Supporting Information (SI)

The scavenging mechanism of hydrazone compounds towards HOO• and CH_3OO• radicals: A computational mechanistic and kinetic study

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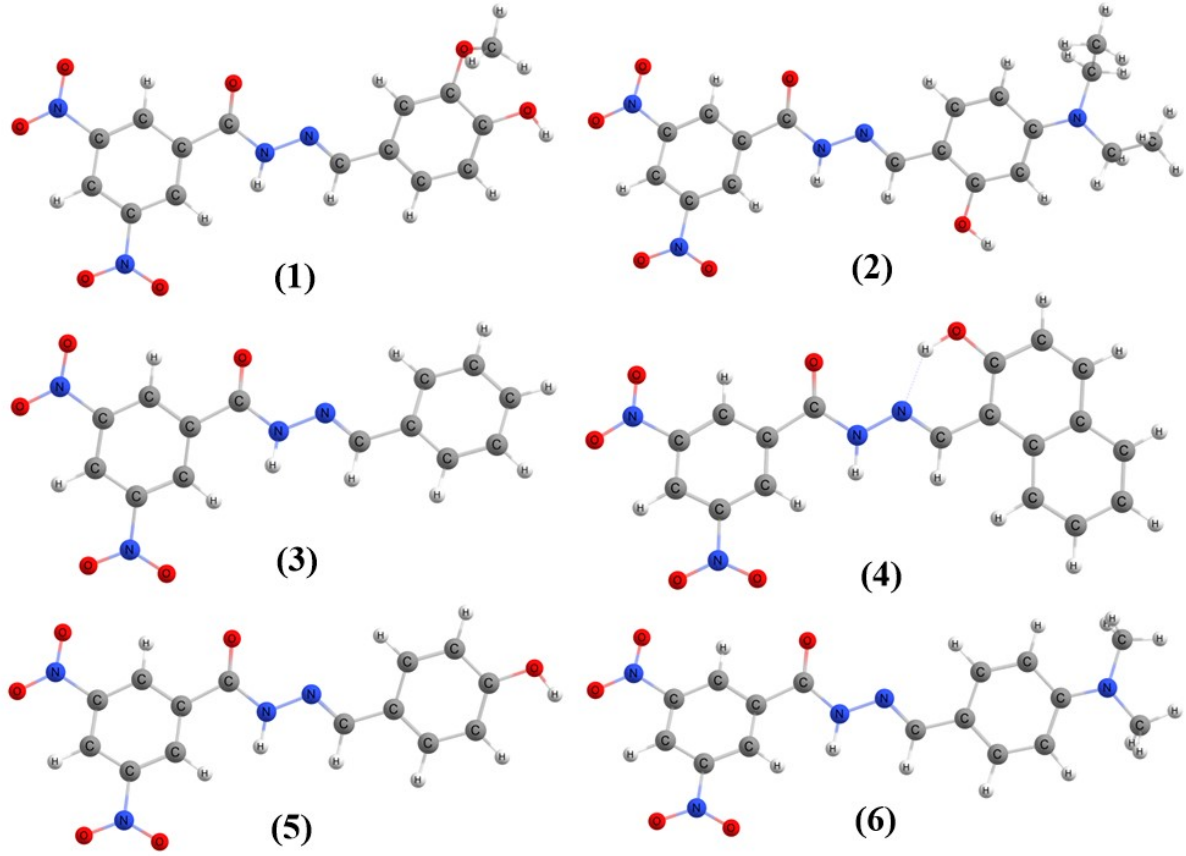

Figure S1. Optimized molecular geometries of hydrazone compounds **1**– **6** computed in the gas phase at the M062X/6-311+G(d,p) level of theory.

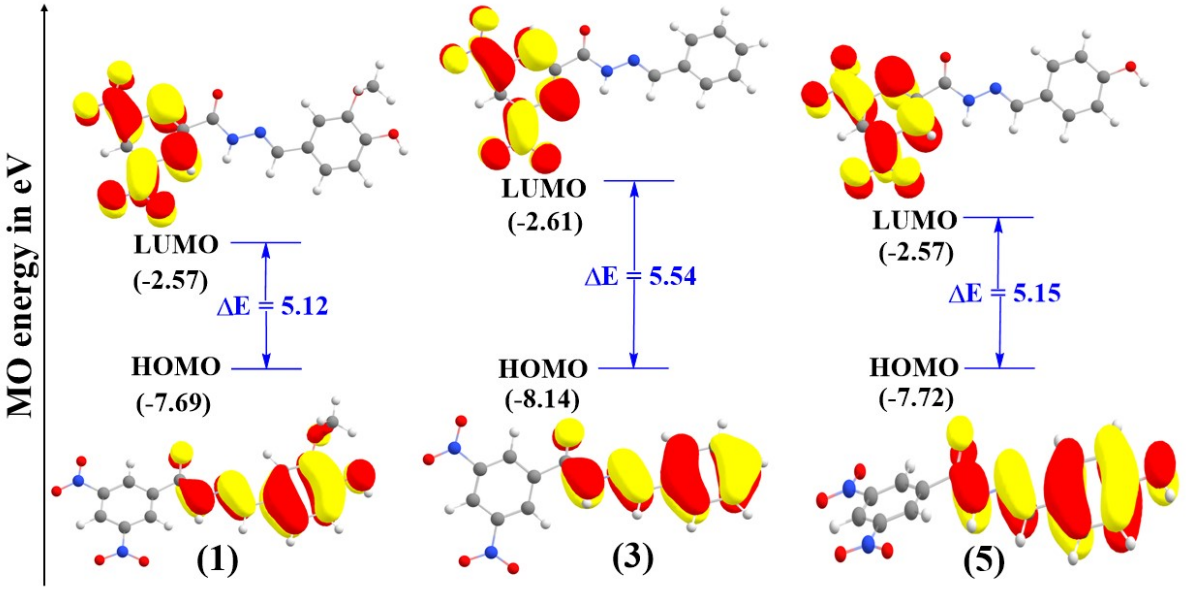

Figure S2. Frontiers molecular orbital (FMO) plots of Compound **1**, **3**, and **5** calculated in the gas phase.

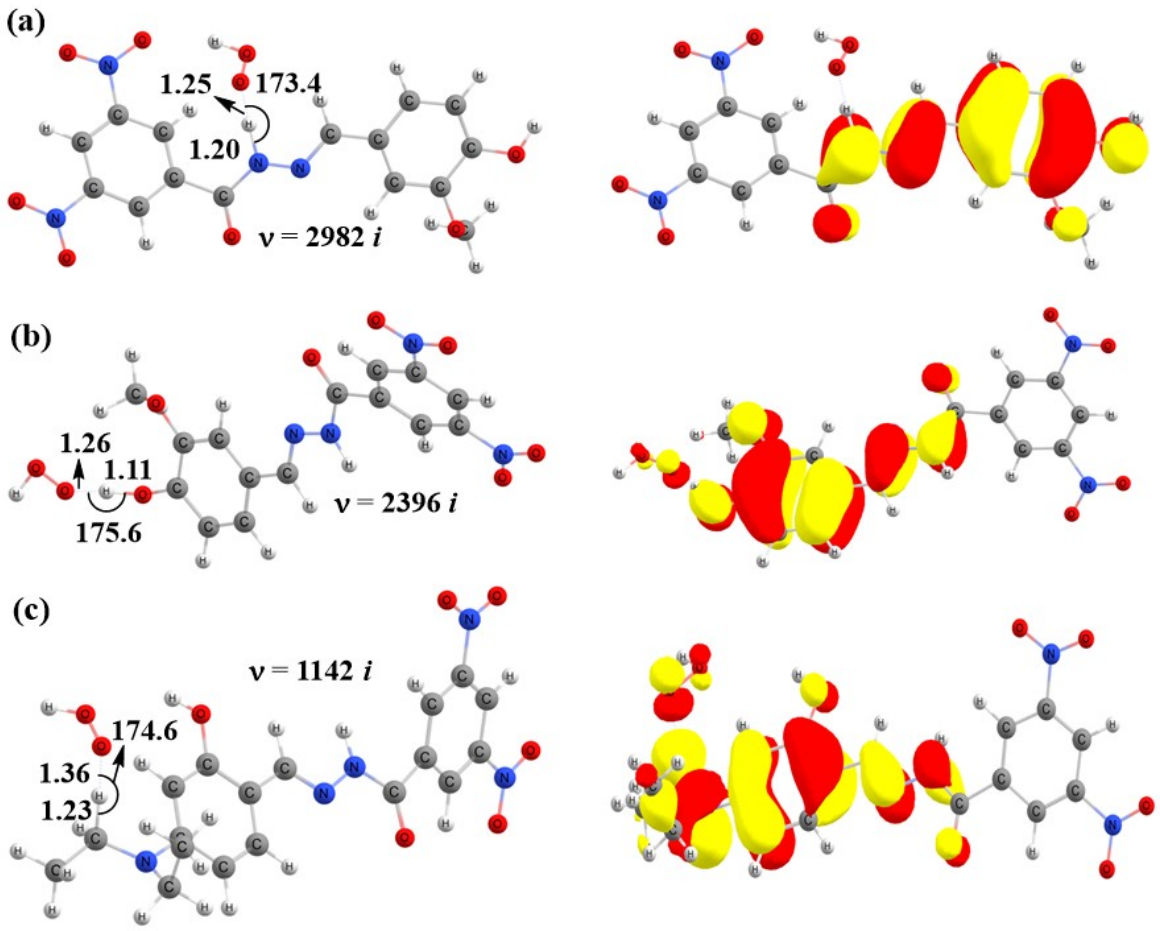

Figure S3. Optimized geometries of transition states of HAT reactions between HOO• and (a) TS-1-N8 (b) TS-1-O4′ (c) TS-2-C7′ and their corresponding SOMO distributions. (Bond angle in °, Bond distance in Å).

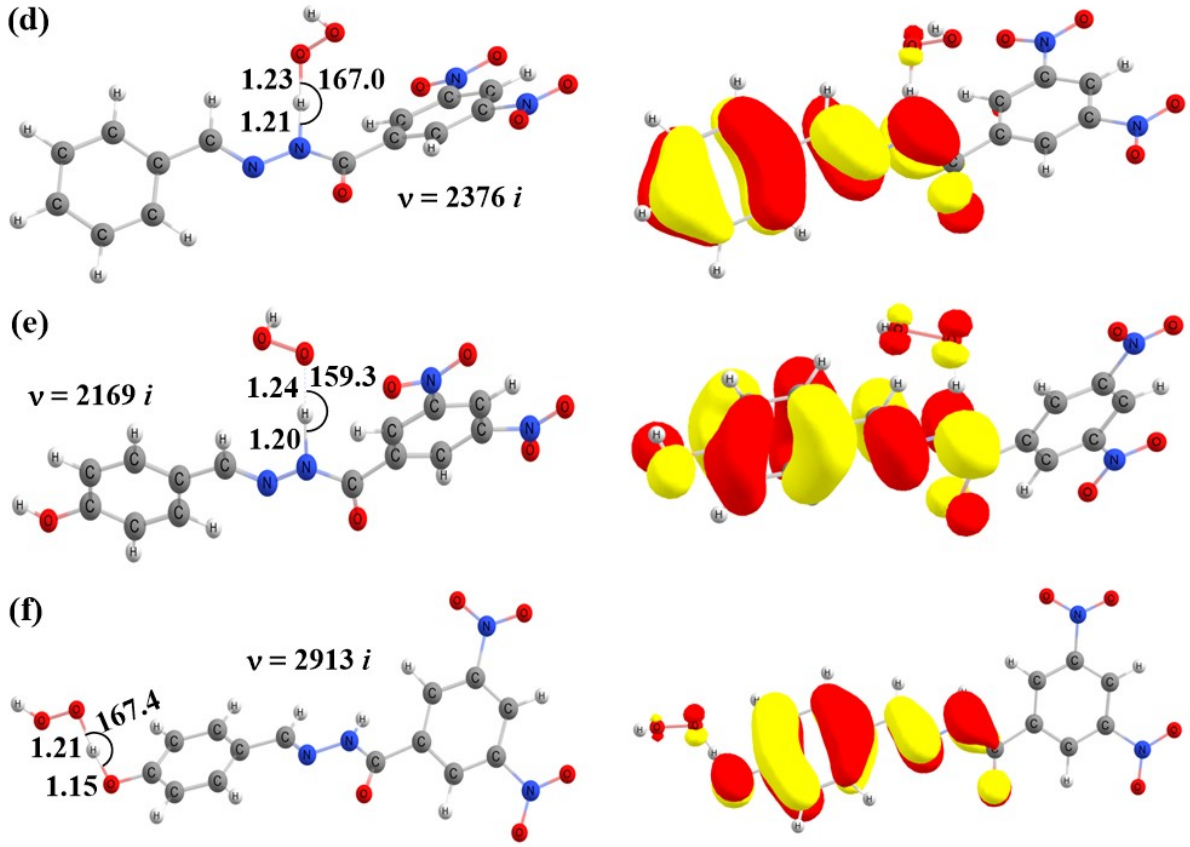

Figure S4. Optimized geometries of transition states of HAT reactions between HOO• and (d) TS-3-N8 (e) TS-5-N8 (f) TS-5-O4′ and their corresponding SOMO distributions. (Bond angle in °, Bond distance in Å).

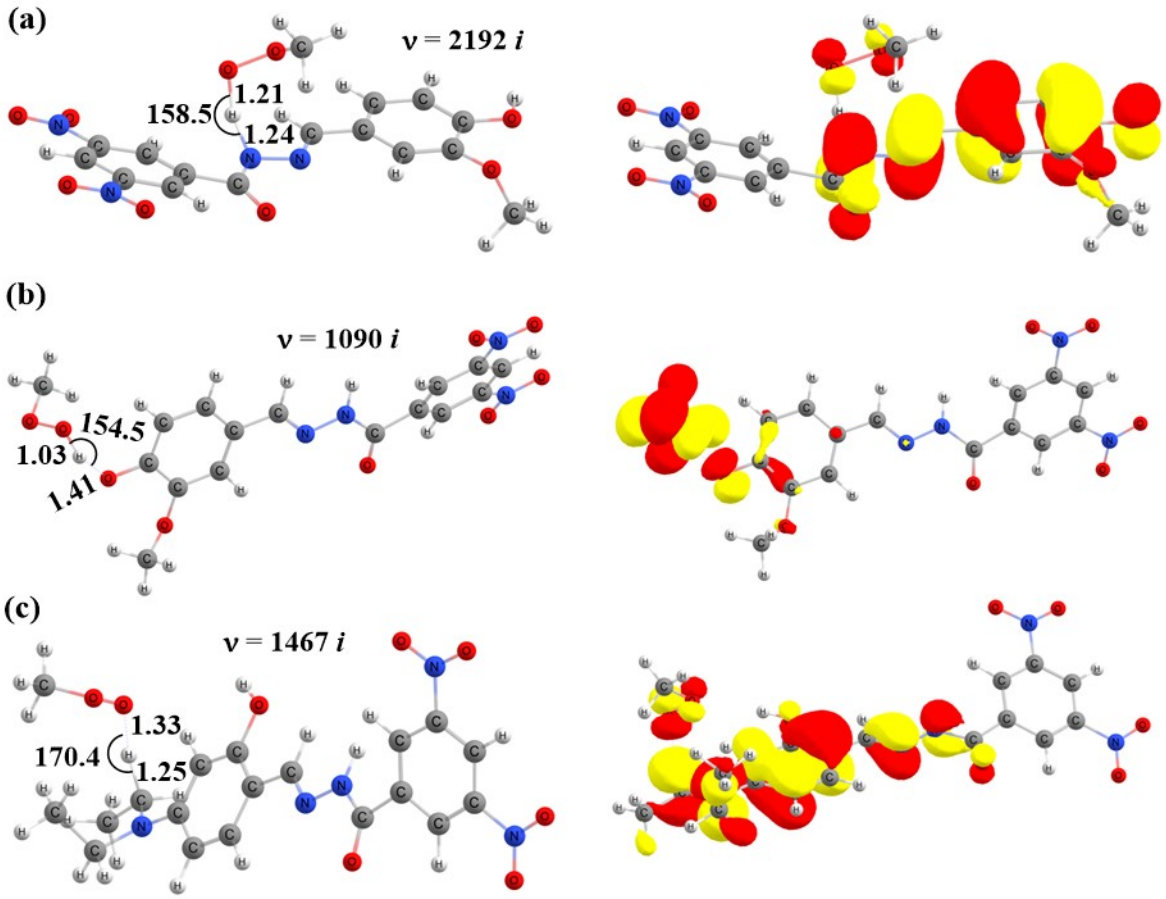

Figure S5. Optimized geometries of transition states of HAT reactions between $CH_3OO^{\bullet}$ and (a) TS-1-N8 (b) TS-1-O4′ (c) TS-2-C7′ ′ and their corresponding SOMO distributions. (Bond angle in °, Bond distance in Å).

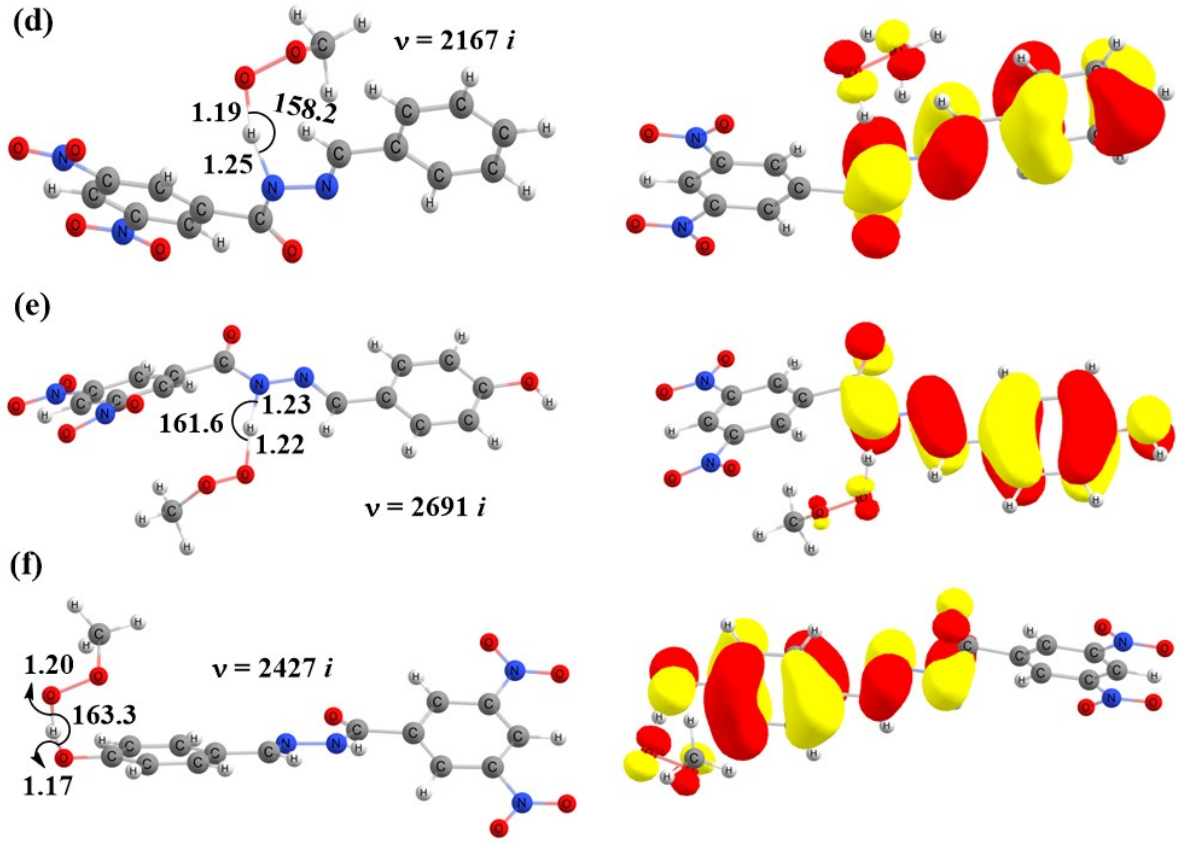

Figure S6. Optimized geometries of transition states of HAT reactions between $CH_3OO^{\bullet}$ and (d) TS-3-N8 (e) TS-5-N8 (f) TS-5-O4′ and their corresponding SOMO distributions. (Bond angle in °, Bond distance in Å).

Table S1. The values of the enthalpies (in Hartree) of e^-, H^+, and $H^{\bullet}$ in the gas phase, water and pentyl ethanoate.

Species	gas phase	water	pentyl ethanoate
$H(e^-)$	0.00120	-0.03885	-0.02403
$H(H^+)$	0.00236	-0.40331	-0.3885
$H(H^{\bullet})$	-0.49577	-0.49364	-0.49541

Table S2. BDE (kcal mol^{-1}) values and Gibbs free energy (ΔG° in kcal mol^{-1} at 298.15 K) values of the reaction corresponding to HAT mechanism of compounds (**1- 6**) with $HOO^{\bullet}$ and $CH_3OO^{\bullet}$ radicals in the gas phase calculated at the M062X/6-311+G (d,p) level of theory.

Compound	Positions	BDE	ΔG°	
			$HOO^{\bullet}$	$CH_3OO^{\bullet}$
1	C2-H	116.8	31.1	32.3
	C4-H	117.2	31.6	32.8
	C6-H	111.9	26.0	27.2
	N8-H	87.9	**1.5**	**2.8**
	C10-H	101.3	15.0	16.2

	C2′-H	114.9	29.1	30.3
	C3′-H	97.2	11.4	12.7
	O4′-H	81.2	**- 4.4**	**-3.2**
	C5′-H	112.0	26.5	27.7
	C6′-H	111.9	26.3	27.5
2	C2-H	116.6	30.6	31.9
	C4-H	117.1	31.5	32.8
	C6-H	112.0	26.0	27.2
	N8-H	84.7	**-1.2**	**0.1**
	C10-H	101.6	15.2	16.4
	O2′-H	84.8	**- 0.2**	**1.0**
	C3′-H	108.9	22.6	23.8
	C5′-H	108.4	22.2	23.4
	C6′-H	112.4	26.6	27.8
	C7′-H	88.5	**2.5**	**3.7**
	C8′-H	100.0	13.5	14.8
3	C2-H	116.8	31.1	32.4
	C4-H	117.2	31.6	32.8
	C6-H	111.9	26.2	27.4
	N8-H	89.4	**3.1**	**4.3**
	C10-H	101.5	14.7	15.9
	C2′-H	112.9	27.4	28.6
	C3′-H	111.3	25.8	27.0
	C4′-H	111.3	25.8	27.0
	C5′-H	111.4	25.9	27.1
	C6′-H	111.3	25.8	27.0
4	C2-H	116.8	30.7	32.0
	C4-H	117.2	31.6	32.9
	C6-H	112.0	25.8	27.0
	N8-H	83.3	**-1.8**	**-0.6**
	C10-H	99.7	13.9	15.1
	O2′-H	96.6	10.7	11.9
	C3′-H	113.8	28.3	29.6
	C4′-H	111.3	25.7	26.9
	C5′-H	111.4	25.7	27.0
	C6′-H	111.8	26.2	27.5
	C7′-H	110.9	25.3	26.5
	C8′-H	108.2	22.9	24.1
5	C2-H	116.8	31.3	32.6
	C4-H	117.1	31.5	32.7
	C6-H	111.9	26.2	27.4
	N8-H	87.9	**2.1**	**3.3**
	C10-H	101.2	14.7	15.9
	C2′-H	113.0	27.5	28.7
	C3′-H	113.7	28.0	29.3

	O4′-H	87.1	**2.0**	**3.2**
	C5′-H	112.3	26.8	28.0
	C6′-H	111.4	25.8	27.0
6	C2-H	116.7	31.0	32.2
	C4-H	117.1	31.5	32.7
	C6-H	112.0	26.1	27.3
	N8-H	84.8	**- 0.6**	**0.6**
	C10-H	100.9	13.0	14.2
	C2′-H	112.3	26.3	27.6
	C3′-H	109.7	24.4	25.6
	C5′-H	134.8	49.8	51.0
	C6′-H	110.7	24.8	26.0
	C7′-H	90.0	5.2	6.5

Table S3. The Gibbs free energy (ΔG° in kcal mol^{-1} at 298.15 K) values of the reaction corresponding to SET and SPLET mechanisms of compounds (**1**- **6**) with $HOO^{\bullet}$ and $CH_3OO^{\bullet}$ radicals in the gas phase calculated at the M062X/6-311+G (d, p) level of theory.

Compound	ΔG°		Sites	ΔG°	
	SET			SPLET	
	$HOO^{\bullet}$	$CH_3OO^{\bullet}$		$HOO^{\bullet}$	$CH_3OO^{\bullet}$
1	160.5	158.8	N8-H	166.0	146.7
			O4′-H	171.4	152.0
2	139.1	137.4	N8-H	171.5	152.1
			O2′-H	175.1	155.7
3	172.2	170.5	N8-H	165.3	145.9
4	157.2	155.5	N8-H	158.2	138.8
			O2′-H	182.9	163.6
5	163.6	161.9	N8-H	166.3	146.9
			O4′-H	174.3	154.9
6	144.0	142.3	N8-H	170.0	150.7

Table S4. Calculated Free Energy (ΔG° in kcal mol^{-1} at 298.15 K) of reaction between Hydrazone Compounds (1-6) with $HOO^{\bullet}$ and $CH_3OO^{\bullet}$ radicals via SET mechanism in the Water solvent.

Compounds[a]	ΔG°	
	$HOO^{\bullet}$	$CH_3OO^{\bullet}$
1	33.0	34.8
2	13.7	15.5
3	40.8	42.6
4	30.2	32.0
5	33.4	35.2
6	15.9	17.7
Anions		

1-O4′	7.1	8.9
2-O2′	4.1	5.9
3-N8	14.7	16.5
4-N8	13.8	15.6
5-O4′	7.6	9.4
6-N8	6.0	7.8

[a] = Neutral molecule

Table S5. Cartesian coordinates of all the reactants, radicals,cationic radicals, and anions including the zero point energy, ZPE, enthalpy, H, free energy, G,imaginary frequency calculated at the M06-2X/6-311+G(d,p) level of theory in the gas phase.

