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Supporting information

Learning to Fly: Thermochemistry of Energetic Materials by Modified Thermogravimetric Analysis and Highly Accurate Quantum Chemical Calculations

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Contents

S1. Characterization of the compounds studied

Table S1 lists the compounds studied. They include the non-energetic species taken as references for thermochemical parameters (entries ##1-11), and the species with typical explosophoric functional groups or structural units, i.e., nitroaromatics (##12-16), alyphatic nitrocompounds (##17, 18), fluorine containing species (#19), nitramines (##20-26), caged nitramines (##27, 28), nitroesters (##29-31), diaziridine (#32), imidazoles (##33-34), pyrazoles (##35-42), pyrazines (##43, 44), triazoles (##45, 46), tetrazoles (##49-50), azasydnones (##51, 52), furazans (##53-57), furoxans (##58-63). All these compounds are comprised of CHNO atoms, except #19, which extends the proposed methodology to CHNOF compounds. Moreover, to cope with some typical difficulties in a common calorimetric experiment, we consider the two species (##47, 49) containing the water molecules in the crystal and #19, which is liquid at room temperature.

Due to the difficulties in determining of the accurate purity values for the materials with common physico-chemical tools, it was measured only for selected compounds (via DSC or NMR with the internal standard). For the rest of materials (denoted as "P" in the corresponding column) the NMR, MS spectra and the elemental analysis results were used for characterization. If the complete characterization of the species was published, the literature reference is given.

Table S1. List of investigated compounds with their purity and phase transition parameters.

#	Compound	Formula	Abbreviation	Purity / mol. %	T_m / °C		ΔH_m (T_m) / kJ mol^{-1}	
					exp.	ref.	exp.	ref.
1	Acetamide	C_2H_5NO	**ACM**	99.8[a]	80.5 ± 0.2[d,f]	80.3[1] 81.8[2]	16.2 ± 0.8[d,e]	15.6[1,3]
2	Carbamide	CH_4N_2O	**Urea**	P	133	132.9[4]	–[c]	–
3	2-Amino-3-methylbutanoic acid	$C_5H_{11}NO_2$	**Val**	P	294[d]	298[5]	–[c]	–
4	Benzoic acid	$C_7H_6O_2$	**BCA**	99.9[a]	122.1 ± 0.4	122.1 ± 0.7[4]	18.1 ± 0.6[d]	17.3[6] 16.2[7] 18.0[8]
5	Naphtalene	$C_{10}H_8$	**NPH**	99.9[a]	80.4 ± 0.3[f]	80.1 ± 0.7[4]	20.2 ± 0.4[d,e]	19.6[9] 19.3[10]
6	Adamantane	$C_{10}H_{16}$	**ADM**	P	267[d]	269[11] 270[12] 279[13]	–	14.0[12] 10.9[14]
7	Anthracene	$C_{14}H_{10}$	**ANT**	99.9[a]	216.3 ± 0.1[d]	217 ± 3[4]	29.3 ± 0.9[d,e]	28.8[15] 29.8[16]
8	Trans-azobenzene	$C_{12}H_{10}N_2$	**tAB**	99.9[a]	67.8 ± 0.5[d]	66.8[17]	27.6 ± 0.3[d]	20.8[17]

						67.9[18]		21.3[19] 22.6[20]
9	Hypoxanthine	$C_5H_4N_4O$	**HPX**	P	405[d]	–	–[c]	–
10	1,3-Dimethylxanthine	$C_7H_8N_4O_2$	**TPL**	99.9[a]	271.1 ± 0.3	269.1 for form II, 273.4 for form I [21] 270.6[22]	25.2 ± 1.8	28.2 for form II, 26.4 for form I [21] 31.2[22]
11	6,7,9,10,17,18,20,21-Octahydrodibenzo[b,k][1,4,7,10,13,16]hexaoxacyclooctadecine	$C_{20}H_{24}O_6$	**D18C6**	99.9[a]	162.1 ± 0.1	162.6[23] 166.9[24]	57.1 ± 1.5	55.4[24] 60.7[25] 56[23]
12	1-Azido-4-nitrobenzene	$C_6H_4N_4O_2$	**4-NPA**	99.9[a]	69.7 ± 0.4	72[26] 73.9[27]	25.1 ± 1.3	17.1 [26]
13	1-Methyl-2,4-dinitrobenzene	$C_7H_6N_2O_4$	**24-DNT**	99.9[a]	69.4 ± 0.3	67.9[28] 71.2[29]	25.3 ± 0.7	20.1[30] 20.9[10]
14	2,4-Dinitroanisole	$C_7H_6N_2O_5$	**DNAN**	99.9[a]	86.2 ± 0.6	87.5 for β-, 96.7 for α-[31] 86.8[32]	21.1 ± 0.8	20.2 [33]
15	2,4,6-Trinitrotoluene	$C_7H_5N_3O_6$	**TNT**	99.8[b]	80.4 ± 0.3[34]	80.7[35]	22.5 ± 0.5[34]	23.4[36]
16	N-Methyl-N-(2,4,6-trinitrophenyl)nitramide	$C_7H_5N_5O_8$	**Tetryl**	99.9[a]	129.0 ± 0.6	128.7-129.1[37] 127.4[38] 129.5[39]	25.3 ± 1.5	22.9[39] 25.9[38]
17	2,2-Dinitroethene-1,1-diamine	$C_2H_4N_4O_4$	**FOX-7**	P	–[g]	–	–[g]	–
18	Tetranitroacetimidic acid	$C_2HN_5O_9$	**TNAA**	99.5[b]	91.0 ± 0.2[40]	91[41]	14.9 ± 1.8[c] [40]	–
19	Bis(2-fluoro-2,2-dinitroethyl)formal	$C_5H_6N_4O_{10}F_2$	**FEFO**	P	–	13.4[42] 14.5[43]	–	–
20	Nitroguanidine	$CH_4N_4O_2$	**NIGU**	P	–	–	–	–
21	2,4-Dinitro-2,4-diazapentane	$C_3H_8N_4O_4$	**DNDAP**	99.8[a]	54.8 ± 0.4[f]	54[44] 54.4[45]	22.3 ± 1.1	16.4[46]
22	1,4-Dinitropiperazine	$C_4H_8N_4O_4$	**DNPP**	99.9[a]	216.2 ±0.3[d,f]	214[46] 215[47]	35.2 ± 1.1[d]	33.8[46]

23	1,3,5-Trinitroperhydro-1,3,5-triazine	$C_3H_6N_6O_6$	**RDX**	P	204.2 ± 0.3[c] [34]	204.0±0.1[39]	27.5 ± 0.9[c][34]	33.9±1.0[48]
24	Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine	$C_4H_8N_8O_8$	**HMX**	P	280[c]	280.8±1.1[48]	–[c,g]	31.9±3.9[48]
25	1,9-diazido-2,4,6,8-tetranitro-2,4,6,8-tetrazanonane	$C_5H_{10}N_{14}O_8$	**DATN**	P	177.4 ± 0.5[c]	176-177[49] 177[50]	–[c]	–
26	cis-2,4,6,8-Tetra-nitro-1H,5H-2,4,6,8-tetraazabicyclo-[3.3.0]-octane	$C_4H_6N_8O_8$	**BC-HMX**	P	–	–	–	–
27	4,10-Dinitro-2,6,8,12-tetraoxa-4,10-diazatetracyclo[5.5.0.05,9.03,11]-dodecane	$C_6H_6N_4O_8$	**TEX**	99.0[b]	–	–	–	–
28	2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane	$C_6H_6N_{12}O_{12}$	**CL-20**	P	–	–	–[g]	–
29	Erythritol tetranitrate	$C_4H_6N_4O_{12}$	**ETN**	99.6[a]	61.2 ± 0.7	60±2[51]	36.9 ± 3.3[d]	32±3[51]
30	Pentaerythritol tetranitrate	$C_5H_8N_4O_{12}$	**PETN**	99.9[a]	140.9±0.3	141.0±0.2[48] 142±2[51]	48.1±1.1	40±7[51] 53.8±3.9[48]
31	2,3-Hydroxymethyl-2,3-dinitro-1,4-butanediol tetranitrate	$C_6H_8N_6O_{16}$	**SMX**	99.4[a]	86.6 ± 0.7	85-86[52]	43.7 ± 3.0	35±6[51]
32	3,3-Pentamethylenediaziridine	$C_6H_{12}N_2$	**PMDA**	P	105[d,f]	–	28[d]	–
33	2,4-Dinitroimidazole	$C_3H_2N_4O_4$	**24-DNI**	P	–	278-280[53] 265-274[54]	–	–
34	4,5-Dinitroimidazole	$C_3H_2N_4O_4$	**45-DNI**	P	179.9 ± 1.0[f]	187-188[55]	23.3 ± 1.6	–
35	3,4-Dinitro-1H-pyrazole	$C_3H_2N_4O_4$	**34-DNP**	99.5[a]	85.9 ± 0.8[f]	87[56] 89[57]	14.2 ± 0.3	–
36	3,5-Dinitro-1H-pyrazole	$C_3H_2N_4O_4$	**35-DNP**	P	169.2 ± 0.3 [58]	168[56] 172[59]	20.7 ± 0.8	–
37	3,5-Dinitropyrazole-1-amine	$C_3H_3N_5O_4$	**1-ADP**	99.7[a]	112.9 ± 0.7[f]	112[60] 113[61]	23.6 ± 2.2	–
38	5-Amino-3,4-dinitro-1H-pyrazole	$C_3H_3N_5O_4$	**5-ADP**	99.5[b]	195[c]	–	–[c]	–
39	3,4,5-Trinitro-1H-pyrazole	$C_3HN_5O_6$	**TNP**	99.8[a]	186.3±0.6[f]	182-184[62] 187[63] 186[56]	24.9±1.9	28.2[64] 28.8[63]

40	1-Methyl-3,4,5-trinitropyrazole	$C_4H_3N_5O_6$	**MTNP**	99.8[a]	90.6 ± 0.5[d,f]	90.8[56] 91.3[65]	19.2 ± 1.7[d]	17[63]
41	3,6-Dinitropyrazolo[4,3-c]pyrazole	$C_4H_2N_6O_4$	**DNPPy**	P	–	–	–	–
42	1,2,9,10-Tetranitrodipyrazolo[1,5-d:5′,1′-f][1,2,3,4]-tetrazine,	$C_6N_{10}O_8$	**TNDPT**	P	195.5 ± 1.6[c]	205[h] [66]	–[c]	–
43	2,6-Diamino-3,5-dinitropyrazine	$C_4H_4N_6O_4$	**ANPZ**	P	–	–	–	–
44	2,6-Diamino-3,5-dinitropyrazine-1-oxide	$C_4H_4N_6O_5$	**LLM-105**	P	–	–	–	–
45	5-Amino-3-nitro-1H-1,2,4-triazole	$C_2H_3N_5O_2$	**ANTA**	P	242.4[c]	–	–[c]	–
46	3-Nitro-1,2,4-triazol-5-one	$C_2H_3N_5O_2$	**NTO**	P	–	–	–	–
47	1H-Tetrazol-5-ylamine hydrate	CH_3N_5	**5-ATZ**	P	205.1 ± 0.2	205[67] 203[68]	–[c]	–
48	1,5-Diaminotetrazole	CH_4N_6	**DAT**	99.9[a]	187.3 ± 0.8	187-188[69]	26.7 ± 1.4[c]	–
49	5,5’-Bi-1H-tetrazole	$C_2H_2N_8$	**BTZ**	P	–	–	–	–
50	5,5'-Bistetrazole-1,1'-diol hydrate	$C_2H_6N_8O_4$	**BTO**	P	–	–	–	–
51	3-Phenyl-1,2,3,4-oxatriazolium-5-olat	$C_7H_5N_3O_2$	**Ph-Azs**	P[70]	81.7 ± 0.5	–	20.8 ± 0.5	–
52	3-(4-Tolyl)-1,2,3,4-oxatriazolium-5-olat	$C_8H_7N_3O_2$	**4-Tol-Azs**	P[70]	98.7 ± 1.1[f]	–	20.5 ± 0.3	–
53	3-Amino-4-nitro-1,2,5-oxadiazole	$C_3H_3N_3O_4$	**ANF**	99.4[a]	123.8 ±0.8[d,f]	121[71]	27.6 ± 1.7[d]	–
54	3,4-Diaminofurazan	$C_2H_4N_4O$	**DAF**	99.9[a]	179.9 ±0.3[d]	179-180[72]	23.1 ± 0.4[d]	
55	3,4-Di(nitramino)furazan	$C_2H_2N_6O_5$	**DNAF**	P	94.2[c]	93[73]	–[c]	–
56	3,3'-Diamino-4,4'-azofurazan	$C_4H_4N_8O_2$	**DAAzF**	P	–	325[74]	–	–
57	3,3'-Diamino-4,4'-azoxyfurazan	$C_4H_4N_8O_3$	**DAAF**	P	253.9 [c]	249[74]	–[c]	–
58	3-Methyl-4-nitro-1,2,5-oxadiazole 2-oxide	$C_3H_3N_3O_4$	**34-MNF**	P	60; 65	67-68[75]	21.3 ± 0.4	–
59	4-Methyl-3-nitro-1,2,5-oxadiazole 2-oxide	$C_3H_3N_3O_4$	**43-MNF**	99.7[a]	40.7 ± 0.3[f]	–	15.1 ± 0.2	–
60	3-Cyano-4-nitrofuroxan	$C_3N_4O_4$	**34-CNF**	99.6[a]	48.1 ± 0.3[d,f]	48-49[76]	22.8 ± 0.9[d]	–
61	Benzotris[1,2,5]oxadiazole, 1,4,7-trioxide	$C_6N_6O_6$	**BTF**	99.3[a]	197.1 ±0.4[d,f]	194-195[77] 196-197[78] 201[79]	22.7 ± 1.6[c,d]	–

62	4-nitro-(4-nitrofurazan-3-yl)furoxan	$C_4N_6O_7$	**NNFF**	P[80]	105.7 ±1.1[d,f]	–	33.0 ± 2.8	–
63	4,4'-Dinitro-3,3'-bisfuroxan	$C_4N_6O_8$	**DNBF**	P[81]	134.5 ± 0.5[c]	–	24.9 ± 3.3[c]	–

[a] The purity is determined by DSC.
[b] The purity determined by NMR with an internal standard.
[c] Melting upon decomposition.
[d] High pressure DSC was used to suppress evaporation.
[e] The enthalpy value was corrected to account for a slight mass loss (<10%).
[f] The melting temperature for pure sample obtained from the Van't-Hoff equation [82].
[g] The phase transition instead of melting observed with the following parameters:
CL-20: the temperature onset 164.3±0.5°C, the enthalpy 6.9±0.9 kJ/mol in agreement with 7.2[83] and 7.9±0.4[84] kJ/mol
HMX: the temperature onset 189.9±2.0°C, the enthalpy 8.3±0.9 kJ/mol in agreement with 9.8±0.8[38] kJ/mol
FOX-7: the temperature onset 120.5±1.2°C, the enthalpy 2.5±0.2 kJ/mol in agreement with 3.2±0.5[85] kJ/mol and the temperature onset 166.0±0.9°C, enthalpy 2.8±0.5 kJ/mol in agreement with 2.6±0.5[85] kJ/mol
[h] The peak temperature was reported in the original paper, while all temperature values in present study correspond to the extrapolated onset of the peak.

