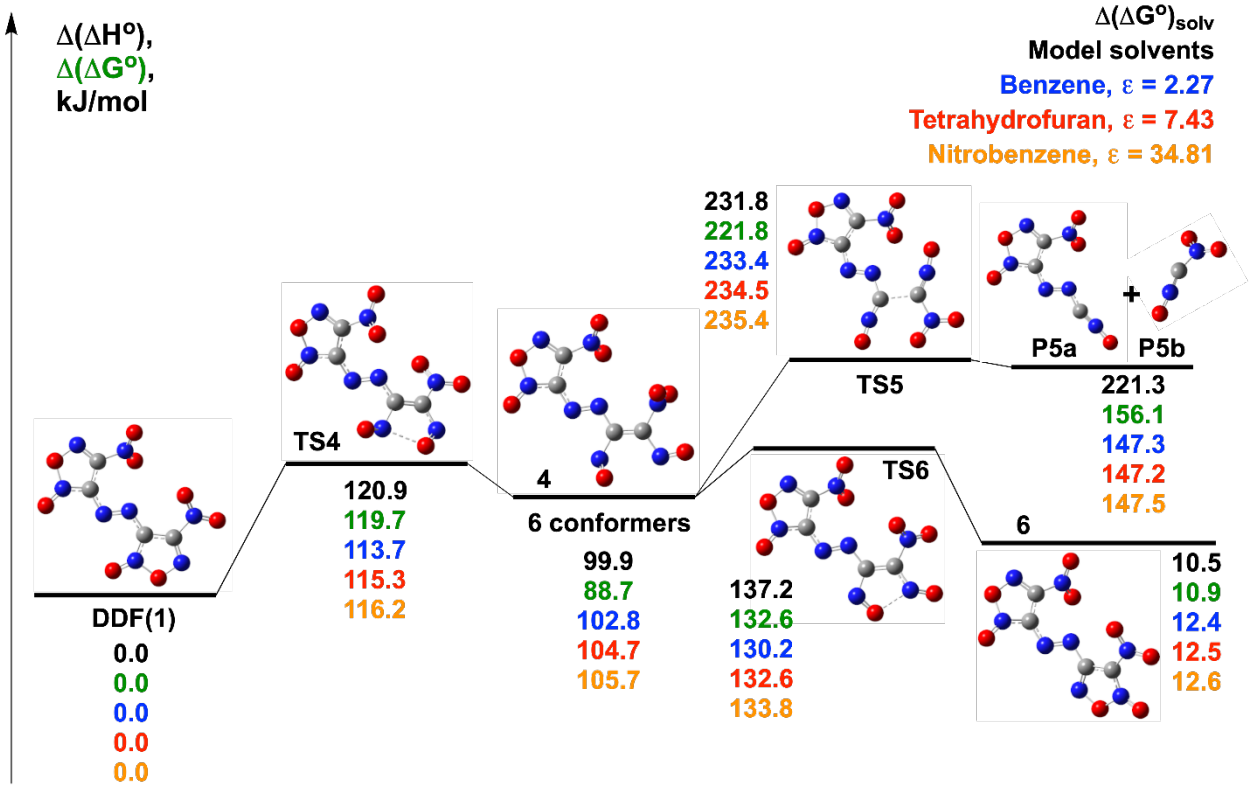

Figure S3. The stationary points on the PES corresponding to the conventional reactions of thermal decomposition of DDF at 298 K in the three model solvents with the dielectric constants of ε = 2.3, 7.4, and 34.8 (cf. Figure 7 in the manuscript). All solvation Gibbs free energy values are calculated at the M06-2X/6-311++G(2df,p) level of theory and are given in kJ mol^{-1}.

5. Raw quantum chemical data: optimized geometries, electronic energies, and thermal corrections to thermodynamic potentials of all compounds under study

M06-2X/6-311++G(2df,p) geometries, zero-point vibrational energies (unscaled) and thermal corrections to thermodynamic potentials, M06-2X/6-311++G(2df,p) and DLPNO-CCSD(T)/aug-cc-pVQZ electronic energies. All values are in Hartrees.