N′-(4-Hydroxy-3-methoxybenzylidene)-3,5-dinitrobenzohydrazide (1)

```
C         5.071834000     -0.255762000     -0.008302000
C         4.113015000     -1.215238000     -0.272735000
C         2.757046000     -0.929844000     -0.339643000
C         2.335424000      0.378472000     -0.125096000
C         3.273612000      1.379186000      0.125270000
C         4.612132000      1.036759000      0.187007000
H         6.124561000     -0.498868000      0.037853000
H         2.070565000     -1.729322000     -0.587743000
H         2.953184000      2.404716000      0.260715000
C         0.890448000      0.807629000     -0.207753000
O         0.590394000      1.928091000     -0.529022000
N        -0.005472000     -0.180297000      0.117325000
H         0.322092000     -1.039188000      0.547388000
N        -1.342543000      0.066004000      0.057682000
C        -2.110578000     -0.856373000      0.482184000
C        -3.566640000     -0.716190000      0.461414000
C        -4.361553000     -1.765257000      0.915466000
C        -5.747275000     -1.652725000      0.906373000
C        -6.350184000     -0.488774000      0.447709000
C        -5.553193000      0.573741000     -0.021469000
C        -4.177735000      0.453425000     -0.009053000
H        -3.901791000     -2.676936000      1.280867000
H        -6.365218000     -2.468445000      1.267704000
H        -3.575148000      1.283129000     -0.359438000
O        -6.128085000      1.738941000     -0.430401000
O        -7.694665000     -0.306552000      0.432923000
H        -8.133047000     -1.073465000      0.812006000
C        -6.819684000      1.653766000     -1.673805000
H        -7.642078000      0.938423000     -1.615946000
H        -7.212273000      2.648697000     -1.872725000
H        -6.126797000      1.366449000     -2.470254000
N         5.609765000      2.098133000      0.470589000
O         5.188847000      3.215899000      0.652225000
O         6.772431000      1.766175000      0.501375000
N         4.553935000     -2.611161000     -0.503260000
O         5.741864000     -2.828354000     -0.476031000
O         3.690083000     -3.437052000     -0.698737000
H        -1.710813000     -1.798029000      0.879174000
Zero-point correction=                           0.273423(Hartree/Particle)
 Thermal correction to Energy=                    0.296701
 Thermal correction to Enthalpy=                  0.297646
 Thermal correction to Gibbs Free Energy=         0.216417
 Sum of electronic and zero-point Energies=          -1323.734896
 Sum of electronic and thermal Energies=             -1323.711618
 Sum of electronic and thermal Enthalpies=           -1323.710673
```

Sum of electronic and thermal Free Energies= -1323.791902

OOH

O	0.054943000	-0.599131000	0.000000000
H	-0.879090000	-0.872954000	0.000000000
O	0.054943000	0.708250000	0.000000000

Zero-point correction= 0.014604(Hartree/Particle)
Thermal correction to Energy= 0.017456
Thermal correction to Enthalpy= 0.018400
Thermal correction to Gibbs Free Energy= -0.007537
Sum of electronic and zero-point Energies= -150.875902
Sum of electronic and thermal Energies= -150.873050
Sum of electronic and thermal Enthalpies= -150.872106
Sum of electronic and thermal Free Energies= -150.898043

CH_3OO

C	-0.988804000	-0.481863000	0.000000000
H	-1.950937000	0.025683000	0.000000000
H	-0.862976000	-1.088013000	0.896509000
H	-0.862976000	-1.088013000	-0.896509000
O	1.201214000	0.070962000	0.000000000
O	0.000000000	0.559228000	0.000000000

Zero-point correction= 0.043745
(Hartree/Particle)
Thermal correction to Energy= 0.047541
Thermal correction to Enthalpy= 0.048485
Thermal correction to Gibbs Free Energy= 0.018132
Sum of electronic and zero-point Energies= -190.144321
Sum of electronic and thermal Energies= -190.140525
Sum of electronic and thermal Enthalpies= -190.139581
Sum of electronic and thermal Free Energies= -190.169934

BHA

C	-2.016291000	1.124905000	0.000089000
C	-1.862870000	-0.252529000	0.000222000
C	-0.579526000	-0.806305000	0.000217000
C	0.573925000	-0.032331000	0.000147000
C	0.397382000	1.367870000	0.000068000
C	-0.871161000	1.921769000	0.000016000
H	-2.990224000	1.594283000	0.000110000
H	-0.523815000	-1.886239000	0.000146000
H	-0.977924000	3.002633000	0.000056000
O	1.508784000	2.175045000	0.000144000
H	1.230312000	3.094301000	-0.001288000
O	-2.891234000	-1.148667000	0.000398000
C	-4.200908000	-0.627868000	-0.000433000
H	-4.869645000	-1.485775000	-0.000699000
H	-4.387634000	-0.022203000	0.892666000
H	-4.386588000	-0.022465000	-0.893928000
C	1.969030000	-0.666837000	-0.000078000
C	2.738540000	-0.237747000	-1.262672000
C	2.738800000	-0.237634000	1.262355000
C	1.893854000	-2.198364000	0.000003000
H	2.201415000	-0.554511000	-2.160658000
H	2.876705000	0.841474000	-1.302204000
H	3.723433000	-0.713570000	-1.269746000
H	3.723930000	-0.712997000	1.268996000
H	2.876536000	0.841640000	1.302069000
H	2.202120000	-0.554846000	2.160436000

```
H        1.383744000     -2.579969000      0.888059000
H        1.383686000     -2.580097000     -0.887962000
H        2.908900000     -2.602250000      0.000000000

Zero-point  correction=                                          0.251543
(Hartree/Particle)
 Thermal correction to Energy=                    0.264988
 Thermal correction to Enthalpy=                  0.265932
 Thermal correction to Gibbs Free Energy=         0.212860
 Sum of electronic and zero-point Energies=          -578.900286
 Sum of electronic and thermal Energies=             -578.886841
 Sum of electronic and thermal Enthalpies=           -578.885897
 Sum of electronic and thermal Free Energies=        -578.938969
```

1-N8-H Radical

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C        5.024186000      0.232235000     -0.007468000
C        4.058177000      1.221653000      0.031045000
C        2.698427000      0.952016000      0.047148000
C        2.282280000     -0.377518000      0.024139000
C        3.224258000     -1.404709000     -0.014751000
C        4.567935000     -1.075703000     -0.029519000
H        6.079706000      0.466438000     -0.019638000
H        1.980528000      1.759329000      0.078405000
H        2.903546000     -2.438774000     -0.032648000
C        0.828240000     -0.760550000      0.036631000
O        0.482270000     -1.914752000      0.027625000
N       -0.029514000      0.365629000      0.072953000
N       -1.279651000      0.022901000     -0.000083000
C       -2.102013000      1.059636000      0.053612000
C       -3.515981000      0.879281000     -0.018204000
C       -4.359167000      2.001612000      0.052864000
C       -5.731009000      1.851520000     -0.015272000
C       -6.287953000      0.579932000     -0.159373000
C       -5.453241000     -0.560016000     -0.223420000
C       -4.088575000     -0.404515000     -0.155826000
H       -3.927703000      2.990199000      0.159805000
H       -6.383434000      2.717201000      0.031863000
H       -3.450421000     -1.277732000     -0.219020000
O       -5.995538000     -1.791460000     -0.414597000
O       -7.614713000      0.368751000     -0.252492000
H       -8.090315000      1.204826000     -0.227973000
C       -6.665272000     -2.330136000      0.724673000
H       -7.502958000     -1.696277000      1.021430000
H       -7.034168000     -3.308382000      0.425195000
H       -5.962581000     -2.440077000      1.555447000
N        5.571848000     -2.165986000     -0.070768000
O        5.155657000     -3.300893000     -0.082403000
O        6.737820000     -1.843003000     -0.089685000
N        4.503160000      2.635170000      0.057114000
O        5.694989000      2.841126000      0.041994000
O        3.643629000      3.486085000      0.091821000
H       -1.687766000      2.063989000      0.156843000
Zero-point correction=                           0.259784(Hartree/Particle)
 Thermal correction to Energy=                    0.282959
 Thermal correction to Enthalpy=                  0.283903
 Thermal correction to Gibbs Free Energy=         0.200758
 Sum of electronic and zero-point Energies=         -1323.098898
 Sum of electronic and thermal Energies=            -1323.075723
 Sum of electronic and thermal Enthalpies=          -1323.074779
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 Sum of electronic and thermal Free Energies=        -1323.157924
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1-O4′-H Radical

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C         5.050780000      0.224300000     -0.008036000
C         4.103751000      1.199546000      0.240865000
C         2.745420000      0.930333000      0.321108000
C         2.309434000     -0.378037000      0.137078000
C         3.235260000     -1.394117000     -0.097601000
C         4.576743000     -1.067200000     -0.173457000
H         6.105855000      0.455216000     -0.064991000
H         2.070219000      1.743311000      0.556313000
H         2.904327000     -2.419025000     -0.210818000
C         0.862391000     -0.789406000      0.236814000
O         0.545716000     -1.898761000      0.574038000
N        -0.030818000      0.206195000     -0.098206000
H         0.301414000      1.057616000     -0.540403000
N        -1.360289000     -0.024262000     -0.012095000
C        -2.134503000      0.898504000     -0.442930000
C        -3.580397000      0.759031000     -0.385880000
C        -4.385526000      1.825199000     -0.884810000
C        -5.739681000      1.737942000     -0.850997000
C        -6.422312000      0.573531000     -0.313750000
C        -5.556574000     -0.508999000      0.192261000
C        -4.175220000     -0.383347000      0.141240000
H        -3.901462000      2.706842000     -1.291331000
H        -6.380623000      2.528709000     -1.220904000
H        -3.562376000     -1.192709000      0.519145000
O        -6.016668000     -1.639498000      0.715122000
O        -7.657528000      0.504262000     -0.286392000
C        -7.410162000     -1.946002000      0.840710000
H        -7.892747000     -1.962004000     -0.134745000
H        -7.426253000     -2.933477000      1.295610000
H        -7.911300000     -1.218898000      1.476893000
N         5.561454000     -2.145358000     -0.439765000
O         5.126748000     -3.261695000     -0.595360000
O         6.726982000     -1.826346000     -0.483629000
N         4.560094000      2.595918000      0.438351000
O         5.749930000      2.799129000      0.402863000
O         3.704963000      3.434413000      0.617138000
H        -1.737699000      1.827252000     -0.868692000

Zero-point correction=                           0.260520(Hartree/Particle)
 Thermal correction to Energy=                    0.283478
 Thermal correction to Enthalpy=                  0.284422
 Thermal correction to Gibbs Free Energy=         0.202544
 Sum of electronic and zero-point Energies=          -1323.109439
 Sum of electronic and thermal Energies=             -1323.086482
 Sum of electronic and thermal Enthalpies=           -1323.085538
 Sum of electronic and thermal Free Energies=        -1323.167415
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1-Cationic Radical

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C         5.070251000      0.190135000      0.044277000
C         4.133597000      1.184627000      0.256947000
C         2.769835000      0.942973000      0.275267000
C         2.319830000     -0.357635000      0.064443000
C         3.232532000     -1.394114000     -0.138484000
C         4.580631000     -1.091937000     -0.150922000
H         6.132484000      0.400004000      0.034504000
```

H	2.110556000	1.774921000	0.489752000
H	2.894810000	-2.413333000	-0.281940000
C	0.874610000	-0.729986000	0.093733000
O	0.463549000	-1.820727000	0.343006000
N	-0.016733000	0.334677000	-0.229881000
H	0.344513000	1.208213000	-0.610394000
N	-1.305820000	0.125670000	-0.144167000
C	-2.121240000	1.069039000	-0.509262000
C	-3.531526000	0.839710000	-0.408075000
C	-4.419281000	1.890467000	-0.813943000
C	-5.768808000	1.716167000	-0.740452000
C	-6.297564000	0.494692000	-0.268214000
C	-5.415848000	-0.565145000	0.177569000
C	-4.051112000	-0.363931000	0.076988000
H	-4.009856000	2.823666000	-1.182384000
H	-6.453370000	2.497238000	-1.052762000
H	-3.388719000	-1.160882000	0.391207000
O	-5.815536000	-1.737824000	0.626387000
O	-7.594062000	0.261639000	-0.234602000
H	-8.112378000	1.007083000	-0.568687000
C	-7.135650000	-2.033754000	1.122508000
H	-7.836852000	-2.140994000	0.298055000
H	-7.018523000	-2.977996000	1.645362000
H	-7.465793000	-1.258296000	1.812471000
N	5.554421000	-2.191725000	-0.382551000
O	5.095934000	-3.293198000	-0.567273000
O	6.723357000	-1.893898000	-0.368996000
N	4.601746000	2.575596000	0.480180000
O	5.792064000	2.756250000	0.503670000
O	3.746093000	3.421980000	0.617151000
H	-1.764905000	2.029205000	-0.889282000

Zero-point correction=	0.273308(Hartree/Particle)
Thermal correction to Energy=	0.296450
Thermal correction to Enthalpy=	0.297394
Thermal correction to Gibbs Free Energy=	0.215456
Sum of electronic and zero-point Energies=	-1323.443486
Sum of electronic and thermal Energies=	-1323.420344
Sum of electronic and thermal Enthalpies=	-1323.419400
Sum of electronic and thermal Free Energies=	-1323.501338

1-N8-H Anion

C	5.038047000	0.235474000	0.035247000
C	4.068761000	1.226752000	0.047669000
C	2.707704000	0.959086000	0.015517000
C	2.279232000	-0.367817000	-0.031589000
C	3.224355000	-1.390710000	-0.045480000
C	4.574413000	-1.067564000	-0.011900000
H	6.092225000	0.466638000	0.060968000
H	1.970903000	1.750914000	0.026170000
H	2.879623000	-2.416569000	-0.082318000
C	0.802777000	-0.756788000	-0.069545000
O	0.542254000	-1.961060000	-0.110121000
N	0.023338000	0.331088000	-0.048341000
N	-1.297988000	0.029430000	-0.088349000
C	-2.083291000	1.039719000	-0.044506000
C	-3.538125000	0.871720000	-0.076857000
C	-4.377436000	1.982218000	0.022174000
C	-5.762859000	1.838820000	0.005251000

C	-6.334549000	0.581301000	-0.115656000
C	-5.502298000	-0.543673000	-0.219273000
C	-4.128717000	-0.396094000	-0.198930000
H	-3.942893000	2.971599000	0.116536000
H	-6.404947000	2.712327000	0.081897000
H	-3.493910000	-1.270917000	-0.283476000
O	-6.060853000	-1.788654000	-0.374146000
O	-7.690991000	0.376008000	-0.142474000
H	-8.129506000	1.228644000	-0.092274000
C	-6.598989000	-2.314249000	0.828486000
H	-7.397264000	-1.672926000	1.212400000
H	-7.004512000	-3.296131000	0.586904000
H	-5.812828000	-2.419092000	1.583320000
N	5.576842000	-2.153772000	-0.025959000
O	5.173196000	-3.294487000	-0.068272000
O	6.750660000	-1.840046000	0.005977000
N	4.523911000	2.631787000	0.098292000
O	5.721810000	2.836784000	0.118793000
O	3.680130000	3.500229000	0.116623000
H	-1.683416000	2.056422000	0.025682000

Zero-point correction=	0.259163(Hartree/Particle)
Thermal correction to Energy=	0.282296
Thermal correction to Enthalpy=	0.283240
Thermal correction to Gibbs Free Energy=	0.201534
Sum of electronic and zero-point Energies=	-1323.229706
Sum of electronic and thermal Energies=	-1323.206574
Sum of electronic and thermal Enthalpies=	-1323.205630
Sum of electronic and thermal Free Energies=	-1323.287335

1-O4′-H Anion

C	5.034021000	0.345381000	-0.021664000
C	4.024908000	1.251826000	0.246724000
C	2.688123000	0.891327000	0.346633000
C	2.330071000	-0.441560000	0.157104000
C	3.325415000	-1.388655000	-0.091508000
C	4.641627000	-0.973577000	-0.185437000
H	6.069167000	0.646590000	-0.090386000
H	1.961220000	1.653013000	0.598088000
H	3.052876000	-2.431303000	-0.196328000
C	0.915992000	-0.969407000	0.276198000
O	0.733032000	-2.127615000	0.594722000
N	-0.035718000	-0.055654000	-0.010040000
H	0.240622000	0.840801000	-0.399013000
N	-1.375921000	-0.349658000	0.058545000
C	-2.138180000	0.613382000	-0.353689000
C	-3.559425000	0.586301000	-0.388584000
C	-4.266908000	1.719286000	-0.848414000
C	-5.636362000	1.743555000	-0.899825000
C	-6.446801000	0.612891000	-0.506451000
C	-5.679422000	-0.536003000	-0.016191000
C	-4.315933000	-0.539618000	0.031261000
H	-3.701759000	2.591816000	-1.170410000
H	-6.171062000	2.613347000	-1.265137000
H	-3.803419000	-1.427081000	0.387205000
O	-6.353606000	-1.679369000	0.348494000
O	-7.690324000	0.603469000	-0.580055000
C	-7.232160000	-1.505678000	1.447580000
H	-7.993901000	-0.758514000	1.220657000
H	-7.699042000	-2.475025000	1.627302000

H	-6.666487000	-1.207954000	2.339295000
N	5.693343000	-1.979287000	-0.465560000
O	5.343250000	-3.126772000	-0.613629000
O	6.837626000	-1.583885000	-0.529413000
N	4.396028000	2.669395000	0.453815000
O	5.569840000	2.956624000	0.371952000
O	3.502196000	3.451949000	0.687936000
H	-1.678247000	1.548816000	-0.711080000

Zero-point correction= 0.259972(Hartree/Particle)
Thermal correction to Energy= 0.282829
Thermal correction to Enthalpy= 0.283774
Thermal correction to Gibbs Free Energy= 0.203260
Sum of electronic and zero-point Energies= -1323.222110
Sum of electronic and thermal Energies= -1323.199253
Sum of electronic and thermal Enthalpies= -1323.198309
Sum of electronic and thermal Free Energies= -1323.278822

N′-(4-(Diethylamino)2-hydroxy-benzylidene)-3,5-dinitrobenzohydrazide (2)

C	-6.098266000	0.289894000	-0.010793000
C	-5.101816000	1.196578000	-0.319031000
C	-3.763106000	0.844805000	-0.415546000
C	-3.398429000	-0.478144000	-0.185818000
C	-4.377013000	-1.426794000	0.108608000
C	-5.695495000	-1.019214000	0.198897000
H	-7.136455000	0.584383000	0.057274000
H	-3.045389000	1.604892000	-0.696977000
H	-4.101475000	-2.463727000	0.254830000
C	-1.978532000	-0.981830000	-0.298105000
O	-1.750455000	-2.125573000	-0.603987000
N	-1.027938000	-0.038546000	-0.019725000
H	-1.298958000	0.846734000	0.395932000
N	0.297321000	-0.352519000	-0.106003000
C	1.110075000	0.548611000	0.290304000
C	2.550530000	0.343836000	0.237219000
C	3.424319000	1.333737000	0.694668000
C	4.803686000	1.164236000	0.654505000
C	5.369132000	-0.013035000	0.135417000
C	4.482891000	-1.018992000	-0.320491000
C	3.120408000	-0.833843000	-0.264321000
H	5.425268000	1.944989000	1.073555000
H	2.451965000	-1.606122000	-0.626842000
N	-6.734810000	-2.025376000	0.528511000
O	-6.363824000	-3.158481000	0.724691000
O	-7.879842000	-1.638185000	0.579668000
N	-5.482850000	2.606771000	-0.567687000
O	-6.657680000	2.882568000	-0.505402000
O	-4.588468000	3.385615000	-0.811946000
H	0.758099000	1.507735000	0.682499000
O	2.870602000	2.470883000	1.205280000
H	3.562773000	3.089908000	1.451332000
H	4.871669000	-1.932786000	-0.747073000
N	6.735488000	-0.200638000	0.057300000
C	7.265948000	-1.563358000	0.123343000
C	7.658645000	-2.141578000	-1.234242000
H	6.523712000	-2.203388000	0.604961000
H	8.132302000	-1.555665000	0.791199000
H	8.001412000	-3.172931000	-1.122009000
H	6.809567000	-2.132211000	-1.919791000
H	8.460917000	-1.560852000	-1.690839000
C	7.643018000	0.877445000	0.426626000

C	8.992754000	0.794081000	-0.278572000
H	7.789227000	0.907142000	1.517778000
H	7.179835000	1.818954000	0.132259000
H	9.601649000	1.652783000	0.010013000
H	9.549400000	-0.106480000	-0.015731000
H	8.858849000	0.815577000	-1.361581000

Zero-point correction= 0.372010(Hartree/Particle)
Thermal correction to Energy= 0.399349
Thermal correction to Enthalpy= 0.400293
Thermal correction to Gibbs Free Energy= 0.310044
Sum of electronic and zero-point Energies= -1421.685489
Sum of electronic and thermal Energies= -1421.658151
Sum of electronic and thermal Enthalpies= -1421.657207
Sum of electronic and thermal Free Energies= -1421.747455

2-N8-H Radical

C	6.047772000	0.237601000	0.051316000
C	5.040829000	1.186567000	0.048454000
C	3.693216000	0.861444000	0.023060000
C	3.331607000	-0.484241000	-0.000368000
C	4.316039000	-1.470899000	0.002019000
C	5.645694000	-1.087682000	0.027515000
H	7.092361000	0.515166000	0.071148000
H	2.939510000	1.636295000	0.021474000
H	4.036229000	-2.516648000	-0.016172000
C	1.891978000	-0.928202000	-0.029724000
O	1.607141000	-2.102470000	-0.047667000
N	0.997526000	0.155769000	-0.032352000
N	-0.240912000	-0.235296000	-0.065372000
C	-1.105055000	0.772832000	-0.064620000
C	-2.495777000	0.514039000	-0.100190000
C	-3.432382000	1.576916000	-0.110333000
C	-4.793971000	1.344243000	-0.139859000
C	-5.305659000	0.026265000	-0.155178000
C	-4.364560000	-1.046792000	-0.161233000
C	-3.020679000	-0.801081000	-0.132600000
H	-5.453072000	2.199390000	-0.202186000
H	-2.312595000	-1.620792000	-0.122157000
N	6.693742000	-2.135425000	0.029469000
O	6.326513000	-3.287357000	0.007260000
O	7.846436000	-1.766246000	0.053170000
N	5.428151000	2.616552000	0.073763000
O	6.611333000	2.870855000	0.093814000
O	4.536066000	3.433913000	0.072711000
H	-0.736520000	1.796828000	-0.035812000
O	-2.926889000	2.830831000	-0.110556000
H	-3.635825000	3.479997000	-0.095807000
H	-4.707551000	-2.070664000	-0.157300000
N	-6.645208000	-0.231617000	-0.166939000
C	-7.136337000	-1.539033000	-0.610477000
C	-7.361380000	-2.537160000	0.523305000
H	-6.434194000	-1.942678000	-1.341906000
H	-8.069089000	-1.368960000	-1.153177000
H	-7.662160000	-3.504401000	0.114991000
H	-6.450588000	-2.677906000	1.107291000
H	-8.143023000	-2.194162000	1.201403000
C	-7.633161000	0.839148000	-0.052300000
C	-8.885225000	0.427950000	0.716023000
H	-7.904756000	1.205131000	-1.051990000
H	-7.177322000	1.664628000	0.489848000

H	-9.551956000	1.288627000	0.790733000
H	-9.437918000	-0.373480000	0.224635000
H	-8.627101000	0.106050000	1.726290000

Zero-point correction= 0.359048(Hartree/Particle)
Thermal correction to Energy= 0.386223
Thermal correction to Enthalpy= 0.387167
Thermal correction to Gibbs Free Energy= 0.295752
Sum of electronic and zero-point Energies= -1421.054498
Sum of electronic and thermal Energies= -1421.027323
Sum of electronic and thermal Enthalpies= -1421.026378
Sum of electronic and thermal Free Energies= -1421.117794

2-O2′-H Radical

C	6.083703000	0.281378000	0.010818000
C	5.091289000	1.200327000	0.294670000
C	3.749541000	0.859893000	0.385682000
C	3.379469000	-0.465313000	0.177552000
C	4.353218000	-1.426273000	-0.092116000
C	5.674728000	-1.028832000	-0.178804000
H	7.124399000	0.568320000	-0.054143000
H	3.036056000	1.631282000	0.647191000
H	4.073720000	-2.464140000	-0.223463000
C	1.958251000	-0.956307000	0.288627000
O	1.709428000	-2.088761000	0.609622000
N	1.006566000	-0.008556000	-0.016422000
H	1.281726000	0.873140000	-0.438871000
N	-0.305976000	-0.313506000	0.082625000
C	-1.127994000	0.589246000	-0.323228000
C	-2.547323000	0.369242000	-0.251842000
C	-3.430891000	1.443007000	-0.737914000
C	-4.856284000	1.225767000	-0.661921000
C	-5.385782000	0.065286000	-0.150263000
C	-4.472847000	-0.958264000	0.317263000
C	-3.109375000	-0.804971000	0.258196000
H	-5.465943000	2.022047000	-1.063519000
H	-2.453114000	-1.586188000	0.623122000
N	6.709783000	-2.048383000	-0.480952000
O	6.331374000	-3.182195000	-0.657599000
O	7.857087000	-1.669358000	-0.530634000
N	5.480114000	2.612409000	0.523456000
O	6.656300000	2.879551000	0.456115000
O	4.589522000	3.397770000	0.758190000
H	-0.799205000	1.547627000	-0.733135000
O	-2.945044000	2.479169000	-1.209951000
H	-4.878814000	-1.860514000	0.755445000
N	-6.740650000	-0.169345000	-0.012132000
C	-7.245188000	-1.536353000	-0.189688000
C	-7.678868000	-2.208210000	1.110007000
H	-6.480256000	-2.136218000	-0.686859000
H	-8.085418000	-1.495982000	-0.889362000
H	-8.026832000	-3.224876000	0.912808000
H	-6.849664000	-2.258450000	1.818352000
H	-8.487575000	-1.654519000	1.587566000
C	-7.664858000	0.911920000	-0.336448000
C	-9.022926000	0.762232000	0.338165000
H	-7.789139000	0.997361000	-1.426989000
H	-7.215226000	1.841675000	0.012758000
H	-9.641680000	1.625961000	0.089208000
H	-9.559238000	-0.130452000	0.012358000

H	-8.909167000	0.723525000	1.423029000

Zero-point correction=	0.358789(Hartree/Particle)
Thermal correction to Energy=	0.385698
Thermal correction to Enthalpy=	0.386642
Thermal correction to Gibbs Free Energy=	0.296580
Sum of electronic and zero-point Energies=	-1421.054080
Sum of electronic and thermal Energies=	-1421.027171
Sum of electronic and thermal Enthalpies=	-1421.026227
Sum of electronic and thermal Free Energies=	-1421.116289

2-C7′-H Radical

C	6.043610000	0.318115000	-0.000057000
C	5.037366000	1.210464000	0.318122000
C	3.702116000	0.843941000	0.406920000
C	3.351316000	-0.479402000	0.158387000
C	4.340107000	-1.414049000	-0.146717000
C	5.654557000	-0.992012000	-0.228406000
H	7.078934000	0.623909000	-0.061811000
H	2.976396000	1.593078000	0.697096000
H	4.075470000	-2.451624000	-0.307749000
C	1.936755000	-0.999247000	0.260941000
O	1.719640000	-2.149700000	0.548906000
N	0.975995000	-0.062139000	-0.005115000
H	1.237613000	0.833618000	-0.403988000
N	-0.344916000	-0.391424000	0.077399000
C	-1.169220000	0.509343000	-0.296937000
C	-2.605977000	0.281212000	-0.252175000
C	-3.496563000	1.294878000	-0.623861000
C	-4.870263000	1.101312000	-0.591900000
C	-5.410768000	-0.133374000	-0.192781000
C	-4.515630000	-1.151640000	0.206611000
C	-3.155642000	-0.936351000	0.169481000
H	-5.522793000	1.932275000	-0.827538000
H	-2.474049000	-1.724382000	0.467410000
N	6.704725000	-1.983194000	-0.568990000
O	6.345609000	-3.117339000	-0.780609000
O	7.845789000	-1.583708000	-0.612754000
N	5.403568000	2.620987000	0.586762000
O	6.575678000	2.909339000	0.531094000
O	4.500765000	3.387330000	0.839343000
H	-0.830476000	1.483302000	-0.662886000
O	-2.960610000	2.490083000	-1.001418000
H	-3.661402000	3.097812000	-1.251943000
H	-4.876938000	-2.113189000	0.539350000
N	-6.786223000	-0.334233000	-0.199361000
C	-7.345956000	-1.454111000	0.562442000
C	-7.278973000	-1.226480000	2.069252000
H	-6.826856000	-2.371044000	0.278593000
H	-8.377360000	-1.585443000	0.244833000
H	-7.695134000	-2.084131000	2.601338000
H	-6.248496000	-1.082345000	2.398056000
H	-7.850316000	-0.337145000	2.342975000
C	-7.630932000	0.571200000	-0.817814000
C	-9.110344000	0.509039000	-0.660420000
H	-7.209301000	1.103322000	-1.658977000
H	-9.548252000	1.412867000	-1.085321000
H	-9.574092000	-0.343800000	-1.177177000
H	-9.413329000	0.457881000	0.389852000

Zero-point correction= 0.357920
(Hartree/Particle)
Thermal correction to Energy= 0.385464
Thermal correction to Enthalpy= 0.386409
Thermal correction to Gibbs Free Energy= 0.294848
Sum of electronic and zero-point Energies= -1421.048951
Sum of electronic and thermal Energies= -1421.021406
Sum of electronic and thermal Enthalpies= -1421.020462
Sum of electronic and thermal Free Energies= -1421.112023

2-Cationic Radical

C	6.016569000	0.289299000	0.097406000
C	5.012346000	1.205000000	0.350946000
C	3.668821000	0.866677000	0.359757000
C	3.310759000	-0.452390000	0.095526000
C	4.294187000	-1.411521000	-0.149599000
C	5.617806000	-1.014712000	-0.150806000
H	7.061009000	0.574151000	0.096438000
H	2.951378000	1.639013000	0.607735000
H	4.027811000	-2.445171000	-0.333404000
C	1.893266000	-0.928974000	0.109826000
O	1.573163000	-2.059026000	0.327192000
N	0.934766000	0.070606000	-0.179712000
H	1.231403000	0.980354000	-0.527485000
N	-0.344031000	-0.234484000	-0.115136000
C	-1.208840000	0.675105000	-0.461821000
C	-2.593629000	0.353822000	-0.388094000
C	-3.576936000	1.331769000	-0.749721000
C	-4.914902000	1.046577000	-0.698562000
C	-5.366557000	-0.240858000	-0.275492000
C	-4.374589000	-1.217449000	0.101641000
C	-3.049935000	-0.921874000	0.037216000
H	-5.621531000	1.825567000	-0.949383000
H	-2.306833000	-1.663147000	0.303910000
N	6.665970000	-2.031925000	-0.427347000
O	6.287380000	-3.155567000	-0.655857000
O	7.811532000	-1.653260000	-0.403666000
N	5.382968000	2.614064000	0.633400000
O	6.558238000	2.877446000	0.661482000
O	4.471846000	3.392377000	0.809922000
H	-0.908652000	1.665797000	-0.804202000
O	-3.088212000	2.524675000	-1.122778000
H	-3.786779000	3.141758000	-1.365972000
H	-4.677528000	-2.204302000	0.416877000
N	-6.668047000	-0.544643000	-0.234532000
C	-7.154968000	-1.787237000	0.399257000
C	-7.017053000	-1.771849000	1.920084000
H	-6.634510000	-2.637520000	-0.044237000
H	-8.203014000	-1.882967000	0.120724000
H	-7.404119000	-2.708329000	2.323898000
H	-5.977850000	-1.667852000	2.233702000
H	-7.588411000	-0.951698000	2.355160000
C	-7.699697000	0.389083000	-0.714834000
C	-8.199921000	1.323606000	0.383614000
H	-8.517010000	-0.220017000	-1.100503000
H	-7.300523000	0.940377000	-1.564381000
H	-8.918501000	2.028262000	-0.036906000
H	-8.702111000	0.765454000	1.174533000
H	-7.377549000	1.887357000	0.828371000