S2. Thermal corrections of the phase change data

The enthalpy data obtained at elevated temperature can be corrected to the standard conditions (298 K) using several approaches. Since the heat capacity values for novel energetic materials are often unknown, semiempirical corrections were considered either with the constant $\Delta c_p^{s\rightarrow g}$:[86]

$$\Delta_s^g H_m^0 = \Delta_s^g H_m(T_{ave}) + 0.032 \cdot (T_{ave} - 298.15), \quad \text{(S1)}$$

or with an estimated solid-state heat capacity by group additivity methods:[86]

$$\Delta_s^g H_m^0 = \Delta_s^g H_m(T_{ave}) + \left[0.75 + 0.15 \cdot c_p^s(estd)\right] \cdot (T_{ave} - 298.15), \quad \text{(S2)}$$

or with a gas-phase heat capacity only:[87]

$$\Delta_s^g H_m^0 = \Delta_s^g H_m(T_{ave}) + \left[-0.9 + 0.176 \cdot c_p^g\right] \cdot (T_{ave} - 298.15), \quad \text{(S3)}$$

The enthalpy of vaporization can be corrected analogously – via adjustment with a constant $\Delta c_p^{l\rightarrow g}$:[88]

$$\Delta_l^g H_m^0 = \Delta_l^g H_m(T_{ave}) + 0.054 \cdot (T_{ave} - 298.15), \quad \text{(S4)}$$

or via an estimated liquid-state heat capacity:[86]

$$\Delta_l^g H_m^0 = \Delta_l^g H_m(T_{ave}) + \left[10.58 + 0.26 \cdot c_p^l(estd)\right] \cdot (T_{ave} - 298.15). \quad \text{(S5)}$$

For a subset of selected compounds we compared the accurate temperature corrections using Eq. (5) with accounting for temperature dependence of the solid-state heat capacity (from DSC data or from literature) and the gas-phase heat capacity (obtained by quantum chemical calculations) with the approximations (S1) - (S5).

Table S2. Thermal adjustment of the sublimation enthalpy data by various methods

	Thermal correction value (second term in Eq. 5)				Error		
Compound	exact $\Delta c_p^{s\rightarrow g}$	Equation S1	Equation S2	Equation S3	Equation S1	Equation S2	Equation S3
ACM	0.5	1.2	0.5	0.5	0.7	0.0	0.0
Urea	0.8	1.2	0.6	0.5	0.4	-0.3	-0.4
Val	4.8	6.3	5.0	5.1	1.6	0.2	0.4
BCA	2.0	2.2	1.6	1.4	0.2	-0.4	-0.6
NPH	1.4	1.1	0.9	0.7	-0.3	-0.5	-0.6
ADM	1.8	1.2	1.0	0.9	-0.6	-0.7	-0.9
ANT	5.8	4.6	4.6	4.3	-1.2	-1.2	-1.4
tAB	0.8	0.5	0.6	0.5	-0.2	-0.2	-0.2
TPL	3.0	6.8	6.4	6.8	3.9	3.4	3.9
DB18C6	5.9	3.6	7.5	7.4	-2.4	1.6	1.5

DNAN	1.2	1.3	1.4	1.4	0.2	0.3	0.2
TNT	1.9	1.1	1.4	1.3	-0.8	-0.5	-0.6
Tetryl	4.0	2.5	3.6	3.6	-1.5	-0.4	-0.5
FOX-7	5.4	5.2	4.4	4.1	-0.2	-1.0	-1.3
NIGU	2.5	3.8	2.3	2.2	1.3	-0.2	-0.4
DNPP	6.4	4.9	5.8	4.6	-1.5	-0.6	-1.8
RDX	4.1	2.4	2.7	2.4	-1.8	-1.5	-1.7
HMX	6.7	4.5	8.1	6.6	-2.2	1.4	-0.1
TEX	4.1	6.9	7.3	7.5	2.8	3.2	3.4
CL-20	19.7	4.7	10.5	9.5	-14.9	-9.2	-10.2
PETN	4.9	2.3	3.7	3.6	-2.6	-1.2	-1.3
5-ADP	4.6	4.0	3.5	3.4	-0.6	-1.1	-1.3
LLM-105	3.4	5.4	5.4	5.9	2.0	2.0	2.5
NTO	1.4	3.2	1.8	1.9	1.8	0.4	0.5
DAF	6.3	4.3	3.0	2.3	-2.0	-3.4	-4.1
DAAzF	3.1	3.3	3.4	3.4	0.2	0.3	0.3
Average deviation					-0.7	-0.4	-0.6
Absolute average deviation					1.8	1.3	1.5
Maximal absolute deviation					14.9	9.2	10.2

Table S3. Thermal corrections to the evaporation enthalpy data by various methods.

	correction			difference	
Corrections	exact $\Delta c_p^{l\rightarrow g}$	Equation S4	Equation S5	Equation S4	Equation S5
ACM	6.6	4.9	4.4	-1.7	-2.3
BCA	11.1	7.0	7.7	-4.0	-3.4
NPH	5.6	4.7	5.4	-0.9	-0.2
tAB	3.0	6.7	10.2	3.7	7.2
DB18C6	45.8	12.4	39.2	-33.4	-6.6

FEFO	5.7	1.6	3.9	-4.1	-1.7
Average deviation (AD)				-6.7	-1.2
Absolute average deviation (AAD)				6.8	3.1
Maximal absolute deviation (MAD)				33.4	7.2

S3. Summary of the experimental sublimation and vaporization enthalpies.

Table S4. Comparison of the experimentally determined sublimation and evaporation enthalpies with the literature data.

#	Compound	ΔH_{ev} (298 K) / kJ mol^{-1}		Details	ΔH_s (298 K) / kJ mol^{-1}				Details
		this study	literature		this study	literature	evaporation + melting	Trouton-Williams equation (4)	
1	**ACM**	65.6 ±2.8	68.6[89] [a] 65.2[90] [a]	Argon flow, β = 0.15-5 K min^{-1}, 3 runs, <T> = 120°C	83.2 ±1.6	80.3[91] 78.3[2] [a]	78.7 ± 3.0	66	Argon flow, β = 0.15-0.3 K min^{-1}, 3 runs, <T> = 64°C
2	**Urea**				97.2 ±1.9	95.5[92] (tr) 96.3[93] (cl) 98.3[94] (to) 76.9[95] (to) 89[96] (ef)		77	Vacuum, β = 0.1-1 K min^{-1}, 4 runs, <T> = 63°C
3	**Val**				135.1 ±2.2	167.8[97] [a]		107	Argon flow, β = 0.5-5 K min^{-1}, 3 runs, <T> = 223°C
4	**BCA**	75.3 ±2.8	73.2[98] [a] (tr) 69.3[99] [a] (tg) 72.4[4] [a] (is) 76.5[100] [a] (ma) 83[101][a] (ch)	Argon flow, β = 1-5 K min^{-1}, 4 runs, <T> = 155°C	94.0 ±1.6	89.7±1.0[102] (cl) 90± 4[4] (re) 89.5±0.2[103] (re) 95.1±1.8[104] (ef)	88.5 ± 3.1	75	Argon flow, β = 0.15-2 K min^{-1}, 8 runs, <T> = 95°C
5	**NPH**	52.5 ±3.0	53.4[14] (ch) 54.8[105] (eb) 50.3[106] (ma)	Argon flow, β = 0.5-5 K min^{-1}, 4 runs, <T> = 112°C	73.4 ±1.2	72.6±0.6 [102] (re) 71± 5[4] (re) 72.8±0.8 [103] (cl)	71.5 ±3.4	66	Argon flow, β = 0.1-0.5 K min^{-1}, 5 runs, <T> = 59°C
6	**ADM**				62.7 ±1.9	59±4[4] (re) 59.1±0.9[107] (re)		102	Argon flow, β = 0.1-5 K min^{-1}, 4 runs, <T> = 61°C

7	**ANT**		77.8[108] [a] (ch) 75.1[109] [a] (ch) 77.5[16] [a] (ds)		103.0 ±2.5	103.4±2.7 [102] (re) 100.4±4.2 [103] (re)		92	Argon flow, β = 0.5-5 K min^{-1}, 4 runs, <T> = 169°C
8	**tAB**	74.1 ±1.6	72.8[19]	Argon flow, β = 1-5 K min^{-1}, 3 runs, <T> = 149°C	92.8 ±1.9	93.8 ±0.4[4] (re)	96.6 ±3.6	64	Vacuum, β = 0.1-2 K min^{-1}, 3 runs, <T> = 42°C
9	**HPX**				161.9 ±2.8	162.5[110] 162.9[111] [a]		128	Argon flow, β = 0.5-5 K min^{-1}, 3 runs, <T> = 349°C
10	**TPL**	106.7 ±2.3		Argon flow, β = 1-5 K min^{-1}, 4 runs, <T> = 311°C	130.8 ±2.3	136.3[112] [a] 138.5[112] [a] 132.5[113] (fs) 129.9[22] [a]	132.0 ±4.1	102	Argon flow, β = 0.5-5 K min^{-1}, 5 runs, <T> = 239°C
11	**D18C6**	130.9 ±15.2	137[24] 154.1[23]	Argon flow, β = 0.5-5 K min^{-1}, 3 runs, <T> = 254°C	167.0 ±5.4	178.4[24] 180.2[24] 190.6[23]	168.6 ±16.7	82	Vacuum, β = 0.2-1 K min^{-1}, 3 runs, <T> = 137°C
12	**4-NPA**	66.7 ±3.1		Argon flow, β = 0.5-5 K min^{-1}, 3 runs, <T> = 117°C		81[26] 79.5[114]	89.7 ±4.4	65	
13	**24-DNT**	77.1 ±3.0	75.3[115] (re) 76[89] [a]	Argon flow, β = 0.5-5 K min^{-1}, 3 runs, <T> = 153°C	100.6 ±2.1	94[115] (re) 96.0[116] [a] 94.5[117] [a] 83.3[118] [a]	99.8 ±3.9	64	Vacuum, β = 0.15-0.5 K min^{-1}, 3 runs, <T> = 50°C
14	**DNAN**	86.4 ±3.5	57.2 (comptd) [119]	Argon flow, β = 0.5-2 K min^{-1}, 3 runs, <T> = 172°C	107.1 ±1.4		104.2 ±4.4	68	Vacuum, β = 0.2-1 K min^{-1}, 4 runs, <T> = 67°C
15	**TNT**	90.7 ±3.7	89.8[115] (re) 86.6±0.4[103] (cl)	Argon flow, β = 1-10 K min^{-1}, 4 runs, <T> =	110.7 ±2.6	114.1[115] (re) 113.2±1.5[120] (ef)	110.2±4.1	67	Vacuum, β = 0.5-5 K min^{-1}, 4 runs, <T> = 60°C

			87.0±1.9[120] (ef)	192°C		106.3±0.4[103] (cl) 118.0±0.8[103] (cl)			
16	**Tetryl**				136.0 ±3.1	133.1[121] 133.8±1.6[120] (ef)		76	Vacuum, β = 0.2-0.5 K min^{-1}, up to DSC growth, 5 runs, <T> = 188 °C
17	**FOX-7**				119.4 ±3.3	116[122][c] 104[123][c] 152[124][c]		90[b]	Vacuum, β = 0.15-1 K min^{-1}, up to DSC growth, 5 runs, <T> = 188 °C
18	**TNAA**				101.2 ±1.7			69	Vacuum, β = 0.05-0.25 K min^{-1}, 5 runs, <T> = 51 °C
19	**FEFO**	93.3 ±7.4	85.1[125]	Vacuum, β = 0.5-2 K min^{-1}, 3 runs, <T> = 54 °C				54	
20	**NIGU**				141.6 ±2.4	142.7 [120] 139.7[126]		83	Vacuum, β = 0.05-1 K min^{-1}, 4 runs, <T> = 145 °C
21	**DNDAP**	75.0 ±2.7		Argon flow, β = 0.5-2 K min^{-1}, 3 runs, <T> = 122°C		102.5[127]	95.6 ±3.8	62	
22	**DNPP**	78.6 ±1.3		Argon flow, β = 0.75-2 K min^{-1}, 3 runs, <T> = 234°C	111.1 ±1.0	112.7±0.8[128][a] (ef) 102.9± 1.2[127] (ef)	113.7±2.4	92	Argon flow, β = 0.75-2 K min^{-1}, 4 runs, <T> = 177°C
23	**RDX**				130.4 ±2.3	128.0±1.3[127] (cl) 127.1[115](re) 150[129][c] (bu)		90	Vacuum, β = 0.15-0.35 K min^{-1}, 5 runs, <T> = 99°C
24	**HMX**				179.1 ±7.0	161.0±0.3[120] (ef) 164.4±1.7 [103](cl)		104	Vacuum, β = 0.1-0.2 K min^{-1}, 3 runs, <T> = 165°C (all data before

						176.1±1.7 [127](cl) 174.7[130] [c] (ef) 180[129] [c] (bu)			phase transition)
25	**DATN**				230.8 ±8.0	195[131] (ri)		85	Vacuum, β = 0.04-0.15 K min^{-1}, 4 runs, <T> = 156 °C
26	**BC-HMX**				134.6 ±2.5			97[b]	Vacuum, β = 0.2-1 K min^{-1}, 4 runs, <T> = 170 °C
27	**TEX**				130.9 ±2.4	~130[132]		104[b]	Argon flow, β = 0.5-5 K min^{-1}, 4 runs, <T> = 240 °C
28	**CL-20**				171.9 ±3.2	157±20[133] (po) 168[129][c] (bu) 226.8±4.6 [127](ph)		95[b]	Vacuum, β = 0.15-0.35 K min^{-1}, 5 runs, <T> = 173 °C
29	**ETN**	92.7 ±2.4		Vacuum, β = 0.2-1 K min^{-1}, 4 runs, <T> = 74 °C	139.5 ±3.0	118.5[51] [a]	127.6±5.7	63	Vacuum, β = 0.1-1 K min^{-1}, 5 runs, <T> = 50 °C
30	**PETN**			-	147.6 ±3.5	150.8 [115] (re) 150.4±1.3[120] (ef) 150.6±1.8[134] (tg?) 149.2[51] [a]	-	78	Vacuum, β = 0.4-1 K min^{-1}, 3 runs, <T> = 97 °C
31	**SMX**				166.3 ±3.5	106[51] [a] 164±20[135] (po)		68	Vacuum, β = 0.1-0.4 K min^{-1}, 4 runs, <T> = 71 °C
32	**PMDA**				85.6 ±1.5			71	Argon flow, β = 0.5-2 K min^{-1}, 3 runs, <T> = 75 °C
33	**24-DNI**				112.1 ±3.2	112.1[136]		102	Vacuum, β = 0.2-1 K min^{-1}, 3 runs, <T> =

									134 °C
34	**45-DNI**				119.0 ±2.0			85	Vacuum, β = 0.2-1 K min^{-1}, 3 runs, <T> = 110 °C
35	**34-DNP**	99.6 ±2.4		Vacuum, β = 0.5-2 K min^{-1}, 6 runs, <T> = 114°C	113.8 ±2.3	112.5±0.8[136] (cl) 141.4[137] (tg)	114.1 ±3.3	68	Vacuum, β = 0.03-0.1 K min^{-1}, 4 runs, <T> = 75°C
36	**35-DNP**	89.3 ±2.0		Argon flow, β = 0.2-2 K min^{-1}, 3 runs, <T> = 199°C	107.8 ±1.3		104.0 ±2.7	83	Argon flow, β = 0.1-25 K min^{-1}, 4 runs, <T> = 145°C
37	**1-ADP**	100.1 ±4.6		Argon flow, β = 1-5 K min^{-1}, 3 runs, <T> = 211°C			119.0 ±6.8	72	
38	**5-ADP**				121.2 ±2.0			88	Vacuum, β = 0.15-0.3 K min^{-1}, 4 runs, <T> = 150 °C
39	**TNP**				121.5 ±1.9			86	Vacuum, β = 0.5-2 K min^{-1}, 3 runs, <T> = 107 °C
40	**MTNP**				104.8 ±1.7			68	Vacuum, β = 0.2-2 K min^{-1}, 4 runs, <T> = 70°C
41	**DNPPy**				134.2 ±4.4			112	Vacuum, β = 0.5-2 K min^{-1}, 3 runs, <T> = 172°C
42	**TNDPT**				122.0 ±3.8			88	Vacuum, β = 0.2-1 K min^{-1}, 4 runs, <T> = 170 °C
43	**ANPZ**				124.7 ±2.3			119	Vacuum, β = 0.1-2 K min^{-1}, 4 runs, <T> = 180 °C
44	**LLM-105**				132.3 ±3.9	135.6[138] (est) 163.8[137]		114	Vacuum, β = 0.5-2 K min^{-1}, 3 runs, <T> = 193 °C