DDF (1)
Zero-point correction= 0.096843 (Hartree/Particle)
Thermal correction to Energy= 0.112621
Thermal correction to Enthalpy= 0.113565
Thermal correction to Gibbs Free Energy= 0.049671
Electronic energy:
M06-2X = -1191.579017
DLPNO-CCSD(T) = -1190.268526883991

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.786794	-0.596437	0.057578
2	6	0	-2.731383	0.114421	-0.103359
3	6	0	-1.537088	-0.647691	-0.030086
4	7	0	-1.958501	-1.903424	0.197115
5	8	0	-3.363522	-1.864031	0.250794
6	7	0	-0.240724	-0.207375	-0.075825
7	7	0	0.639746	-1.097323	-0.045266
8	6	0	1.903179	-0.561532	-0.046562
9	6	0	2.460601	0.735486	0.090941
10	7	0	2.958353	-1.361492	-0.251944
11	7	0	3.737390	0.735592	-0.020178
12	8	0	4.099309	-0.553063	-0.242391
13	8	0	-1.414289	-2.950719	0.368970
14	8	0	3.090903	-2.532508	-0.443212
15	7	0	1.764442	1.976544	0.445982
16	8	0	1.103067	1.916634	1.451909
17	8	0	1.936516	2.919980	-0.274342
18	7	0	-2.845857	1.548181	-0.380794
19	8	0	-3.859659	2.089384	-0.034857
20	8	0	-1.898355	2.036328	-0.945908

R1
Zero-point correction= 0.081418 (Hartree/Particle)
Thermal correction to Energy= 0.094455
Thermal correction to Enthalpy= 0.095399
Thermal correction to Gibbs Free Energy= 0.038211
Electronic energy:

M06-2X = -986.4070542
DLPNO-CCSD(T) = -985.294659864916

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-4.188156	1.095697	-0.244405
2	6	0	-2.977331	1.421789	-0.341425
3	6	0	-2.071564	0.353133	-0.145741
4	7	0	-2.871900	-0.708105	0.093335
5	8	0	-4.191649	-0.270738	0.037676
6	7	0	-0.706044	0.374352	-0.175147
7	7	0	-0.132614	-0.723564	0.017059
8	6	0	1.235066	-0.602447	-0.003522
9	6	0	2.166170	0.466424	-0.007327
10	7	0	1.992798	-1.705415	-0.058118
11	7	0	3.381941	0.063633	-0.061902
12	8	0	3.329190	-1.290581	-0.101832
13	8	0	-2.668504	-1.861583	0.329121
14	8	0	1.758951	-2.876770	-0.091866
15	7	0	1.883711	1.895365	0.151511
16	8	0	1.262516	2.184445	1.142524
17	8	0	2.305470	2.630584	-0.699154

TS2
Zero-point correction= 0.093754 (Hartree/Particle)
Thermal correction to Energy= 0.109468
Thermal correction to Enthalpy= 0.110412
Thermal correction to Gibbs Free Energy= 0.047234
Electronic energy:
M06-2X = -1191.4889258
DLPNO-CCSD(T) = -1190.177763867115

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.792690	-0.560638	0.068137
2	6	0	2.698454	0.109757	0.195658
3	6	0	1.530728	-0.699294	0.072231
4	7	0	2.004690	-1.938313	-0.133067
5	8	0	3.384391	-1.876873	-0.151026
6	7	0	0.244486	-0.265958	0.119098
7	7	0	-0.653589	-1.130458	-0.021754
8	6	0	-1.907486	-0.570986	-0.000224
9	6	0	-2.438089	0.743824	-0.017726
10	7	0	-2.983752	-1.363739	0.079949
11	7	0	-3.718248	0.762186	0.047985
12	8	0	-4.111062	-0.532905	0.114858
13	8	0	1.475772	-2.997162	-0.297099
14	8	0	-3.146016	-2.546138	0.138285

15	7	0	-1.704355	2.000061	-0.194259
16	8	0	-1.011885	2.055958	-1.179737
17	8	0	-1.869387	2.846683	0.640849
18	7	0	2.654334	1.669813	-0.066512
19	8	0	2.697824	1.414494	1.199283
20	8	0	2.985934	2.672133	-0.564996

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2 (the lowest conformer out of 8)
Zero-point correction= 0.094625 (Hartree/Particle)
Thermal correction to Energy= 0.111051
Thermal correction to Enthalpy= 0.111995
Thermal correction to Gibbs Free Energy= 0.046609
Electronic energy:
M06-2X = -1191.5996801
DLPNO-CCSD(T) = -1190.288902500324