```
Zero-point correction=                           0.372544(Hartree/Particle)
 Thermal correction to Energy=                    0.399725
 Thermal correction to Enthalpy=                  0.400669
 Thermal correction to Gibbs Free Energy=         0.310059
 Sum of electronic and zero-point Energies=          -1421.428459
 Sum of electronic and thermal Energies=             -1421.401278
 Sum of electronic and thermal Enthalpies=           -1421.400334
 Sum of electronic and thermal Free Energies=        -1421.490944
```

2-N8-H Anion

```
C        6.086055000      0.234328000      0.013352000
C        5.077813000      1.186231000     -0.005579000
C        3.728141000      0.864131000     -0.006479000
C        3.352245000     -0.479690000      0.012458000
C        4.337726000     -1.463790000      0.031855000
C        5.674328000     -1.086670000      0.031734000
H        7.130193000      0.508175000      0.013684000
H        2.959636000      1.625375000     -0.021578000
H        4.033267000     -2.502798000      0.046713000
C        1.892382000     -0.928452000      0.013826000
O        1.682212000     -2.144952000      0.032898000
N        1.071777000      0.126174000     -0.006644000
N       -0.238925000     -0.229157000     -0.003489000
C       -1.061810000      0.753672000     -0.025878000
C       -2.505458000      0.500860000     -0.020503000
C       -3.431481000      1.545448000     -0.064102000
C       -4.808088000      1.314662000     -0.062930000
C       -5.314841000      0.013239000      0.002946000
C       -4.391344000     -1.044909000      0.049939000
C       -3.031499000     -0.797130000      0.031629000
H       -5.470416000      2.169052000     -0.146523000
H       -2.319297000     -1.613318000      0.074433000
N        6.719042000     -2.131753000      0.052192000
O        6.361385000     -3.288585000      0.067067000
O        7.880074000     -1.771456000      0.052899000
N        5.477834000      2.608541000     -0.025595000
O        6.667269000      2.860680000     -0.025367000
O        4.601316000      3.443780000     -0.041165000
H       -0.707985000      1.785024000     -0.048163000
O       -2.946953000      2.825868000     -0.129065000
H       -3.683146000      3.441043000     -0.109067000
H       -4.747082000     -2.065206000      0.127233000
N       -6.696875000     -0.263599000      0.033780000
C       -7.160744000     -1.377136000     -0.796601000
C       -7.656615000     -2.574993000      0.010804000
H       -6.343195000     -1.689376000     -1.449592000
H       -7.958895000     -1.016812000     -1.458276000
H       -7.971422000     -3.383017000     -0.655463000
H       -6.861844000     -2.949272000      0.658417000
H       -8.501001000     -2.300960000      0.645408000
C       -7.612201000      0.857863000      0.139224000
C       -8.994027000      0.449266000      0.639285000
H       -7.710344000      1.390398000     -0.823821000
H       -7.189640000      1.562718000      0.856968000
H       -9.619472000      1.337199000      0.755724000
H       -9.502119000     -0.224662000     -0.053195000
H       -8.913135000     -0.049260000      1.607384000
```

```
Zero-point correction=                           0.357413(Hartree/Particle)
 Thermal correction to Energy=                    0.384581
```

```
 Thermal correction to Enthalpy=                  0.385525
 Thermal correction to Gibbs Free Energy=         0.294921
 Sum of electronic and zero-point Energies=          -1421.171689
 Sum of electronic and thermal Energies=             -1421.144521
 Sum of electronic and thermal Enthalpies=           -1421.143577
 Sum of electronic and thermal Free Energies=        -1421.234180
```

2-O2′-H Anion

```
C         6.054018000      0.397030000     -0.082630000
C         5.017146000      1.255598000      0.232605000
C         3.704963000      0.833016000      0.398505000
C         3.404125000     -0.517375000      0.234362000
C         4.430412000     -1.417189000     -0.058277000
C         5.718713000     -0.940295000     -0.221470000
H         7.068344000      0.747976000     -0.204314000
H         2.953216000      1.560320000      0.678447000
H         4.203581000     -2.472485000     -0.142136000
C         2.025163000     -1.113712000      0.429614000
O         1.922323000     -2.273438000      0.783102000
N         1.016753000     -0.260211000      0.166909000
H         1.221463000      0.641569000     -0.253594000
N        -0.304997000     -0.622840000      0.301373000
C        -1.125057000      0.286239000     -0.121076000
C        -2.545691000      0.188424000     -0.093862000
C        -3.298663000      1.313607000     -0.626091000
C        -4.740053000      1.166281000     -0.583513000
C        -5.363938000      0.052077000     -0.067641000
C        -4.581313000     -1.026650000      0.450555000
C        -3.212921000     -0.936819000      0.423268000
H        -5.294779000      1.987473000     -1.018132000
H        -2.607741000     -1.744588000      0.823694000
N         6.802375000     -1.896086000     -0.547731000
O         6.502024000     -3.060751000     -0.671912000
O         7.922127000     -1.447464000     -0.670986000
N         5.333546000      2.689196000      0.421834000
O         6.481544000      3.034880000      0.244952000
O         4.426091000      3.423934000      0.739223000
H        -0.751431000      1.228902000     -0.543427000
O        -2.757908000      2.334553000     -1.106617000
H        -5.067907000     -1.884907000      0.896236000
N        -6.772645000     -0.073225000      0.001054000
C        -7.330277000     -1.361299000     -0.413837000
C        -7.999288000     -2.131797000      0.723757000
H        -6.530208000     -1.968177000     -0.841932000
H        -8.052563000     -1.192671000     -1.223997000
H        -8.385785000     -3.090717000      0.365322000
H        -7.278730000     -2.322910000      1.521044000
H        -8.826342000     -1.563599000      1.153011000
C        -7.564388000      1.084141000     -0.374613000
C        -8.995047000      1.018722000      0.151326000
H        -7.578159000      1.222704000     -1.470041000
H        -7.080850000      1.963442000      0.051743000
H        -9.521757000      1.941726000     -0.102786000
H        -9.558381000      0.187730000     -0.279108000
H        -8.994229000      0.906660000      1.237902000
```

```
Zero-point correction=                           0.358367(Hartree/Particle)
 Thermal correction to Energy=                    0.385145
 Thermal correction to Enthalpy=                  0.386089
 Thermal correction to Gibbs Free Energy=         0.296837
```

```
 Sum of electronic and zero-point Energies=          -1421.166904
 Sum of electronic and thermal Energies=             -1421.140126
 Sum of electronic and thermal Enthalpies=           -1421.139182
 Sum of electronic and thermal Free Energies=        -1421.228434
```

2-C7′-H Anion

```
C         6.042610000      0.392397000     -0.022580000
C         4.980251000      1.256927000      0.223765000
C         3.662333000      0.821356000      0.298019000
C         3.371355000     -0.525899000      0.103863000
C         4.419739000     -1.426968000     -0.126674000
C         5.716035000     -0.941030000     -0.191302000
H         7.061958000      0.744622000     -0.069894000
H         2.901964000      1.554158000      0.534667000
H         4.202097000     -2.480230000     -0.239932000
C         1.988296000     -1.117652000      0.194519000
O         1.845298000     -2.312334000      0.374625000
N         0.981381000     -0.221755000      0.044021000
H         1.199319000      0.731205000     -0.227518000
N        -0.330860000     -0.592331000      0.100316000
C        -1.163212000      0.376578000     -0.133163000
C        -2.576023000      0.210322000     -0.126668000
C        -3.440076000      1.304458000     -0.358043000
C        -4.808517000      1.178828000     -0.377225000
C        -5.434791000     -0.091775000     -0.172749000
C        -4.563325000     -1.190018000      0.130620000
C        -3.205587000     -1.035864000      0.137672000
H        -5.409253000      2.070427000     -0.491566000
H        -2.565650000     -1.883058000      0.355068000
N         6.821812000     -1.894158000     -0.444548000
O         6.534990000     -3.061868000     -0.581919000
O         7.948009000     -1.446322000     -0.501145000
N         5.264947000      2.675336000      0.431176000
O         6.427862000      3.032909000      0.363437000
O         4.325529000      3.419575000      0.654351000
H        -0.791370000      1.384805000     -0.348721000
O        -2.849125000      2.528585000     -0.549409000
H        -3.540289000      3.170683000     -0.729575000
H        -4.959560000     -2.168109000      0.362719000
N        -6.783260000     -0.205066000     -0.236677000
C        -7.393926000     -1.464746000      0.190072000
C        -7.545433000     -1.526442000      1.707993000
H        -6.798259000     -2.295247000     -0.183885000
H        -8.366435000     -1.548018000     -0.288653000
H        -8.028514000     -2.458637000      2.011685000
H        -6.568588000     -1.462035000      2.191487000
H        -8.149411000     -0.682555000      2.047407000
C        -7.648888000      0.883954000     -0.435615000
C        -9.080816000      0.613493000     -0.801434000
H        -7.192925000      1.683759000     -1.002034000
H        -9.550107000      1.573598000     -1.026577000
H        -9.233376000     -0.030094000     -1.691515000
H        -9.670401000      0.168649000      0.010866000

Zero-point correction=                          0.355073(Hartree/Particle)
 Thermal correction to Energy=                   0.382798
 Thermal correction to Enthalpy=                 0.383743
 Thermal correction to Gibbs Free Energy=        0.292059
 Sum of electronic and zero-point Energies=         -1421.089910
 Sum of electronic and thermal Energies=            -1421.062184
```

```
 Sum of electronic and thermal Enthalpies=          -1421.061240
 Sum of electronic and thermal Free Energies=       -1421.152923
```

N′-benzylidene-3,5-dinitrobenzohydrazide (3)

```
C       -3.012016000      1.308332000      0.120306000
C       -1.682578000      0.942958000      0.274067000
C       -1.345460000     -0.405110000      0.204807000
C       -2.340677000     -1.362037000      0.009403000
C       -3.648720000     -0.940539000     -0.144315000
C       -4.024551000      0.392179000     -0.092820000
H       -0.952172000      1.716444000      0.474748000
H       -2.087416000     -2.414652000     -0.013551000
H       -5.055456000      0.698057000     -0.207860000
N       -3.363491000      2.746101000      0.196838000
O       -4.531707000      3.036336000      0.097027000
O       -2.452339000      3.528867000      0.349768000
N       -4.706306000     -1.957154000     -0.368740000
O       -5.841550000     -1.554816000     -0.478274000
O       -4.356697000     -3.112099000     -0.428090000
C        0.060978000     -0.919037000      0.392468000
O        0.269647000     -2.021093000      0.828205000
N        1.038503000     -0.028700000      0.018651000
H        0.792198000      0.804566000     -0.505899000
N        2.348577000     -0.361171000      0.163523000
C        3.202395000      0.453246000     -0.313132000
H        2.894772000      1.375022000     -0.822595000
C        5.136109000     -0.944928000      0.425160000
C        4.643604000      0.203170000     -0.205470000
C        5.535346000      1.131500000     -0.744274000
C        6.907029000      0.919882000     -0.657006000
C        7.392032000     -0.221827000     -0.030447000
C        6.503619000     -1.152254000      0.509389000
H        4.434583000     -1.658962000      0.839477000
H        5.153998000      2.022241000     -1.233012000
H        7.593720000      1.644455000     -1.077353000
H        8.460140000     -0.389561000      0.038895000
H        6.883174000     -2.041905000      0.997330000
Zero-point correction=                           0.236491(Hartree/Particle)
 Thermal correction to Energy=                    0.255816
 Thermal correction to Enthalpy=                  0.256760
 Thermal correction to Gibbs Free Energy=         0.184402
 Sum of electronic and zero-point Energies=          -1134.040564
 Sum of electronic and thermal Energies=             -1134.021239
 Sum of electronic and thermal Enthalpies=           -1134.020295
 Sum of electronic and thermal Free Energies=        -1134.092653
```

3-N8-H Radical

```
C        2.932375000      1.318751000     -0.000023000
C        1.603139000      0.925057000      0.000082000
C        1.312449000     -0.437679000      0.000123000
C        2.345537000     -1.374184000      0.000072000
C        3.652912000     -0.922777000     -0.000035000
C        3.985805000      0.422182000     -0.000081000
H        0.814097000      1.663710000      0.000139000
H        2.122336000     -2.433756000      0.000124000
H        5.015304000      0.752994000     -0.000161000
N        3.244390000      2.767920000     -0.000074000
O        4.412107000      3.082631000     -0.000076000
O        2.309109000      3.535398000     -0.000119000
```

N	4.753660000	-1.916292000	-0.000072000
O	5.884772000	-1.487085000	-0.000412000
O	4.443446000	-3.084639000	0.000240000
C	-0.098136000	-0.954848000	0.000204000
O	-0.338299000	-2.134654000	0.000223000
N	-1.062513000	0.088005000	0.000277000
N	-2.273752000	-0.379410000	0.000101000
C	-3.192096000	0.573872000	0.000242000
H	-2.876489000	1.618576000	0.000490000
C	-5.029549000	-1.089166000	-0.000241000
C	-4.589971000	0.249436000	0.000068000
C	-5.534546000	1.290653000	0.000203000
C	-6.889355000	1.003052000	0.000034000
C	-7.314330000	-0.324406000	-0.000275000
C	-6.384125000	-1.366214000	-0.000411000
H	-4.290714000	-1.880937000	-0.000336000
H	-5.192149000	2.319820000	0.000437000
H	-7.615481000	1.806320000	0.000138000
H	-8.374214000	-0.549706000	-0.000408000
H	-6.724912000	-2.394169000	-0.000653000

Zero-point correction=	0.222475(Hartree/Particle)
Thermal correction to Energy=	0.241786
Thermal correction to Enthalpy=	0.242730
Thermal correction to Gibbs Free Energy=	0.168503
Sum of electronic and zero-point Energies=	-1133.402243
Sum of electronic and thermal Energies=	-1133.382932
Sum of electronic and thermal Enthalpies=	-1133.381988
Sum of electronic and thermal Free Energies=	-1133.456215

3-Cationic Radical

C	2.980946000	1.308264000	-0.117881000
C	1.651302000	0.930611000	-0.193430000
C	1.338884000	-0.424713000	-0.112182000
C	2.351572000	-1.377787000	0.021976000
C	3.658989000	-0.939561000	0.096493000
C	4.012908000	0.399383000	0.028858000
H	0.915442000	1.709901000	-0.350651000
H	2.123251000	-2.435976000	0.068124000
H	5.047309000	0.716251000	0.085386000
N	3.302188000	2.756103000	-0.203061000
O	4.466248000	3.059390000	-0.179907000
O	2.361913000	3.514973000	-0.284885000
N	4.739839000	-1.950296000	0.254381000
O	5.869497000	-1.531646000	0.296947000
O	4.394106000	-3.104186000	0.328335000
C	-0.051318000	-0.937273000	-0.213191000
O	-0.371774000	-2.033710000	-0.535349000
N	-1.078178000	0.024930000	0.157460000
H	-0.819868000	0.899901000	0.619814000
N	-2.317032000	-0.295553000	-0.018718000
C	-3.243438000	0.556333000	0.388472000
H	-2.968977000	1.500474000	0.866099000
C	-5.002705000	-0.986425000	-0.411799000
C	-4.606125000	0.240206000	0.202763000
C	-5.592898000	1.168201000	0.640523000
C	-6.924159000	0.880930000	0.469167000
C	-7.298190000	-0.331055000	-0.137853000
C	-6.337872000	-1.258711000	-0.574856000
H	-4.239614000	-1.682503000	-0.737127000

H	-5.282389000	2.096822000	1.106324000
H	-7.684594000	1.577901000	0.796647000
H	-8.350710000	-0.553893000	-0.270615000
H	-6.654864000	-2.184163000	-1.037923000

Zero-point correction= 0.235899(Hartree/Particle)
Thermal correction to Energy= 0.255282
Thermal correction to Enthalpy= 0.256226
Thermal correction to Gibbs Free Energy= 0.183437
Sum of electronic and zero-point Energies= -1133.731032
Sum of electronic and thermal Energies= -1133.711649
Sum of electronic and thermal Enthalpies= -1133.710705
Sum of electronic and thermal Free Energies= -1133.783494

3-N8-H Anion

C	2.941599000	1.319729000	0.000040000
C	1.609712000	0.930577000	-0.000016000
C	1.302048000	-0.430243000	-0.000039000
C	2.335178000	-1.364266000	-0.000017000
C	3.650913000	-0.921024000	-0.000016000
C	3.995836000	0.419247000	0.000030000
H	0.805228000	1.653635000	-0.000048000
H	2.083655000	-2.417490000	0.000000000
H	5.025132000	0.744771000	0.000054000
N	3.269207000	2.760903000	0.000138000
O	4.444007000	3.072559000	0.000555000
O	2.351020000	3.550292000	-0.000231000
N	4.746688000	-1.913127000	-0.000058000
O	5.887784000	-1.494850000	-0.000976000
O	4.446634000	-3.086129000	0.000823000
C	-0.132899000	-0.952629000	-0.000033000
O	-0.282982000	-2.175895000	0.000002000
N	-1.010271000	0.059637000	-0.000073000
N	-2.295413000	-0.365890000	-0.000007000
C	-3.175920000	0.565237000	-0.000189000
H	-2.875970000	1.618005000	-0.000408000
C	-5.068847000	-1.074473000	-0.000027000
C	-4.606384000	0.251301000	-0.000085000
C	-5.550532000	1.284464000	-0.000057000
C	-6.914616000	1.009741000	0.000039000
C	-7.362027000	-0.306916000	0.000105000
C	-6.428008000	-1.345283000	0.000072000
H	-4.332435000	-1.869518000	-0.000055000
H	-5.204506000	2.313420000	-0.000106000
H	-7.628568000	1.826299000	0.000062000
H	-8.423903000	-0.525085000	0.000181000
H	-6.768149000	-2.375302000	0.000112000

Zero-point correction= 0.222308
(Hartree/Particle)
Thermal correction to Energy= 0.241406
Thermal correction to Enthalpy= 0.242350
Thermal correction to Gibbs Free Energy= 0.169892
Sum of electronic and zero-point Energies= -1133.536853
Sum of electronic and thermal Energies= -1133.517755
Sum of electronic and thermal Enthalpies= -1133.516810
Sum of electronic and thermal Free Energies= -1133.589269

N′-((2-Hydroxynaphthalen-1-yl)methylene)-3,5-dinitrobenzohydrazide (4)

C	-5.075169000	0.630657000	0.112773000
C	-4.002555000	1.421352000	-0.253976000
C	-2.716967000	0.924846000	-0.410306000
C	-2.488473000	-0.427969000	-0.179301000
C	-3.547456000	-1.263016000	0.175079000
C	-4.807779000	-0.712839000	0.321035000
H	-6.070920000	1.037187000	0.226243000
H	-1.937065000	1.600683000	-0.737465000
H	-3.380361000	-2.322375000	0.325454000
C	-1.139856000	-1.077284000	-0.346485000
O	-1.030206000	-2.245375000	-0.621547000
N	-0.073431000	-0.233673000	-0.157220000
H	-0.202556000	0.680923000	0.261564000
N	1.185386000	-0.729603000	-0.294518000
C	2.171296000	0.030487000	0.010651000
C	3.544218000	-0.430151000	-0.084870000
C	4.639525000	0.465848000	0.195152000
C	5.969268000	-0.031012000	0.146662000
C	6.189314000	-1.396568000	-0.189298000
C	5.153891000	-2.231210000	-0.468665000
C	3.816010000	-1.758652000	-0.422689000
H	1.981674000	1.044452000	0.367799000
C	5.545639000	2.650001000	0.776066000
C	4.469289000	1.838446000	0.512016000
C	7.059505000	0.826012000	0.423932000
C	6.859736000	2.145125000	0.737296000
H	5.378960000	3.694224000	1.012768000
H	3.483423000	2.282153000	0.541786000
H	8.062249000	0.414526000	0.380804000
H	7.699043000	2.796011000	0.947754000
H	5.304018000	-3.271056000	-0.729893000
H	7.209390000	-1.763751000	-0.223071000
O	2.883887000	-2.667375000	-0.709769000
H	1.990700000	-2.267881000	-0.667282000
N	-5.933110000	-1.597606000	0.713216000
O	-7.023220000	-1.085300000	0.820517000
O	-5.677758000	-2.763635000	0.898941000
N	-4.237888000	2.863687000	-0.501261000
O	-3.272865000	3.538662000	-0.783199000
O	-5.372572000	3.264376000	-0.399743000

Zero-point correction= 0.288306
(Hartree/Particle)
Thermal correction to Energy= 0.311238
Thermal correction to Enthalpy= 0.312183
Thermal correction to Gibbs Free Energy= 0.231720
Sum of electronic and zero-point Energies= -1362.838282
Sum of electronic and thermal Energies= -1362.815350
Sum of electronic and thermal Enthalpies= -1362.814406
Sum of electronic and thermal Free Energies= -1362.894868

4-N8-H Radical

C	-5.047227000	0.657905000	-0.000087000
C	-3.924129000	1.465955000	-0.000083000
C	-2.631694000	0.965363000	0.000032000
C	-2.452934000	-0.416543000	0.000171000
C	-3.558225000	-1.266236000	0.000137000
C	-4.824817000	-0.709453000	0.000014000
H	-6.046339000	1.071414000	-0.000135000
H	-1.784310000	1.636453000	0.000004000

H	-3.421133000	-2.340324000	0.000200000
C	-1.088378000	-1.040981000	0.000297000
O	-0.940801000	-2.240727000	0.000274000
N	-0.048159000	-0.090076000	0.000484000
N	1.109830000	-0.671535000	0.000153000
C	2.165431000	0.137416000	0.000314000
C	3.467932000	-0.399039000	0.000065000
C	4.639862000	0.464522000	0.000067000
C	5.929072000	-0.120204000	-0.000135000
C	6.053929000	-1.545923000	-0.000377000
C	4.968946000	-2.362093000	-0.000389000
C	3.658673000	-1.814522000	-0.000161000
H	1.980371000	1.208263000	0.000633000
C	5.693817000	2.652055000	0.000282000
C	4.556691000	1.872372000	0.000259000
C	7.078197000	0.694793000	-0.000119000
C	6.968274000	2.065652000	0.000097000
H	5.597948000	3.731124000	0.000439000
H	3.596342000	2.369282000	0.000374000
H	8.052975000	0.219425000	-0.000284000
H	7.854048000	2.688294000	0.000112000
H	5.055158000	-3.440925000	-0.000564000
H	7.051400000	-1.972546000	-0.000553000
O	2.673549000	-2.680286000	-0.000155000
H	1.797194000	-2.195086000	-0.000091000
N	-6.002958000	-1.609773000	-0.000033000
O	-7.095448000	-1.089818000	0.000099000
O	-5.789404000	-2.799620000	-0.000242000
N	-4.117304000	2.935525000	-0.000208000
O	-3.122849000	3.624746000	-0.001035000
O	-5.255550000	3.344381000	0.000405000

Zero-point correction= 0.274983(Hartree/Particle)
Thermal correction to Energy= 0.297563
Thermal correction to Enthalpy= 0.298507
Thermal correction to Gibbs Free Energy= 0.218064
Sum of electronic and zero-point Energies= -1362.209373
Sum of electronic and thermal Energies= -1362.186793
Sum of electronic and thermal Enthalpies= -1362.185849
Sum of electronic and thermal Free Energies= -1362.266292

4-O2′-H Radical

C	-5.013703000	0.662829000	0.129387000
C	-3.889506000	1.456026000	0.000474000
C	-2.618168000	0.937314000	-0.196979000
C	-2.459547000	-0.443124000	-0.263129000
C	-3.571998000	-1.277423000	-0.156794000
C	-4.814764000	-0.706100000	0.046623000
H	-5.996897000	1.086902000	0.281451000
H	-1.793191000	1.626354000	-0.325363000
H	-3.458714000	-2.351348000	-0.239302000
C	-1.131401000	-1.112913000	-0.515579000
O	-1.060202000	-2.173141000	-1.073081000
N	-0.045864000	-0.399765000	-0.044895000
H	-0.195339000	0.414868000	0.543470000
N	1.205495000	-0.871308000	-0.222172000
C	2.148182000	-0.146453000	0.259876000
C	3.536903000	-0.547075000	0.179171000
C	4.570536000	0.434133000	0.077999000
C	5.931519000	0.015873000	0.045897000
C	6.252876000	-1.393876000	0.083954000

C	5.297028000	-2.333188000	0.168436000
C	3.877549000	-1.976196000	0.278743000
H	1.918947000	0.806495000	0.749030000
C	5.318446000	2.743545000	-0.118575000
C	4.299030000	1.821851000	-0.030427000
C	6.949322000	0.971631000	-0.049241000
C	6.655212000	2.320825000	-0.121632000
H	5.085015000	3.798174000	-0.197537000
H	3.276030000	2.172816000	-0.063337000
H	7.980160000	0.635713000	-0.071170000
H	7.453935000	3.048705000	-0.193955000
H	5.521192000	-3.392207000	0.203003000
H	7.300719000	-1.672120000	0.036399000
O	3.031972000	-2.836167000	0.501772000
N	-5.997661000	-1.593208000	0.176190000
O	-7.070268000	-1.058510000	0.338495000
O	-5.802899000	-2.783566000	0.112562000
N	-4.049236000	2.927813000	0.066998000
O	-3.042071000	3.595668000	-0.014124000
O	-5.169793000	3.357571000	0.201280000

Zero-point correction= 0.274442(Hartree/Particle)
Thermal correction to Energy= 0.297425
Thermal correction to Enthalpy= 0.298369
Thermal correction to Gibbs Free Energy= 0.216717
Sum of electronic and zero-point Energies= -1362.188631
Sum of electronic and thermal Energies= -1362.165648
Sum of electronic and thermal Enthalpies= -1362.164704
Sum of electronic and thermal Free Energies= -1362.246356

4-Cationic Radical

C	-5.117636000	0.572115000	0.064143000
C	-4.061425000	1.419424000	-0.216680000
C	-2.750716000	0.982710000	-0.309464000
C	-2.481629000	-0.367625000	-0.102319000
C	-3.520082000	-1.260130000	0.169302000
C	-4.807484000	-0.765671000	0.252559000
H	-6.136371000	0.933498000	0.130282000
H	-1.993361000	1.709845000	-0.574807000
H	-3.325202000	-2.316172000	0.311780000
C	-1.110887000	-0.940923000	-0.200128000
O	-0.868023000	-2.090865000	-0.421962000
N	-0.052042000	-0.018962000	0.008744000
H	-0.218591000	0.922880000	0.353949000
N	1.173112000	-0.480681000	-0.121965000
C	2.210615000	0.257466000	0.119992000
C	3.515963000	-0.314234000	-0.037968000
C	4.703195000	0.461725000	0.177942000
C	5.975226000	-0.160855000	0.037684000
C	6.054270000	-1.549255000	-0.325040000
C	4.945822000	-2.299063000	-0.544086000
C	3.661332000	-1.716430000	-0.411428000
H	2.095726000	1.290223000	0.441396000
C	5.841137000	2.544536000	0.725410000
C	4.672228000	1.833169000	0.523003000
C	7.142295000	0.573516000	0.246423000
C	7.081105000	1.919437000	0.590310000
H	5.789396000	3.593453000	0.988263000
H	3.735219000	2.361341000	0.631584000
H	8.102438000	0.082459000	0.136333000

H	7.993529000	2.480235000	0.749811000
H	4.990638000	-3.344443000	-0.819933000
H	7.037614000	-1.996069000	-0.425092000
O	2.656108000	-2.503696000	-0.634459000
H	1.787569000	-2.036924000	-0.526093000
N	-5.914522000	-1.711675000	0.555928000
O	-7.026773000	-1.247658000	0.603082000
O	-5.608508000	-2.866045000	0.732113000
N	-4.335748000	2.862044000	-0.435835000
O	-3.375510000	3.573467000	-0.633782000
O	-5.486566000	3.212935000	-0.395431000

Zero-point correction= 0.287233(Hartree/Particle)
Thermal correction to Energy= 0.310221
Thermal correction to Enthalpy= 0.311165
Thermal correction to Gibbs Free Energy= 0.230083
Sum of electronic and zero-point Energies= -1362.552391
Sum of electronic and thermal Energies= -1362.529402
Sum of electronic and thermal Enthalpies= -1362.528458
Sum of electronic and thermal Free Energies= -1362.609540

4-N8-H Anion

C	-5.059303000	0.651949000	0.000061000
C	-3.936811000	1.465454000	-0.000095000
C	-2.640799000	0.971090000	-0.000200000
C	-2.444446000	-0.409913000	-0.000129000
C	-3.547869000	-1.259571000	0.000045000
C	-4.823419000	-0.711644000	0.000128000
H	-6.059261000	1.059034000	0.000126000
H	-1.782772000	1.629643000	-0.000323000
H	-3.383309000	-2.329817000	0.000099000
C	-1.059032000	-1.038319000	-0.000255000
O	-0.987485000	-2.269948000	-0.000510000
N	-0.096630000	-0.107194000	-0.000043000
N	1.132948000	-0.669451000	-0.000221000
C	2.144037000	0.126868000	0.000038000
C	3.499888000	-0.411771000	0.000001000
C	4.651918000	0.444180000	0.000083000
C	5.960101000	-0.120970000	0.000068000
C	6.101423000	-1.533841000	-0.000048000
C	5.004298000	-2.342633000	-0.000144000
C	3.692918000	-1.799278000	-0.000122000
H	1.963448000	1.200663000	0.000404000
C	5.677621000	2.658404000	0.000257000
C	4.558747000	1.864163000	0.000175000
C	7.096540000	0.724065000	0.000162000
C	6.969300000	2.088467000	0.000259000
H	5.566117000	3.736878000	0.000314000
H	3.587918000	2.339977000	0.000171000
H	8.079065000	0.261984000	0.000154000
H	7.846163000	2.725188000	0.000333000
H	5.088912000	-3.422932000	-0.000249000
H	7.099686000	-1.959480000	-0.000072000
O	2.691682000	-2.675462000	-0.000231000
H	1.823346000	-2.159203000	-0.000380000
N	-5.995464000	-1.613110000	0.000300000
O	-7.098560000	-1.104010000	-0.000441000
O	-5.789318000	-2.805923000	0.001149000
N	-4.147260000	2.928644000	-0.000137000
O	-3.167856000	3.640495000	-0.000095000

O	-5.292856000	3.333052000	-0.000070000

Zero-point correction= 0.274150
(Hartree/Particle)
Thermal correction to Energy= 0.296610
Thermal correction to Enthalpy= 0.297555
Thermal correction to Gibbs Free Energy= 0.218080
Sum of electronic and zero-point Energies= -1362.346708
Sum of electronic and thermal Energies= -1362.324247
Sum of electronic and thermal Enthalpies= -1362.323303
Sum of electronic and thermal Free Energies= -1362.402778

4-O2′-H Anion

C	-4.904749000	0.762144000	0.184185000
C	-3.752412000	1.453207000	-0.140817000
C	-2.533769000	0.829471000	-0.373671000
C	-2.452068000	-0.556988000	-0.270274000
C	-3.601594000	-1.289495000	0.031250000
C	-4.788120000	-0.616539000	0.262315000
H	-5.843660000	1.267097000	0.358232000
H	-1.683186000	1.435810000	-0.657725000
H	-3.547887000	-2.370368000	0.068579000
C	-1.195063000	-1.362067000	-0.544541000
O	-1.298923000	-2.500614000	-0.951419000
N	-0.054593000	-0.691695000	-0.277998000
H	-0.115003000	0.215188000	0.177620000
N	1.194337000	-1.241510000	-0.473556000
C	2.141795000	-0.427770000	-0.131087000
C	3.548358000	-0.676048000	-0.107736000
C	4.444899000	0.437019000	0.065483000
C	5.829685000	0.210559000	0.322019000
C	6.309341000	-1.144513000	0.363624000
C	5.488244000	-2.190589000	0.145806000
C	4.050003000	-2.039644000	-0.136421000
H	1.842077000	0.569646000	0.224972000
C	4.931655000	2.839776000	0.157041000
C	4.048433000	1.799480000	-0.041679000
C	6.710766000	1.285907000	0.516409000
C	6.281989000	2.596365000	0.451940000
H	4.576203000	3.860669000	0.062245000
H	3.032861000	2.046403000	-0.323283000
H	7.754782000	1.061402000	0.717149000
H	6.972868000	3.417230000	0.602524000
H	5.849867000	-3.213346000	0.166372000
H	7.365555000	-1.302832000	0.568906000
O	3.362211000	-3.043767000	-0.340669000
N	-6.002392000	-1.395655000	0.599335000
O	-7.027988000	-0.775456000	0.784362000
O	-5.893493000	-2.597461000	0.670140000
N	-3.832870000	2.925889000	-0.261667000
O	-2.818473000	3.518674000	-0.553845000
O	-4.908361000	3.445154000	-0.057501000

Zero-point correction= 0.274065
(Hartree/Particle)
Thermal correction to Energy= 0.296996
Thermal correction to Enthalpy= 0.297941
Thermal correction to Gibbs Free Energy= 0.216861
Sum of electronic and zero-point Energies= -1362.306124

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 Sum of electronic and thermal Energies=            -1362.283193
 Sum of electronic and thermal Enthalpies=          -1362.282248
 Sum of electronic and thermal Free Energies=       -1362.363328
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N′-(4-Hydroxybenzylidene)-3,5-dinitrobenzohydrazide (5)