						103.3[139] (ri)			
45	**ANTA**				127.8 ±3.3			97	Vacuum, β = 0.2-1 K min^{-1}, 3 runs, <T> = 158 °C
46	**NTO**				122.8 ±2.3	107.9[129]		102	Vacuum, β = 0.2-1 K min^{-1}, 3 runs, <T> = 126 °C
47	**5-ATZ**				116.0 ±2.0	116.3±1.2[140] [a]	-	90	Vacuum, β = 0.2-1 K min^{-1}, 4 runs, <T> = 110°C
48	**DAT**				109.6 ±2.2			87	Vacuum, β = 0.2-2 K min^{-1}, 4 runs, <T> = 125°C
49	**BTZ**				142.5 ±2.8			101[b]	Vacuum, β = 0.3-1 K min^{-1}, 3 runs, <T> = 166°C
50	**BTO**				141.2 ±2.7			95	Vacuum, β = 0.2-1 K min^{-1}, 3 runs, <T> = 178°C
51	**Ph-Azs**	80.5 ±3.3		Argon flow, β = 0.5-2 K min^{-1}, 3 runs, <T> = 152°C	109.5 ±1.7		98.2 ± 3.8	67	Vacuum, β = 0.1-0.5 K min^{-1}, 4 runs, <T> = 44°C
52	**4-Tol-Azs**	77.1 ±3.6		Argon flow, β = 1-10 K min^{-1}, 3 runs, <T> = 160°C	97.1 ±2.4		93.7 ± 3.9	70	Vacuum, β = 0.2-2 K min^{-1}, 3 runs, <T> = 66°C
53	**ANF**				93.3 ±2.2		90.0 ±4.7	74	Argon flow, β = 0.5-5 K min^{-1}, 3 runs, <T> = 92°C
54	**DAF**	89.2 ±2.2		Argon flow, β = 0.5-5 K min^{-1}, 4 runs, <T> = 206°C	109.4 ±4.1		103.9 ±2.6	85	Argon flow, β = 0.5-5 K min^{-1}, 4 runs, <T> = 160°C
55	**DNAF**				133.3 ±2.9			69	Vacuum, β = 0.1-1 K min^{-1}, 3 runs, <T> =

									69°C
56	**DAAzF**				96.4 ±3.7	103.5[141] (calc) 99.6[142] (co)		109	Vacuum, β = 0.1-2 K min^{-1}, 3 runs, <T> = 127°C
57	**DAAF**				117.1 ±2.3	117.2[141] (calc) 82.3[143]		99	Vacuum, β = 0.2-2 K min^{-1}, 3 runs, <T> = 153°C
58	**34-MNF**	67.5 ±1.8		Argon flow, β = 0.5-5 K min^{-1}, 3 runs, <T> = 102°C			86.6 ±2.2	64	
59	**43-MNF**	61.8 ±2.8		Argon flow, β = 0.5-5 K min^{-1}, 3 runs, <T> = 81°C			76.6 ±3.1	59	
60	**34-CNF**	72.5 ±2.6		Argon flow, β = 0.5-2 K min^{-1}, 3 runs, <T> = 91°C			94.0 ±3.5	60	
61	**BTF**	95.4 ±4.6		Argon flow, β = 0.5-5 K min^{-1}, 3 runs, <T> = 218°C	107.1 ±0.9	175.2±2.5[79][a]	108.9 ±6.2	88	Vacuum, β = 0.2-1 K min^{-1}, 3 runs, <T> = 114 °C
62	**NNFF**	87.7 ±3.1		Argon flow, β = 0.5-5 K min^{-1}, 3 runs, <T> = 123°C	119.6 ±1.9			71	Vacuum, β = 0.3-1 K min^{-1}, 3 runs, <T> = 54 °C
63	**DNBF**				106.5 ±2.4			77	Vacuum, β = 0.5-1 K min^{-1}, 3 runs, <T> = 69 °C

[a]Corrected to RT with Eqs. (S1) and (S4).
[b]The onset temperature used in Eq.(4) instead of melting point.
[c]Corrected to RT with Eq.(S1) and phase transition enthalpy added.

Methods:
re – the values recommended upon the analysis of the available literature

bu – corrected to RT data from the pressure-time dependence obtained in burning tests
cl – calorimetric technique.
tr –transpiration
is – isoteniscope
ma – manometry
ch – gas chromatography
tg – thermogravimetric
ds- DSC
ef - Knudsen effusion method
eb – ebulliometer
ph - supposed to be equal to the experimental value of the activation energy of the phase transition.
po – calculated by the Politzer approach
ri – calculated by the Rice approach
to – torsion-effusion method
fs – fast scanning calorimetry

S4. Summary of the data fit with the modified Westwell-Trouton equation

```
Residuals:
   Min     1Q Median     3Q    Max
-28160  -5573   1113   7456  29514

Coefficients:
   Estimate Std. Error t value Pr(>|t|)
Nh  3268.12     494.72   6.606 4.33e-08 ***
Nn  5294.95     965.86   5.482 1.93e-06 ***
Tm   151.13      12.38  12.211 9.99e-16 ***
No  3298.10     605.52   5.447 2.18e-06 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 12860 on 44 degrees of freedom
Multiple R-squared:  0.9895,    Adjusted R-squared:  0.9885
F-statistic:  1036 on 4 and 44 DF,  p-value: < 2.2e-16
```

S5. Quantum chemical calculations of the gas-phase enthalpies of formation: Summary and literature data. Raw quantum chemical data: optimized geometries, electronic energies, and thermal corrections to thermodynamic potentials of all compounds under study

Table S5. The results of quantum chemical calculations of $^{\Delta_f H_m^0(g)}$ along with the literature data. All value are calculated either with W1-F12 or W2-F12 multi-level techniques, except otherwise noted. All values are given in kJ/mol.

Compound	Present study	Literature (Method/Basis)
ACM	-234.8	-238.8 ±0.8[144] -236.5 (W3X-L) [145] -230.6 (G4MP2) [146]
Urea	-233.2	
Val	-466.6	-476.5 (G4) -475.8 (isodesmic) [147]
BCA	-296.9	-298.6 (G4MP2) [146] -294.1±1.6 [148]
NPH	146.4	150.6±1.5 (review)[149] 146.2 (W1-F12) 146.9 (G4) [150]
ADM	-135.9	-132.2±2.2 (exp) [107]
ANT	225.8	229.4±2.9 (review)[149] 225.5 (W1-F12) 224.3 (G4) [150]
tAB	407.6	405.5 ±1.3 (experiment) [19]
HPX	50.6	52.4 ±1.4 (experiment) 46 ± 4.6 (G4) [110]
TPL	-228.7	-232 ±8 (G3B3) [151]
DB18C6	–	
4-NPA	400.4	389.7 ±5.2 (experiment)[26] 393.9 (isodesmic) 384.3 (G4) [152]
24-DNT	30.5	32.5±4 (isodesmic) 31.5(recommended) [152]
DNAN	-75.9	
TNT	48.8	24.1 ±3.5 (experiment)[29] 50.1±4 (isodesmic) 23.0 (G4) [152]
Tetryl	164.2	165.7±4 (G4(MP2)+isodesmic) [152]
FOX-7	10.0	3.1±6.0[141]
TNAA	-16.3	-38.1 (G4) -16.3 ±6.3 (G4+isodesmic) [40] -134.6 (isodesmic) [41] -174.9[153]
FEFO	–	
NIGU	51.3	48.7±4 (G4+isodesmic) [154]
DNDA-5	41.3	51.0 ±0.8 (experiment) [127] 37.8±7 (G4+isodesmic) [154]
DNPP	84.7	58 ±3 (experiment) [128] 49.8±2.1 (experiment) [127] 64.7±5 68.3 (G4) [155]
RDX	197.9	185.8 (B3LYP/6-31G(d,p)) [156] 196.2 (G4) [155] 190.8±5 [141] 195.0 ±1.7 (experiment) [127]

HMX	259.9	247.7±7 253.9 (G4) [155] 261.9 ±2.5 (experiment) [127]
DATN	848.6	864.8 [131]
BC-HMX	318.7	
TEX	-400.0	-400.0 ±6.3 [157] -448.4 (B3LYP 6-31+G**) [158]
CL-20	548.5	-548.5 ±6.3 [157] 601.7 ±4.6 (experiment) [127] 523.1 (G4) [155] 522.8±10 [141] 691.3 (B3LYP+6-31G*) [159]
ETN	-356.7	
PETN	-395.5	-413.6 ±4[141]
SMX	-375.3[a]	-469 -674 [160] -415.7 ± 15 [135]
PMDA	128.5	
2,4-DNI	137.2	133.5 (G4MP2-SFM) [161]
4,5-DNI	160.6	
3,4-DNP	210.3	205.0 (B3P86/6-311G (d, p))[162]
3,5-DNP	190.6	
1-ADP	305.3	243.8 (MP2/6-311++G**)[61]
5-ADP	196.5	165.7 (B3P86/6-311G (d, p))[162]
TNP	253.6	142.7 (PM3)[163]
MTNP	233.0	230.1 (B3P86/6-311G (d, p))[162] -15.1 (PM3) [163]
DNPPy	414.5	
TNDPT	897.5	847.4 (MP2/6–311++G**)[66]
ANPZ	119.9	98.3 (CBS-4M)[164]
LLM-105	112.5	108.4 (ccCA-PS3) 94.1 (G4) [138] 126.8 (CBS-4M)[164]
ANTA	201.2	
NTO	-4.2	-14 (G4) -6.5 (isodesmic)[152] -3.8(B3LYP/6-31G(d,p)//B3LYP/6-31G(d,p))[156]
5-ATZ	329.0	325.1 (W1) [165] 325.3 ±3 [141]
DAT	424.6	
BTZ	674.2	665.1 ±5[141]
BTO	669.7	689.1 (CBS-4M) [166]
Ph-Azs	175.1	

4-Tol-Azs	140.9	
ANF	220.1	
DAF	198.7	
DNAF	347.9	
DAAzF	653.3	639.3 ±7 [141]
DAAF	616.4	605 ±5 [141]
DNAAF	811.3[b]	798.3 (isodesmic) [167]
34-MNF	188.2	
43-MNF	196.6	
34-CNF	421.3	
BTF	730.9	752.7 ±4.6 (experiment)[79] 489.5 (B3LYP/6-31G*)[168]
NNFF	521.2	
DNBF	514.7	525.6 (CBS-4M) [169]

[a] W1-F12 atomization energies of the reactants and DLPNO-CCSD(T) enthalpy of the isodesmic reaction SMX + C_4H_{10} -> ETN + $C_6H_{12}(NO_2)_2$. [b] W1-F12 atomization energies of the reactants and DLPNO-CCSD(T) enthalpy of the isodesmic reaction DNAAF + (azoxy bisfurazan) -> 2 (azoxy bis(furazano)nitraminofurazan).

The raw computational data: B3LYP-D3BJ/def2-TZVPP geometries, zero-point vibrational energies (unscaled) and thermal corrections to thermodynamic potentials, W1-F12 and W2-F12 electronic energies. The species are named in accordance with Table 1 from the manuscript.

ACM

Zero-point correction= 0.072408 (Hartree/Particle)
Thermal correction to Energy= 0.077721
Thermal correction to Enthalpy= 0.078665
Thermal correction to Gibbs Free Energy= 0.043873

Electronic energy:

B3LYP = -209.3125834
W1-F12 = -209.31995003
W2-F12 = -209.32102852

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.075472	0.145704	-0.002324
2	8	0	-0.352171	1.329201	0.000092
3	6	0	1.358981	-0.346721	-0.000251
4	1	0	1.886660	0.119859	-0.830609
5	1	0	1.837704	-0.013833	0.920423
6	1	0	1.452321	-1.429241	-0.077571
7	7	0	-1.035135	-0.823209	-0.000501
8	1	0	-2.000258	-0.540754	0.007793
9	1	0	-0.814171	-1.801080	-0.001817

Urea

Zero-point correction= 0.062932 (Hartree/Particle)
Thermal correction to Energy= 0.067406
Thermal correction to Enthalpy= 0.068350
Thermal correction to Gibbs Free Energy= 0.037275

Electronic energy:

B3LYP = -225.3828217
W1-F12 = -225.39371507
W2-F12 = -225.39481251

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.143468
2	8	0	0.000000	0.000000	1.357738
3	7	0	0.000000	1.160155	-0.608746
4	1	0	-0.200216	1.988011	-0.073352
5	1	0	-0.411182	1.136624	-1.526779
6	7	0	0.000000	-1.160155	-0.608746

7	1	0	0.411182	-1.136624	-1.526779
8	1	0	0.200216	-1.988011	-0.073352

Val

Zero-point correction= 0.162341 (Hartree/Particle)
Thermal correction to Energy= 0.172007
Thermal correction to Enthalpy= 0.172951
Thermal correction to Gibbs Free Energy= 0.127638

Electronic energy:

B3LYP = -402.574404
W1-F12 = -402.57033900
W2-F12 = -402.57221050

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.271138	0.393450	-0.065944
2	1	0	1.758162	1.312634	-0.403340
3	6	0	1.261501	0.408903	1.460561
4	1	0	0.847964	-0.520300	1.859203
5	1	0	2.274708	0.509855	1.850918
6	1	0	0.665239	1.241157	1.831997
7	6	0	2.065306	-0.784328	-0.626713
8	1	0	1.665104	-1.738331	-0.288789
9	1	0	2.057357	-0.785772	-1.718621
10	1	0	3.104575	-0.720419	-0.301387
11	6	0	-0.165970	0.518443	-0.645461
12	1	0	-0.114480	0.241526	-1.707309
13	6	0	-1.153057	-0.456488	-0.030018
14	8	0	-2.178837	-0.149937	0.520867
15	8	0	-0.780683	-1.745732	-0.186656
16	1	0	-1.468683	-2.286981	0.226151
17	7	0	-0.665765	1.871665	-0.439139

18	1	0	-0.463866	2.463428	-1.231391
19	1	0	-1.663084	1.867025	-0.271693

BCA

Zero-point correction= 0.114475 (Hartree/Particle)
Thermal correction to Energy= 0.121645
Thermal correction to Enthalpy= 0.122589
Thermal correction to Gibbs Free Energy= 0.082332

Electronic energy:

B3LYP = -421.025426
W1-F12 = -421.01269127
W2-F12 = -421.01464817

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.431375	-1.717610	0.000000
2	1	0	2.422436	-2.150046	0.000000
3	6	0	1.277963	-0.340234	0.000000
4	6	0	0.000000	0.220347	0.000000
5	8	0	-1.395968	2.135370	0.000000
6	8	0	0.820598	2.464456	0.000000
7	6	0	0.310323	-2.542054	0.000000
8	6	0	-0.964574	-1.986783	0.000000
9	6	0	-1.123001	-0.608227	0.000000
10	1	0	0.430618	-3.617077	0.000000
11	1	0	-1.834973	-2.628437	0.000000
12	1	0	-2.109707	-0.170716	0.000000
13	1	0	2.133763	0.319076	0.000000
14	6	0	-0.112535	1.699090	0.000000
15	1	0	-1.356491	3.101413	0.000000