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.608700	-1.010062	-0.191737
2	6	0	-2.604604	-0.208854	-0.332295
3	6	0	-1.363817	-0.889399	-0.141691
4	7	0	-1.695918	-2.161433	0.123185
5	8	0	-3.081592	-2.241734	0.103945
6	7	0	-0.118876	-0.335640	-0.183118
7	7	0	0.849197	-1.109310	0.009295
8	6	0	2.044424	-0.430039	-0.007697
9	6	0	2.434292	0.932409	0.012897
10	7	0	3.196265	-1.106745	-0.076818
11	7	0	3.706235	1.084658	-0.041364
12	8	0	4.232070	-0.162869	-0.105553
13	8	0	-1.069581	-3.153012	0.363607
14	8	0	3.481807	-2.266598	-0.132294
15	7	0	1.572190	2.103431	0.195164
16	8	0	0.892504	2.087698	1.190447
17	8	0	1.636852	2.961780	-0.641845
18	7	0	-3.718481	1.766087	0.365958
19	8	0	-2.724411	1.077953	-0.618392
20	8	0	-3.909542	2.816581	0.016179

TS3
Zero-point correction= 0.091714 (Hartree/Particle)
Thermal correction to Energy= 0.108456
Thermal correction to Enthalpy= 0.109400
Thermal correction to Gibbs Free Energy= 0.043577
Electronic energy:
M06-2X = -1191.4872961
DLPNO-CCSD(T) = -1190.177822264954

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	-4.027011	-0.353338	1.065794
2	6	0	-3.128891	0.007061	0.092019
3	6	0	-1.957444	-0.678631	-0.128604
4	7	0	-1.456293	-1.799718	-0.167681
5	8	0	-3.727074	-1.315794	1.743663
6	7	0	-0.389516	0.287685	-0.169325
7	7	0	0.494672	-0.448042	-0.160743
8	6	0	1.856671	-0.396936	-0.102534
9	6	0	2.813029	0.626359	0.132278
10	7	0	2.577214	-1.513544	-0.321088
11	7	0	4.011119	0.180339	0.067332
12	8	0	3.919566	-1.139474	-0.216076
13	8	0	-0.350763	-2.281615	-0.028323
14	8	0	2.316162	-2.639377	-0.572929
15	7	0	2.549428	2.025213	0.481856
16	8	0	1.412288	2.241565	0.824511
17	8	0	3.467337	2.787493	0.405977
18	7	0	-3.421277	1.122517	-0.752954
19	8	0	-4.413308	1.774369	-0.545136
20	8	0	-2.607776	1.340971	-1.644348

R3a

Zero-point correction= 0.050294 (Hartree/Particle)
Thermal correction to Energy= 0.059068
Thermal correction to Enthalpy= 0.060012
Thermal correction to Gibbs Free Energy= 0.014415

Electronic energy:

M06-2X = -650.4854103
DLPNO-CCSD(T) = -649.766104627904

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.096964	2.601620	-0.296718
2	7	0	-0.767613	1.847165	-0.056821
3	6	0	-0.616429	0.445556	-0.003707
4	6	0	0.442703	-0.494358	-0.007210
5	7	0	-1.726944	-0.292504	0.031386
6	7	0	0.020316	-1.706827	0.025824
7	8	0	-1.327101	-1.637321	0.047225
8	8	0	-2.895785	-0.044708	0.038024
9	7	0	1.879730	-0.221556	0.041474
10	8	0	2.178223	0.826511	0.559409
11	8	0	2.610310	-1.057291	-0.413473

R3b

Zero-point correction= 0.039731 (Hartree/Particle)
Thermal correction to Energy= 0.047646

Thermal correction to Enthalpy= 0.048590
Thermal correction to Gibbs Free Energy= 0.004838
Electronic energy:
M06-2X = -541.0324068
DLPNO-CCSD(T) = -540.434234899041

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.157343	-0.208186	-0.000082
2	6	0	-1.018904	-0.018049	-0.000032
3	6	0	0.358728	0.250670	0.000029
4	7	0	0.897303	1.412783	0.000157
5	8	0	0.473956	2.527155	0.000259
6	8	0	-3.326455	-0.404847	-0.000133
7	7	0	1.314470	-0.878671	-0.000047
8	8	0	2.485974	-0.607385	0.000006
9	8	0	0.814031	-1.974574	-0.000155

TS4
Zero-point correction= 0.092528 (Hartree/Particle)
Thermal correction to Energy= 0.108731
Thermal correction to Enthalpy= 0.109676
Thermal correction to Gibbs Free Energy= 0.045241
Electronic energy:
M06-2X = -1191.5317165
DLPNO-CCSD(T) = -1190.218549643899