```
C        3.436635000      1.297299000      0.121502000
C        2.104638000      0.941275000      0.275381000
C        1.757499000     -0.404199000      0.205170000
C        2.746038000     -1.367968000      0.009371000
C        4.057143000     -0.955816000     -0.144114000
C        4.442643000      0.374114000     -0.092148000
H        1.379796000      1.719733000      0.476809000
H        2.484955000     -2.418663000     -0.013819000
H        5.475673000      0.672611000     -0.207174000
N        5.107414000     -1.979807000     -0.368975000
O        6.245522000     -1.585553000     -0.479182000
O        4.749880000     -3.132348000     -0.428054000
N        3.798353000      2.732400000      0.198396000
O        4.968595000      3.014577000      0.098436000
O        2.892936000      3.521836000      0.351646000
C        0.347036000     -0.908451000      0.392048000
O        0.131945000     -2.010712000      0.825679000
N       -0.622736000     -0.010823000      0.021363000
N       -1.937344000     -0.333317000      0.164029000
C       -2.782116000      0.492719000     -0.310619000
H       -2.461896000      1.413642000     -0.814498000
C       -6.481032000      1.008275000     -0.658887000
C       -6.978430000     -0.135760000     -0.041809000
C       -6.101857000     -1.084490000      0.493162000
C       -4.738743000     -0.885612000      0.409553000
C       -4.222819000      0.262008000     -0.209749000
C       -5.107296000      1.199811000     -0.739219000
H       -7.162282000      1.743739000     -1.073904000
H       -6.517034000     -1.964957000      0.967209000
H       -4.049728000     -1.613922000      0.820240000
H       -0.369639000      0.821922000     -0.500570000
H       -4.722306000      2.092658000     -1.220891000
O       -8.306158000     -0.388947000      0.072483000
H       -8.815142000      0.324017000     -0.323010000
Zero-point  correction=                                  0.240564
(Hartree/Particle)
 Thermal correction to Energy=                  0.261175
 Thermal correction to Enthalpy=                0.262119
 Thermal correction to Gibbs Free Energy=       0.186875
 Sum of electronic and zero-point Energies=         -1209.261902
 Sum of electronic and thermal Energies=            -1209.241291
 Sum of electronic and thermal Enthalpies=          -1209.240347
 Sum of electronic and thermal Free Energies=       -1209.315591
```

5-N8-H Radical

```
C       -3.360904000      1.302045000      0.000009000
C       -2.026670000      0.925603000     -0.000124000
C       -1.717570000     -0.433076000     -0.000148000
C       -2.738524000     -1.382554000     -0.000061000
C       -4.051947000     -0.948334000      0.000060000
C       -4.402807000      0.391945000      0.000100000
H       -1.246563000      1.673642000     -0.000225000
H       -2.500729000     -2.438920000     -0.000093000
H       -5.436506000      0.709080000      0.000202000
N       -5.139615000     -1.955907000      0.000126000
```

O	-6.276510000	-1.541702000	0.000210000
O	-4.814806000	-3.120346000	0.000109000
N	-3.691843000	2.746786000	0.000052000
O	-4.863648000	3.046650000	0.000335000
O	-2.767039000	3.527019000	-0.000200000
C	-0.299019000	-0.931815000	-0.000254000
O	-0.047991000	-2.110582000	-0.000345000
N	0.647293000	0.121280000	-0.000281000
N	1.866098000	-0.326698000	-0.000182000
C	2.771679000	0.639612000	-0.000167000
H	2.440881000	1.679761000	-0.000215000
C	6.459226000	1.121412000	0.000084000
C	6.901042000	-0.205946000	0.000164000
C	5.981462000	-1.265083000	0.000158000
C	4.633292000	-0.998369000	0.000053000
C	4.165781000	0.336391000	-0.000043000
C	5.104070000	1.384719000	-0.000020000
H	7.179180000	1.932841000	0.000102000
H	6.361283000	-2.278805000	0.000234000
H	3.906908000	-1.801703000	0.000038000
H	4.754962000	2.411446000	-0.000079000
O	8.206998000	-0.533665000	0.000258000
H	8.756346000	0.256139000	0.000221000

Zero-point correction= 0.227212
(Hartree/Particle)
Thermal correction to Energy= 0.247606
Thermal correction to Enthalpy= 0.248550
Thermal correction to Gibbs Free Energy= 0.172294
Sum of electronic and zero-point Energies= -1208.625878
Sum of electronic and thermal Energies= -1208.605484
Sum of electronic and thermal Enthalpies= -1208.604540
Sum of electronic and thermal Free Energies= -1208.680795

5-O4′-H Radical

C	-3.376237000	1.295445000	-0.124400000
C	-2.042322000	0.942190000	-0.264266000
C	-1.694419000	-0.403011000	-0.189953000
C	-2.682340000	-1.369428000	-0.003059000
C	-3.995377000	-0.959317000	0.136298000
C	-4.382282000	0.370042000	0.079476000
H	-1.318695000	1.723522000	-0.459342000
H	-2.421219000	-2.420032000	0.025726000
H	-5.417174000	0.666696000	0.184031000
N	-5.045942000	-1.985805000	0.351385000
O	-6.185057000	-1.593027000	0.450298000
O	-4.685295000	-3.137010000	0.413870000
N	-3.738941000	2.730587000	-0.205452000
O	-4.910128000	3.010411000	-0.117665000
O	-2.832112000	3.519956000	-0.349561000
C	-0.283653000	-0.902236000	-0.361488000
O	-0.048739000	-2.002169000	-0.782793000
N	0.689087000	0.005162000	0.015856000
N	1.990274000	-0.311911000	-0.128819000
C	2.847498000	0.524663000	0.336472000
H	2.534110000	1.449332000	0.833679000
C	6.521139000	1.026848000	0.652033000
C	7.058108000	-0.169765000	0.013629000
C	6.088324000	-1.126173000	-0.513652000

C	4.751216000	-0.905433000	-0.411592000
C	4.263754000	0.275145000	0.219108000
C	5.175361000	1.226370000	0.743476000
H	7.238662000	1.737505000	1.043683000
H	6.489133000	-2.014491000	-0.986885000
H	4.029953000	-1.613633000	-0.801406000
H	0.429994000	0.844730000	0.525189000
H	4.785033000	2.119844000	1.220209000
O	8.273362000	-0.362130000	-0.075170000

Zero-point correction= 0.227163
(Hartree/Particle)
Thermal correction to Energy= 0.247434
Thermal correction to Enthalpy= 0.248378
Thermal correction to Gibbs Free Energy= 0.173290
Sum of electronic and zero-point Energies= -1208.627005
Sum of electronic and thermal Energies= -1208.606734
Sum of electronic and thermal Enthalpies= -1208.605790
Sum of electronic and thermal Free Energies= -1208.680879

5-Cationic Radical

C	-3.416373000	1.286898000	-0.126778000
C	-2.078483000	0.937818000	-0.202075000
C	-1.735586000	-0.409338000	-0.116704000
C	-2.727399000	-1.382899000	0.020350000
C	-4.044596000	-0.973684000	0.093633000
C	-4.428399000	0.356686000	0.023301000
H	-1.358538000	1.731126000	-0.361659000
H	-2.474757000	-2.435336000	0.068180000
H	-5.469259000	0.650813000	0.079416000
N	-5.102680000	-2.007041000	0.254962000
O	-6.241837000	-1.613788000	0.298081000
O	-4.733022000	-3.153540000	0.331168000
N	-3.769651000	2.726524000	-0.215686000
O	-4.940405000	3.004900000	-0.193638000
O	-2.847287000	3.507112000	-0.299287000
C	-0.330986000	-0.892827000	-0.215349000
O	-0.001415000	-1.985951000	-0.548697000
N	0.664119000	0.078538000	0.160785000
N	1.918323000	-0.220758000	0.002970000
C	2.822926000	0.641613000	0.412985000
H	2.537470000	1.586588000	0.881590000
C	6.504127000	1.004822000	0.524502000
C	6.898055000	-0.218771000	-0.076111000
C	5.933871000	-1.163856000	-0.516709000
C	4.609652000	-0.892496000	-0.362264000
C	4.191000000	0.336107000	0.240405000
C	5.174383000	1.270988000	0.677275000
H	7.257916000	1.711427000	0.853571000
H	6.287505000	-2.082693000	-0.967100000
H	3.854735000	-1.596994000	-0.688693000
H	0.385394000	0.947873000	0.617638000
H	4.857338000	2.201593000	1.134332000
O	8.157043000	-0.545141000	-0.257022000
H	8.773655000	0.129659000	0.057904000

Zero-point correction= 0.240988
(Hartree/Particle)
Thermal correction to Energy= 0.261348
Thermal correction to Enthalpy= 0.262292
Thermal correction to Gibbs Free Energy= 0.187248

```
 Sum of electronic and zero-point Energies=          -1208.966368
 Sum of electronic and thermal Energies=             -1208.946008
 Sum of electronic and thermal Enthalpies=           -1208.945064
 Sum of electronic and thermal Free Energies=        -1209.020108
```

5-N8-H Anion

```
C       -3.372871000      1.304817000      0.000059000
C       -2.036946000      0.929858000      0.000044000
C       -1.714289000     -0.427557000      0.000001000
C       -2.737444000     -1.372531000     -0.000031000
C       -4.057993000     -0.943387000     -0.000023000
C       -4.417498000      0.393016000      0.000023000
H       -1.240091000      1.661272000      0.000055000
H       -2.474203000     -2.422893000     -0.000049000
H       -5.450251000      0.707301000      0.000037000
N       -5.143099000     -1.947050000     -0.000071000
O       -6.288746000     -1.541069000     -0.000157000
O       -4.830703000     -3.116844000     -0.000032000
N       -3.715767000      2.742238000      0.000115000
O       -4.893822000      3.041664000      0.000135000
O       -2.806138000      3.541666000      0.000111000
C       -0.273560000     -0.934398000      0.000030000
O       -0.111139000     -2.157053000      0.000131000
N        0.590794000      0.086619000     -0.000074000
N        1.884237000     -0.323680000      0.000066000
C        2.749985000      0.619125000     -0.000286000
H        2.434405000      1.667683000     -0.000701000
C        6.486320000      1.119131000     -0.000144000
C        6.945077000     -0.191228000      0.000081000
C        6.033561000     -1.247075000      0.000186000
C        4.674498000     -0.988009000      0.000067000
C        4.186493000      0.329408000     -0.000160000
C        5.115915000      1.370448000     -0.000272000
H        7.194427000      1.943399000     -0.000215000
H        6.413215000     -2.262047000      0.000345000
H        3.952428000     -1.796259000      0.000146000
H        4.762280000      2.396522000     -0.000449000
O        8.282631000     -0.503684000      0.000219000
H        8.790493000      0.310979000     -0.000122000

Zero-point  correction=                                          0.226286
(Hartree/Particle)
 Thermal correction to Energy=                    0.246806
 Thermal correction to Enthalpy=                  0.247750
 Thermal correction to Gibbs Free Energy=         0.172143
 Sum of electronic and zero-point Energies=          -1208.756473
 Sum of electronic and thermal Energies=             -1208.735953
 Sum of electronic and thermal Enthalpies=           -1208.735009
 Sum of electronic and thermal Free Energies=        -1208.810616
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5-O4′-H Anion

```
C       -3.301468000      1.334168000     -0.118101000
C       -1.996363000      0.898568000     -0.301525000
C       -1.720444000     -0.465135000     -0.228191000
C       -2.766872000     -1.363533000     -0.009259000
C       -4.048104000     -0.874346000      0.171730000
C       -4.358164000      0.475459000      0.123696000
H       -1.230619000      1.630083000     -0.525841000
```

H	-2.560351000	-2.426285000	0.005115000
H	-5.367730000	0.835449000	0.258164000
N	-5.153001000	-1.830220000	0.419553000
O	-6.264877000	-1.369250000	0.564994000
O	-4.875281000	-3.005980000	0.462550000
N	-3.585289000	2.784102000	-0.203132000
O	-4.733854000	3.137775000	-0.051645000
O	-2.650853000	3.524535000	-0.414651000
C	-0.350467000	-1.070654000	-0.446211000
O	-0.257080000	-2.211561000	-0.856120000
N	0.669660000	-0.244060000	-0.134943000
N	1.983751000	-0.615143000	-0.283420000
C	2.823246000	0.258325000	0.180627000
H	2.436303000	1.183219000	0.638897000
C	6.405743000	1.118589000	0.691410000
C	7.121980000	-0.017781000	0.136317000
C	6.268900000	-1.067660000	-0.407633000
C	4.907052000	-0.985786000	-0.395382000
C	4.237679000	0.140326000	0.156084000
C	5.039727000	1.178747000	0.693548000
H	7.005910000	1.921132000	1.106021000
H	6.773924000	-1.930137000	-0.829570000
H	4.300966000	-1.786025000	-0.808894000
H	0.468292000	0.636344000	0.329624000
H	4.542236000	2.048937000	1.119285000
O	8.363262000	-0.091918000	0.124639000

Zero-point correction=	0.227040
(Hartree/Particle)	
Thermal correction to Energy=	0.247290
Thermal correction to Enthalpy=	0.248234
Thermal correction to Gibbs Free Energy=	0.173628
Sum of electronic and zero-point Energies=	-1208.744482
Sum of electronic and thermal Energies=	-1208.724232
Sum of electronic and thermal Enthalpies=	-1208.723288
Sum of electronic and thermal Free Energies=	-1208.797893

N′-(4-(Dimethylamino)benzylidene)-3,5-dinitrobenzohydrazide (6)

C	-4.247340000	1.276284000	-0.152639000
C	-2.912813000	0.928216000	-0.304042000
C	-2.552324000	-0.411449000	-0.198227000
C	-3.531256000	-1.378068000	0.029070000
C	-4.845447000	-0.973951000	0.178271000
C	-5.243736000	0.350455000	0.092212000
H	-2.195794000	1.706907000	-0.530871000
H	-3.259879000	-2.425195000	0.078802000
H	-6.278790000	0.642560000	0.204499000
N	-5.884966000	-2.000678000	0.436578000
O	-7.026172000	-1.614022000	0.543853000
O	-5.517387000	-3.148388000	0.523540000
N	-4.623198000	2.705039000	-0.267552000
O	-5.795872000	2.979029000	-0.170184000
O	-3.726517000	3.498931000	-0.446832000
C	-1.137717000	-0.908593000	-0.379878000
O	-0.919231000	-2.021116000	-0.788320000
N	-0.176553000	0.004367000	-0.037126000
N	1.144085000	-0.305910000	-0.176751000
C	1.975134000	0.548117000	0.277156000
H	1.633485000	1.474689000	0.757376000
C	5.659505000	1.166210000	0.625694000
C	6.224668000	0.019241000	0.030901000

C	5.338191000	-0.963133000	-0.472165000
C	3.971666000	-0.794337000	-0.396370000
C	3.416429000	0.352071000	0.186026000
C	4.285016000	1.319174000	0.693181000
H	6.291629000	1.940069000	1.037138000
H	5.724961000	-1.865491000	-0.924307000
H	3.307793000	-1.556593000	-0.787357000
H	-0.436395000	0.848976000	0.461920000
H	3.879140000	2.213905000	1.155337000
N	7.585554000	-0.140173000	-0.060895000
C	8.130122000	-1.400127000	-0.529287000
C	8.460446000	0.809051000	0.598045000
H	7.828170000	-2.241054000	0.106932000
H	7.809526000	-1.609051000	-1.553426000
H	9.216179000	-1.339115000	-0.527008000
H	9.494538000	0.524325000	0.416941000
H	8.316206000	1.816564000	0.198124000
H	8.292952000	0.839567000	1.681984000

Zero-point correction= 0.309908
(Hartree/Particle)
Thermal correction to Energy= 0.333707
Thermal correction to Enthalpy= 0.334652
Thermal correction to Gibbs Free Energy= 0.251826
Sum of electronic and zero-point Energies= -1267.913163
Sum of electronic and thermal Energies= -1267.889363
Sum of electronic and thermal Enthalpies= -1267.888419
Sum of electronic and thermal Free Energies= -1267.971244

6-N8-H Radical

C	-4.178134000	1.275256000	0.000078000
C	-2.836503000	0.925564000	-0.000014000
C	-2.499112000	-0.426457000	-0.000081000
C	-3.501145000	-1.395357000	-0.000071000
C	-4.823684000	-0.988000000	0.000015000
C	-5.201970000	0.344591000	0.000101000
H	-2.069584000	1.687180000	-0.000033000
H	-3.240376000	-2.446201000	-0.000127000
H	-6.241627000	0.640953000	0.000192000
N	-5.890604000	-2.016761000	0.000012000
O	-7.036376000	-1.626357000	0.000223000
O	-5.543705000	-3.175087000	-0.000198000
N	-4.539005000	2.712430000	0.000157000
O	-5.717163000	2.988742000	0.000513000
O	-3.631531000	3.512846000	-0.000131000
C	-1.068066000	-0.896841000	-0.000149000
O	-0.803075000	-2.075214000	-0.000165000
N	-0.151654000	0.170894000	-0.000209000
N	1.078735000	-0.245585000	-0.000197000
C	1.964979000	0.740450000	-0.000278000
H	1.611363000	1.773271000	-0.000304000
C	5.640921000	1.299685000	-0.000125000
C	6.146788000	-0.027824000	0.000003000
C	5.208701000	-1.098577000	-0.000011000
C	3.860749000	-0.854656000	-0.000112000
C	3.355992000	0.468562000	-0.000204000
C	4.287250000	1.529401000	-0.000214000
H	6.317575000	2.142046000	-0.000103000
H	5.554339000	-2.122475000	-0.000004000
H	3.153112000	-1.674901000	-0.000145000
H	3.921266000	2.550726000	-0.000290000

N	7.482940000	-0.268951000	0.000119000
C	7.981391000	-1.635506000	0.000759000
C	8.425602000	0.838010000	-0.000118000
H	7.647025000	-2.178080000	0.889657000
H	7.648018000	-2.178604000	-0.888199000
H	9.068083000	-1.615591000	0.001372000
H	9.437659000	0.441806000	-0.000442000
H	8.300996000	1.463206000	-0.889146000
H	8.301515000	1.463223000	0.888980000

Zero-point correction= 0.297142
(Hartree/Particle)
Thermal correction to Energy= 0.320659
Thermal correction to Enthalpy= 0.321603
Thermal correction to Gibbs Free Energy= 0.238379
Sum of electronic and zero-point Energies= -1267.281893
Sum of electronic and thermal Energies= -1267.258375
Sum of electronic and thermal Enthalpies= -1267.257431
Sum of electronic and thermal Free Energies= -1267.340656

6-Cationic Radical

C	-4.250073000	1.247600000	-0.171160000
C	-2.900840000	0.941156000	-0.242121000
C	-2.510820000	-0.389384000	-0.117825000
C	-3.469259000	-1.389534000	0.051382000
C	-4.800047000	-1.023682000	0.119683000
C	-5.229981000	0.289537000	0.011061000
H	-2.205356000	1.750185000	-0.427588000
H	-3.178724000	-2.430338000	0.125820000
H	-6.279564000	0.549986000	0.062439000
N	-5.821368000	-2.086237000	0.315310000
O	-6.974056000	-1.731792000	0.356321000
O	-5.415373000	-3.218607000	0.419743000
N	-4.654037000	2.669646000	-0.303354000
O	-5.834400000	2.909065000	-0.283036000
O	-3.761844000	3.480997000	-0.417168000
C	-1.084975000	-0.829867000	-0.209072000
O	-0.744923000	-1.925564000	-0.540087000
N	-0.139958000	0.160964000	0.153228000
N	1.142068000	-0.107219000	0.027148000
C	2.005313000	0.772777000	0.432254000
H	1.700569000	1.722764000	0.878449000
C	5.698841000	1.194195000	0.589956000
C	6.159370000	-0.037256000	0.016860000
C	5.179206000	-0.994183000	-0.414490000
C	3.850149000	-0.734780000	-0.281787000
C	3.399287000	0.489716000	0.287699000
C	4.362405000	1.437865000	0.716277000
H	6.407082000	1.937594000	0.926267000
H	5.491798000	-1.932191000	-0.850352000
H	3.112543000	-1.458084000	-0.606984000
H	-0.447003000	1.025101000	0.595125000
H	4.029252000	2.373186000	1.151662000
N	7.467153000	-0.287609000	-0.111926000
C	7.937570000	-1.549459000	-0.694767000
C	8.468275000	0.691502000	0.325591000
H	7.586454000	-2.395079000	-0.101067000
H	7.581521000	-1.648554000	-1.721660000
H	9.022608000	-1.551141000	-0.698572000