NPH

Zero-point correction= 0.145946 (Hartree/Particle)
Thermal correction to Energy= 0.152816
Thermal correction to Enthalpy= 0.153760
Thermal correction to Gibbs Free Energy= 0.116005

Electronic energy:

B3LYP = -386.0731871
W1-F12 = -386.00216480
W2-F12 = -386.00298561

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	2.422511	0.705726
2	6	0	0.000000	1.239453	1.396737
3	6	0	0.000000	0.000000	0.713642
4	6	0	0.000000	0.000000	-0.713642
5	6	0	0.000000	1.239453	-1.396737
6	6	0	0.000000	2.422511	-0.705726
7	1	0	0.000000	-1.236812	2.479353
8	1	0	0.000000	3.362991	1.240009
9	1	0	0.000000	1.236812	2.479353
10	6	0	0.000000	-1.239453	1.396737
11	6	0	0.000000	-1.239453	-1.396737
12	1	0	0.000000	1.236812	-2.479353
13	1	0	0.000000	3.362991	-1.240009
14	6	0	0.000000	-2.422511	-0.705726
15	6	0	0.000000	-2.422511	0.705726
16	1	0	0.000000	-1.236812	-2.479353
17	1	0	0.000000	-3.362991	-1.240009
18	1	0	0.000000	-3.362991	1.240009

ADM

Zero-point correction= 0.241082 (Hartree/Particle)
Thermal correction to Energy= 0.248139
Thermal correction to Enthalpy= 0.249083
Thermal correction to Gibbs Free Energy= 0.212597

Electronic energy:

B3LYP = -390.9193707
W1-F12 = -390.85144214
W2-F12 = -390.85182455

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.772083
2	1	0	0.621614	0.621614	2.422078
3	1	0	-0.621614	-0.621614	2.422078
4	6	0	0.888119	-0.888119	0.888119
5	1	0	1.518891	-1.518891	1.518891
6	6	0	-0.888119	0.888119	0.888119
7	1	0	-1.518891	1.518891	1.518891
8	6	0	0.000000	1.772083	0.000000
9	1	0	0.621614	2.422078	0.621614
10	1	0	-0.621614	2.422078	-0.621614
11	6	0	1.772083	0.000000	0.000000
12	1	0	2.422078	-0.621614	-0.621614
13	1	0	2.422078	0.621614	0.621614
14	6	0	0.888119	0.888119	-0.888119
15	1	0	1.518891	1.518891	-1.518891
16	6	0	0.000000	0.000000	-1.772083
17	1	0	-0.621614	0.621614	-2.422078
18	1	0	0.621614	-0.621614	-2.422078
19	6	0	0.000000	-1.772083	0.000000
20	1	0	-0.621614	-2.422078	0.621614

21	1	0	0.621614	-2.422078	-0.621614
22	6	0	-1.772083	0.000000	0.000000
23	1	0	-2.422078	-0.621614	0.621614
24	1	0	-2.422078	0.621614	-0.621614
25	6	0	-0.888119	-0.888119	-0.888119
26	1	0	-1.518891	-1.518891	-1.518891

ANT

Zero-point correction= 0.192113 (Hartree/Particle)
Thermal correction to Energy= 0.201642
Thermal correction to Enthalpy= 0.202586
Thermal correction to Gibbs Free Energy= 0.158547

Electronic energy:

B3LYP = -539.7814526
W1-F12 = -539.68570002
W2-F12 = -539.68679622

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	3.643606	0.710558
2	6	0	0.000000	2.468408	1.401217
3	6	0	0.000000	1.217729	0.719568
4	6	0	0.000000	1.217729	-0.719568
5	6	0	0.000000	2.468408	-1.401217
6	6	0	0.000000	3.643606	-0.710558
7	6	0	0.000000	0.000000	1.398166
8	6	0	0.000000	0.000000	-1.398166
9	6	0	0.000000	-1.217729	-0.719568
10	6	0	0.000000	-1.217729	0.719568
11	6	0	0.000000	-2.468408	1.401217
12	1	0	0.000000	-2.466419	2.483718
13	6	0	0.000000	-3.643606	0.710558

14	6	0	0.000000	-3.643606	-0.710558
15	6	0	0.000000	-2.468408	-1.401217
16	1	0	0.000000	0.000000	2.481517
17	1	0	0.000000	4.585927	1.241494
18	1	0	0.000000	2.466419	2.483718
19	1	0	0.000000	2.466419	-2.483718
20	1	0	0.000000	4.585927	-1.241494
21	1	0	0.000000	0.000000	-2.481517
22	1	0	0.000000	-4.585927	1.241494
23	1	0	0.000000	-4.585927	-1.241494
24	1	0	0.000000	-2.466419	-2.483718

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tAB

Zero-point correction= 0.188765 (Hartree/Particle)
Thermal correction to Energy= 0.199755
Thermal correction to Enthalpy= 0.200700
Thermal correction to Gibbs Free Energy= 0.149455

Electronic energy:

B3LYP = -573.0244777
W1-F12 = -572.94482100
W2-F12 = -572.94604016

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.188045	4.519639	0.000000
2	6	0	1.099487	3.997333	0.000000
3	6	0	1.287357	2.622075	0.000000
4	6	0	0.188045	1.763973	0.000000
5	6	0	-1.108601	2.290374	0.000000
6	6	0	-1.288436	3.662265	0.000000
7	1	0	-0.338348	5.590787	0.000000
8	1	0	1.954518	4.659436	0.000000

9	1	0	2.277557	2.188081	0.000000
10	1	0	-1.949395	1.613471	0.000000
11	1	0	-2.289549	4.072379	0.000000
12	7	0	0.492373	0.383116	0.000000
13	7	0	-0.492373	-0.383116	0.000000
14	6	0	-0.188045	-1.763973	0.000000
15	6	0	1.108601	-2.290374	0.000000
16	6	0	-1.287357	-2.622075	0.000000
17	6	0	1.288436	-3.662265	0.000000
18	1	0	1.949395	-1.613471	0.000000
19	6	0	-1.099487	-3.997333	0.000000
20	1	0	-2.277557	-2.188081	0.000000
21	6	0	0.188045	-4.519639	0.000000
22	1	0	2.289549	-4.072379	0.000000
23	1	0	-1.954518	-4.659436	0.000000
24	1	0	0.338348	-5.590787	0.000000

HPX

Zero-point correction= 0.099172 (Hartree/Particle)
Thermal correction to Energy= 0.105944
Thermal correction to Enthalpy= 0.106888
Thermal correction to Gibbs Free Energy= 0.067727

Electronic energy:

B3LYP = -487.4084128
W1-F12 = -487.40981432
W2-F12 = -487.41148885

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.640451	-1.042847	0.000000
2	6	0	0.000000	0.622157	0.000000
3	6	0	-0.878734	-0.456292	0.000000

4	7	0	-0.589942	-1.781682	0.000000
5	8	0	2.358831	1.131919	0.000000
6	7	0	-0.692923	1.810337	0.000000
7	7	0	-2.127451	0.100479	0.000000
8	6	0	1.418430	0.369400	0.000000
9	6	0	0.686559	-2.010858	0.000000
10	1	0	1.046714	-3.031955	0.000000
11	1	0	2.614185	-1.309535	0.000000
12	1	0	-2.994926	-0.408410	0.000000
13	6	0	-1.952762	1.466326	0.000000
14	1	0	-2.788530	2.146137	0.000000

TPL

Zero-point correction= 0.158870 (Hartree/Particle)
Thermal correction to Energy= 0.170354
Thermal correction to Enthalpy= 0.171298
Thermal correction to Gibbs Free Energy= 0.120662

Electronic energy:

B3LYP = -641.360894
W1-F12 = -641.36135072
W2-F12 = -641.36403980

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.743402	-1.470007	0.000000
2	6	0	0.000000	0.767858	0.000000
3	6	0	1.299940	0.319032	0.000000
4	7	0	1.570884	-1.020167	0.000000
5	8	0	-2.304841	0.213648	0.000000
6	7	0	0.098107	2.148904	0.000000
7	7	0	2.187231	1.340135	0.000000
8	6	0	-1.128258	-0.109604	0.000000

9	6	0	0.567490	-1.971568	0.000000
10	6	0	1.421896	2.426366	0.000000
11	1	0	1.789933	3.438933	0.000000
12	8	0	0.822990	-3.158466	0.000000
13	6	0	-1.837431	-2.441283	0.000000
14	1	0	-2.457881	-2.296362	0.881736
15	1	0	-2.457881	-2.296362	-0.881736
16	1	0	-1.402810	-3.433043	0.000000
17	1	0	2.516923	-1.364457	0.000000
18	6	0	-1.004178	3.095083	0.000000
19	1	0	-1.623278	2.950410	-0.882273
20	1	0	-1.623278	2.950410	0.882273
21	1	0	-0.593416	4.101655	0.000000

4-NPA

Zero-point correction= 0.105076 (Hartree/Particle)
Thermal correction to Energy= 0.114593
Thermal correction to Enthalpy= 0.115537
Thermal correction to Gibbs Free Energy= 0.068828

Electronic energy:

B3LYP = -600.61401
W1-F12 = -600.61748790

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.142698	0.416970	0.000000
2	1	0	2.113959	0.891997	0.000000
3	6	0	0.000000	1.195969	0.000000
4	6	0	-1.242007	0.576780	0.000000
5	7	0	-2.453102	1.404803	0.000000
6	8	0	-3.532193	0.831414	0.000000
7	8	0	-2.310989	2.618686	0.000000

8	6	0	1.033775	-0.977281	0.000000
9	6	0	-0.224493	-1.584483	0.000000
10	6	0	-1.366158	-0.806907	0.000000
11	1	0	-0.286520	-2.662638	0.000000
12	1	0	-2.348295	-1.252396	0.000000
13	1	0	0.056934	2.273011	0.000000
14	7	0	2.140864	-1.845463	0.000000
15	7	0	3.270338	-1.353768	0.000000
16	7	0	4.348541	-1.030867	0.000000

24-DNT

Zero-point correction= 0.131766 (Hartree/Particle)
Thermal correction to Energy= 0.142772
Thermal correction to Enthalpy= 0.143716
Thermal correction to Gibbs Free Energy= 0.093613

Electronic energy:

B3LYP = -680.8787573
W1-F12 = -680.90415550

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.212544	1.197388	-0.047244
2	6	0	-0.954979	-0.179976	-0.008104
3	6	0	0.326751	-0.705559	0.006674
4	6	0	1.392823	0.171093	0.008027
5	6	0	1.201858	1.543634	-0.031483
6	6	0	-0.091407	2.034070	-0.068239
7	1	0	0.484668	-1.771208	0.018006
8	1	0	2.056388	2.201849	-0.038065
9	7	0	-2.053970	-1.166154	0.014449
10	8	0	-1.827541	-2.266537	-0.458795
11	8	0	-3.113071	-0.824855	0.516373

12	7	0	2.763127	-0.369913	0.045628
13	8	0	3.682083	0.432829	0.025196
14	8	0	2.890043	-1.581392	0.095016
15	6	0	-2.580222	1.811770	-0.093883
16	1	0	-3.221392	1.321264	-0.823994
17	1	0	-3.081007	1.716170	0.868485
18	1	0	-2.500143	2.867008	-0.346671
19	1	0	-0.248424	3.102503	-0.115108

DNAN

Zero-point correction= 0.136384 (Hartree/Particle)
Thermal correction to Energy= 0.148525
Thermal correction to Enthalpy= 0.149469
Thermal correction to Gibbs Free Energy= 0.096586

Electronic energy:

B3LYP = -756.1147135
W1-F12 = -756.15671416

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.168803	-0.733395	-0.018556
2	6	0	0.651856	0.577607	0.000172
3	6	0	-0.704721	0.822812	-0.003680
4	6	0	-1.576140	-0.252772	0.015682
5	6	0	-1.107504	-1.557750	0.012733
6	6	0	0.254583	-1.795033	-0.012978
7	1	0	-1.075943	1.834850	-0.016634
8	1	0	-1.812981	-2.373740	0.023970
9	7	0	1.545176	1.746925	0.029532
10	8	0	1.211177	2.709582	-0.642959
11	8	0	2.531033	1.687547	0.740596
12	7	0	-3.020675	-0.002499	0.036182

13	8	0	-3.760569	-0.974943	0.039263
14	8	0	-3.393497	1.159703	0.048894
15	1	0	0.611095	-2.811938	-0.033025
16	8	0	2.491744	-0.887926	-0.082375
17	6	0	3.041241	-2.202387	-0.131646
18	1	0	4.116261	-2.063499	-0.176143
19	1	0	2.781127	-2.766984	0.764851
20	1	0	2.701110	-2.735859	-1.020738

TNT

Zero-point correction= 0.133802 (Hartree/Particle)
Thermal correction to Energy= 0.147509
Thermal correction to Enthalpy= 0.148453
Thermal correction to Gibbs Free Energy= 0.091568

Electronic energy:

B3LYP = -885.4577427
W1-F12 = -885.52480482

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.054344	-1.266422	0.000000
2	6	0	-0.025558	-0.505740	-1.176724
3	6	0	0.011003	0.876507	-1.204430
4	6	0	0.042931	1.551012	0.000000
5	6	0	0.011003	0.876507	1.204430
6	6	0	-0.025558	-0.505740	1.176724
7	1	0	0.012558	1.412350	-2.139870
8	1	0	0.012558	1.412350	2.139870
9	7	0	-0.023114	-1.169259	-2.498563
10	8	0	-0.693026	-0.653885	-3.375266
11	8	0	0.667986	-2.164950	-2.622937
12	7	0	-0.023114	-1.169259	2.498563

13	8	0	-0.693026	-0.653885	3.375266
14	8	0	0.667986	-2.164950	2.622937
15	7	0	0.102694	3.026042	0.000000
16	8	0	0.125293	3.581568	1.083737
17	8	0	0.125293	3.581568	-1.083737
18	6	0	-0.189987	-2.760432	0.000000
19	1	0	-0.717121	-3.102623	-0.884928
20	1	0	0.792877	-3.229993	0.000000
21	1	0	-0.717121	-3.102623	0.884928

Tetryl

Zero-point correction= 0.152519 (Hartree/Particle)
Thermal correction to Energy= 0.170022
Thermal correction to Enthalpy= 0.170966
Thermal correction to Gibbs Free Energy= 0.105005

Electronic energy:

B3LYP = -1145.3921458
W1-F12 = -1145.49793952

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.508001	0.130517	0.139397
2	6	0	0.125499	-1.120284	0.171903
3	6	0	1.493345	-1.260192	0.057015
4	6	0	2.268642	-0.117083	-0.024657
5	6	0	1.709521	1.144991	-0.019888
6	6	0	0.331134	1.245047	0.027735
7	1	0	1.946470	-2.238608	0.055825
8	1	0	2.327388	2.026813	-0.077795
9	7	0	-0.644016	-2.365988	0.389758
10	8	0	-0.243854	-3.360380	-0.178135
11	8	0	-1.588061	-2.307121	1.157749