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	3.961595	-0.388516	0.079840
2	6	0	2.733928	0.164918	-0.172885
3	6	0	1.618182	-0.549558	0.154881
4	7	0	1.848243	-1.900614	0.581144
5	8	0	3.907528	-1.292570	0.892844
6	7	0	0.319688	-0.129918	0.007306
7	7	0	-0.525176	-0.989392	-0.305491
8	6	0	-1.816541	-0.538428	-0.245051
9	6	0	-2.496508	0.611071	0.236616
10	7	0	-2.780945	-1.289463	-0.804584
11	7	0	-3.754689	0.569626	-0.001323
12	8	0	-3.982723	-0.596197	-0.657327
13	8	0	1.154900	-2.435243	1.361194
14	8	0	-2.792375	-2.337628	-1.369114
15	7	0	-1.951401	1.706210	1.045163
16	8	0	-2.280328	2.819034	0.744276
17	8	0	-1.242567	1.355673	1.955312
18	7	0	2.702492	1.369079	-0.988369
19	8	0	3.697607	2.045964	-0.993187
20	8	0	1.666332	1.596330	-1.576144

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4 (the lowest conformer out of 6)
Zero-point correction= 0.092453 (Hartree/Particle)
Thermal correction to Energy= 0.109972
Thermal correction to Enthalpy= 0.110916
Thermal correction to Gibbs Free Energy= 0.042719
Electronic energy:
M06-2X = -1191.5336385
DLPNO-CCSD(T) = -1190.227726359043

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.892835	0.635817	-0.164476
2	6	0	-2.553242	0.138255	0.018560
3	6	0	-1.477487	0.908293	-0.157447
4	7	0	-1.590438	2.299633	-0.615424
5	8	0	-4.736150	-0.154133	0.123894
6	7	0	-0.211606	0.330418	-0.064299
7	7	0	0.709785	1.174800	-0.091759
8	6	0	1.954628	0.615985	-0.011594
9	6	0	2.504064	-0.693200	-0.032948
10	7	0	3.015252	1.422177	0.175760
11	7	0	3.774756	-0.692450	0.126448
12	8	0	4.142515	0.608486	0.269259
13	8	0	-2.336848	2.959409	0.026243
14	8	0	3.150719	2.599843	0.286028
15	7	0	1.812793	-1.953650	-0.327296
16	8	0	1.169369	-1.948834	-1.345180
17	8	0	1.974175	-2.852671	0.450163
18	7	0	-2.405427	-1.296332	0.327139
19	8	0	-2.517679	-2.048171	-0.603955
20	8	0	-2.227818	-1.571290	1.485790

TS5
Zero-point correction= 0.091853 (Hartree/Particle)
Thermal correction to Energy= 0.109109
Thermal correction to Enthalpy= 0.110054
Thermal correction to Gibbs Free Energy= 0.042320
Electronic energy:
M06-2X = -1191.4833343
DLPNO-CCSD(T) = -1190.176775123636

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.939208	-1.564930	0.478584
2	6	0	-2.462413	-0.541200	0.183433
3	6	0	-1.393615	1.040372	0.058089
4	7	0	-1.856263	2.142682	0.034302

5	8	0	-1.232360	-2.456178	0.786859
6	7	0	-0.117832	0.480600	0.100490
7	7	0	0.813571	1.295822	-0.042713
8	6	0	2.040388	0.673061	-0.026384
9	6	0	2.505733	-0.665613	-0.091699
10	7	0	3.150329	1.411536	0.098967
11	7	0	3.782988	-0.743131	-0.012261
12	8	0	4.234617	0.528623	0.117164
13	8	0	-2.502601	3.122420	0.029961
14	8	0	3.364865	2.581158	0.208851
15	7	0	1.726012	-1.879709	-0.359590
16	8	0	0.986998	-1.807906	-1.309875
17	8	0	1.917706	-2.817153	0.362636
18	7	0	-3.871911	-0.257279	-0.116207
19	8	0	-4.625999	-1.191215	-0.064263
20	8	0	-4.137520	0.885393	-0.382787

P5a

Zero-point correction= 0.065964 (Hartree/Particle)
Thermal correction to Energy= 0.077460
Thermal correction to Enthalpy= 0.078404
Thermal correction to Gibbs Free Energy= 0.026006
Electronic energy:
M06-2X = -818.4697444
DLPNO-CCSD(T) = -817.55277719