H	9.458171000	0.294864000	0.125322000
H	8.347680000	1.627677000	-0.222099000
H	8.374197000	0.877192000	1.396959000

Zero-point correction= 0.310265
(Hartree/Particle)
Thermal correction to Energy= 0.333975
Thermal correction to Enthalpy= 0.334919
Thermal correction to Gibbs Free Energy= 0.251584
Sum of electronic and zero-point Energies= -1267.648334
Sum of electronic and thermal Energies= -1267.624623
Sum of electronic and thermal Enthalpies= -1267.623679
Sum of electronic and thermal Free Energies= -1267.707014

6-N8-H Anion

C	-4.191274000	1.281338000	0.020021000
C	-2.849509000	0.928303000	0.002146000
C	-2.504475000	-0.423697000	-0.008729000
C	-3.512156000	-1.385213000	-0.001515000
C	-4.839555000	-0.977689000	0.016237000
C	-5.220951000	0.352548000	0.027487000
H	-2.064320000	1.672256000	-0.003602000
H	-3.231592000	-2.431013000	-0.010203000
H	-6.258595000	0.649854000	0.041282000
N	-5.908032000	-1.998839000	0.023702000
O	-7.060255000	-1.611912000	0.040280000
O	-5.576940000	-3.163516000	0.012893000
N	-4.557763000	2.712733000	0.031820000
O	-5.740660000	2.992750000	0.045396000
O	-3.661703000	3.527329000	0.027386000
C	-1.055583000	-0.906525000	-0.029020000
O	-0.873953000	-2.127266000	-0.037586000
N	-0.209748000	0.128454000	-0.033779000
N	1.092443000	-0.258120000	-0.053664000
C	1.939090000	0.702003000	-0.055315000
H	1.601193000	1.743708000	-0.040874000
C	5.668913000	1.280698000	-0.083596000
C	6.190309000	-0.020643000	-0.116550000
C	5.267709000	-1.085453000	-0.109908000
C	3.903258000	-0.856184000	-0.094046000
C	3.380608000	0.443947000	-0.076204000
C	4.294928000	1.497306000	-0.069810000
H	6.325910000	2.139526000	-0.069182000
H	5.614505000	-2.109908000	-0.118614000
H	3.205025000	-1.685400000	-0.090325000
H	3.924274000	2.517692000	-0.046316000
N	7.575453000	-0.257643000	-0.172952000
C	8.034477000	-1.568303000	0.245950000
C	8.442634000	0.842753000	0.195701000
H	7.720071000	-1.821111000	1.270008000
H	7.660193000	-2.341446000	-0.426560000
H	9.122965000	-1.592965000	0.196731000
H	9.479402000	0.512772000	0.132497000
H	8.321541000	1.675507000	-0.499295000
H	8.250509000	1.214228000	1.214504000

Zero-point correction= 0.296077
(Hartree/Particle)
Thermal correction to Energy= 0.319388
Thermal correction to Enthalpy= 0.320332

```
 Thermal correction to Gibbs Free Energy=         0.238194
 Sum of electronic and zero-point Energies=          -1267.402413
 Sum of electronic and thermal Energies=             -1267.379103
 Sum of electronic and thermal Enthalpies=           -1267.378159
 Sum of electronic and thermal Free Energies=        -1267.460296
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Table S6. Cartesian coordinates of all the transition states and products of HAT reactions with HOO• and CH_3OO• radicals including the zero point energy, ZPE, enthalpy, H, free energy, G,imaginary frequency calculated at the M06-2X/6-311+G(d,p) level of theory in the gas phase.

TS-1-O4′-H +HOO•

```
C         5.853897000      0.091886000     -0.115678000
C         4.962192000      1.121228000      0.119477000
C         3.597224000      0.920051000      0.263188000
C         3.095991000     -0.373757000      0.160902000
C         3.965331000     -1.442105000     -0.057112000
C         5.316041000     -1.182403000     -0.199306000
H         6.915219000      0.270032000     -0.223059000
H         2.968282000      1.773595000      0.482263000
H         3.583993000     -2.454500000     -0.106112000
C         1.636782000     -0.713030000      0.335502000
O         1.287961000     -1.788932000      0.743145000
N         0.776685000      0.302881000     -0.017640000
H         1.127481000      1.114386000     -0.516546000
N        -0.560470000      0.134011000      0.121880000
C        -1.308032000      1.066454000     -0.321417000
C        -2.764582000      0.989491000     -0.216641000
C        -3.537216000      2.059848000     -0.709050000
C        -4.907875000      2.002882000     -0.638252000
C        -5.562964000      0.894488000     -0.061912000
C        -4.771914000     -0.167063000      0.477023000
C        -3.386254000     -0.109420000      0.366767000
H        -3.047823000      2.919338000     -1.153153000
H        -5.535148000      2.795034000     -1.027828000
H        -2.797705000     -0.929586000      0.759216000
O        -5.279984000     -1.265568000      1.051815000
O        -6.880229000      0.864449000     -0.033890000
H        -7.266998000      0.029410000     -0.648386000
C        -6.507449000     -1.213859000      1.784605000
H        -7.360808000     -1.398987000      1.133462000
H        -6.429206000     -2.008163000      2.524266000
H        -6.621220000     -0.249173000      2.280076000
N         6.240374000     -2.316743000     -0.447945000
O         5.750962000     -3.418188000     -0.529413000
O         7.416251000     -2.054620000     -0.553002000
N         5.488608000      2.502241000      0.231059000
O         6.683933000      2.647821000      0.138599000
O         4.680538000      3.387563000      0.403031000
H        -0.889932000      1.961583000     -0.797007000
O        -8.794507000     -1.366582000     -0.771166000
H        -9.555090000     -1.029493000     -1.266632000
O        -7.714231000     -0.858237000     -1.421697000
Zero-point  correction=                                  0.284435
(Hartree/Particle)
 Thermal correction to Energy=                  0.310873
 Thermal correction to Enthalpy=                0.311817
 Thermal correction to Gibbs Free Energy=       0.220999
 Sum of electronic and zero-point Energies=          -1474.598757
 Sum of electronic and thermal Energies=             -1474.572320
 Sum of electronic and thermal Enthalpies=           -1474.571375
```

Sum of electronic and thermal Free Energies= -1474.662194

TS-1-N8-H +HOO•

C	4.891763000	0.153610000	0.286944000
C	3.805723000	0.968564000	0.550379000
C	2.497939000	0.528131000	0.457780000
C	2.254483000	-0.775350000	0.045601000
C	3.315419000	-1.639983000	-0.206361000
C	4.606619000	-1.151700000	-0.081835000
H	5.909566000	0.511797000	0.363279000
H	1.686368000	1.188267000	0.725319000
H	3.138695000	-2.667715000	-0.498568000
C	0.841343000	-1.264813000	-0.083226000
O	0.509184000	-2.378457000	0.223079000
N	-0.015836000	-0.318121000	-0.656749000
H	0.376938000	0.739571000	-1.067322000
N	-1.302359000	-0.414997000	-0.359224000
C	-2.081072000	0.565023000	-0.683339000
C	-3.513368000	0.468196000	-0.502895000
C	-4.312366000	1.569341000	-0.824933000
C	-5.689300000	1.501528000	-0.680451000
C	-6.285631000	0.333000000	-0.215013000
C	-5.487389000	-0.780990000	0.123506000
C	-4.119413000	-0.705956000	-0.023494000
H	-3.851906000	2.479599000	-1.191756000
H	-6.311079000	2.353160000	-0.936494000
H	-3.515445000	-1.569040000	0.230963000
O	-6.066698000	-1.940803000	0.536292000
O	-7.622009000	0.196049000	-0.068879000
H	-8.070434000	0.998711000	-0.351167000
C	-6.612042000	-1.896942000	1.853450000
H	-7.402604000	-1.147826000	1.924752000
H	-7.025019000	-2.884942000	2.044411000
H	-5.822812000	-1.681557000	2.579585000
N	5.743380000	-2.059775000	-0.368479000
O	5.475142000	-3.187455000	-0.710448000
O	6.857252000	-1.606952000	-0.237702000
N	4.037369000	2.380786000	0.911864000
O	5.160857000	2.711191000	1.194087000
O	3.073371000	3.124814000	0.891196000
H	-1.670643000	1.498250000	-1.073813000
O	0.326516000	2.769579000	-0.384548000
H	1.165303000	3.099320000	-0.019360000
O	0.721253000	1.904185000	-1.382876000

Zero-point correction= 0.285532
(Hartree/Particle)
Thermal correction to Energy= 0.311524
Thermal correction to Enthalpy= 0.312468
Thermal correction to Gibbs Free Energy= 0.224886
Sum of electronic and zero-point Energies= -1474.596043
Sum of electronic and thermal Energies= -1474.570051
Sum of electronic and thermal Enthalpies= -1474.569107
Sum of electronic and thermal Free Energies= -1474.656689

TS-2-O2′-H +HOO•

C	-5.774225000	0.501775000	-0.235931000
C	-4.559582000	1.160625000	-0.284532000
C	-3.343187000	0.507125000	-0.179757000
C	-3.333779000	-0.872912000	0.002007000
C	-4.533788000	-1.578886000	0.037688000

C	-5.720488000	-0.874092000	-0.074358000
H	-6.715233000	1.027578000	-0.323180000
H	-2.430200000	1.084638000	-0.268712000
H	-4.533139000	-2.656573000	0.145444000
C	-2.041155000	-1.647704000	0.090278000
O	-1.954966000	-2.793816000	-0.268933000
N	-1.018186000	-0.897918000	0.611877000
H	-1.206118000	0.051931000	0.919706000
N	0.284346000	-1.239582000	0.450741000
C	1.089934000	-0.344387000	0.900121000
C	2.509136000	-0.401077000	0.680624000
C	3.266516000	0.804257000	0.826817000
C	4.647487000	0.790864000	0.637062000
C	5.321650000	-0.389702000	0.300141000
C	4.538702000	-1.580210000	0.110281000
C	3.181848000	-1.571856000	0.293287000
H	5.153103000	1.739482000	0.737362000
H	2.603724000	-2.478200000	0.157810000
N	-7.001918000	-1.619970000	-0.020082000
O	-6.937591000	-2.816108000	0.138837000
O	-8.019551000	-0.976606000	-0.137462000
N	-4.548031000	2.631524000	-0.455071000
O	-5.607243000	3.177926000	-0.644018000
O	-3.471866000	3.188734000	-0.386816000
H	0.705728000	0.534333000	1.417567000
O	2.664573000	1.939044000	1.136912000
H	1.800747000	2.089937000	0.537219000
H	5.018085000	-2.506975000	-0.168839000
N	6.679232000	-0.433830000	0.162504000
C	7.350786000	-1.603361000	-0.400969000
C	7.130858000	-1.778803000	-1.904009000
H	7.038032000	-2.498829000	0.141672000
H	8.415402000	-1.483528000	-0.196930000
H	7.534935000	-0.929750000	-2.456621000
H	7.631098000	-2.684611000	-2.252983000
H	6.069007000	-1.859344000	-2.142233000
C	7.480865000	0.765249000	0.382781000
C	7.542208000	1.696956000	-0.828301000
H	8.486315000	0.438306000	0.653506000
H	7.084100000	1.289322000	1.254057000
H	8.073920000	2.615317000	-0.571001000
H	8.069796000	1.222034000	-1.657081000
H	6.539686000	1.961675000	-1.168869000
O	-0.426470000	2.209703000	0.276036000
H	-0.856409000	3.047925000	0.049557000
O	0.781439000	2.247448000	-0.386631000

Zero-point correction= 0.384604
(Hartree/Particle)
Thermal correction to Energy= 0.414760
Thermal correction to Enthalpy= 0.415704
Thermal correction to Gibbs Free Energy= 0.318141
Sum of electronic and zero-point Energies= -1572.554594
Sum of electronic and thermal Energies= -1572.524438
Sum of electronic and thermal Enthalpies= -1572.523494
Sum of electronic and thermal Free Energies= -1572.621057

TS-2-N8-H +HOO•

C	-5.995917000	0.077303000	-0.089661000
C	-5.030382000	1.030595000	-0.357443000
C	-3.684682000	0.728949000	-0.495047000
C	-3.282248000	-0.598692000	-0.363130000

C	-4.226703000	-1.591666000	-0.112394000
C	-5.555245000	-1.230287000	0.025675000
H	-7.039172000	0.339055000	0.019712000
H	-2.986619000	1.527259000	-0.711916000
H	-3.919488000	-2.626506000	-0.029643000
C	-1.849047000	-1.041817000	-0.502372000
O	-1.564971000	-2.189978000	-0.727962000
N	-0.929958000	0.002522000	-0.389929000
H	-1.253229000	0.848701000	0.341407000
N	0.353281000	-0.368229000	-0.297030000
C	1.187774000	0.627442000	-0.194846000
C	2.595590000	0.381651000	-0.093962000
C	3.505085000	1.454264000	-0.014487000
C	4.871727000	1.241661000	0.069248000
C	5.402615000	-0.065227000	0.068226000
C	4.482520000	-1.149809000	0.002726000
C	3.133944000	-0.920379000	-0.075533000
H	5.513468000	2.105086000	0.181883000
H	2.441580000	-1.751484000	-0.138028000
N	-6.558171000	-2.285072000	0.305101000
O	-6.152445000	-3.418306000	0.420351000
O	-7.713757000	-1.938577000	0.399625000
N	-5.460995000	2.439912000	-0.512619000
O	-6.618062000	2.694303000	-0.266701000
O	-4.627350000	3.237301000	-0.875326000
H	0.837482000	1.658759000	-0.192497000
O	2.982428000	2.703256000	-0.007756000
H	3.681937000	3.360414000	0.042063000
H	4.841752000	-2.168142000	-0.016048000
N	6.749615000	-0.303306000	0.128118000
C	7.238161000	-1.600439000	0.600011000
C	7.556339000	-2.590552000	-0.518419000
H	6.498334000	-2.022180000	1.282929000
H	8.130560000	-1.415903000	1.203204000
H	6.686281000	-2.751100000	-1.157026000
H	8.368637000	-2.225794000	-1.147525000
H	7.855816000	-3.551740000	-0.094726000
C	7.713992000	0.791951000	0.086101000
C	9.027708000	0.415346000	-0.591460000
H	7.905645000	1.167357000	1.101564000
H	7.275302000	1.605264000	-0.488924000
H	9.675989000	1.292826000	-0.619710000
H	9.565170000	-0.372516000	-0.062444000
H	8.849489000	0.087896000	-1.617118000
O	-0.302015000	1.445689000	2.095786000
H	-0.441470000	0.865995000	2.857253000
O	-1.517732000	1.449335000	1.455822000

Zero-point correction= 0.384289
(Hartree/Particle)
Thermal correction to Energy= 0.414705
Thermal correction to Enthalpy= 0.415649
Thermal correction to Gibbs Free Energy= 0.317420
Sum of electronic and zero-point Energies= -1572.552220
Sum of electronic and thermal Energies= -1572.521804
Sum of electronic and thermal Enthalpies= -1572.520860
Sum of electronic and thermal Free Energies= -1572.619089

TS-2-C7′-H +HOO•

C	6.612159000	0.502594000	-0.014027000
C	5.545618000	1.314357000	0.322812000
C	4.242279000	0.848627000	0.419492000

C	3.989074000	-0.494797000	0.160610000
C	5.041321000	-1.350431000	-0.163245000
C	6.319763000	-0.830589000	-0.252739000
H	7.621068000	0.885689000	-0.082089000
H	3.465774000	1.539045000	0.723701000
H	4.853717000	-2.403284000	-0.333160000
C	2.617993000	-1.117671000	0.271342000
O	2.485518000	-2.281550000	0.553109000
N	1.587605000	-0.250213000	0.019219000
H	1.778662000	0.662821000	-0.380697000
N	0.297233000	-0.675719000	0.115308000
C	-0.596995000	0.156247000	-0.252133000
C	-2.014367000	-0.185917000	-0.184701000
C	-2.978058000	0.747011000	-0.577657000
C	-4.335172000	0.446750000	-0.521922000
C	-4.760704000	-0.800522000	-0.064515000
C	-3.799028000	-1.746372000	0.335381000
C	-2.457376000	-1.435201000	0.270003000
H	-5.047391000	1.214054000	-0.795512000
H	-1.710756000	-2.164880000	0.560191000
N	7.437134000	-1.737539000	-0.613886000
O	7.161019000	-2.893528000	-0.831700000
O	8.544364000	-1.253305000	-0.666568000
N	5.808362000	2.745771000	0.602763000
O	6.955284000	3.120674000	0.540794000
O	4.853089000	3.439971000	0.870001000
H	-0.342187000	1.151633000	-0.627596000
O	-2.550518000	1.967945000	-0.999184000
H	-3.309745000	2.536608000	-1.163799000
H	-4.106138000	-2.733544000	0.653746000
N	-6.130790000	-1.123901000	-0.023379000
C	-6.650767000	-1.665915000	1.237352000
C	-6.956140000	-0.558671000	2.245875000
H	-5.909725000	-2.349680000	1.646265000
H	-7.540779000	-2.256871000	1.018312000
H	-7.311853000	-0.988718000	3.184029000
H	-6.056026000	0.025830000	2.447833000
H	-7.719226000	0.124957000	1.866926000
C	-7.019221000	-0.355964000	-0.812660000
C	-8.436694000	-0.882752000	-0.922332000
H	-6.570165000	-0.168499000	-1.791386000
H	-7.115318000	0.782375000	-0.353508000
H	-8.986325000	-0.271279000	-1.638483000
H	-8.444562000	-1.917461000	-1.276849000
H	-8.970645000	-0.835370000	0.028136000
O	-6.581584000	2.790151000	-0.992860000
H	-7.328890000	3.123146000	-1.505802000
O	-7.170722000	2.083385000	0.043653000

Zero-point correction= 0.383981
(Hartree/Particle)

Thermal correction to Energy=	0.414364
Thermal correction to Enthalpy=	0.415308
Thermal correction to Gibbs Free Energy=	0.316737
Sum of electronic and zero-point Energies=	-1572.553231
Sum of electronic and thermal Energies=	-1572.522849
Sum of electronic and thermal Enthalpies=	-1572.521905
Sum of electronic and thermal Free Energies=	-1572.620475

TS-3-N8-H +HOO•

C	3.041587000	1.159600000	-0.450457000
C	1.706239000	0.831695000	-0.617421000

C	1.323683000	-0.496917000	-0.449885000
C	2.272068000	-1.468547000	-0.139634000
C	3.589446000	-1.080344000	0.024734000
C	4.011735000	0.230687000	-0.120616000
H	0.997460000	1.606529000	-0.877538000
H	1.980555000	-2.505070000	-0.026275000
H	5.046977000	0.513144000	0.013094000
N	3.452952000	2.571458000	-0.634523000
O	4.609191000	2.843515000	-0.407381000
O	2.603564000	3.351926000	-0.997671000
N	4.598420000	-2.108050000	0.375405000
O	5.745422000	-1.740766000	0.486511000
O	4.203267000	-3.240805000	0.526623000
C	-0.097781000	-0.949892000	-0.598216000
O	-0.391826000	-2.082090000	-0.875006000
N	-1.029980000	0.086420000	-0.400327000
H	-0.696538000	0.876177000	0.455731000
N	-2.305110000	-0.273777000	-0.449709000
C	-3.184155000	0.343709000	0.243693000
H	-2.869997000	1.071185000	0.999727000
C	-5.080928000	-0.865706000	-0.834194000
C	-4.611269000	0.086556000	0.079743000
C	-5.520304000	0.815669000	0.850895000
C	-6.885937000	0.602490000	0.709417000
C	-7.347333000	-0.342509000	-0.200321000
C	-6.443007000	-1.075818000	-0.969740000
H	-4.365828000	-1.432827000	-1.418170000
H	-5.154036000	1.552607000	1.557878000
H	-7.587414000	1.171126000	1.307293000
H	-8.411725000	-0.512188000	-0.310377000
H	-6.806496000	-1.814355000	-1.673783000
O	0.445765000	0.692894000	2.216629000
H	-0.066445000	0.424320000	2.991648000
O	-0.430977000	1.471946000	1.497402000

Zero-point correction= 0.247746
(Hartree/Particle)
Thermal correction to Energy= 0.270224
Thermal correction to Enthalpy= 0.271168
Thermal correction to Gibbs Free Energy= 0.190542
Sum of electronic and zero-point Energies= -1284.900868
Sum of electronic and thermal Energies= -1284.878390
Sum of electronic and thermal Enthalpies= -1284.877446
Sum of electronic and thermal Free Energies= -1284.958071

TS-4-N8-H +HOO•

C	-4.995983000	0.485739000	0.032891000
C	-3.886983000	1.237535000	-0.312559000
C	-2.636425000	0.685347000	-0.520916000
C	-2.463976000	-0.679641000	-0.319812000
C	-3.551959000	-1.476882000	0.025080000
C	-4.790144000	-0.875762000	0.184577000
H	-5.969444000	0.933232000	0.181792000
H	-1.819192000	1.312470000	-0.846835000
H	-3.428058000	-2.543150000	0.169324000
C	-1.113708000	-1.325473000	-0.436610000
O	-0.976580000	-2.511255000	-0.596834000
N	-0.060077000	-0.409691000	-0.367924000
H	-0.191402000	0.538181000	0.317101000
N	1.153277000	-0.964676000	-0.282124000
C	2.155260000	-0.135446000	-0.176742000
C	3.496193000	-0.618518000	-0.103230000

C	4.605505000	0.298205000	0.060409000
C	5.925511000	-0.218068000	0.103754000
C	6.128507000	-1.627272000	-0.000980000
C	5.089364000	-2.492090000	-0.138848000
C	3.757388000	-2.006302000	-0.194553000
H	1.952205000	0.932410000	-0.136545000
C	5.530645000	2.527045000	0.340042000
C	4.442351000	1.696957000	0.188853000
C	7.024117000	0.652868000	0.257767000
C	6.836110000	2.008961000	0.372682000
H	5.373588000	3.594522000	0.437548000
H	3.457716000	2.144701000	0.178173000
H	8.022230000	0.229372000	0.285891000
H	7.682480000	2.673739000	0.491385000
H	5.232474000	-3.562230000	-0.214982000
H	7.145160000	-2.004188000	0.035292000
O	2.818011000	-2.922422000	-0.338294000
H	1.924704000	-2.495112000	-0.347914000
N	-5.951430000	-1.719487000	0.557941000
O	-7.016768000	-1.162232000	0.691025000
O	-5.750373000	-2.902381000	0.700027000
N	-4.026447000	2.702226000	-0.433214000
O	-3.001301000	3.359689000	-0.418323000
O	-5.138898000	3.154957000	-0.525029000
O	-0.130308000	2.580652000	0.216635000
H	-0.994220000	3.027359000	0.245261000
O	-0.242049000	1.545104000	1.109659000

Zero-point correction= 0.300492
(Hartree/Particle)

Thermal correction to Energy=	0.326086
Thermal correction to Enthalpy=	0.327030
Thermal correction to Gibbs Free Energy=	0.240707
Sum of electronic and zero-point Energies=	-1513.706375
Sum of electronic and thermal Energies=	-1513.680781
Sum of electronic and thermal Enthalpies=	-1513.679837
Sum of electronic and thermal Free Energies=	-1513.766159

TS-5-N8-H +HOO•

C	-3.490796000	1.166980000	-0.321146000
C	-2.162303000	0.810795000	-0.490894000
C	-1.813080000	-0.533192000	-0.376338000
C	-2.791181000	-1.489002000	-0.109242000
C	-4.099772000	-1.073793000	0.060331000
C	-4.488239000	0.251907000	-0.037734000
H	-1.436936000	1.580328000	-0.721407000
H	-2.526422000	-2.536475000	-0.038325000
H	-5.517436000	0.555316000	0.096328000
N	-5.139152000	-2.088524000	0.357558000
O	-6.276964000	-1.695122000	0.475338000
O	-4.775970000	-3.236820000	0.462391000
N	-3.864226000	2.595019000	-0.455727000
O	-5.009498000	2.891883000	-0.205464000
O	-2.997932000	3.362472000	-0.806849000
C	-0.404066000	-1.030253000	-0.551235000
O	-0.162677000	-2.183495000	-0.789444000
N	0.562801000	-0.016701000	-0.452668000
N	1.825953000	-0.451383000	-0.391321000
C	2.709442000	0.490028000	-0.247200000
H	2.408192000	1.537412000	-0.185591000
C	6.398779000	0.964520000	0.033196000
C	6.849539000	-0.353442000	-0.057564000

C	5.939140000	-1.407850000	-0.205635000
C	4.589212000	-1.142609000	-0.261536000
C	4.117663000	0.181393000	-0.175810000
C	5.040220000	1.223958000	-0.026241000
H	7.109806000	1.775516000	0.149720000
H	6.323323000	-2.417843000	-0.271303000
H	3.870864000	-1.945749000	-0.373078000
H	0.293092000	0.829375000	0.349565000
H	4.684637000	2.246086000	0.045732000
O	8.158872000	-0.678855000	-0.006463000
H	8.698387000	0.110781000	0.095306000
O	1.323645000	1.293066000	2.069073000
H	1.178331000	0.690922000	2.812433000
O	0.096671000	1.365476000	1.456170000

Zero-point correction= 0.252757
(Hartree/Particle)
Thermal correction to Energy= 0.276301
Thermal correction to Enthalpy= 0.277245
Thermal correction to Gibbs Free Energy= 0.194369
Sum of electronic and zero-point Energies= -1360.126079
Sum of electronic and thermal Energies= -1360.102535
Sum of electronic and thermal Enthalpies= -1360.101591
Sum of electronic and thermal Free Energies= -1360.184467

TS-5-O4′-H +HOO•

C	4.260868000	1.395532000	0.120058000
C	2.949141000	0.965230000	0.254905000
C	2.681983000	-0.398973000	0.196516000
C	3.727332000	-1.306990000	0.030981000
C	5.014949000	-0.821410000	-0.104207000
C	5.321855000	0.529231000	-0.063930000
H	2.178197000	1.704159000	0.433230000
H	3.528917000	-2.371482000	0.015811000
H	6.338059000	0.885364000	-0.165325000
N	6.126295000	-1.786108000	-0.297425000
O	7.241195000	-1.327863000	-0.392844000
O	5.835797000	-2.957659000	-0.347196000
N	4.537327000	2.850414000	0.183819000
O	5.690696000	3.198228000	0.100092000
O	3.584538000	3.586737000	0.311335000
C	1.300837000	-0.979356000	0.364713000
O	1.132712000	-2.084902000	0.805931000
N	0.283594000	-0.140111000	-0.036771000
N	-1.004176000	-0.532367000	0.096989000
C	-1.897344000	0.236770000	-0.395595000
H	-1.633358000	1.167652000	-0.911106000
C	-5.605755000	0.494852000	-0.788187000
C	-6.045089000	-0.678583000	-0.120568000
C	-5.081914000	-1.546098000	0.462383000
C	-3.744367000	-1.262453000	0.364858000
C	-3.312405000	-0.089211000	-0.290983000
C	-4.258097000	0.779183000	-0.854861000
H	-6.346355000	1.149025000	-1.231529000
H	-5.443192000	-2.431085000	0.971167000
H	-3.000285000	-1.922398000	0.794132000
H	0.497565000	0.703121000	-0.560137000
H	-3.922460000	1.678755000	-1.360005000
O	-7.308335000	-0.979164000	-0.045480000
H	-7.916754000	-0.012638000	0.083082000
O	-9.692064000	0.995075000	-0.061726000
H	-10.248250000	1.180500000	0.707141000

O	-8.422704000	1.022034000	0.447483000

Zero-point correction= 0.251960
(Hartree/Particle)
Thermal correction to Energy= 0.275811
Thermal correction to Enthalpy= 0.276755
Thermal correction to Gibbs Free Energy= 0.191565
Sum of electronic and zero-point Energies= -1360.121209
Sum of electronic and thermal Energies= -1360.097358
Sum of electronic and thermal Enthalpies= -1360.096414
Sum of electronic and thermal Free Energies= -1360.181604

TS-6-N8-H +HOO•

C	-4.230680000	1.121699000	-0.325961000
C	-2.894339000	0.790915000	-0.485412000
C	-2.518853000	-0.545200000	-0.360400000
C	-3.480381000	-1.517822000	-0.094987000
C	-4.798294000	-1.127735000	0.064268000
C	-5.212221000	0.189283000	-0.043373000
H	-2.183103000	1.574186000	-0.713833000
H	-3.194722000	-2.559244000	-0.017488000
H	-6.247722000	0.473517000	0.082855000
N	-5.819492000	-2.160884000	0.358818000
O	-6.965551000	-1.789310000	0.470810000
O	-5.436317000	-3.302492000	0.467713000
N	-4.632319000	2.540457000	-0.473030000
O	-5.779330000	2.819997000	-0.208884000
O	-3.786566000	3.319465000	-0.847685000
C	-1.098438000	-1.018808000	-0.523169000
O	-0.841078000	-2.171824000	-0.753177000
N	-0.154310000	0.006421000	-0.425061000
N	1.121360000	-0.391942000	-0.359545000
C	1.981152000	0.578592000	-0.248856000
H	1.648663000	1.617954000	-0.214801000
C	5.655373000	1.172334000	-0.015663000
C	6.180910000	-0.142435000	-0.066468000
C	5.262095000	-1.221469000	-0.170539000
C	3.908721000	-0.993497000	-0.222154000
C	3.389868000	0.315469000	-0.177654000
C	4.295143000	1.383184000	-0.070737000
H	6.315965000	2.023404000	0.066406000
H	5.622121000	-2.239763000	-0.208353000
H	3.216523000	-1.823556000	-0.299701000
H	-0.443920000	0.862618000	0.310170000
H	3.913520000	2.398103000	-0.029123000
N	7.523091000	-0.367009000	-0.015082000
C	8.040034000	-1.723394000	-0.075385000
C	8.443884000	0.750330000	0.097148000
H	7.678892000	-2.324799000	0.764540000
H	7.751251000	-2.217500000	-1.008016000
H	9.125677000	-1.691082000	-0.029276000
H	9.461800000	0.369978000	0.127506000
H	8.355432000	1.425999000	-0.759346000
H	8.264298000	1.322478000	1.012674000
O	0.546386000	1.445112000	2.051994000
H	0.390401000	0.886342000	2.825764000
O	-0.673449000	1.484478000	1.419651000

Zero-point correction= 0.322297
(Hartree/Particle)
Thermal correction to Energy= 0.349105
Thermal correction to Enthalpy= 0.350049