12	7	0	-0.231526	2.609417	-0.080432
13	8	0	-1.197454	2.763699	-0.802787
14	8	0	0.340228	3.480968	0.549087
15	7	0	3.738014	-0.250184	-0.112946
16	8	0	4.384127	0.779484	-0.184409
17	8	0	4.193471	-1.378959	-0.106586
18	7	0	-1.892475	0.289310	0.251947
19	7	0	-2.708080	-0.338530	-0.676532
20	8	0	-2.151593	-0.969937	-1.559442
21	8	0	-3.900582	-0.184509	-0.522732
22	6	0	-2.541059	1.037878	1.318875
23	1	0	-1.762537	1.404402	1.982261
24	1	0	-3.109372	1.872487	0.916655
25	1	0	-3.200112	0.375528	1.876262

FOX-7

Zero-point correction= 0.091023 (Hartree/Particle)
Thermal correction to Energy= 0.100337
Thermal correction to Enthalpy= 0.101282
Thermal correction to Gibbs Free Energy= 0.056861

Electronic energy:

B3LYP = -598.6044501
W1-F12 = -598.66029515
W2-F12 = -598.66334834

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	1.368590
2	6	0	0.000000	0.000000	-0.050505
3	7	0	0.231326	1.195182	-0.801368
4	8	0	0.682014	1.115405	-1.925912

5	8	0	0.000000	2.286983	-0.244575
6	7	0	-0.231326	-1.195182	-0.801368
7	8	0	-0.682014	-1.115405	-1.925912
8	8	0	0.000000	-2.286983	-0.244575
9	7	0	-0.034495	1.143654	2.063831
10	1	0	0.186501	1.140479	3.042979
11	1	0	-0.064691	2.003541	1.529422
12	7	0	0.034495	-1.143654	2.063831
13	1	0	-0.186501	-1.140479	3.042979
14	1	0	0.064691	-2.003541	1.529422

TNAA

Zero-point correction= 0.080971 (Hartree/Particle)
Thermal correction to Energy= 0.095214
Thermal correction to Enthalpy= 0.096158
Thermal correction to Gibbs Free Energy= 0.037432

Electronic energy:

B3LYP = -1027.5733512
W1-F12 = -1027.73720234

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.709575	-0.413988	0.064722
2	6	0	-0.751136	0.000188	0.001913
3	7	0	-0.921456	1.490130	-0.392216
4	8	0	-1.259127	1.723819	-1.522665
5	8	0	-0.689885	2.258637	0.505552
6	7	0	-1.441873	-0.890968	-1.059042
7	8	0	-2.505693	-1.380074	-0.785771
8	8	0	-0.799479	-0.997205	-2.076717
9	7	0	1.574278	0.535477	-0.034190
10	7	0	-1.458549	-0.146602	1.363338

11	8	0	-2.577786	0.293273	1.412048
12	8	0	-0.816724	-0.676957	2.240012
13	7	0	2.941791	0.156569	0.009930
14	8	0	3.254022	-1.037984	0.170943
15	8	0	3.721817	1.052973	-0.114641
16	8	0	0.864678	-1.697593	0.190940
17	1	0	1.855456	-1.840564	0.227837

FEFO

Zero-point correction= 0.161405 (Hartree/Particle)
Thermal correction to Energy= 0.182030
Thermal correction to Enthalpy= 0.182974
Thermal correction to Gibbs Free Energy= 0.105651

Electronic energy:

B3LYP = -1365.1863583

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.800938	0.115872	0.605309
2	1	0	-2.061570	0.264751	1.649012
3	1	0	-1.148655	0.929032	0.288224
4	6	0	-3.070723	0.148123	-0.232332
5	7	0	-3.884071	1.451176	-0.033881
6	8	0	-3.435043	2.256128	0.752735
7	8	0	-4.881316	1.547902	-0.708237
8	7	0	-4.026252	-0.996774	0.185694
9	8	0	-4.446637	-0.903527	1.319858
10	8	0	-4.239388	-1.860476	-0.623695
11	9	0	-2.831946	0.037019	-1.540189
12	6	0	2.068989	-0.527747	-0.800153
13	1	0	1.845280	-0.080065	-1.774297
14	1	0	2.464952	-1.532899	-0.957071

15	6	0	3.129396	0.319258	-0.128908
16	9	0	2.767365	1.588524	0.017427
17	7	0	3.483177	-0.258128	1.267770
18	8	0	3.939660	-1.382719	1.236857
19	8	0	3.268129	0.437310	2.223192
20	7	0	4.464028	0.315970	-0.918107
21	8	0	5.341565	1.000011	-0.450013
22	8	0	4.495937	-0.345414	-1.933439
23	8	0	-1.189837	-1.153989	0.478510
24	8	0	0.957668	-0.519119	0.062240
25	6	0	-0.148992	-1.257469	-0.435670
26	1	0	-0.423853	-0.873266	-1.426206
27	1	0	0.094595	-2.320231	-0.498670

NIGU

Zero-point correction= 0.077186 (Hartree/Particle)
Thermal correction to Energy= 0.084022
Thermal correction to Enthalpy= 0.084966
Thermal correction to Gibbs Free Energy= 0.046044

Electronic energy:

B3LYP = -410.0606893
W1-F12 = -410.09054736
W2-F12 = -410.09238290

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.065026	-0.078484	0.005637
2	7	0	1.232293	1.250750	0.022966
3	1	0	2.120519	1.649210	-0.221493
4	1	0	0.379940	1.795839	-0.010786
5	7	0	2.185736	-0.848440	-0.071131
6	1	0	3.051111	-0.482619	0.285830

7	1	0	2.030346	-1.834947	0.052841
8	7	0	-0.062624	-0.769748	0.046336
9	7	0	-1.263902	-0.102441	0.003228
10	8	0	-1.329542	1.142259	0.008227
11	8	0	-2.247032	-0.813186	-0.026978

DNDAP

Zero-point correction= 0.141881 (Hartree/Particle)
Thermal correction to Energy= 0.153517
Thermal correction to Enthalpy= 0.154462
Thermal correction to Gibbs Free Energy= 0.102282

Electronic energy:

B3LYP = -639.1058288
W1-F12 = -639.14978242
W2-F12 = -639.15318517

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.179420	2.036933	0.112451
2	1	0	-1.430566	2.024623	-0.946800
3	1	0	-1.999429	1.601932	0.672153
4	1	0	-1.008665	3.065422	0.423431
5	6	0	0.000000	0.000000	1.147736
6	1	0	0.887765	-0.029486	1.770292
7	1	0	-0.887765	0.029486	1.770292
8	6	0	1.179420	-2.036933	0.112451
9	1	0	1.008665	-3.065422	0.423431
10	1	0	1.430566	-2.024623	-0.946800
11	1	0	1.999429	-1.601932	0.672153
12	7	0	0.000000	-1.226438	0.377894
13	7	0	0.000000	1.226438	0.377894
14	7	0	1.171794	1.605948	-0.212268

15	8	0	1.149390	2.627371	-0.879017
16	8	0	2.152744	0.891764	-0.020530
17	7	0	-1.171794	-1.605948	-0.212268
18	8	0	-2.152744	-0.891764	-0.020530
19	8	0	-1.149390	-2.627371	-0.879017

DNPP

Zero-point correction= 0.150196 (Hartree/Particle)
Thermal correction to Energy= 0.161011
Thermal correction to Enthalpy= 0.161956
Thermal correction to Gibbs Free Energy= 0.111574

Electronic energy:

B3LYP = -677.1899974
W1-F12 = -677.26748870

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.411377	0.641762	-1.183272
2	1	0	0.131996	1.262158	-2.030081
3	1	0	1.476278	0.415002	-1.276657
4	6	0	0.268441	-0.712233	1.257189
5	1	0	1.359566	-0.715687	1.335777
6	1	0	-0.122217	-1.242000	2.122076
7	6	0	-0.411377	-0.641762	-1.183272
8	1	0	-0.131996	-1.262158	-2.030081
9	1	0	-1.476278	-0.415002	-1.276657
10	6	0	-0.268441	0.712233	1.257189
11	1	0	-1.359566	0.715687	1.335777
12	1	0	0.122217	1.242000	2.122076
13	7	0	-0.164517	-1.394407	0.043149
14	7	0	0.164517	1.394407	0.043149
15	7	0	-0.001861	2.750607	-0.024938

16	7	0	0.001861	-2.750607	-0.024938
17	8	0	-0.411377	3.303114	0.987944
18	8	0	0.288838	3.301539	-1.078205
19	8	0	0.411377	-3.303114	0.987944
20	8	0	-0.288838	-3.301539	-1.078205

RDX (aaa conformer)

Zero-point correction= 0.141019 (Hartree/Particle)
Thermal correction to Energy= 0.153647
Thermal correction to Enthalpy= 0.154592
Thermal correction to Gibbs Free Energy= 0.100581

Electronic energy:

B3LYP = -897.8299788
W1-F12 = -897.92329127
DLPNO-CCSD(T) = -896.4187140

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	1.395192	0.808607
2	7	0	-1.208272	-0.697596	0.808607
3	7	0	1.208272	-0.697596	0.808607
4	6	0	-1.230375	0.710358	1.172863
5	6	0	0.000000	-1.420715	1.172863
6	6	0	1.230375	0.710358	1.172863
7	1	0	2.074543	1.197738	0.705339
8	1	0	1.322862	0.763755	2.257673
9	1	0	-2.074543	1.197738	0.705339
10	1	0	0.000000	-2.395475	0.705339
11	1	0	0.000000	-1.527510	2.257673
12	1	0	-1.322862	0.763755	2.257673
13	7	0	0.000000	2.165907	-0.379262
14	8	0	-1.085081	2.489469	-0.812850

15	8	0	1.085081	2.489469	-0.812850
16	7	0	-1.875731	-1.082954	-0.379262
17	8	0	-2.698484	-0.305027	-0.812850
18	8	0	-1.613403	-2.184443	-0.812850
19	7	0	1.875731	-1.082954	-0.379262
20	8	0	2.698484	-0.305027	-0.812850
21	8	0	1.613403	-2.184443	-0.812850

RDX (aae conformer)

Zero-point correction= 0.142593 (Hartree/Particle)
Thermal correction to Energy= 0.155143
Thermal correction to Enthalpy= 0.156087
Thermal correction to Gibbs Free Energy= 0.101490

Electronic energy:

B3LYP = -897.8303348
DLPNO-CCSD(T) = -896.41998406

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.132221	1.253084	0.000000
2	7	0	0.785558	-0.678259	1.209726
3	7	0	0.785558	-0.678259	-1.209726
4	6	0	0.756006	0.764681	1.234562
5	6	0	1.342066	-1.269770	0.000000
6	6	0	0.756006	0.764681	-1.234562
7	1	0	0.193586	1.113846	-2.087198
8	1	0	1.791644	1.112402	-1.306771
9	1	0	0.193586	1.113846	2.087198
10	1	0	1.172724	-2.337162	0.000000
11	1	0	2.410891	-1.061807	0.000000
12	1	0	1.791644	1.112402	1.306771
13	7	0	-0.242253	2.598729	0.000000

14	8	0	-0.403105	3.119892	1.087152
15	8	0	-0.403105	3.119892	-1.087152
16	7	0	-0.337703	-1.341019	1.786411
17	8	0	-1.055792	-0.673684	2.498829
18	8	0	-0.427245	-2.527701	1.565443
19	7	0	-0.337703	-1.341019	-1.786411
20	8	0	-1.055792	-0.673684	-2.498829
21	8	0	-0.427245	-2.527701	-1.565443

HMX (crown conformer)

Zero-point correction= 0.190912 (Hartree/Particle)
Thermal correction to Energy= 0.208261
Thermal correction to Enthalpy= 0.209205
Thermal correction to Gibbs Free Energy= 0.144153

Electronic energy:

B3LYP = -1197.1084085
W1-F12 = -1197.23049313
DLPNO-CCSD(T) = -1195.2254780

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.262117	1.278449	-1.065014
2	1	0	1.282494	1.093693	-2.140853
3	1	0	2.043149	1.981299	-0.803123
4	6	0	-1.262117	-1.278449	-1.065014
5	1	0	-2.043149	-1.981299	-0.803123
6	1	0	-1.282494	-1.093693	-2.140853
7	6	0	1.262117	-1.278449	-1.065014
8	1	0	2.043149	-1.981299	-0.803123
9	1	0	1.282494	-1.093693	-2.140853
10	6	0	-1.262117	1.278449	-1.065014
11	1	0	-1.282494	1.093693	-2.140853

12	1	0	-2.043149	1.981299	-0.803123
13	7	0	0.000000	-1.883775	-0.695320
14	7	0	-1.511585	0.000000	-0.436765
15	7	0	1.511585	0.000000	-0.436765
16	7	0	0.000000	1.883775	-0.695320
17	7	0	-1.895746	0.000000	0.902965
18	7	0	1.895746	0.000000	0.902965
19	7	0	0.000000	3.206973	-0.227568
20	7	0	0.000000	-3.206973	-0.227568
21	8	0	-1.083630	3.725295	-0.052902
22	8	0	1.083630	3.725295	-0.052902
23	8	0	2.043942	1.089626	1.419460
24	8	0	2.043942	-1.089626	1.419460
25	8	0	-1.083630	-3.725295	-0.052902
26	8	0	1.083630	-3.725295	-0.052902
27	8	0	-2.043942	-1.089626	1.419460
28	8	0	-2.043942	1.089626	1.419460

HMX (chair conformer)

Zero-point correction= 0.191510 (Hartree/Particle)
Thermal correction to Energy= 0.208772
Thermal correction to Enthalpy= 0.209716
Thermal correction to Gibbs Free Energy= 0.144247

Electronic energy:

B3LYP = -1197.112482
DLPNO-CCSD(T) = -1195.23082782

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.236143	0.323749	-1.181711
2	6	0	-1.236138	-0.323739	1.181696
3	6	0	-1.131717	1.201500	-0.874425

4	1	0	0.678961	-0.262065	-1.909298
5	1	0	-0.678954	0.262072	1.909283
6	1	0	2.038335	0.852093	-1.686505
7	1	0	-2.038330	-0.852083	1.686490
8	1	0	-1.521471	2.205133	-1.002220
9	1	0	-1.272735	0.651405	-1.803343
10	6	0	1.131719	-1.201496	0.874406
11	1	0	1.272737	-0.651412	1.803331
12	1	0	1.521469	-2.205132	1.002190
13	7	0	1.866903	-0.549146	-0.219207
14	7	0	0.276679	1.249630	-0.598687
15	7	0	-0.276677	-1.249619	0.598666
16	7	0	-1.866899	0.549161	0.219196
17	7	0	-3.231531	0.434530	0.018048
18	8	0	-3.653492	0.953676	-1.003814
19	8	0	-3.888966	-0.122299	0.873930
20	7	0	3.231534	-0.434515	-0.018056
21	8	0	3.888971	0.122317	-0.873934
22	8	0	3.653493	-0.953667	1.003805
23	7	0	0.759140	2.284045	0.190178
24	8	0	-0.066805	3.034820	0.674986
25	8	0	1.966241	2.321741	0.341649
26	7	0	-0.759140	-2.284028	-0.190205
27	8	0	-1.966250	-2.321786	-0.341590
28	8	0	0.066796	-3.034863	-0.674937

DATN

Zero-point correction= 0.245495 (Hartree/Particle)
Thermal correction to Energy= 0.270265
Thermal correction to Enthalpy= 0.271209
Thermal correction to Gibbs Free Energy= 0.185309

Electronic energy:

B3LYP = -1564.9775035

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.214140	-0.591672	0.562740
2	1	0	4.272229	-0.357880	1.620528
3	1	0	5.211367	-0.689183	0.144006
4	6	0	0.139310	0.702685	-0.156170
5	1	0	-0.217106	-0.283726	-0.431296
6	1	0	0.544098	1.197792	-1.031298
7	6	0	2.506294	1.279810	0.637348
8	1	0	2.302132	2.193056	0.094161
9	1	0	2.889054	1.516715	1.623192
10	6	0	-2.268961	0.805549	0.697623
11	1	0	-2.199480	0.343614	1.678153
12	1	0	-3.013596	1.592997	0.713732
13	7	0	1.240578	0.582550	0.787601
14	7	0	-0.997190	1.432002	0.349129
15	7	0	3.544347	0.538393	-0.056960
16	7	0	-2.620463	-0.247953	-0.230779
17	7	0	-0.917621	2.808774	0.351897
18	7	0	3.478926	0.508670	-1.448942
19	7	0	-3.262260	0.157035	-1.402569
20	7	0	1.066009	-0.251920	1.864479
21	8	0	-3.155084	1.331830	-1.696603
22	8	0	-3.839693	-0.705770	-2.038290
23	8	0	4.225191	-0.271281	-2.009631
24	8	0	2.702267	1.276541	-1.990608
25	8	0	-0.003896	-0.844581	1.928120
26	8	0	1.971311	-0.330810	2.674652
27	8	0	0.151460	3.286410	-0.005186
28	8	0	-1.886866	3.434047	0.734412
29	7	0	3.442083	-1.835982	0.431547

30	7	0	3.909457	-2.684807	-0.330621
31	7	0	4.240079	-3.542357	-0.978786
32	6	0	-2.918027	-1.583825	0.257088
33	1	0	-2.838897	-2.281878	-0.570883
34	1	0	-2.155149	-1.804350	0.996925
35	7	0	-4.215527	-1.674632	0.934682
36	7	0	-5.146118	-2.146383	0.275175
37	7	0	-6.069257	-2.573896	-0.203558

BC-HMX

Zero-point correction= 0.166186 (Hartree/Particle)
Thermal correction to Energy= 0.182813
Thermal correction to Enthalpy= 0.183757
Thermal correction to Gibbs Free Energy= 0.119309

Electronic energy:

B3LYP = -1195.8942716
W1-F12 = -1196.02804802

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.046783	-1.231214	-1.336921
2	7	0	-1.380803	-1.118006	0.219225
3	7	0	-1.928293	-2.361552	-0.055135
4	7	0	-1.380765	1.118048	0.219260
5	7	0	2.112384	1.816719	-0.121278
6	7	0	-1.928226	2.361611	-0.055111
7	7	0	1.011336	1.157457	0.506442
8	7	0	2.112299	-1.816812	-0.121247
9	7	0	1.011292	-1.157476	0.506459
10	8	0	3.144069	1.826167	0.511411
11	8	0	-1.163961	-3.209287	-0.467829
12	8	0	-1.163875	3.209321	-0.467818

13	8	0	-3.117669	2.476736	0.177583
14	8	0	1.897995	2.351180	-1.185971
15	8	0	1.897882	-2.351178	-1.185980
16	8	0	3.143998	-1.826315	0.511423
17	8	0	-3.117737	-2.476651	0.177574
18	6	0	-0.094534	0.780525	-0.359941
19	6	0	-0.094554	-0.780515	-0.359944
20	6	0	1.349050	-0.000008	1.336034
21	6	0	-2.307957	0.000034	0.338814
22	1	0	0.046790	1.231222	-1.336919
23	1	0	2.388853	-0.000025	1.632029
24	1	0	0.705881	0.000012	2.212786
25	1	0	-3.058300	0.000059	-0.454668
26	1	0	-2.812220	0.000027	1.300472

ETN

Zero-point correction= 0.157688 (Hartree/Particle)
Thermal correction to Energy= 0.177374
Thermal correction to Enthalpy= 0.178318
Thermal correction to Gibbs Free Energy= 0.101136

Electronic energy:

B3LYP = -1277.7555946
W1-F12 = -1277.94067950
DLPNO-CCSD(T) = -1275.819200983

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.860053	-0.513859	0.194609
2	6	0	-0.664190	0.349801	-0.163217
3	1	0	-1.789192	-1.485908	-0.288771
4	1	0	-1.934216	-0.644554	1.273399
5	6	0	0.664190	-0.349801	0.163217

6	1	0	-0.696790	0.616910	-1.217442
7	6	0	1.860053	0.513859	-0.194609
8	1	0	0.696790	-0.616910	1.217442
9	1	0	1.934216	0.644554	-1.273399
10	1	0	1.789192	1.485908	0.288771
11	8	0	-2.996762	0.205595	-0.300896
12	8	0	-0.710977	1.541921	0.631387
13	8	0	0.710977	-1.541921	-0.631387
14	8	0	2.996762	-0.205595	0.300896
15	7	0	-4.246438	-0.419783	-0.004137
16	8	0	-4.201977	-1.464170	0.589289
17	8	0	-5.176211	0.207936	-0.405817
18	7	0	-0.982372	2.779592	-0.086678
19	8	0	-1.002842	2.733262	-1.282022
20	8	0	-1.127695	3.687842	0.665239
21	7	0	0.982372	-2.779592	0.086678
22	8	0	1.002842	-2.733262	1.282022
23	8	0	1.127695	-3.687842	-0.665239
24	7	0	4.246438	0.419783	0.004137
25	8	0	4.201977	1.464170	-0.589289
26	8	0	5.176211	-0.207936	0.405817

PETN

Zero-point correction= 0.186948 (Hartree/Particle)
Thermal correction to Energy= 0.207781
Thermal correction to Enthalpy= 0.208726
Thermal correction to Gibbs Free Energy= 0.132084

Electronic energy:

B3LYP = -1317.0937455
W1-F12 = -1317.27303193
DLPNO-CCSD(T) = -1315.07923547

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.867608	0.867630	0.923858
2	1	0	0.246069	1.502191	1.551209
3	1	0	1.501954	0.246116	1.551451
4	8	0	1.681254	1.680979	0.063712
5	7	0	2.562192	2.561914	0.761606
6	8	0	2.526902	2.526855	1.961397
7	8	0	3.223033	3.222529	0.020557
8	6	0	-0.867608	0.867630	-0.923858
9	1	0	-0.246069	1.502191	-1.551209
10	1	0	-1.501954	0.246116	-1.551451
11	6	0	0.867608	-0.867630	-0.923858
12	1	0	0.246069	-1.502191	-1.551209
13	1	0	1.501954	-0.246116	-1.551451
14	6	0	-0.867608	-0.867630	0.923858
15	1	0	-1.501954	-0.246116	1.551451
16	1	0	-0.246069	-1.502191	1.551209
17	8	0	-1.681254	-1.680979	0.063712
18	8	0	1.681254	-1.680979	-0.063712
19	8	0	-1.681254	1.680979	-0.063712
20	7	0	2.562192	-2.561914	-0.761606
21	8	0	3.223033	-3.222529	-0.020557
22	8	0	2.526902	-2.526855	-1.961397
23	7	0	-2.562192	-2.561914	0.761606
24	8	0	-2.526902	-2.526855	1.961397
25	8	0	-3.223033	-3.222529	0.020557
26	7	0	-2.562192	2.561914	-0.761606
27	8	0	-3.223033	3.222529	-0.020557
28	8	0	-2.526902	2.526855	-1.961397
29	6	0	0.000000	0.000000	0.000000

SMX

Zero-point correction= 0.219298 (Hartree/Particle)
Thermal correction to Energy= 0.246214
Thermal correction to Enthalpy= 0.247158
Thermal correction to Gibbs Free Energy= 0.156395

Electronic energy:

B3LYP = -1765.5783172
DLPNO-CCSD(T) = -1762.89786073

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.617727	0.445539	1.183629
2	6	0	-0.680481	-0.223720	0.151063
3	1	0	-1.758984	-0.248095	2.012736
4	1	0	-1.185991	1.360518	1.572915
5	6	0	0.821987	-0.112597	0.627505
6	6	0	1.732945	-1.111482	-0.084288
7	1	0	1.431911	-2.132367	0.122781
8	1	0	1.720211	-0.924989	-1.154973
9	8	0	-2.895015	0.721083	0.638893
10	8	0	3.035222	-0.873983	0.459576
11	7	0	-3.284909	2.132857	0.675613
12	8	0	-2.587750	2.885663	1.290062
13	8	0	-4.296368	2.307532	0.081130
14	7	0	4.049150	-1.730483	-0.095367
15	8	0	3.687621	-2.520596	-0.922098
16	8	0	5.122214	-1.512932	0.368409
17	7	0	-0.763813	0.564096	-1.189887
18	8	0	-1.027875	1.745025	-1.112429
19	8	0	-0.531414	-0.051494	-2.205011
20	7	0	0.811795	-0.499118	2.139479
21	8	0	0.729285	-1.680296	2.405813
22	8	0	0.852071	0.410068	2.939827

23	6	0	-1.059710	-1.676659	-0.131248
24	1	0	-0.476177	-2.076630	-0.953032
25	1	0	-0.890101	-2.273324	0.762263
26	6	0	1.389512	1.319530	0.556303
27	1	0	0.649836	2.063789	0.827314
28	1	0	2.243793	1.407503	1.219868
29	8	0	1.801065	1.495880	-0.802063
30	8	0	-2.444433	-1.680264	-0.480131
31	7	0	2.017894	2.876839	-1.170784
32	8	0	1.870593	3.692645	-0.306661
33	8	0	2.328119	2.983923	-2.312678
34	7	0	-2.928335	-2.986606	-0.832009
35	8	0	-2.136913	-3.888672	-0.770217
36	8	0	-4.077187	-2.973976	-1.137042

C4H10

Zero-point correction= 0.131652 (Hartree/Particle)
Thermal correction to Energy= 0.137428
Thermal correction to Enthalpy= 0.138372
Thermal correction to Gibbs Free Energy= 0.103652

Electronic energy:

B3LYP = -158.5388223
W1-F12 = -158.49528974
DLPNO-CCSD(T) = -158.204411

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.876958	-0.518934	0.186545
2	6	0	-0.664093	0.331020	-0.180313
3	1	0	-1.850704	-1.482178	-0.327235
4	1	0	-1.905191	-0.719859	1.259519
5	6	0	0.664093	-0.331020	0.180313

6	1	0	-0.677138	0.546023	-1.253194
7	6	0	1.876958	0.518934	-0.186545
8	1	0	0.677138	-0.546023	1.253194
9	1	0	1.905191	0.719859	-1.259519
10	1	0	1.850704	1.482178	0.327235
11	1	0	-2.810741	-0.023990	-0.083306
12	1	0	-0.728990	1.300533	0.322933
13	1	0	0.728990	-1.300533	-0.322933
14	1	0	2.810741	0.023990	0.083306

C6H12(NO2)2

Zero-point correction= 0.193757 (Hartree/Particle)
Thermal correction to Energy= 0.206500
Thermal correction to Enthalpy= 0.207444
Thermal correction to Gibbs Free Energy= 0.156269

Electronic energy:

B3LYP = -646.3950873
W1-F12 = -646.42229632
DLPNO-CCSD(T) = -645.31409231

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.571160	1.496583	-1.034853
2	6	0	-0.140740	0.778711	0.104074
3	1	0	1.637458	1.530683	-0.820823
4	1	0	0.420717	1.014294	-1.995248
5	6	0	0.140740	-0.778711	0.104074
6	6	0	-0.140740	-1.469092	1.434533
7	1	0	0.464773	-1.060601	2.236051
8	1	0	-1.191646	-1.353074	1.684049
9	7	0	-1.675048	0.901436	-0.133545
10	8	0	-2.058741	1.310649	-1.210188

11	8	0	-2.405210	0.563681	0.782026
12	7	0	1.675048	-0.901436	-0.133545
13	8	0	2.405210	-0.563681	0.782026
14	8	0	2.058741	-1.310649	-1.210188
15	6	0	0.140740	1.469092	1.434533
16	1	0	-0.464773	1.060601	2.236051
17	1	0	1.191646	1.353074	1.684049
18	6	0	-0.571160	-1.496583	-1.034853
19	1	0	-0.420717	-1.014294	-1.995248
20	1	0	-0.209368	-2.518640	-1.109029
21	1	0	0.209368	2.518640	-1.109029
22	1	0	-0.079879	2.532108	1.342591
23	1	0	0.079879	-2.532108	1.342591
24	1	0	-1.637458	-1.530683	-0.820823

PMDA

Zero-point correction= 0.179448 (Hartree/Particle)
Thermal correction to Energy= 0.186623
Thermal correction to Enthalpy= 0.187567
Thermal correction to Gibbs Free Energy= 0.148394

Electronic energy:

B3LYP = -345.4819524
W1-F12 = -345.44356115
W2-F12 = -345.44408480

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.288110	-1.261780	0.235953
2	6	0	-2.080937	0.015584	-0.049563
3	6	0	-1.268763	1.264309	0.300515
4	6	0	0.078791	1.278995	-0.428676
5	6	0	0.838592	-0.002034	-0.171095

6	6	0	0.056150	-1.252946	-0.498164
7	1	0	-1.833089	2.166678	0.058900
8	1	0	-2.348172	0.043031	-1.111252
9	1	0	-3.019112	0.009147	0.508378
10	1	0	-1.111627	-1.341694	1.313070
11	1	0	-1.864210	-2.142451	-0.052707
12	1	0	-0.085777	1.379600	-1.506312
13	1	0	0.684388	2.126046	-0.103115
14	1	0	-0.115854	-1.278902	-1.578498
15	1	0	0.656213	-2.130414	-0.252215
16	1	0	-1.083514	1.285569	1.377926
17	7	0	1.695220	0.022744	0.997192
18	1	0	1.791343	-0.921993	1.362932
19	7	0	2.261731	-0.067843	-0.393476
20	1	0	2.616414	0.868312	-0.576945

24-DNI

Zero-point correction= 0.076174 (Hartree/Particle)
Thermal correction to Energy= 0.084707
Thermal correction to Enthalpy= 0.085651
Thermal correction to Gibbs Free Energy= 0.041197

Electronic energy:

B3LYP = -635.494867
W1-F12 = -635.56009325
W2-F12 = -635.56316575

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.067080	-0.111881	0.000000
2	7	0	0.000000	0.717108	0.000000
3	6	0	0.695911	-1.440644	0.000000
4	1	0	1.274562	-2.345026	0.000000

5	6	0	-1.019566	-0.091374	0.000000
6	7	0	-0.660829	-1.406167	0.000000
7	7	0	2.435135	0.368752	0.000000
8	8	0	3.299132	-0.500986	0.000000
9	8	0	2.622581	1.566518	0.000000
10	7	0	-2.420178	0.273588	0.000000
11	8	0	-3.202845	-0.674699	0.000000
12	8	0	-2.706691	1.448199	0.000000
13	1	0	-1.311433	-2.176806	0.000000

45-DNI

Zero-point correction= 0.076107 (Hartree/Particle)
Thermal correction to Energy= 0.084814
Thermal correction to Enthalpy= 0.085758
Thermal correction to Gibbs Free Energy= 0.040478

Electronic energy:

B3LYP = -635.4867166
W1-F12 = -635.55194529
W2-F12 = -635.55502848

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.645816	0.478874	-0.029328
2	7	0	-0.872649	1.805394	-0.067285
3	6	0	0.703138	0.213526	-0.005310
4	6	0	0.323789	2.366493	-0.072310
5	7	0	1.308499	1.441593	-0.031448
6	7	0	-1.758112	-0.468614	-0.047608
7	8	0	-1.785590	-1.254328	-0.974816
8	8	0	-2.564529	-0.371042	0.854991
9	1	0	2.308677	1.571515	-0.011794
10	7	0	1.476785	-0.979523	0.090656

11	8	0	2.695851	-0.839223	0.016931
12	8	0	0.880272	-2.028169	0.246494
13	1	0	0.514961	3.425280	-0.105527