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.698991	-0.360027	-0.055867
2	7	0	-3.849079	-0.239246	-0.088004
3	7	0	-1.387073	-0.065978	-0.111603
4	7	0	-0.609053	-1.026289	0.102480
5	6	0	0.708844	-0.650581	0.046031
6	6	0	1.433809	0.566342	-0.031753
7	7	0	1.652954	-1.603357	0.023335
8	7	0	2.700355	0.381621	-0.097725
9	8	0	2.890016	-0.961304	-0.073133
10	8	0	-5.039372	-0.202832	-0.103388
11	8	0	1.630641	-2.796650	0.049653
12	7	0	0.908381	1.930919	0.071429
13	8	0	0.230589	2.140552	1.044856
14	8	0	1.215954	2.697971	-0.799219

P5b

Zero-point correction= 0.025267 (Hartree/Particle)
Thermal correction to Energy= 0.030586
Thermal correction to Enthalpy= 0.031530
Thermal correction to Gibbs Free Energy= -0.004841
Electronic energy:

M06-2X = -373.0242743
DLPNO-CCSD(T) = -372.627782427409

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.436938	0.000073	0.051578
2	6	0	0.319196	0.000063	0.354918
3	8	0	2.598130	-0.000056	-0.156679
4	7	0	-1.065459	-0.000015	0.028200
5	8	0	-1.581266	-1.081682	-0.089642
6	8	0	-1.581305	1.081640	-0.089672

TS6
Zero-point correction= 0.092552 (Hartree/Particle)
Thermal correction to Energy= 0.108906
Thermal correction to Enthalpy= 0.109850
Thermal correction to Gibbs Free Energy= 0.044206
Electronic energy:
M06-2X = -1191.5249537
DLPNO-CCSD(T) = -1190.212530285139

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.766566	-0.649976	-0.162428
2	6	0	-2.533588	-0.064308	-0.085416
3	6	0	-1.427703	-0.837220	0.162913
4	7	0	-1.720043	-2.166668	0.421408
5	8	0	-4.806046	-0.162090	0.124611
6	7	0	-0.140755	-0.345402	0.053361
7	7	0	0.756506	-1.210123	-0.004620
8	6	0	2.013302	-0.658457	-0.028299
9	6	0	2.569116	0.635262	0.143962
10	7	0	3.064125	-1.438520	-0.320993
11	7	0	3.839238	0.651396	-0.025599
12	8	0	4.198746	-0.622581	-0.323745
13	8	0	-2.869251	-2.355970	0.742384
14	8	0	3.195476	-2.597313	-0.573952
15	7	0	1.882823	1.853720	0.584079
16	8	0	1.251278	1.739549	1.604542
17	8	0	2.030718	2.833893	-0.091379
18	7	0	-2.420124	1.311111	-0.608044
19	8	0	-3.107043	2.118404	-0.041866
20	8	0	-1.668027	1.484805	-1.530481

6
Zero-point correction= 0.097069 (Hartree/Particle)
Thermal correction to Energy= 0.112776
Thermal correction to Enthalpy= 0.113720

Thermal correction to Gibbs Free Energy= 0.050110

Electronic energy:

M06-2X = -1191.5746457

DLPNO-CCSD(T) = -1190.264759916173

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.610003	-0.645092	0.321554
2	6	0	-2.567478	0.054156	-0.123710
3	6	0	-1.401080	-0.620950	0.315449
4	7	0	-1.717855	-1.664967	1.008401
5	8	0	-4.794982	-0.558625	0.234670
6	7	0	-0.081945	-0.165895	0.161978
7	7	0	0.722067	-1.088055	-0.051022
8	6	0	2.027135	-0.656330	-0.113589
9	6	0	2.731252	0.542263	0.167131
10	7	0	2.961429	-1.493515	-0.588896
11	7	0	3.979637	0.452533	-0.107504
12	8	0	4.173936	-0.800970	-0.591136
13	8	0	-3.073962	-1.722975	1.036065
14	8	0	2.945564	-2.614761	-0.992183
15	7	0	2.220799	1.751536	0.820691
16	8	0	1.618814	1.555099	1.846032
17	8	0	2.469859	2.799524	0.293333
18	7	0	-2.704543	1.212773	-0.956948
19	8	0	-3.801183	1.698760	-1.063818
20	8	0	-1.678807	1.590191	-1.479144