```
 Thermal correction to Gibbs Free Energy=         0.259484
 Sum of electronic and zero-point Energies=          -1418.780458
 Sum of electronic and thermal Energies=             -1418.753650
 Sum of electronic and thermal Enthalpies=           -1418.752706
 Sum of electronic and thermal Free Energies=        -1418.843270
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TS-BHA(O-H) +HOO•

```
C        2.052221000     -0.970760000     -0.595280000
C        2.104425000      0.294316000     -0.002997000
C        0.929801000      1.040595000      0.186883000
C       -0.316455000      0.572064000     -0.183058000
C       -0.371037000     -0.722766000     -0.793585000
C        0.817503000     -1.455441000     -0.986969000
H        2.943887000     -1.559435000     -0.760990000
H        1.052659000      2.010356000      0.649413000
H        0.727893000     -2.422753000     -1.469574000
O       -1.509863000     -1.255938000     -1.203838000
H       -1.828999000     -2.012738000     -0.473986000
O        3.239471000      0.888457000      0.418745000
C        4.461511000      0.196390000      0.244217000
H        5.234475000      0.848368000      0.642995000
H        4.459553000     -0.748043000      0.796017000
H        4.655117000      0.004320000     -0.814919000
C       -1.584766000      1.398442000      0.026274000
C       -2.258681000      1.659575000     -1.334276000
C       -2.551536000      0.648725000      0.961601000
C       -1.272855000      2.756794000      0.665411000
H       -1.581547000      2.202419000     -1.999516000
H       -2.554512000      0.729813000     -1.817065000
H       -3.150372000      2.274160000     -1.182728000
H       -3.428020000      1.276369000      1.145574000
H       -2.890852000     -0.292616000      0.533224000
H       -2.072605000      0.434205000      1.919748000
H       -0.822530000      2.646613000      1.655344000
H       -0.607288000      3.358220000      0.040622000
H       -2.205640000      3.311741000      0.786056000
O       -1.034652000     -2.140451000      1.432290000
H       -0.195565000     -2.605636000      1.288651000
O       -1.919511000     -2.737438000      0.594279000
Zero-point  correction=                                  0.263479
(Hartree/Particle)
 Thermal correction to Energy=                  0.279668
 Thermal correction to Enthalpy=                0.280612
 Thermal correction to Gibbs Free Energy=       0.220035
 Sum of electronic and zero-point Energies=          -729.772984
 Sum of electronic and thermal Energies=             -729.756795
 Sum of electronic and thermal Enthalpies=           -729.755851
 Sum of electronic and thermal Free Energies=        -729.816428
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TS-1-O4′-H +CH_3OO•

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C        6.130419000      0.450907000     -0.158068000
C        5.145158000      1.298399000      0.312071000
C        3.818731000      0.914462000      0.445063000
C        3.455468000     -0.379225000      0.084223000
C        4.423899000     -1.270794000     -0.375737000
C        5.730032000     -0.832257000     -0.494522000
H        7.159478000      0.769603000     -0.252847000
H        3.112122000      1.624493000      0.855669000
H        4.152043000     -2.288510000     -0.626881000
C        2.050710000     -0.914463000      0.219379000
```

O	1.844680000	-2.086243000	0.401103000
N	1.073101000	0.043464000	0.109038000
H	1.309837000	0.973644000	-0.220586000
N	-0.235818000	-0.303522000	0.239563000
C	-1.093953000	0.607556000	0.006524000
C	-2.530197000	0.357484000	0.124426000
C	-3.432479000	1.386345000	-0.127050000
C	-4.800055000	1.174855000	-0.022731000
C	-5.293237000	-0.082473000	0.338647000
C	-4.375116000	-1.137537000	0.606773000
C	-3.019916000	-0.898712000	0.495176000
H	-3.072564000	2.370620000	-0.406819000
H	-5.511926000	1.964644000	-0.225432000
H	-2.337422000	-1.715281000	0.699953000
O	-4.795216000	-2.393151000	0.902611000
O	-6.594685000	-0.338186000	0.420315000
H	-7.531256000	0.706190000	0.244135000
C	-5.719195000	-2.516034000	1.975362000
H	-6.704033000	-2.133347000	1.690302000
H	-5.791313000	-3.579505000	2.192813000
H	-5.357108000	-1.978917000	2.856414000
N	6.758090000	-1.775162000	-1.000799000
O	6.387416000	-2.884783000	-1.302369000
O	7.892645000	-1.363071000	-1.076705000
N	5.524191000	2.677984000	0.698695000
O	6.690677000	2.977864000	0.607181000
O	4.635188000	3.408876000	1.075413000
H	-0.791670000	1.619587000	-0.290465000
C	-7.791954000	1.107286000	-2.471522000
H	-8.378614000	0.698908000	-3.293158000
H	-6.857834000	0.548402000	-2.355853000
H	-7.585488000	2.166657000	-2.635432000
O	-7.943574000	1.511905000	-0.247693000
O	-8.597267000	0.936622000	-1.318026000

Zero-point correction= 0.313239
(Hartree/Particle)
Thermal correction to Energy= 0.341170
Thermal correction to Enthalpy= 0.342115
Thermal correction to Gibbs Free Energy= 0.246961
Sum of electronic and zero-point Energies= -1513.843619
Sum of electronic and thermal Energies= -1513.815687
Sum of electronic and thermal Enthalpies= -1513.814743
Sum of electronic and thermal Free Energies= -1513.909896

TS-1-N8-H +$CH_3OO^{\bullet}$

C	5.080018000	0.061410000	0.146776000
C	4.163047000	1.044405000	0.471921000
C	2.808933000	0.794489000	0.628957000
C	2.347425000	-0.508799000	0.456815000
C	3.241428000	-1.530982000	0.144349000
C	4.580889000	-1.221010000	-0.008860000
H	6.131481000	0.282047000	0.024357000
H	2.148948000	1.610072000	0.894638000
H	2.888502000	-2.547822000	0.026754000
C	0.899683000	-0.889397000	0.608803000
O	0.558761000	-2.031336000	0.772172000
N	0.029409000	0.212649000	0.582624000
H	0.361835000	1.059594000	-0.256924000
N	-1.266238000	-0.111219000	0.478950000
C	-2.062185000	0.911068000	0.393834000
C	-3.490053000	0.730652000	0.254586000

C	-4.318645000	1.855036000	0.195970000
C	-5.691073000	1.707489000	0.069290000
C	-6.252215000	0.435574000	-0.007577000
C	-5.425459000	-0.706560000	0.054979000
C	-4.061786000	-0.551640000	0.180799000
H	-3.884793000	2.847159000	0.247023000
H	-6.335078000	2.579281000	0.017310000
H	-3.431378000	-1.432304000	0.215058000
O	-5.962312000	-1.950297000	-0.072994000
O	-7.578726000	0.224134000	-0.154247000
H	-8.043529000	1.063670000	-0.218970000
C	-6.703433000	-2.396554000	1.061347000
H	-7.554998000	-1.741549000	1.253968000
H	-7.057263000	-3.396180000	0.819175000
H	-6.054327000	-2.439060000	1.940662000
N	5.531041000	-2.305709000	-0.353839000
O	5.072453000	-3.413661000	-0.507638000
O	6.698117000	-2.004950000	-0.457923000
N	4.656345000	2.428259000	0.668408000
O	5.825394000	2.635410000	0.438535000
O	3.855539000	3.252749000	1.045002000
H	-1.672404000	1.929848000	0.433251000
C	-0.759338000	0.337543000	-2.764270000
H	-1.755307000	0.335178000	-3.205196000
H	-0.597840000	-0.573748000	-2.181080000
H	0.008732000	0.441631000	-3.531806000
O	0.513508000	1.566099000	-1.340447000
O	-0.726473000	1.469097000	-1.902150000

Zero-point correction= 0.313752
(Hartree/Particle)

Thermal correction to Energy=	0.341249
Thermal correction to Enthalpy=	0.342193
Thermal correction to Gibbs Free Energy=	0.249897
Sum of electronic and zero-point Energies=	-1513.869137
Sum of electronic and thermal Energies=	-1513.841639
Sum of electronic and thermal Enthalpies=	-1513.840695
Sum of electronic and thermal Free Energies=	-1513.932991

TS-2-O2′-H +$CH_3OO^{\bullet}$

C	6.228973000	0.445548000	0.218649000
C	5.201232000	1.331460000	0.481717000
C	3.877110000	0.937310000	0.606744000
C	3.562713000	-0.410086000	0.457642000
C	4.573724000	-1.338120000	0.211252000
C	5.875204000	-0.887699000	0.087636000
H	7.255054000	0.774371000	0.125904000
H	3.133116000	1.686146000	0.847895000
H	4.338155000	-2.391558000	0.126157000
C	2.165518000	-0.955834000	0.610094000
O	1.970430000	-2.084606000	0.981239000
N	1.172223000	-0.063125000	0.281466000
H	1.403244000	0.796929000	-0.207328000
N	-0.128605000	-0.421175000	0.408626000
C	-0.988054000	0.413719000	-0.059312000
C	-2.402061000	0.152835000	0.034119000
C	-3.306954000	1.014976000	-0.668800000
C	-4.689316000	0.832932000	-0.535596000
C	-5.213911000	-0.200731000	0.243617000
C	-4.287487000	-1.076795000	0.909171000
C	-2.934021000	-0.900412000	0.797665000
H	-5.312774000	1.526681000	-1.079495000

H	-2.251222000	-1.564405000	1.314775000
N	6.949387000	-1.872783000	-0.190753000
O	6.618245000	-3.027787000	-0.319248000
O	8.078627000	-1.447578000	-0.270883000
N	5.531134000	2.766929000	0.649313000
O	6.693543000	3.081721000	0.553663000
O	4.610593000	3.521900000	0.867610000
H	-0.682522000	1.341387000	-0.549594000
O	-2.824816000	1.950153000	-1.445834000
H	-2.269741000	1.434042000	-2.318888000
H	-4.653226000	-1.892552000	1.515561000
N	-6.560524000	-0.416618000	0.356159000
C	-7.100543000	-1.363268000	1.328233000
C	-6.989090000	-0.894658000	2.779615000
H	-6.615908000	-2.334492000	1.199989000
H	-8.149585000	-1.515417000	1.071350000
H	-7.376921000	-1.661012000	3.454240000
H	-5.951363000	-0.692091000	3.050247000
H	-7.561245000	0.020824000	2.935790000
C	-7.502301000	0.455041000	-0.336999000
C	-7.766896000	1.778015000	0.383041000
H	-8.435041000	-0.100070000	-0.450988000
H	-7.128749000	0.634227000	-1.347124000
H	-8.404932000	2.419992000	-0.227965000
H	-8.271699000	1.607152000	1.335407000
H	-6.833467000	2.307488000	0.581361000
C	-1.498924000	-1.597986000	-2.637742000
H	-2.088673000	-2.439507000	-2.276870000
H	-0.691482000	-1.368703000	-1.939311000
H	-1.093270000	-1.805112000	-3.630014000
O	-1.734270000	0.621105000	-3.085268000
O	-2.403922000	-0.509206000	-2.722437000

Zero-point correction= 0.412096
(Hartree/Particle)
Thermal correction to Energy= 0.443700
Thermal correction to Enthalpy= 0.444645
Thermal correction to Gibbs Free Energy= 0.342236
Sum of electronic and zero-point Energies= -1611.824056
Sum of electronic and thermal Energies= -1611.792452
Sum of electronic and thermal Enthalpies= -1611.791508
Sum of electronic and thermal Free Energies= -1611.893917

TS-2-N8-H +$CH_3OO^{\bullet}$

C	-5.937984000	0.160875000	-0.202213000
C	-4.953405000	1.097626000	-0.459309000
C	-3.614326000	0.770175000	-0.602382000
C	-3.238956000	-0.567007000	-0.488093000
C	-4.203089000	-1.543295000	-0.247280000
C	-5.523934000	-1.156728000	-0.103460000
H	-6.975559000	0.442535000	-0.088314000
H	-2.898884000	1.555106000	-0.811080000
H	-3.916612000	-2.584953000	-0.176636000
C	-1.813725000	-1.035265000	-0.627978000
O	-1.551069000	-2.191032000	-0.844687000
N	-0.878509000	-0.003534000	-0.523809000
H	-1.181523000	0.831124000	0.278854000
N	0.395641000	-0.405144000	-0.409930000
C	1.248775000	0.572720000	-0.291637000
C	2.647750000	0.297569000	-0.142560000
C	3.579547000	1.350319000	-0.056938000
C	4.935549000	1.107787000	0.083286000

C	5.433894000	-0.211614000	0.158319000
C	4.493523000	-1.275904000	0.057893000
C	3.154731000	-1.014568000	-0.080983000
H	5.603694000	1.958140000	0.118787000
H	2.445273000	-1.830895000	-0.148355000
N	-6.547648000	-2.194059000	0.165675000
O	-6.164674000	-3.336391000	0.268898000
O	-7.696049000	-1.825602000	0.264433000
N	-5.355517000	2.517260000	-0.596275000
O	-6.508415000	2.791068000	-0.351714000
O	-4.504682000	3.303150000	-0.943970000
H	0.919184000	1.610787000	-0.304151000
O	3.090608000	2.611171000	-0.133028000
H	3.797709000	3.253059000	-0.025347000
H	4.821033000	-2.303825000	0.095411000
N	6.765442000	-0.459270000	0.336870000
C	7.290304000	-1.820565000	0.258204000
C	7.359138000	-2.375991000	-1.164626000
H	6.690503000	-2.472479000	0.897630000
H	8.289047000	-1.802335000	0.696311000
H	6.380045000	-2.349411000	-1.645428000
H	8.050954000	-1.794221000	-1.775324000
H	7.706358000	-3.411202000	-1.147999000
C	7.725496000	0.634875000	0.421742000
C	8.128619000	1.212639000	-0.935917000
H	8.607674000	0.252692000	0.937629000
H	7.314039000	1.413698000	1.067825000
H	8.777272000	2.080948000	-0.801461000
H	8.672206000	0.472581000	-1.524991000
H	7.251318000	1.519579000	-1.508307000
C	-0.270488000	-0.020326000	2.837598000
H	0.699691000	-0.134691000	3.319955000
H	-0.491806000	-0.893531000	2.216425000
H	-1.059014000	0.129114000	3.577164000
O	-1.357559000	1.359764000	1.404330000
O	-0.159033000	1.134306000	2.018451000

Zero-point correction= 0.412289
(Hartree/Particle)
Thermal correction to Energy= 0.444085
Thermal correction to Enthalpy= 0.445029
Thermal correction to Gibbs Free Energy= 0.342212
Sum of electronic and zero-point Energies= -1611.824759
Sum of electronic and thermal Energies= -1611.792963
Sum of electronic and thermal Enthalpies= -1611.792019
Sum of electronic and thermal Free Energies= -1611.894836

TS-2-C7′-H +$CH_3OO^•$

C	-6.891409000	0.574724000	0.016285000
C	-5.800606000	1.398131000	-0.189027000
C	-4.504325000	0.918940000	-0.311178000
C	-4.284058000	-0.451666000	-0.217018000
C	-5.361012000	-1.317233000	-0.029498000
C	-6.631237000	-0.784072000	0.092755000
H	-7.894360000	0.968688000	0.106640000
H	-3.706598000	1.624241000	-0.506960000
H	-5.198478000	-2.387041000	0.011227000
C	-2.922550000	-1.086198000	-0.371540000
O	-2.804795000	-2.208231000	-0.794508000
N	-1.883259000	-0.280491000	0.013199000
H	-2.067798000	0.579701000	0.519233000
N	-0.598777000	-0.718467000	-0.104511000

C	0.300458000	0.042376000	0.384924000
C	1.712540000	-0.319512000	0.310209000
C	2.683864000	0.540734000	0.831376000
C	4.036180000	0.220561000	0.774166000
C	4.448158000	-0.975350000	0.184141000
C	3.479316000	-1.847289000	-0.345417000
C	2.142489000	-1.516195000	-0.276437000
H	4.766663000	0.935703000	1.135421000
H	1.389960000	-2.191335000	-0.666236000
N	-7.775395000	-1.703777000	0.308668000
O	-7.527461000	-2.883686000	0.388312000
O	-8.874418000	-1.205335000	0.391786000
N	-6.028098000	2.858797000	-0.293880000
O	-7.168681000	3.248876000	-0.211856000
O	-5.052964000	3.559131000	-0.450515000
H	0.053638000	0.988936000	0.874466000
O	2.261861000	1.712438000	1.379955000
H	3.021955000	2.241372000	1.640461000
H	3.771866000	-2.798862000	-0.767966000
N	5.812617000	-1.319145000	0.144056000
C	6.360472000	-1.803013000	-1.124163000
C	6.774029000	-0.660162000	-2.049256000
H	5.603918000	-2.415119000	-1.610316000
H	7.206099000	-2.457548000	-0.910012000
H	7.126833000	-1.054121000	-3.004638000
H	5.928036000	0.006591000	-2.227187000
H	7.574528000	-0.070986000	-1.599180000
C	6.685263000	-0.740441000	1.093770000
C	8.088149000	-1.308835000	1.154687000
H	6.199057000	-0.731268000	2.073174000
H	6.818220000	0.493877000	0.917097000
H	8.627599000	-0.820019000	1.966223000
H	8.073196000	-2.385075000	1.351720000
H	8.646995000	-1.132599000	0.233665000
C	7.826049000	2.595064000	-0.975342000
H	7.610828000	2.801092000	-2.024391000
H	8.581401000	1.808116000	-0.890824000
H	8.182971000	3.498248000	-0.475721000
O	6.832133000	1.826439000	0.910040000
O	6.602229000	2.169821000	-0.405619000

Zero-point correction= 0.411759
(Hartree/Particle)
Thermal correction to Energy= 0.443588
Thermal correction to Enthalpy= 0.444532
Thermal correction to Gibbs Free Energy= 0.341493
Sum of electronic and zero-point Energies= -1611.817943
Sum of electronic and thermal Energies= -1611.786114
Sum of electronic and thermal Enthalpies= -1611.785169
Sum of electronic and thermal Free Energies= -1611.888208

TS-3-N8-H +$CH_3OO^{\bullet}$

C	3.195388000	1.232546000	-0.344403000
C	1.876605000	0.868225000	-0.565292000
C	1.542045000	-0.483444000	-0.517440000
C	2.524487000	-1.438308000	-0.262769000
C	3.822772000	-1.015456000	-0.041562000
C	4.196582000	0.317755000	-0.073268000
H	1.145858000	1.636018000	-0.784045000
H	2.271098000	-2.490765000	-0.241481000
H	5.217977000	0.627165000	0.101025000
N	3.554055000	2.669535000	-0.407095000

O	4.692480000	2.966708000	-0.128211000
O	2.683127000	3.442961000	-0.732689000
N	4.866428000	-2.029678000	0.242689000
O	5.995609000	-1.628494000	0.406852000
O	4.514632000	-3.185268000	0.291275000
C	0.143149000	-0.985927000	-0.745790000
O	-0.082741000	-2.136584000	-1.012144000
N	-0.832638000	0.023797000	-0.654451000
H	-0.607405000	0.814647000	0.291498000
N	-2.090199000	-0.433511000	-0.626877000
C	-2.987148000	0.486165000	-0.446419000
H	-2.703557000	1.535535000	-0.348137000
C	-4.834466000	-1.181543000	-0.506545000
C	-4.397366000	0.145958000	-0.378290000
C	-5.332141000	1.169117000	-0.182072000
C	-6.687305000	0.874488000	-0.119502000
C	-7.114938000	-0.443079000	-0.252558000
C	-6.187570000	-1.468229000	-0.446596000
H	-4.099593000	-1.963545000	-0.654484000
H	-4.989046000	2.192899000	-0.077952000
H	-7.408297000	1.668155000	0.032358000
H	-8.172355000	-0.674653000	-0.204288000
H	-6.527208000	-2.491637000	-0.549198000
C	-1.693364000	-0.298858000	2.662738000
H	-2.689097000	-0.446190000	3.078695000
H	-0.948022000	-0.205398000	3.453527000
H	-1.435554000	-1.119958000	1.987250000
O	-0.531744000	1.200460000	1.414497000
O	-1.763702000	0.919001000	1.929667000

Zero-point correction= 0.276647
(Hartree/Particle)
Thermal correction to Energy= 0.300235
Thermal correction to Enthalpy= 0.301179
Thermal correction to Gibbs Free Energy= 0.217581
Sum of electronic and zero-point Energies= -1324.173063
Sum of electronic and thermal Energies= -1324.149475
Sum of electronic and thermal Enthalpies= -1324.148531
Sum of electronic and thermal Free Energies= -1324.232129

TS-4-N8-H +$CH_3OO^{\bullet}$

C	-5.112383000	0.556736000	-0.120486000
C	-4.024686000	1.348529000	-0.441152000
C	-2.741932000	0.847082000	-0.593518000
C	-2.536718000	-0.520097000	-0.419252000
C	-3.608917000	-1.355136000	-0.110679000
C	-4.865982000	-0.797013000	0.036422000
H	-6.103552000	0.972555000	-0.001893000
H	-1.939829000	1.524689000	-0.856451000
H	-3.455172000	-2.420201000	0.009342000
C	-1.187639000	-1.164432000	-0.561399000
O	-1.056410000	-2.355262000	-0.687555000
N	-0.124285000	-0.251400000	-0.566960000
H	-0.258725000	0.664733000	0.215075000
N	1.077617000	-0.831000000	-0.471792000
C	2.102913000	-0.021267000	-0.457315000
C	3.432996000	-0.532741000	-0.342143000
C	4.558058000	0.367473000	-0.205009000
C	5.871464000	-0.166322000	-0.189698000
C	6.049190000	-1.579256000	-0.276107000
C	4.991485000	-2.429013000	-0.359850000
C	3.665496000	-1.922992000	-0.389757000

H	1.933799000	1.047973000	-0.550582000
C	5.515640000	2.583820000	0.060669000
C	4.414305000	1.766921000	-0.056874000
C	6.985160000	0.692907000	-0.070724000
C	6.816596000	2.050452000	0.046034000
H	5.374641000	3.652004000	0.174496000
H	3.432585000	2.218936000	-0.010065000
H	7.978499000	0.257329000	-0.067954000
H	7.673772000	2.705622000	0.137634000
H	5.115530000	-3.502857000	-0.416077000
H	7.060135000	-1.972792000	-0.264439000
O	2.707685000	-2.831549000	-0.484452000
H	1.822699000	-2.391546000	-0.490365000
N	-6.006081000	-1.682418000	0.375976000
O	-7.094259000	-1.164853000	0.480414000
O	-5.766734000	-2.857842000	0.525264000
N	-4.246117000	2.800964000	-0.638376000
O	-3.304502000	3.456555000	-1.020568000
O	-5.353085000	3.226957000	-0.403396000
C	0.883177000	0.085935000	2.820150000
H	1.900517000	-0.036548000	3.189559000
H	0.506670000	-0.854846000	2.409537000
H	0.222139000	0.448130000	3.608674000
O	-0.277919000	1.287200000	1.280218000
O	0.967600000	1.059329000	1.785787000

Zero-point correction= 0.328740
(Hartree/Particle)
Thermal correction to Energy= 0.355881
Thermal correction to Enthalpy= 0.356825
Thermal correction to Gibbs Free Energy= 0.265138
Sum of electronic and zero-point Energies= -1552.975937
Sum of electronic and thermal Energies= -1552.948796
Sum of electronic and thermal Enthalpies= -1552.947852
Sum of electronic and thermal Free Energies= -1553.039538

TS-5-N8-H +$CH_3OO^{\bullet}$

C	-3.311299000	0.953554000	-0.689592000
C	-1.980247000	0.607123000	-0.864577000
C	-1.589875000	-0.696740000	-0.569942000
C	-2.532463000	-1.635902000	-0.153910000
C	-3.846216000	-1.231976000	0.005015000
C	-4.271291000	0.063876000	-0.244459000
H	-1.276530000	1.349761000	-1.214680000
H	-2.237094000	-2.658165000	0.047625000
H	-5.301146000	0.361626000	-0.101814000
N	-4.847587000	-2.219895000	0.472729000
O	-5.987863000	-1.834364000	0.594513000
O	-4.453903000	-3.339748000	0.700940000
N	-3.718002000	2.350801000	-0.963141000
O	-4.823796000	2.684099000	-0.600215000
O	-2.914364000	3.062386000	-1.518686000
C	-0.162657000	-1.148962000	-0.690378000
O	0.127741000	-2.284426000	-0.957552000
N	0.749970000	-0.103781000	-0.477438000
N	2.030232000	-0.484411000	-0.440520000
C	2.868634000	0.438369000	-0.084771000
H	2.518583000	1.432406000	0.204541000
C	6.534801000	0.983389000	0.350677000
C	7.037507000	-0.274607000	0.013991000
C	6.170089000	-1.312763000	-0.349918000
C	4.811746000	-1.090778000	-0.377072000