34-DNP

Zero-point correction= 0.075452 (Hartree/Particle)
Thermal correction to Energy= 0.084284
Thermal correction to Enthalpy= 0.085228
Thermal correction to Gibbs Free Energy= 0.038934

Electronic energy:

B3LYP = -635.4675432
W1-F12 = -635.53259701
W2-F12 = -635.53561033

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.354282	1.493941	0.013982
2	7	0	0.331002	2.362177	0.035529
3	1	0	0.376872	3.367117	0.054127
4	1	0	2.389622	1.782185	0.000312
5	6	0	0.771734	0.242968	0.000007
6	6	0	-0.615269	0.489403	0.010349
7	7	0	-0.882522	1.772803	0.033454
8	7	0	1.466256	-1.009248	-0.072358
9	8	0	0.789963	-2.008671	-0.249331
10	8	0	2.683915	-0.975277	0.036584
11	7	0	-1.716783	-0.474622	0.051126
12	8	0	-2.412740	-0.550579	-0.940065
13	8	0	-1.838219	-1.098590	1.085972

35-DNP

Zero-point correction= 0.075446 (Hartree/Particle)

Thermal correction to Energy= 0.084071
Thermal correction to Enthalpy= 0.085016
Thermal correction to Gibbs Free Energy= 0.040315

Electronic energy:

B3LYP = -635.4753566
W1-F12 = -635.53994866
W2-F12 = -635.54292669

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.069189	-0.057812	0.000000
2	7	0	-0.587450	-1.325874	0.000000
3	1	0	-1.133329	-2.174049	0.000000
4	6	0	0.000000	0.804696	0.000000
5	6	0	1.090107	-0.077418	0.000000
6	7	0	0.735517	-1.357227	0.000000
7	7	0	2.496547	0.300336	0.000000
8	8	0	3.326865	-0.584673	0.000000
9	8	0	2.717480	1.502756	0.000000
10	7	0	-2.485233	0.186183	0.000000
11	8	0	-2.853005	1.345327	0.000000
12	8	0	-3.204408	-0.806433	0.000000
13	1	0	-0.003295	1.877512	0.000000

1-ADP

Zero-point correction= 0.092591 (Hartree/Particle)
Thermal correction to Energy= 0.102504
Thermal correction to Enthalpy= 0.103448
Thermal correction to Gibbs Free Energy= 0.056004

Electronic energy:

B3LYP = -690.8221844
W1-F12 = -690.88555275

W2-F12 = -690.88865474

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.935727	-0.255372	-0.033880
2	7	0	-0.577540	1.066508	-0.025309
3	6	0	0.232754	-0.999883	-0.023670
4	6	0	1.217654	-0.024153	-0.010692
5	7	0	0.722796	1.222560	-0.019690
6	7	0	2.649257	-0.241540	0.019117
7	8	0	3.375255	0.732842	0.057300
8	8	0	3.009311	-1.410552	0.004287
9	7	0	-2.287033	-0.715671	0.016927
10	8	0	-2.463321	-1.915194	-0.079685
11	8	0	-3.174219	0.124459	0.169460
12	1	0	0.332820	-2.067892	-0.012516
13	7	0	-1.390985	2.177300	-0.175324
14	1	0	-2.294031	1.969823	0.236643
15	1	0	-0.918548	2.957979	0.264378

5-ADP

Zero-point correction= 0.091775 (Hartree/Particle)
Thermal correction to Energy= 0.102068
Thermal correction to Enthalpy= 0.103012
Thermal correction to Gibbs Free Energy= 0.054777

Electronic energy:

B3LYP = -690.8645528
W1-F12 = -690.92793711
W2-F12 = -690.93110247

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.510256	-0.841756	0.036166
2	7	0	-0.857820	-2.024010	0.025499
3	1	0	-1.252750	-2.946508	0.076857
4	6	0	-0.498501	0.128946	0.025753
5	6	0	0.706698	-0.612511	0.005484
6	7	0	0.504819	-1.897581	0.008122
7	7	0	-0.706681	1.518669	-0.089676
8	8	0	0.260123	2.239555	-0.270114
9	8	0	-1.878223	1.917102	-0.013793
10	7	0	2.079694	-0.106718	0.060447
11	8	0	2.801226	-0.367570	-0.880711
12	8	0	2.375103	0.517836	1.060167
13	7	0	-2.846780	-0.689696	0.081683
14	1	0	-3.164569	0.264957	-0.007928
15	1	0	-3.448802	-1.426557	-0.240258

TNP

Zero-point correction= 0.077434 (Hartree/Particle)
Thermal correction to Energy= 0.088875
Thermal correction to Enthalpy= 0.089820
Thermal correction to Gibbs Free Energy= 0.037794

Electronic energy:

B3LYP = -840.0388949
W1-F12 = -840.14418816
W2-F12 = -840.14846355

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.085713	-0.612046	0.000000
2	7	0	-0.617159	-1.882590	0.000000
3	1	0	-1.179218	-2.721518	0.000000

4	6	0	0.011341	0.216899	0.000000
5	6	0	1.097553	-0.672529	0.000000
6	7	0	0.703463	-1.937848	0.000000
7	7	0	0.013353	1.679327	0.000000
8	8	0	0.011341	2.211264	1.088321
9	8	0	0.011341	2.211264	-1.088321
10	7	0	2.510583	-0.324740	0.000000
11	8	0	2.745768	0.873321	0.000000
12	8	0	3.317171	-1.228228	0.000000
13	7	0	-2.494779	-0.334351	0.000000
14	8	0	-2.824708	0.834524	0.000000
15	8	0	-3.231926	-1.311022	0.000000

MTNP

Zero-point correction= 0.104922 (Hartree/Particle)
Thermal correction to Energy= 0.117971
Thermal correction to Enthalpy= 0.118915
Thermal correction to Gibbs Free Energy= 0.063383

Electronic energy:

B3LYP = -879.3715799
W1-F12 = -879.46730380
W2-F12 = -879.47174409

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.792580	-0.712659	0.000000
2	7	0	1.742020	0.269165	0.000000
3	6	0	-0.439008	-0.090708	0.000000
4	6	0	-0.126804	1.269248	0.000000
5	7	0	1.184462	1.469733	0.000000
6	7	0	-1.756406	-0.726287	0.000000
7	8	0	-2.236971	-0.957065	1.087972

8	8	0	-2.236971	-0.957065	-1.087972
9	7	0	-1.054987	2.386814	0.000000
10	8	0	-2.236971	2.079630	0.000000
11	8	0	-0.593809	3.508178	0.000000
12	7	0	1.076545	-2.123097	0.000000
13	8	0	0.110561	-2.862428	0.000000
14	8	0	2.250712	-2.463105	0.000000
15	6	0	3.201010	0.169883	0.000000
16	1	0	3.536756	-0.362463	0.884639
17	1	0	3.536756	-0.362463	-0.884639
18	1	0	3.565971	1.190874	0.000000

DNPPy

Zero-point correction= 0.093215 (Hartree/Particle)
Thermal correction to Energy= 0.103715
Thermal correction to Enthalpy= 0.104660
Thermal correction to Gibbs Free Energy= 0.056292

Electronic energy:

B3LYP = -783.1141741
W1-F12 = -783.18238765
W2-F12 = -783.18566511

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.333642	1.042678	0.000000
2	6	0	0.019098	0.694093	0.000000
3	6	0	-0.019098	-0.694093	0.000000
4	7	0	-1.333642	-1.042678	0.000000
5	7	0	-2.131747	0.031249	0.000000
6	7	0	2.131747	-0.031249	0.000000
7	6	0	1.333642	-1.088155	0.000000
8	6	0	-1.333642	1.088155	0.000000

9	7	0	-1.821220	2.442384	0.000000
10	8	0	-3.015393	2.648655	0.000000
11	8	0	-0.935836	3.297473	0.000000
12	7	0	1.821220	-2.442384	0.000000
13	8	0	3.015393	-2.648655	0.000000
14	8	0	0.935836	-3.297473	0.000000
15	1	0	1.733470	1.966020	0.000000
16	1	0	-1.733470	-1.966020	0.000000

ANPZ

Zero-point correction= 0.115263 (Hartree/Particle)
Thermal correction to Energy= 0.126874
Thermal correction to Enthalpy= 0.127819
Thermal correction to Gibbs Free Energy= 0.077171

Electronic energy:

B3LYP = -784.4244385
W1-F12 = -784.47765122
W2-F12 = -784.48123233

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.158121	1.241696
2	6	0	0.000000	1.131169	-0.193852
3	6	0	0.000000	-1.131169	-0.193852
4	6	0	0.000000	-1.158121	1.241696
5	7	0	0.000000	2.342805	-1.018148
6	8	0	0.000000	2.229561	-2.221903
7	8	0	0.000000	3.426414	-0.418516
8	7	0	0.000000	-2.342805	-1.018148
9	8	0	0.000000	-3.426414	-0.418516
10	8	0	0.000000	-2.229561	-2.221903
11	7	0	0.000000	2.277250	1.968257

12	1	0	0.000000	3.165917	1.494189
13	1	0	0.000000	2.193144	2.969500
14	7	0	0.000000	0.000000	-0.838578
15	7	0	0.000000	0.000000	1.901960
16	7	0	0.000000	-2.277250	1.968257
17	1	0	0.000000	-2.193144	2.969500
18	1	0	0.000000	-3.165917	1.494189

LLM-105

Zero-point correction= 0.119203 (Hartree/Particle)
Thermal correction to Energy= 0.131586
Thermal correction to Enthalpy= 0.132531
Thermal correction to Gibbs Free Energy= 0.080511

Electronic energy:

B3LYP = -859.6204907
W1-F12 = -859.69129033
W2-F12 = -859.69536880

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.200019	0.978531
2	6	0	0.000000	1.130469	-0.436446
3	6	0	0.000000	-1.130469	-0.436446
4	6	0	0.000000	-1.200019	0.978531
5	7	0	0.000000	2.352898	-1.248689
6	8	0	0.000000	2.247182	-2.451844
7	8	0	0.000000	3.425496	-0.633876
8	7	0	0.000000	-2.352898	-1.248689
9	8	0	0.000000	-3.425496	-0.633876
10	8	0	0.000000	-2.247182	-2.451844
11	7	0	0.000000	2.265408	1.765140
12	1	0	0.000000	3.178600	1.343765

13	1	0	0.000000	2.078026	2.758234
14	7	0	0.000000	-2.265408	1.765140
15	1	0	0.000000	-2.078026	2.758234
16	1	0	0.000000	-3.178600	1.343765
17	7	0	0.000000	0.000000	1.644070
18	7	0	0.000000	0.000000	-1.086721
19	8	0	0.000000	0.000000	2.941340

ANTA

Zero-point correction= 0.077885 (Hartree/Particle)
Thermal correction to Energy= 0.085428
Thermal correction to Enthalpy= 0.086372
Thermal correction to Gibbs Free Energy= 0.044796

Electronic energy:

B3LYP = -502.3319039
W1-F12 = -502.37112720
W2-F12 = -502.37310281

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.390155	0.106711	-0.001599
2	7	0	1.823438	-0.187885	0.003707
3	7	0	-0.038864	1.343687	-0.015752
4	7	0	-1.381818	1.149263	-0.018095
5	6	0	-1.667342	-0.178807	-0.000234
6	7	0	-0.543973	-0.868844	0.013083
7	8	0	2.584413	0.762019	0.036493
8	8	0	2.138403	-1.363015	-0.025595
9	1	0	-1.999275	1.941385	-0.071614
10	7	0	-2.929554	-0.697365	-0.057101
11	1	0	-2.962557	-1.690076	0.111642
12	1	0	-3.662189	-0.182760	0.402886

NTO

Zero-point correction= 0.065825 (Hartree/Particle)
Thermal correction to Energy= 0.072892
Thermal correction to Enthalpy= 0.073836
Thermal correction to Gibbs Free Energy= 0.033702

Electronic energy:

B3LYP = -522.2186539
W1-F12 = -522.27081546
W2-F12 = -522.27333393

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.405289	0.000000
2	7	0	0.810218	1.602539	0.000000
3	7	0	-1.288370	0.395443	0.000000
4	7	0	-1.596082	-0.925137	0.000000
5	6	0	-0.489431	-1.772699	0.000000
6	7	0	0.553688	-0.839203	0.000000
7	8	0	-0.446266	-2.974953	0.000000
8	8	0	2.020741	1.402458	0.000000
9	8	0	0.250682	2.677685	0.000000
10	1	0	1.536339	-1.052290	0.000000
11	1	0	-2.557177	-1.220267	0.000000

5-ATZ

Zero-point correction= 0.063068 (Hartree/Particle)
Thermal correction to Energy= 0.067975
Thermal correction to Enthalpy= 0.068919
Thermal correction to Gibbs Free Energy= 0.035120

Electronic energy:

B3LYP = -313.7557239

W1-F12 = -313.76663149

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.621357	-0.043508	-0.003522
2	7	0	-1.485948	0.574839	0.004407
3	7	0	-0.120171	-1.130869	0.009688
4	7	0	-1.411133	-0.699429	0.008601
5	7	0	-0.197292	1.024435	-0.005354
6	1	0	0.000338	2.008284	-0.059131
7	7	0	1.987750	0.003468	-0.077526
8	1	0	2.443019	0.743010	0.432364
9	1	0	2.416062	-0.897350	0.069181

DAT

Zero-point correction= 0.079926 (Hartree/Particle)
Thermal correction to Energy= 0.086085
Thermal correction to Enthalpy= 0.087029
Thermal correction to Gibbs Free Energy= 0.050269

Electronic energy:

B3LYP = -369.1086825
W1-F12 = -369.12026832
W2-F12 = -369.12106271

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.224681	-0.715635	0.005140
2	7	0	-0.203895	0.631730	0.010662
3	7	0	1.103356	1.040522	0.003121
4	7	0	1.798890	-0.029376	-0.006850
5	7	0	1.019212	-1.149906	-0.005384

6	7	0	-1.363340	-1.453563	0.065972
7	1	0	-2.208461	-0.989698	-0.224160
8	1	0	-1.267533	-2.415170	-0.212430
9	7	0	-1.302055	1.471692	-0.014877
10	1	0	-1.327152	2.017143	0.839472
11	1	0	-1.213949	2.103845	-0.802222

BTZ

Zero-point correction= 0.073894 (Hartree/Particle)
Thermal correction to Energy= 0.080780
Thermal correction to Enthalpy= 0.081725
Thermal correction to Gibbs Free Energy= 0.042034

Electronic energy:

B3LYP = -515.5413664
W1-F12 = -515.56636622

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.009975	0.719456	0.000000
2	7	0	0.672316	2.787262	0.000000
3	7	0	-1.077572	1.488415	0.000000
4	7	0	-0.614951	2.763199	0.000000
5	7	0	1.077572	1.507326	0.000000
6	6	0	0.009975	-0.719456	0.000000
7	7	0	1.077572	-1.488415	0.000000
8	7	0	-1.077572	-1.507326	0.000000
9	7	0	0.614951	-2.763199	0.000000
10	7	0	-0.672316	-2.787262	0.000000
11	1	0	-2.053756	-1.255529	0.000000
12	1	0	2.053756	1.255529	0.000000

BTO

Zero-point correction= 0.080937 (Hartree/Particle)
Thermal correction to Energy= 0.089917
Thermal correction to Enthalpy= 0.090861
Thermal correction to Gibbs Free Energy= 0.046544

Electronic energy:

B3LYP = -665.9311065
W1-F12 = -665.98965514

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.012039	0.711494	0.000000
2	7	0	0.703994	2.766652	0.000000
3	7	0	-1.073829	1.498533	0.000000
4	7	0	-0.597014	2.760046	0.000000
5	7	0	1.073829	1.492424	0.000000
6	6	0	0.012039	-0.711494	0.000000
7	7	0	1.073829	-1.498533	0.000000
8	7	0	-1.073829	-1.492424	0.000000
9	7	0	0.597014	-2.760046	0.000000
10	7	0	-0.703994	-2.766652	0.000000
11	8	0	2.381718	1.131362	0.000000
12	8	0	-2.381718	-1.131362	0.000000
13	1	0	2.371471	0.148506	0.000000
14	1	0	-2.371471	-0.148506	0.000000

Ph-Azs

Zero-point correction= 0.118288 (Hartree/Particle)
Thermal correction to Energy= 0.127054
Thermal correction to Enthalpy= 0.127998
Thermal correction to Gibbs Free Energy= 0.082104

Electronic energy:

B3LYP = -584.6296639

W1-F12 = -584.63103737
W2-F12 = -584.63319377

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.051753	2.522444	0.000000
2	7	0	0.978235	1.513353	0.000000
3	7	0	-1.223854	1.170458	0.000000
4	7	0	0.000000	0.677564	0.000000
5	8	0	0.394192	2.715039	0.000000
6	8	0	-1.803212	3.443566	0.000000
7	6	0	0.242871	-0.734506	0.000000
8	6	0	-0.849059	-1.591001	0.000000
9	6	0	1.550893	-1.205715	0.000000
10	6	0	-0.618241	-2.959814	0.000000
11	1	0	-1.847244	-1.183009	0.000000
12	6	0	1.760520	-2.575463	0.000000
13	1	0	2.378853	-0.514192	0.000000
14	6	0	0.680445	-3.453293	0.000000
15	1	0	-1.458715	-3.639242	0.000000
16	1	0	2.771538	-2.957394	0.000000
17	1	0	0.853007	-4.520531	0.000000

Tol-Azs

Zero-point correction= 0.145045 (Hartree/Particle)
Thermal correction to Energy= 0.155734
Thermal correction to Enthalpy= 0.156678
Thermal correction to Gibbs Free Energy= 0.105981

Electronic energy:

B3LYP = -623.9300195
W1-F12 = -623.96032703

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.159197	-0.416976	0.003214
2	7	0	1.707800	1.322982	0.000542
3	7	0	1.883798	-0.898563	0.000708
4	7	0	1.119679	0.178342	-0.000245
5	8	0	3.013430	1.031933	0.002233
6	8	0	4.229482	-0.936545	0.003507
7	6	0	-0.310977	0.088027	-0.001691
8	6	0	-0.899854	-1.168051	-0.005192
9	6	0	-1.078830	1.248684	-0.003325
10	6	0	-2.285156	-1.256357	-0.008340
11	1	0	-0.279535	-2.050728	-0.007560
12	6	0	-2.457797	1.133703	-0.006452
13	1	0	-0.603969	2.217902	-0.004406
14	6	0	-3.087359	-0.115806	-0.006706
15	1	0	-2.747192	-2.234808	-0.014125
16	1	0	-3.058476	2.034107	-0.010830
17	6	0	-4.587578	-0.217918	0.013204
18	1	0	-5.042711	0.496898	-0.673098
19	1	0	-4.922895	-1.216686	-0.262028
20	1	0	-4.977325	-0.000943	1.010809

ANF

Zero-point correction= 0.064986 (Hartree/Particle)
Thermal correction to Energy= 0.072228
Thermal correction to Enthalpy= 0.073172
Thermal correction to Gibbs Free Energy= 0.032759

Electronic energy:

B3LYP = -522.1313267
W1-F12 = -522.18429138
W2-F12 = -522.18662923

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.399843	-1.512225	0.013474
2	6	0	-0.948597	0.661566	-0.012223
3	6	0	0.101506	-0.313363	-0.005824
4	8	0	-1.723255	-1.342687	0.020516
5	7	0	-2.083778	0.004094	0.006910
6	7	0	1.523739	-0.074013	0.001471
7	8	0	2.279237	-1.018164	-0.049137
8	8	0	1.851188	1.111308	0.063798
9	7	0	-0.838049	2.003100	-0.072881
10	1	0	-1.658431	2.559929	0.086531
11	1	0	0.069147	2.400499	0.097524

DAF

Zero-point correction= 0.079131 (Hartree/Particle)
Thermal correction to Energy= 0.085284
Thermal correction to Enthalpy= 0.086228
Thermal correction to Gibbs Free Energy= 0.049486

Electronic energy:

B3LYP = -372.9392806
W1-F12 = -372.95526847
W2-F12 = -372.95645727

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.231554	-0.717313	0.000554
2	6	0	0.232208	0.717082	-0.000590
3	7	0	-0.997289	-1.135845	0.000758
4	8	0	-1.778941	0.000760	0.000469

5	7	0	-0.996240	1.136716	-0.001169
6	7	0	1.351195	-1.523594	0.069227
7	1	0	1.142611	-2.506602	-0.024934
8	1	0	2.094449	-1.239753	-0.552811
9	7	0	1.352587	1.522372	-0.069260
10	1	0	1.144782	2.505645	0.023949
11	1	0	2.095337	1.238481	0.553364

DNAF

Zero-point correction= 0.084625 (Hartree/Particle)
Thermal correction to Energy= 0.095204
Thermal correction to Enthalpy= 0.096148
Thermal correction to Gibbs Free Energy= 0.047456

Electronic energy:

B3LYP = -782.0629457
W1-F12 = -782.15339585

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.042924	0.717420	0.962926
2	6	0	0.042924	-0.717420	0.962926
3	7	0	-0.064128	1.121556	2.201552
4	8	0	0.000000	0.000000	2.968867
5	7	0	0.064128	-1.121556	2.201552
6	7	0	0.000000	1.655704	-0.052384
7	1	0	0.212843	2.613962	0.184917
8	7	0	0.000000	-1.655704	-0.052384
9	1	0	-0.212843	-2.613962	0.184917
10	7	0	-0.875540	1.576959	-1.136368
11	8	0	-0.928723	2.570844	-1.826177
12	8	0	-1.460638	0.525258	-1.289766
13	7	0	0.875540	-1.576959	-1.136368

14	8	0	0.928723	-2.570844	-1.826177
15	8	0	1.460638	-0.525258	-1.289766

DAAzF

Zero-point correction= 0.113970 (Hartree/Particle)
Thermal correction to Energy= 0.125634
Thermal correction to Enthalpy= 0.126578
Thermal correction to Gibbs Free Energy= 0.076102

Electronic energy:

B3LYP = -743.4078607
W1-F12 = -743.44465733

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.453287	2.456132	-0.050502
2	7	0	-0.546269	0.317300	-0.004094
3	7	0	0.546269	-0.317300	-0.004094
4	7	0	1.453287	-2.456132	-0.050502
5	6	0	0.783137	2.523712	0.024927
6	6	0	-0.783137	-2.523712	0.024927
7	6	0	-0.393885	1.687040	-0.006057
8	6	0	0.393885	-1.687040	-0.006057
9	7	0	2.066269	2.118624	0.111137
10	1	0	2.257568	1.140190	-0.015847
11	1	0	2.800384	2.794043	-0.003363
12	7	0	0.393885	3.772231	-0.009191
13	8	0	-1.002586	3.713212	-0.053183
14	8	0	1.002586	-3.713212	-0.053183
15	7	0	-2.066269	-2.118624	0.111137
16	1	0	-2.257568	-1.140190	-0.015847
17	1	0	-2.800384	-2.794043	-0.003363
18	7	0	-0.393885	-3.772231	-0.009191

DAAF

Zero-point correction= 0.119410 (Hartree/Particle)
Thermal correction to Energy= 0.131463
Thermal correction to Enthalpy= 0.132407
Thermal correction to Gibbs Free Energy= 0.079994

Electronic energy:

B3LYP = -818.6159881
W1-F12 = -818.67080523

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.631574	-1.321278	-0.287926
2	7	0	-0.390923	-0.543388	-0.234240
3	7	0	0.292997	0.519008	-0.043320
4	7	0	2.311461	1.530076	-0.435399
5	6	0	-2.513626	0.864593	0.202123
6	6	0	2.648241	-0.568824	0.262173
7	6	0	-1.797241	-0.341655	-0.104398
8	6	0	1.670727	0.436427	-0.098857
9	7	0	-2.017953	2.083237	0.497434
10	1	0	-1.045445	2.245136	0.298640
11	1	0	-2.653258	2.860913	0.521431
12	7	0	-3.790501	0.566240	0.187693
13	8	0	-3.847118	-0.791694	-0.112455
14	8	0	3.618490	1.250037	-0.339651
15	7	0	2.444619	-1.794872	0.815449
16	1	0	1.620009	-2.274687	0.482976
17	1	0	3.273914	-2.360621	0.903062
18	7	0	3.835733	-0.048957	0.090940
19	8	0	0.026023	-1.676398	-0.536239

34-MNF

Zero-point correction= 0.079466 (Hartree/Particle)
Thermal correction to Energy= 0.088149
Thermal correction to Enthalpy= 0.089093
Thermal correction to Gibbs Free Energy= 0.044562

Electronic energy:

B3LYP =-581.2789124
W1-F12 = -581.33433187
W2-F12 = -581.33730925

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.562771	0.000000
2	6	0	-0.136516	-0.846341	0.000000
3	7	0	1.230911	0.972603	0.000000
4	8	0	1.998711	-0.121481	0.000000
5	7	0	1.105645	-1.315578	0.000000
6	7	0	-1.089539	1.533169	0.000000
7	8	0	-0.804904	2.709470	0.000000
8	8	0	-2.215221	1.054413	0.000000
9	6	0	-1.307727	-1.758349	0.000000
10	1	0	-1.928564	-1.583642	0.877222
11	1	0	-1.928564	-1.583642	-0.877222
12	1	0	-0.959200	-2.788424	0.000000
13	8	0	1.615496	-2.407917	0.000000

34-MNF

Zero-point correction= 0.079613 (Hartree/Particle)
Thermal correction to Energy= 0.088085
Thermal correction to Enthalpy= 0.089029
Thermal correction to Gibbs Free Energy= 0.045297

Electronic energy:

B3LYP = -581.2766975
W1-F12 = -581.33107150
W2-F12 = -581.33409331

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.132988	0.000000
2	6	0	-0.691557	-1.111380	0.000000
3	7	0	1.317808	-0.108332	0.000000
4	8	0	1.430745	-1.544315	0.000000
5	7	0	0.168532	-2.085653	0.000000
6	8	0	2.319714	0.545654	0.000000
7	7	0	-0.530314	1.462992	0.000000
8	8	0	0.246700	2.398462	0.000000
9	8	0	-1.754188	1.538248	0.000000
10	6	0	-2.153714	-1.370655	0.000000
11	1	0	-2.621874	-0.924091	0.875657
12	1	0	-2.621874	-0.924091	-0.875657
13	1	0	-2.320557	-2.444971	0.000000

34-CNF

Zero-point correction= 0.050100 (Hartree/Particle)
Thermal correction to Energy= 0.058863
Thermal correction to Enthalpy= 0.059807
Thermal correction to Gibbs Free Energy= 0.014835

Electronic energy:

B3LYP = -634.1967524
W1-F12 = -634.26511485
W2-F12 = -634.26807240

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.115135	-0.712835	0.000000
2	6	0	0.000000	0.701210	0.000000
3	7	0	-1.340085	-1.120915	0.000000
4	8	0	-2.121183	-0.028084	0.000000
5	7	0	-1.256997	1.172601	0.000000
6	7	0	0.993645	-1.668069	0.000000
7	8	0	0.717205	-2.845409	0.000000
8	8	0	2.103155	-1.163675	0.000000
9	6	0	1.102658	1.573121	0.000000
10	7	0	1.978016	2.320622	0.000000
11	8	0	-1.767576	2.249837	0.000000

BTF

Zero-point correction= 0.086722 (Hartree/Particle)
Thermal correction to Energy= 0.099321
Thermal correction to Enthalpy= 0.100265
Thermal correction to Gibbs Free Energy= 0.047555

Electronic energy:

B3LYP =-1008.4731726
W1-F12 = -1008.56090455

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.416690	0.000000
2	6	0	-1.249528	0.726628	0.000000
3	6	0	-1.227001	-0.708444	0.000000
4	6	0	-0.004595	-1.445476	0.000000
5	6	0	1.226956	-0.708607	0.000000
6	6	0	1.253981	0.718701	0.000000
7	7	0	-0.213745	-2.731929	0.000000
8	7	0	2.481887	-1.133838	0.000000
9	7	0	2.472840	1.180517	0.000000

10	7	0	-0.258867	2.716079	0.000000
11	7	0	-2.259028	1.550994	0.000000
12	7	0	-2.222961	-1.582222	0.000000
13	8	0	-1.743141	2.804212	0.000000
14	8	0	-1.557037	-2.911656	0.000000
15	8	0	3.299796	0.107800	0.000000
16	8	0	3.036786	-2.196750	0.000000
17	8	0	-3.420890	-1.530768	0.000000
18	8	0	0.384515	3.727892	0.000000

NNFF

Zero-point correction= 0.079347 (Hartree/Particle)
Thermal correction to Energy= 0.092632
Thermal correction to Enthalpy= 0.093576
Thermal correction to Gibbs Free Energy= 0.035993

Electronic energy:

B3LYP = -1007.4629609
W1-F12 = -1007.58855748

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.556437	1.629179	-0.714607
2	7	0	-0.550431	-1.571494	-1.309883
3	6	0	1.907934	0.090089	0.065421
4	6	0	-1.880608	-0.406847	-0.003161
5	6	0	0.591850	0.339058	-0.384216
6	6	0	-0.571158	-0.512048	-0.550324
7	7	0	2.662626	1.140011	0.032383
8	8	0	1.907583	2.147531	-0.439614
9	8	0	-1.801102	-2.114352	-1.222169
10	7	0	-2.614083	-1.389303	-0.422023
11	7	0	-2.385019	0.586079	0.938820

12	8	0	-3.574902	0.612168	1.150392
13	8	0	-1.529883	1.300702	1.438295
14	7	0	2.413405	-1.170651	0.608555
15	8	0	3.611098	-1.334807	0.623883
16	8	0	1.554338	-1.938509	1.010008
17	8	0	-0.275714	2.373736	-1.148174

DNBF

Zero-point correction= 0.083177 (Hartree/Particle)
Thermal correction to Energy= 0.097451
Thermal correction to Enthalpy= 0.098395
Thermal correction to Gibbs Free Energy= 0.040222

Electronic energy:

B3LYP = -1082.6645102
W1-F12 = -1082.80078235

1	7	0	1.240654	1.206632	0.878017
2	7	0	-1.240654	-1.206632	0.878017
3	6	0	-0.596630	1.824535	-0.149138
4	6	0	0.596630	-1.824535	-0.149138
5	6	0	0.132717	0.707531	0.323126
6	6	0	-0.132717	-0.707531	0.323126
7	7	0	-0.001753	2.951052	0.073497
8	8	0	1.151824	2.664487	0.702286
9	8	0	-1.151824	-2.664487	0.702286
10	7	0	0.001753	-2.951052	0.073497
11	7	0	1.861338	-1.783017	-0.881500
12	8	0	2.444310	-2.826253	-1.058682
13	8	0	2.199885	-0.672452	-1.260194
14	7	0	-1.861338	1.783017	-0.881500
15	8	0	-2.444310	2.826253	-1.058682
16	8	0	-2.199885	0.672452	-1.260194
17	8	0	-2.199885	-0.744020	1.424837

18	8	0	2.199885	0.744020	1.424837

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