C	4.287535000	0.173821000	-0.045813000
C	5.167890000	1.199764000	0.319772000
H	7.212526000	1.781528000	0.634467000
H	6.593566000	-2.277283000	-0.599636000
H	4.125827000	-1.883673000	-0.649699000
H	0.432895000	0.693030000	0.398024000
H	4.772918000	2.175502000	0.581235000
O	8.357989000	-0.556059000	0.024031000
H	8.864794000	0.216655000	0.290455000
C	-1.859269000	1.466142000	2.317109000
H	-2.724782000	2.119986000	2.206454000
H	-1.460457000	1.525776000	3.330903000
H	-2.123052000	0.431128000	2.078433000
O	0.234706000	1.189921000	1.494797000
O	-0.896716000	1.949049000	1.391608000

Zero-point correction= 0.280594
(Hartree/Particle)

Thermal correction to Energy=	0.305476
Thermal correction to Enthalpy=	0.306420
Thermal correction to Gibbs Free Energy=	0.220777
Sum of electronic and zero-point Energies=	-1399.392633
Sum of electronic and thermal Energies=	-1399.367751
Sum of electronic and thermal Enthalpies=	-1399.366807
Sum of electronic and thermal Free Energies=	-1399.452450

TS-5-O4′-H +$CH_3OO^{\bullet}$

C	-4.536136000	1.246989000	0.111038000
C	-3.210446000	0.975585000	-0.193784000
C	-2.806465000	-0.351194000	-0.304900000
C	-3.734425000	-1.378271000	-0.135708000
C	-5.041632000	-1.049628000	0.172821000
C	-5.481663000	0.257716000	0.304365000
H	-2.539047000	1.807050000	-0.367146000
H	-3.432310000	-2.411699000	-0.251749000
H	-6.511241000	0.490868000	0.539738000
N	-6.026226000	-2.142680000	0.369873000
O	-7.163771000	-1.818699000	0.620963000
O	-5.619032000	-3.275438000	0.267193000
N	-4.958783000	2.663018000	0.227424000
O	-6.125597000	2.874762000	0.455190000
O	-4.101068000	3.506549000	0.089679000
C	-1.400911000	-0.761186000	-0.664523000
O	-1.173871000	-1.797309000	-1.230670000
N	-0.433599000	0.141856000	-0.279908000
N	0.864927000	-0.095792000	-0.579420000
C	1.727410000	0.713252000	-0.098019000
H	1.433024000	1.557939000	0.535958000
C	5.415556000	1.326835000	-0.060847000
C	5.893784000	0.270350000	-0.877850000
C	4.959195000	-0.651621000	-1.424747000
C	3.616859000	-0.506263000	-1.186732000
C	3.149465000	0.549544000	-0.372496000
C	4.062061000	1.453893000	0.182832000
H	6.135530000	2.014767000	0.364582000
H	5.345602000	-1.452728000	-2.043223000
H	2.895598000	-1.195266000	-1.609500000
H	-0.670716000	0.904672000	0.346584000
H	3.701365000	2.261759000	0.810632000
O	7.162529000	0.135517000	-1.136258000
H	7.768939000	0.113612000	-0.138415000
C	6.641027000	-1.572244000	1.882144000

H	5.677654000	-1.575571000	2.390287000
H	7.410935000	-2.036189000	2.500791000
H	6.573918000	-2.081399000	0.918420000
O	8.128388000	-0.112913000	0.985898000
O	6.962977000	-0.200614000	1.677467000

Zero-point correction= 0.280478
(Hartree/Particle)
Thermal correction to Energy= 0.305337
Thermal correction to Enthalpy= 0.306281
Thermal correction to Gibbs Free Energy= 0.218940
Sum of electronic and zero-point Energies= -1399.394843
Sum of electronic and thermal Energies= -1399.369984
Sum of electronic and thermal Enthalpies= -1399.369040
Sum of electronic and thermal Free Energies= -1399.456381

TS-6-N8-H +$CH_3OO^{\bullet}$

C	-4.256596000	1.153392000	-0.386677000
C	-2.923722000	0.825684000	-0.578094000
C	-2.547960000	-0.513713000	-0.497163000
C	-3.505836000	-1.492216000	-0.240546000
C	-4.820424000	-1.105497000	-0.048452000
C	-5.234454000	0.214273000	-0.113178000
H	-2.213853000	1.612576000	-0.797816000
H	-3.219995000	-2.535485000	-0.195212000
H	-6.267286000	0.495776000	0.038443000
N	-5.837341000	-2.145331000	0.237290000
O	-6.980948000	-1.776300000	0.378638000
O	-5.453358000	-3.289574000	0.310277000
N	-4.658981000	2.576083000	-0.487306000
O	-5.803866000	2.847545000	-0.206265000
O	-3.815763000	3.366246000	-0.844055000
C	-1.129308000	-0.980985000	-0.691208000
O	-0.873663000	-2.132336000	-0.934771000
N	-0.188789000	0.049760000	-0.600746000
N	1.087155000	-0.355273000	-0.542029000
C	1.947607000	0.612373000	-0.414073000
H	1.614225000	1.651177000	-0.369511000
C	5.620953000	1.197350000	-0.126725000
C	6.145669000	-0.116718000	-0.188525000
C	5.227344000	-1.192341000	-0.320680000
C	3.874382000	-0.961530000	-0.387699000
C	3.356733000	0.346688000	-0.331851000
C	4.261298000	1.410979000	-0.197286000
H	6.281128000	2.046478000	-0.023645000
H	5.586428000	-2.210562000	-0.368870000
H	3.182818000	-1.789744000	-0.488103000
H	-0.460900000	0.871096000	0.232420000
H	3.880688000	2.425878000	-0.146579000
N	7.487535000	-0.343891000	-0.121466000
C	8.003224000	-1.699682000	-0.195588000
C	8.407456000	0.770818000	0.017141000
H	7.629203000	-2.313893000	0.629430000
H	7.727574000	-2.179183000	-1.139883000
H	9.088167000	-1.670039000	-0.133005000
H	9.424535000	0.389065000	0.057915000
H	8.332456000	1.457047000	-0.832364000
H	8.215373000	1.332550000	0.936649000
C	0.517460000	-0.032351000	2.746461000
H	1.497228000	-0.160932000	3.205050000
H	0.276296000	-0.893742000	2.116155000
H	-0.253441000	0.110918000	3.505375000

O	-0.592930000	1.383813000	1.365250000
O	0.619196000	1.134659000	1.943203000

Zero-point correction= 0.350484
(Hartree/Particle)
Thermal correction to Energy= 0.378584
Thermal correction to Enthalpy= 0.379528
Thermal correction to Gibbs Free Energy= 0.285318
Sum of electronic and zero-point Energies= -1458.049919
Sum of electronic and thermal Energies= -1458.021820
Sum of electronic and thermal Enthalpies= -1458.020876
Sum of electronic and thermal Free Energies= -1458.115086

TS-BHA(O-H) +$CH_3OO^{\bullet}$

C	-1.326516000	-1.962613000	-0.302986000
C	-2.320898000	-1.045901000	0.042304000
C	-2.022300000	0.325739000	0.139952000
C	-0.755793000	0.824825000	-0.081529000
C	0.261874000	-0.115344000	-0.450185000
C	-0.052893000	-1.487858000	-0.554154000
H	-1.532756000	-3.020532000	-0.386603000
H	-2.845057000	0.973863000	0.409834000
H	0.743646000	-2.165997000	-0.835651000
O	1.489397000	0.283111000	-0.705222000
H	2.198646000	-0.453925000	-0.277640000
O	-3.604154000	-1.374258000	0.299910000
C	-3.969912000	-2.739275000	0.227390000
H	-5.028039000	-2.779534000	0.473339000
H	-3.812789000	-3.133660000	-0.780622000
H	-3.402910000	-3.335104000	0.948330000
C	-0.435157000	2.313419000	0.050229000
C	0.626383000	2.516277000	1.147654000
C	0.083073000	2.856788000	-1.294538000
C	-1.675528000	3.125891000	0.439143000
H	0.260333000	2.141197000	2.107085000
H	1.556276000	2.005316000	0.903739000
H	0.834618000	3.584372000	1.257262000
H	0.279621000	3.928587000	-1.200776000
H	1.002774000	2.359691000	-1.598233000
H	-0.667215000	2.716800000	-2.077472000
H	-2.464181000	3.048665000	-0.313879000
H	-2.080599000	2.812590000	1.404877000
H	-1.397242000	4.178856000	0.521719000
C	5.159957000	-1.175048000	0.530403000
H	6.032041000	-1.395544000	-0.083864000
H	5.140266000	-1.814421000	1.415258000
H	5.154687000	-0.124059000	0.827984000
O	2.903312000	-1.227433000	0.432500000
O	4.035711000	-1.449991000	-0.286785000

Zero-point correction= 0.291585
(Hartree/Particle)
Thermal correction to Energy= 0.309660
Thermal correction to Enthalpy= 0.310604
Thermal correction to Gibbs Free Energy= 0.242665
Sum of electronic and zero-point Energies= -769.034940
Sum of electronic and thermal Energies= -769.016866
Sum of electronic and thermal Enthalpies= -769.015922
Sum of electronic and thermal Free Energies= -769.083860

P-1-N8-H +$HOO^{\bullet}$

C	4.913029000	0.020743000	0.280522000
C	3.872582000	0.919278000	0.438056000
C	2.542263000	0.567277000	0.285970000

C	2.233227000	-0.745788000	-0.059407000
C	3.248457000	-1.686563000	-0.216070000
C	4.560787000	-1.279675000	-0.043442000
H	5.946640000	0.314387000	0.402919000
H	1.763608000	1.300791000	0.446766000
H	3.012593000	-2.712488000	-0.470694000
C	0.807869000	-1.179246000	-0.256873000
O	0.487680000	-2.338299000	-0.297310000
N	-0.056220000	-0.074795000	-0.444399000
H	0.476228000	1.568446000	-1.287101000
N	-1.309473000	-0.369349000	-0.276976000
C	-2.111862000	0.676720000	-0.427713000
C	-3.524285000	0.534335000	-0.307736000
C	-4.339094000	1.671670000	-0.454126000
C	-5.711788000	1.564465000	-0.351661000
C	-6.298341000	0.321530000	-0.104335000
C	-5.491418000	-0.830170000	0.055593000
C	-4.125594000	-0.717874000	-0.048521000
H	-3.881506000	2.634446000	-0.650464000
H	-6.343928000	2.438106000	-0.471349000
H	-3.510567000	-1.603085000	0.059980000
O	-6.069100000	-2.045122000	0.246652000
O	-7.629176000	0.147411000	-0.013637000
H	-8.088548000	0.979699000	-0.163409000
C	-6.627408000	-2.241877000	1.545333000
H	-7.420853000	-1.518933000	1.743291000
H	-7.039583000	-3.248257000	1.548854000
H	-5.845529000	-2.161323000	2.305748000
N	5.646999000	-2.273825000	-0.219142000
O	5.321974000	-3.399857000	-0.514531000
O	6.781265000	-1.887286000	-0.053210000
N	4.195127000	2.324712000	0.769794000
O	5.345908000	2.589350000	1.015853000
O	3.279398000	3.123061000	0.771090000
H	-1.684746000	1.662249000	-0.623130000
O	0.394236000	3.054298000	-0.159346000
H	1.259432000	3.428951000	0.059848000
O	0.629214000	2.519053000	-1.460530000

Zero-point correction= 0.290396(Hartree/Particle)
Thermal correction to Energy= 0.317283
Thermal correction to Enthalpy= 0.318228
Thermal correction to Gibbs Free Energy= 0.228081
Sum of electronic and zero-point Energies= -1474.623806
Sum of electronic and thermal Energies= -1474.596919
Sum of electronic and thermal Enthalpies= -1474.595975
Sum of electronic and thermal Free Energies= -1474.686121

P-1-O4′-H +HOO•

C	5.960213000	0.125752000	0.004187000
C	5.044790000	1.129800000	0.256902000
C	3.678025000	0.904919000	0.329194000
C	3.200231000	-0.387013000	0.132995000
C	4.092969000	-1.431264000	-0.106440000
C	5.444686000	-1.148020000	-0.174212000
H	7.022643000	0.322017000	-0.046346000
H	3.028988000	1.737862000	0.568141000
H	3.729200000	-2.443815000	-0.229773000
C	1.740545000	-0.751355000	0.223837000
O	1.384827000	-1.851685000	0.549827000
N	0.880406000	0.276450000	-0.106338000
H	1.241025000	1.120604000	-0.540241000

N	-0.454562000	0.086221000	-0.027384000
C	-1.201213000	1.034034000	-0.449990000
C	-2.652107000	0.929769000	-0.397613000
C	-3.429138000	2.024385000	-0.883296000
C	-4.784374000	1.970345000	-0.855560000
C	-5.495068000	0.814420000	-0.344891000
C	-4.664731000	-0.291976000	0.165061000
C	-3.276182000	-0.199340000	0.113437000
H	-2.922401000	2.899344000	-1.276074000
H	-5.404342000	2.780226000	-1.219450000
H	-2.687262000	-1.028630000	0.486012000
O	-5.146523000	-1.410120000	0.679073000
O	-6.736545000	0.777019000	-0.350129000
H	-8.390875000	0.045403000	-0.614607000
C	-6.546506000	-1.661066000	0.887133000
H	-7.068674000	-1.751305000	-0.063728000
H	-6.572882000	-2.606163000	1.422811000
H	-7.002052000	-0.870479000	1.478030000
N	6.394695000	-2.255870000	-0.445321000
O	5.923808000	-3.355353000	-0.614603000
O	7.570327000	-1.975305000	-0.478867000
N	5.545818000	2.508895000	0.467595000
O	6.741762000	2.672961000	0.439452000
O	4.717718000	3.373626000	0.648810000
H	-0.779327000	1.956560000	-0.864600000
O	-9.406695000	-0.806677000	0.710591000
H	-10.215356000	-0.319938000	0.905299000
O	-9.200684000	-0.490954000	-0.662878000

Zero-point correction= 0.290180
(Hartree/Particle)

Thermal correction to Energy=	0.317502
Thermal correction to Enthalpy=	0.318447
Thermal correction to Gibbs Free Energy=	0.225382
Sum of electronic and zero-point Energies=	-1474.629862
Sum of electronic and thermal Energies=	-1474.602539
Sum of electronic and thermal Enthalpies=	-1474.601595
Sum of electronic and thermal Free Energies=	-1474.694660

P-2-N8-H +HOO•

C	5.961036000	-0.009917000	-0.386214000
C	4.952465000	-0.918226000	-0.651712000
C	3.605903000	-0.613785000	-0.523285000
C	3.246916000	0.669426000	-0.115632000
C	4.233709000	1.619494000	0.142509000
C	5.562096000	1.256238000	0.009611000
H	7.004880000	-0.273341000	-0.485458000
H	2.862822000	-1.365575000	-0.753250000
H	3.956947000	2.622857000	0.440550000
C	1.810309000	1.099274000	0.027731000
O	1.518015000	2.267923000	0.109842000
N	0.922037000	0.014086000	0.093480000
H	1.328349000	-1.570856000	0.936944000
N	-0.324335000	0.382654000	0.037496000
C	-1.185877000	-0.621992000	0.155327000
C	-2.572157000	-0.356597000	0.109913000
C	-3.515171000	-1.411573000	0.223711000
C	-4.875096000	-1.173617000	0.186891000
C	-5.379441000	0.138500000	0.028532000
C	-4.432119000	1.204283000	-0.071905000
C	-3.090690000	0.954630000	-0.035039000
H	-5.539686000	-2.013999000	0.332137000

H	-2.378305000	1.765641000	-0.124180000
N	6.611940000	2.262794000	0.294679000
O	6.246338000	3.360398000	0.646664000
O	7.763312000	1.916245000	0.156693000
N	5.335036000	-2.276468000	-1.103886000
O	6.512355000	-2.555942000	-1.080607000
O	4.445331000	-3.010092000	-1.467509000
H	-0.831656000	-1.642289000	0.290623000
O	-3.012730000	-2.651402000	0.382991000
H	-3.717807000	-3.299946000	0.464052000
H	-4.769830000	2.220704000	-0.207517000
N	-6.714771000	0.400101000	-0.026767000
C	-7.209753000	1.758595000	0.214773000
C	-7.378152000	2.595144000	-1.051801000
H	-6.534398000	2.253434000	0.914572000
H	-8.165638000	1.666545000	0.735237000
H	-6.443632000	2.651486000	-1.611942000
H	-8.135896000	2.168569000	-1.709073000
H	-7.684366000	3.610073000	-0.789544000
C	-7.711954000	-0.669489000	-0.035415000
C	-8.922234000	-0.361184000	-0.911329000
H	-8.032060000	-0.885444000	0.992695000
H	-7.245010000	-1.567444000	-0.432542000
H	-9.595515000	-1.219844000	-0.896915000
H	-9.486781000	0.504126000	-0.562368000
H	-8.614297000	-0.184997000	-1.943316000
O	0.372612000	-1.989589000	2.489337000
H	0.904550000	-1.784811000	3.266365000
O	1.368424000	-2.349077000	1.534827000

Zero-point correction= 0.388888
(Hartree/Particle)

Thermal correction to Energy=	0.420306
Thermal correction to Enthalpy=	0.421250
Thermal correction to Gibbs Free Energy=	0.318978
Sum of electronic and zero-point Energies=	-1572.574241
Sum of electronic and thermal Energies=	-1572.542823
Sum of electronic and thermal Enthalpies=	-1572.541879
Sum of electronic and thermal Free Energies=	-1572.644150

P-2-O2′-H +HOO•

C	5.864319000	0.353088000	0.160120000
C	4.708742000	1.109964000	0.218401000
C	3.439133000	0.558481000	0.167491000
C	3.311893000	-0.820681000	0.025017000
C	4.450746000	-1.621826000	-0.028135000
C	5.693952000	-1.016737000	0.037659000
H	6.846756000	0.802542000	0.208369000
H	2.585636000	1.220258000	0.256564000
H	4.356943000	-2.697270000	-0.114828000
C	1.973888000	-1.516934000	-0.037838000
O	1.854583000	-2.688839000	0.210360000
N	0.945924000	-0.687694000	-0.419093000
H	1.124172000	0.291838000	-0.634329000
N	-0.342002000	-1.077414000	-0.331585000
C	-1.170954000	-0.152558000	-0.693089000
C	-2.581204000	-0.284756000	-0.538263000
C	-3.362319000	0.967736000	-0.590930000
C	-4.786867000	0.864367000	-0.526288000
C	-5.418790000	-0.351138000	-0.347643000
C	-4.600995000	-1.550833000	-0.227482000
C	-3.237867000	-1.504849000	-0.312356000

H	-5.323570000	1.800909000	-0.559704000
H	-2.648518000	-2.411405000	-0.240910000
N	6.907404000	-1.867493000	-0.029502000
O	6.740764000	-3.058180000	-0.150398000
O	7.977454000	-1.307531000	0.040742000
N	4.824993000	2.581659000	0.335607000
O	5.927175000	3.039532000	0.516538000
O	3.803065000	3.227504000	0.233608000
H	-0.811835000	0.795170000	-1.087441000
O	-2.768251000	2.063286000	-0.643786000
H	-1.132762000	2.464272000	0.144409000
H	-5.081088000	-2.509922000	-0.096406000
N	-6.779953000	-0.486025000	-0.307317000
C	-7.419139000	-1.675044000	0.257687000
C	-7.164677000	-1.866894000	1.752865000
H	-7.114387000	-2.563496000	-0.301600000
H	-8.489592000	-1.562897000	0.080466000
H	-7.530500000	-1.010724000	2.321129000
H	-7.677959000	-2.762600000	2.108923000
H	-6.099586000	-1.977496000	1.964440000
C	-7.630049000	0.676577000	-0.535699000
C	-7.885910000	1.512845000	0.718757000
H	-8.576619000	0.312523000	-0.941075000
H	-7.171742000	1.281980000	-1.318923000
H	-8.437440000	2.419755000	0.462798000
H	-8.479139000	0.952864000	1.444335000
H	-6.946366000	1.801219000	1.193668000
O	0.686401000	2.358747000	-0.388580000
H	1.145847000	3.207530000	-0.339844000
O	-0.288216000	2.467837000	0.645459000

Zero-point correction= 0.389699
(Hartree/Particle)

Thermal correction to Energy=	0.420451
Thermal correction to Enthalpy=	0.421395
Thermal correction to Gibbs Free Energy=	0.322868
Sum of electronic and zero-point Energies=	-1572.587609
Sum of electronic and thermal Energies=	-1572.556857
Sum of electronic and thermal Enthalpies=	-1572.555913
Sum of electronic and thermal Free Energies=	-1572.654440

P-2-C7′-H +HOO•

C	6.575227000	0.509619000	0.010317000
C	5.498490000	1.317114000	0.324242000
C	4.197277000	0.843031000	0.408348000
C	3.956893000	-0.504761000	0.160128000
C	5.019545000	-1.356086000	-0.140397000
C	6.295410000	-0.828039000	-0.218204000
H	7.582230000	0.899204000	-0.048129000
H	3.411897000	1.530928000	0.694949000
H	4.841570000	-2.412011000	-0.301359000
C	2.588778000	-1.136535000	0.259204000
O	2.461767000	-2.298799000	0.551085000
N	1.556186000	-0.279457000	-0.014705000
H	1.746252000	0.631387000	-0.419991000
N	0.266787000	-0.712262000	0.069132000
C	-0.627040000	0.113007000	-0.315360000
C	-2.042925000	-0.232874000	-0.263600000
C	-3.006429000	0.694960000	-0.670527000
C	-4.360566000	0.387401000	-0.631501000
C	-4.794505000	-0.849040000	-0.153367000
C	-3.833469000	-1.790744000	0.259072000
C	-2.491069000	-1.478805000	0.194791000

H	-5.064600000	1.146635000	-0.939742000
H	-1.747350000	-2.206462000	0.497355000
N	7.424024000	-1.730678000	-0.554213000
O	7.159616000	-2.891488000	-0.760663000
O	8.528144000	-1.238539000	-0.599551000
N	5.747442000	2.753074000	0.593000000
O	6.892422000	3.135681000	0.542056000
O	4.783989000	3.443152000	0.840861000
H	-0.371834000	1.107127000	-0.694326000
O	-2.586357000	1.918716000	-1.089709000
H	-3.349950000	2.494207000	-1.209703000
H	-4.130729000	-2.774886000	0.592973000
N	-6.171161000	-1.146050000	-0.101028000
C	-6.674465000	-1.820497000	1.100982000
C	-6.859044000	-0.840303000	2.257307000
H	-5.974739000	-2.604093000	1.381263000
H	-7.612113000	-2.314540000	0.848291000
H	-7.199933000	-1.363814000	3.152360000
H	-5.913923000	-0.342302000	2.484344000
H	-7.595591000	-0.073457000	2.006313000
C	-7.061703000	-0.402440000	-0.859241000
C	-8.520422000	-0.739266000	-0.850939000
H	-6.640588000	-0.031070000	-1.787128000
H	-6.994141000	1.525710000	0.057039000
H	-9.045172000	-0.059904000	-1.523021000
H	-8.714233000	-1.762870000	-1.201740000
H	-8.976743000	-0.641483000	0.138163000
O	-6.210559000	3.000426000	-0.810865000
H	-6.872306000	3.640312000	-1.097505000
O	-6.816629000	2.443918000	0.351380000

Zero-point correction= 0.387794
(Hartree/Particle)

Thermal correction to Energy=	0.419463
Thermal correction to Enthalpy=	0.420407
Thermal correction to Gibbs Free Energy=	0.317190
Sum of electronic and zero-point Energies=	-1572.569219
Sum of electronic and thermal Energies=	-1572.537550
Sum of electronic and thermal Enthalpies=	-1572.536606
Sum of electronic and thermal Free Energies=	-1572.639823

P-3-N8-H +HOO•

C	3.062551000	1.088764000	-0.451358000
C	1.685486000	0.976627000	-0.359072000
C	1.131668000	-0.294017000	-0.240291000
C	1.946802000	-1.422738000	-0.231055000
C	3.316101000	-1.249068000	-0.319182000
C	3.911520000	-0.002812000	-0.425753000
H	1.070940000	1.865999000	-0.378589000
H	1.517503000	-2.412734000	-0.146530000
H	4.985079000	0.110813000	-0.488179000
N	3.655954000	2.439595000	-0.583111000
O	4.862939000	2.516749000	-0.564558000
O	2.892494000	3.369923000	-0.701921000
N	4.190127000	-2.445156000	-0.293997000
O	5.382532000	-2.260969000	-0.379709000
O	3.650247000	-3.522536000	-0.189796000
C	-0.339513000	-0.495523000	-0.105120000
O	-0.879209000	-1.564200000	-0.255976000
N	-1.039804000	0.678119000	0.285000000
H	-0.098782000	1.661334000	1.746363000
N	-2.310603000	0.627764000	0.119691000

C	-3.200084000	-0.196256000	0.512727000
H	-2.922426000	-0.951786000	1.249486000
C	-5.010531000	0.835013000	-0.863065000
C	-4.586522000	-0.132986000	0.054226000
C	-5.495447000	-1.073904000	0.541192000
C	-6.817891000	-1.052246000	0.114653000
C	-7.235156000	-0.088695000	-0.796458000
C	-6.330173000	0.854655000	-1.283479000
H	-4.299729000	1.565372000	-1.231701000
H	-5.162973000	-1.824786000	1.249809000
H	-7.519926000	-1.785088000	0.492562000
H	-8.266186000	-0.069083000	-1.128541000
H	-6.659150000	1.605171000	-1.991712000
O	0.850538000	0.312687000	2.622586000
H	0.638473000	0.223899000	3.559084000
O	0.617285000	1.701814000	2.405259000

Zero-point correction= 0.252784
(Hartree/Particle)

Thermal correction to Energy=	0.276261
Thermal correction to Enthalpy=	0.277205
Thermal correction to Gibbs Free Energy=	0.193535
Sum of electronic and zero-point Energies=	-1284.922337
Sum of electronic and thermal Energies=	-1284.898860
Sum of electronic and thermal Enthalpies=	-1284.897915
Sum of electronic and thermal Free Energies=	-1284.981586

P-4-N8-H +HOO•

C	-4.970249000	0.522795000	-0.100144000
C	-3.796352000	1.226066000	-0.306513000
C	-2.549133000	0.626876000	-0.305378000
C	-2.463152000	-0.742182000	-0.064888000
C	-3.619719000	-1.491793000	0.134853000
C	-4.842004000	-0.840307000	0.114217000
H	-5.936991000	1.007548000	-0.105323000
H	-1.663720000	1.215457000	-0.502920000
H	-3.560913000	-2.559563000	0.306176000
C	-1.130290000	-1.431740000	-0.029292000
O	-1.017051000	-2.630867000	-0.107728000
N	-0.076749000	-0.515162000	0.133473000
H	-0.180104000	1.159209000	1.058070000
N	1.092428000	-1.054149000	-0.030285000
C	2.118340000	-0.213230000	0.091686000
C	3.439228000	-0.674207000	-0.045190000
C	4.563526000	0.244069000	0.065596000
C	5.879148000	-0.261880000	-0.062704000
C	6.073936000	-1.659197000	-0.303906000
C	5.032755000	-2.524841000	-0.416351000
C	3.699266000	-2.057597000	-0.290181000
H	1.896623000	0.832884000	0.286328000
C	5.501846000	2.456026000	0.393397000
C	4.404366000	1.626408000	0.294044000
C	6.984979000	0.603752000	0.042554000
C	6.803545000	1.948551000	0.269086000
H	5.351091000	3.514201000	0.569230000
H	3.420321000	2.065655000	0.393404000
H	7.982397000	0.190325000	-0.059115000
H	7.655830000	2.611523000	0.349505000
H	5.174726000	-3.581845000	-0.600101000
H	7.091115000	-2.024401000	-0.399259000
O	2.755545000	-2.961201000	-0.409275000
H	1.859838000	-2.532143000	-0.308685000

N	-6.076801000	-1.630867000	0.337247000
O	-7.128263000	-1.033703000	0.303305000
O	-5.944824000	-2.815660000	0.536550000
N	-3.871625000	2.687337000	-0.527708000
O	-2.823141000	3.298433000	-0.583148000
O	-4.967908000	3.178661000	-0.635733000
O	0.121186000	2.651272000	-0.023546000
H	-0.671738000	3.195218000	-0.136890000
O	-0.079228000	2.106868000	1.278971000

Zero-point correction= 0.305525
(Hartree/Particle)
Thermal correction to Energy= 0.331932
Thermal correction to Enthalpy= 0.332876
Thermal correction to Gibbs Free Energy= 0.244062
Sum of electronic and zero-point Energies= -1513.734411
Sum of electronic and thermal Energies= -1513.708004
Sum of electronic and thermal Enthalpies= -1513.707060
Sum of electronic and thermal Free Energies= -1513.795874

P-5-N8-H +HOO•

C	-3.363412000	1.050185000	-0.545742000
C	-2.043968000	0.640565000	-0.431632000
C	-1.786508000	-0.678978000	-0.064569000
C	-2.841790000	-1.560445000	0.165996000
C	-4.137740000	-1.091580000	0.050758000
C	-4.437592000	0.214227000	-0.302093000
H	-1.250492000	1.346632000	-0.642710000
H	-2.644991000	-2.591587000	0.431284000
H	-5.458337000	0.561279000	-0.386010000
N	-5.261469000	-2.023538000	0.309324000
O	-6.382092000	-1.583607000	0.191193000
O	-4.978679000	-3.156961000	0.620963000
N	-3.640589000	2.447135000	-0.955997000
O	-4.785847000	2.828715000	-0.873397000
O	-2.704217000	3.103023000	-1.347459000
C	-0.390006000	-1.218358000	0.059885000
O	-0.163726000	-2.400511000	0.071279000
N	0.583007000	-0.204488000	0.229050000
N	1.790495000	-0.624027000	-0.000938000
C	2.723964000	0.279862000	0.268032000
H	2.441955000	1.244248000	0.694139000
C	6.403171000	0.738470000	0.095256000
C	6.802704000	-0.496707000	-0.428640000
C	5.856091000	-1.489484000	-0.726017000
C	4.522550000	-1.247577000	-0.503296000
C	4.097623000	-0.005230000	0.024368000
C	5.063118000	0.977123000	0.318643000
H	7.144864000	1.496989000	0.321590000
H	6.205543000	-2.432085000	-1.127490000
H	3.776168000	-2.000841000	-0.723068000
H	0.164826000	1.428403000	1.014655000
H	4.741900000	1.930139000	0.724535000
O	8.091485000	-0.795358000	-0.670199000
H	8.662595000	-0.056299000	-0.438703000
O	1.199724000	2.520988000	2.136267000
H	0.869067000	2.535694000	3.041468000
O	0.003047000	2.321136000	1.388168000

Zero-point correction= 0.257044
(Hartree/Particle)
Thermal correction to Energy= 0.281671
Thermal correction to Enthalpy= 0.282615

Thermal correction to Gibbs Free Energy= 0.195780
Sum of electronic and zero-point Energies= -1360.145691
Sum of electronic and thermal Energies= -1360.121064
Sum of electronic and thermal Enthalpies= -1360.120120
Sum of electronic and thermal Free Energies= -1360.206955

P-5-O4′-H +HOO•

C	-4.236131000	1.369642000	-0.136762000
C	-2.931034000	0.938914000	-0.322692000
C	-2.646757000	-0.416010000	-0.183024000
C	-3.669655000	-1.316337000	0.113682000
C	-4.951203000	-0.829963000	0.294484000
C	-5.274085000	0.512344000	0.175906000
H	-2.181881000	1.668755000	-0.602714000
H	-3.460046000	-2.375760000	0.194220000
H	-6.285716000	0.868970000	0.315376000
N	-6.038021000	-1.785164000	0.626499000
O	-7.148635000	-1.327268000	0.761644000
O	-5.732171000	-2.948346000	0.739038000
N	-4.531012000	2.814704000	-0.287888000
O	-5.680574000	3.160206000	-0.158954000
O	-3.594898000	3.544805000	-0.525981000
C	-1.274173000	-0.997955000	-0.394841000
O	-1.115067000	-2.131855000	-0.756175000
N	-0.237237000	-0.121245000	-0.125796000
N	1.034574000	-0.514703000	-0.318571000
C	1.959111000	0.300444000	0.046343000
H	1.724037000	1.269311000	0.499949000
C	5.667686000	0.610600000	0.135324000
C	6.091774000	-0.649990000	-0.458481000
C	5.049973000	-1.581053000	-0.872184000
C	3.735195000	-1.280120000	-0.712510000
C	3.350297000	-0.036598000	-0.131724000
C	4.340498000	0.888508000	0.283120000
H	6.439065000	1.299073000	0.458617000
H	5.377629000	-2.515783000	-1.310722000
H	2.956245000	-1.967967000	-1.018349000
H	-0.425919000	0.761858000	0.339139000
H	4.028597000	1.828411000	0.726591000
O	7.290809000	-0.927693000	-0.615285000
H	8.525250000	0.288226000	-0.081630000
O	8.414616000	0.915027000	1.680765000
H	9.154159000	0.565717000	2.190487000
O	8.976105000	1.025061000	0.376134000

Zero-point correction= 0.256956
(Hartree/Particle)
Thermal correction to Energy= 0.281539
Thermal correction to Enthalpy= 0.282483
Thermal correction to Gibbs Free Energy= 0.195519
Sum of electronic and zero-point Energies= -1360.149023
Sum of electronic and thermal Energies= -1360.124440
Sum of electronic and thermal Enthalpies= -1360.123496
Sum of electronic and thermal Free Energies= -1360.210460

P-6-N8-H +HOO•

C	-4.115992000	0.979064000	-0.595452000
C	-2.780577000	0.623565000	-0.483767000
C	-2.467893000	-0.674474000	-0.084308000
C	-3.486821000	-1.588767000	0.177719000
C	-4.801547000	-1.173659000	0.063902000

C	-5.155319000	0.109783000	-0.319263000
H	-2.015890000	1.352742000	-0.720171000
H	-3.246714000	-2.604434000	0.465639000
H	-6.189213000	0.415082000	-0.402112000
N	-5.885628000	-2.140858000	0.356336000
O	-7.024308000	-1.748657000	0.237714000
O	-5.557940000	-3.254757000	0.694478000
N	-4.451431000	2.351385000	-1.041820000
O	-5.608296000	2.695238000	-0.947104000
O	-3.548443000	3.028486000	-1.473665000
C	-1.048487000	-1.158300000	0.042058000
O	-0.787099000	-2.335959000	0.050908000
N	-0.124910000	-0.109405000	0.202995000
N	1.107511000	-0.493171000	0.047307000
C	2.000749000	0.453605000	0.307429000
H	1.671082000	1.429431000	0.669150000
C	5.670827000	1.009904000	0.266805000
C	6.160969000	-0.245485000	-0.186917000
C	5.213025000	-1.271219000	-0.469599000
C	3.871436000	-1.051858000	-0.311098000
C	3.382470000	0.200224000	0.138613000
C	4.323689000	1.216054000	0.421405000
H	6.356060000	1.814008000	0.493065000
H	5.548165000	-2.239372000	-0.813198000
H	3.156431000	-1.836898000	-0.525185000
H	-0.618679000	1.496912000	0.926466000
H	3.965696000	2.179739000	0.767987000
N	7.489858000	-0.461433000	-0.345230000
C	7.973996000	-1.752020000	-0.812589000
C	8.444360000	0.596334000	-0.050105000
H	7.692025000	-2.552575000	-0.123037000
H	7.577831000	-1.985945000	-1.804622000
H	9.058438000	-1.720935000	-0.875851000
H	9.449667000	0.228714000	-0.237653000
H	8.273206000	1.470281000	-0.685017000
H	8.380235000	0.904182000	0.997410000
O	0.276638000	2.676796000	2.084497000
H	-0.058109000	2.613426000	2.985920000
O	-0.882720000	2.360541000	1.317558000

Zero-point correction= 0.326912
(Hartree/Particle)
Thermal correction to Energy= 0.354656
Thermal correction to Enthalpy= 0.355600
Thermal correction to Gibbs Free Energy= 0.262082
Sum of electronic and zero-point Energies= -1418.802611
Sum of electronic and thermal Energies= -1418.774867
Sum of electronic and thermal Enthalpies= -1418.773923
Sum of electronic and thermal Free Energies= -1418.867441

P-BHA +HOO•

C	2.055368000	0.984434000	0.682229000
C	2.130968000	-0.237063000	-0.014006000
C	0.972945000	-1.020761000	-0.236433000
C	-0.268007000	-0.643642000	0.200109000
C	-0.379120000	0.631980000	0.922468000
C	0.831775000	1.396039000	1.136260000
H	2.936714000	1.585568000	0.860736000
H	1.127624000	-1.942452000	-0.781793000
H	0.715167000	2.326539000	1.679630000
O	-1.465632000	1.077919000	1.345032000
H	-2.122966000	2.377090000	0.210852000
O	3.265070000	-0.750643000	-0.507747000

C	4.476648000	-0.034495000	-0.326225000
H	5.248982000	-0.633119000	-0.801527000
H	4.423790000	0.945859000	-0.806221000
H	4.703060000	0.082025000	0.736503000
C	-1.513387000	-1.484118000	-0.050109000
C	-2.155117000	-1.868565000	1.296906000
C	-2.515849000	-0.681506000	-0.902141000
C	-1.177745000	-2.776228000	-0.803148000
H	-1.455244000	-2.447990000	1.905622000
H	-2.462475000	-0.985821000	1.854834000
H	-3.036037000	-2.488948000	1.110434000
H	-3.374390000	-1.317989000	-1.134188000
H	-2.872492000	0.201993000	-0.376642000
H	-2.058237000	-0.357614000	-1.839487000
H	-0.756269000	-2.572261000	-1.791048000
H	-0.478346000	-3.403983000	-0.244108000
H	-2.095743000	-3.349724000	-0.947567000
O	-1.185450000	2.235557000	-1.405857000
H	-0.534304000	2.941488000	-1.490542000
O	-2.196452000	2.867528000	-0.629046000

Zero-point correction= 0.268255
(Hartree/Particle)

Thermal correction to Energy=	0.285720
Thermal correction to Enthalpy=	0.286664
Thermal correction to Gibbs Free Energy=	0.222055
Sum of electronic and zero-point Energies=	-729.797021
Sum of electronic and thermal Energies=	-729.779556
Sum of electronic and thermal Enthalpies=	-729.778612
Sum of electronic and thermal Free Energies=	-729.843221

P-1-O4′-H +$CH_3OO^{\bullet}$

C	-6.115433000	0.455120000	0.181489000
C	-5.136370000	1.298064000	-0.309409000
C	-3.812180000	0.912537000	-0.456440000
C	-3.445443000	-0.378157000	-0.088205000
C	-4.407272000	-1.265274000	0.394049000
C	-5.711294000	-0.824808000	0.525819000
H	-7.143252000	0.775177000	0.286548000
H	-3.112423000	1.619495000	-0.883944000
H	-4.133634000	-2.280541000	0.653144000
C	-2.044844000	-0.913804000	-0.236790000
O	-1.831385000	-2.084368000	-0.402612000
N	-1.058861000	0.049664000	-0.154014000
H	-1.289321000	0.986817000	0.161553000
N	0.235262000	-0.301590000	-0.309744000
C	1.112541000	0.607305000	-0.110652000
C	2.531843000	0.326157000	-0.265575000
C	3.463138000	1.379331000	-0.022840000
C	4.797589000	1.165321000	-0.152242000
C	5.323396000	-0.129062000	-0.542306000
C	4.337279000	-1.194936000	-0.783212000
C	2.979841000	-0.935233000	-0.639272000
H	3.091579000	2.356483000	0.266478000
H	5.528782000	1.945137000	0.028730000
H	2.272833000	-1.735105000	-0.822604000
O	4.656004000	-2.430061000	-1.142982000
O	6.545667000	-0.327750000	-0.668035000
H	7.720678000	1.020279000	-0.130625000
C	6.001902000	-2.889957000	-1.324365000
H	6.572934000	-2.787537000	-0.403546000

H	5.890720000	-3.936663000	-1.595967000
H	6.496082000	-2.334617000	-2.119074000
N	-6.732922000	-1.763139000	1.054307000
O	-6.357391000	-2.869657000	1.360749000
O	-7.865664000	-1.349492000	1.141177000
N	-5.519437000	2.674498000	-0.704747000
O	-6.684596000	2.974488000	-0.603412000
O	-4.633674000	3.400845000	-1.097242000
H	0.830857000	1.625151000	0.181327000
C	7.466503000	1.239188000	2.535987000
H	7.845739000	0.770117000	3.445033000
H	6.545709000	0.736959000	2.218541000
H	7.269506000	2.299120000	2.718159000
O	8.070502000	1.757814000	0.402758000
O	8.487756000	1.079800000	1.579528000

Zero-point correction= 0.318348
(Hartree/Particle)

Thermal correction to Energy=	0.346970
Thermal correction to Enthalpy=	0.347915
Thermal correction to Gibbs Free Energy=	0.249681
Sum of electronic and zero-point Energies=	-1513.893754
Sum of electronic and thermal Energies=	-1513.865131
Sum of electronic and thermal Enthalpies=	-1513.864187
Sum of electronic and thermal Free Energies=	-1513.962421

P-1-N8-H +$CH_3OO^{\bullet}$

C	5.043448000	0.010828000	-0.474280000
C	4.061195000	-0.903167000	-0.809722000
C	2.706951000	-0.644864000	-0.665544000
C	2.313073000	0.594645000	-0.166391000
C	3.272296000	1.549076000	0.170092000
C	4.609663000	1.232587000	0.014304000
H	6.094653000	-0.215407000	-0.588849000
H	1.984387000	-1.396953000	-0.951518000
H	2.969582000	2.518710000	0.545120000
C	0.867308000	0.968447000	0.006023000
O	0.532742000	2.102207000	0.237294000
N	-0.002120000	-0.144536000	-0.073841000
H	0.386756000	-1.817623000	0.821789000
N	-1.252731000	0.206374000	-0.125607000
C	-2.086601000	-0.824291000	-0.122853000
C	-3.495462000	-0.616295000	-0.158072000
C	-4.351396000	-1.732036000	-0.132137000
C	-5.721184000	-1.561151000	-0.159341000
C	-6.263121000	-0.275082000	-0.209654000
C	-5.414918000	0.857184000	-0.245167000
C	-4.052090000	0.681251000	-0.214191000
H	-3.928050000	-2.728439000	-0.081318000
H	-6.385178000	-2.418713000	-0.129793000
H	-3.403697000	1.549094000	-0.223090000
O	-5.947157000	2.107573000	-0.242743000
O	-7.588006000	-0.041527000	-0.217230000
H	-8.075949000	-0.868758000	-0.156210000
C	-6.551666000	2.500582000	-1.474444000
H	-7.384333000	1.842235000	-1.728797000
H	-6.918403000	3.513088000	-1.322657000
H	-5.807714000	2.494714000	-2.276038000
N	5.631541000	2.243007000	0.380489000
O	5.233408000	3.301878000	0.806646000
O	6.791425000	1.935504000	0.227456000
N	4.479791000	-2.216923000	-1.353977000

O	5.666715000	-2.444030000	-1.397474000
O	3.604601000	-2.968505000	-1.717440000
H	-1.697318000	-1.841763000	-0.087354000
C	-0.222460000	-1.089721000	3.276461000
H	-1.066164000	-0.708272000	3.852850000
H	0.332249000	-0.252909000	2.838058000
H	0.435428000	-1.682716000	3.915053000
O	0.272028000	-2.480696000	1.531199000
O	-0.793486000	-1.898615000	2.268891000

Zero-point correction= 0.318279
(Hartree/Particle)
Thermal correction to Energy= 0.346758
Thermal correction to Enthalpy= 0.347702
Thermal correction to Gibbs Free Energy= 0.251477
Sum of electronic and zero-point Energies= -1513.884681
Sum of electronic and thermal Energies= -1513.856203
Sum of electronic and thermal Enthalpies= -1513.855258
Sum of electronic and thermal Free Energies= -1513.951484

P-2-O2′-H +$CH_3OO^{\bullet}$

C	-6.108000000	0.243974000	-0.390616000
C	-5.077290000	1.025550000	-0.877493000
C	-3.752067000	0.615869000	-0.875218000
C	-3.439987000	-0.637597000	-0.357328000
C	-4.453850000	-1.464474000	0.124888000
C	-5.756364000	-1.000612000	0.106395000
H	-7.134727000	0.583490000	-0.402432000
H	-3.006121000	1.272378000	-1.305415000
H	-4.220060000	-2.453195000	0.499428000
C	-2.041979000	-1.201228000	-0.340128000
O	-1.842085000	-2.387234000	-0.378999000
N	-1.049764000	-0.248751000	-0.266938000
H	-1.283392000	0.717398000	-0.053909000
N	0.249818000	-0.622066000	-0.279126000
C	1.097392000	0.328239000	-0.083029000
C	2.506898000	0.058169000	-0.070245000
C	3.425856000	1.178676000	0.208791000
C	4.833193000	0.909822000	0.190890000
C	5.332644000	-0.354397000	-0.043809000
C	4.386528000	-1.430161000	-0.297215000
C	3.033805000	-1.218306000	-0.307974000
H	5.466945000	1.765637000	0.370318000
H	2.351685000	-2.038692000	-0.496605000
N	-6.833695000	-1.874030000	0.634007000
O	-6.504722000	-2.950492000	1.073523000
O	-7.962905000	-1.443888000	0.587617000
N	-5.405652000	2.357352000	-1.440038000
O	-6.567053000	2.689825000	-1.430559000
O	-4.485209000	3.017138000	-1.866621000
H	0.782008000	1.358268000	0.090091000
O	2.972914000	2.315712000	0.433349000
H	1.651516000	2.659209000	1.662239000
H	4.753499000	-2.432357000	-0.466724000
N	6.669193000	-0.652757000	-0.007947000
C	7.197760000	-1.881104000	-0.600217000
C	7.039038000	-1.959667000	-2.118914000
H	6.742145000	-2.751742000	-0.121051000
H	8.256623000	-1.918343000	-0.340940000
H	7.457837000	-2.896435000	-2.492711000
H	5.988357000	-1.915142000	-2.411750000
H	7.556352000	-1.132072000	-2.605957000

C	7.630903000	0.386925000	0.338451000
C	8.036902000	1.274023000	-0.839308000
H	8.510800000	-0.108899000	0.753651000
H	7.206224000	0.985966000	1.145584000
H	8.669937000	2.094304000	-0.494815000
H	8.600331000	0.702821000	-1.579640000
H	7.158083000	1.697455000	-1.328998000
C	0.309870000	0.455685000	3.215676000
H	0.690808000	-0.509827000	3.549165000
H	-0.454101000	0.304504000	2.445038000
H	-0.118388000	1.003366000	4.059353000
O	0.935051000	2.413839000	2.280376000
O	1.423613000	1.134769000	2.694413000

Zero-point correction= 0.416656
(Hartree/Particle)
Thermal correction to Energy= 0.449128
Thermal correction to Enthalpy= 0.450073
Thermal correction to Gibbs Free Energy= 0.345786
Sum of electronic and zero-point Energies= -1611.845428
Sum of electronic and thermal Energies= -1611.812956
Sum of electronic and thermal Enthalpies= -1611.812011
Sum of electronic and thermal Free Energies= -1611.916298

P-2-N8-H +$CH_3OO^{\bullet}$

C	-5.885972000	0.087131000	-0.535289000
C	-4.858674000	0.974329000	-0.801289000
C	-3.518861000	0.639364000	-0.680292000
C	-3.186306000	-0.652815000	-0.278932000
C	-4.192601000	-1.581101000	-0.017127000
C	-5.513246000	-1.188499000	-0.144565000
H	-6.924213000	0.373476000	-0.629656000
H	-2.758112000	1.373199000	-0.909122000
H	-3.936720000	-2.590611000	0.278825000
C	-1.758610000	-1.111490000	-0.136936000
O	-1.492786000	-2.284597000	-0.023859000
N	-0.847387000	-0.044352000	-0.103097000
H	-1.225423000	1.530080000	0.884951000
N	0.391062000	-0.444692000	-0.118101000
C	1.270186000	0.544627000	-0.004631000
C	2.651553000	0.252285000	0.000357000
C	3.611371000	1.292926000	0.106711000
C	4.965247000	1.026341000	0.129576000
C	5.446744000	-0.303338000	0.057442000
C	4.483620000	-1.351761000	-0.068375000
C	3.147372000	-1.072354000	-0.089591000
H	5.648992000	1.862487000	0.188979000
H	2.420898000	-1.871420000	-0.173206000
N	-6.583749000	-2.172316000	0.143379000
O	-6.240732000	-3.279699000	0.487433000
O	-7.727838000	-1.799150000	0.014920000
N	-5.212672000	2.343490000	-1.244082000
O	-6.386410000	2.637683000	-1.248040000
O	-4.304648000	3.071603000	-1.572750000
H	0.931833000	1.574103000	0.096754000
O	3.130911000	2.550826000	0.167817000
H	3.842998000	3.183257000	0.299341000
H	4.801001000	-2.380782000	-0.141879000
N	6.776688000	-0.576617000	0.116137000
C	7.277554000	-1.935652000	-0.095830000
C	7.250713000	-2.377765000	-1.558576000
H	6.708407000	-2.626868000	0.529097000

H	8.300903000	-1.958626000	0.279739000
H	6.243726000	-2.309892000	-1.973026000
H	7.908804000	-1.754313000	-2.165203000
H	7.588366000	-3.412637000	-1.642747000
C	7.761111000	0.496329000	0.233272000
C	8.083432000	1.181257000	-1.094973000
H	8.666650000	0.058800000	0.655184000
H	7.404851000	1.219749000	0.969364000
H	8.759256000	2.023097000	-0.931130000
H	8.569220000	0.486270000	-1.781197000
H	7.176965000	1.552194000	-1.576718000
C	-0.888569000	0.573700000	3.311896000
H	-0.110204000	0.136255000	3.938756000
H	-1.385382000	-0.216551000	2.738376000
H	-1.617954000	1.102568000	3.929668000
O	-1.204783000	2.122446000	1.665280000
O	-0.218569000	1.474200000	2.456462000

Zero-point correction= 0.417072
(Hartree/Particle)

Thermal correction to Energy=	0.449712
Thermal correction to Enthalpy=	0.450656
Thermal correction to Gibbs Free Energy=	0.344481
Sum of electronic and zero-point Energies=	-1611.843833
Sum of electronic and thermal Energies=	-1611.811193
Sum of electronic and thermal Enthalpies=	-1611.810249
Sum of electronic and thermal Free Energies=	-1611.916425

P-2-C7′-H +$CH_3OO^{\bullet}$

C	6.796189000	0.562452000	-0.031907000
C	5.696310000	1.385465000	0.119180000
C	4.402749000	0.901555000	0.251150000
C	4.194971000	-0.473968000	0.224654000
C	5.281195000	-1.338293000	0.093670000
C	6.548247000	-0.800739000	-0.041671000
H	7.796793000	0.960177000	-0.131247000
H	3.596941000	1.608702000	0.401871000
H	5.128096000	-2.410200000	0.106183000
C	2.837017000	-1.111703000	0.396773000
O	2.723825000	-2.211181000	0.876622000
N	1.795913000	-0.336193000	-0.040710000
H	1.979571000	0.497475000	-0.589662000
N	0.513352000	-0.778451000	0.084897000
C	-0.385638000	-0.050393000	-0.452920000
C	-1.795789000	-0.417864000	-0.376670000
C	-2.766165000	0.411980000	-0.947271000
C	-4.114910000	0.080318000	-0.894959000
C	-4.529041000	-1.076480000	-0.236646000
C	-3.562876000	-1.916422000	0.343986000
C	-2.225940000	-1.586827000	0.264504000
H	-4.841120000	0.766693000	-1.311797000
H	-1.474105000	-2.238404000	0.693672000
N	7.702481000	-1.719942000	-0.197531000
O	7.465542000	-2.904613000	-0.218038000
O	8.798048000	-1.216515000	-0.295162000
N	5.910341000	2.851496000	0.152678000
O	7.048452000	3.247212000	0.063715000
O	4.927649000	3.550156000	0.263105000
H	-0.139440000	0.872270000	-0.986585000
O	-2.349871000	1.565158000	-1.538277000
H	-3.112914000	2.109458000	-1.756104000
H	-3.859335000	-2.842314000	0.818429000

N	-5.897673000	-1.413567000	-0.167136000
C	-6.435036000	-1.756394000	1.154090000
C	-6.762355000	-0.503790000	1.965276000
H	-5.698616000	-2.360170000	1.680187000
H	-7.318783000	-2.379706000	1.016078000
H	-7.125704000	-0.774169000	2.958601000
H	-5.870278000	0.118217000	2.069854000
H	-7.530893000	0.091005000	1.464829000
C	-6.770950000	-0.924646000	-1.125837000
C	-8.208152000	-1.345006000	-1.109547000
H	-6.305618000	-0.764590000	-2.092644000
H	-6.961347000	1.137823000	-0.726387000
H	-8.724627000	-0.882814000	-1.951077000
H	-8.323144000	-2.433678000	-1.209757000
H	-8.731449000	-1.044528000	-0.197280000
C	-6.447065000	3.046711000	1.356049000
H	-5.629014000	3.207951000	2.059491000
H	-7.256285000	2.493914000	1.841392000
H	-6.818714000	4.005903000	0.988296000
O	-6.913468000	2.115073000	-0.665626000
O	-5.883613000	2.294943000	0.303267000

Zero-point correction= 0.415849
(Hartree/Particle)
Thermal correction to Energy= 0.448682
Thermal correction to Enthalpy= 0.449627
Thermal correction to Gibbs Free Energy= 0.344272
Sum of electronic and zero-point Energies= -1611.834064
Sum of electronic and thermal Energies= -1611.801230
Sum of electronic and thermal Enthalpies= -1611.800286
Sum of electronic and thermal Free Energies= -1611.905641

P-3-N8-H +$CH_3OO^{\bullet}$

C	3.209850000	1.251637000	-0.406438000
C	1.885124000	0.843961000	-0.384400000
C	1.607794000	-0.512836000	-0.233006000
C	2.649973000	-1.431442000	-0.111506000
C	3.952027000	-0.966531000	-0.136492000
C	4.271348000	0.373948000	-0.281948000
H	1.094988000	1.574799000	-0.489251000
H	2.437923000	-2.487500000	-0.000911000
H	5.297285000	0.715658000	-0.298246000
N	3.506145000	2.694550000	-0.574736000
O	4.668329000	3.026475000	-0.547717000
O	2.563889000	3.437327000	-0.728293000
N	5.062392000	-1.940764000	-0.003463000
O	6.188588000	-1.500841000	-0.034470000
O	4.762768000	-3.104550000	0.126548000
C	0.204258000	-1.045467000	-0.215245000
O	-0.027969000	-2.226199000	-0.179825000
N	-0.778754000	-0.023699000	-0.176859000
H	-0.764655000	1.197587000	1.416015000
N	-1.963838000	-0.470649000	-0.471675000
C	-2.905683000	0.455808000	-0.383609000
H	-2.634579000	1.484143000	-0.146098000
C	-4.676477000	-1.193314000	-0.921533000
C	-4.284164000	0.118434000	-0.590100000
C	-5.257831000	1.120541000	-0.438334000
C	-6.597927000	0.820396000	-0.617193000
C	-6.976904000	-0.479399000	-0.948925000
C	-6.016708000	-1.482613000	-1.099713000
H	-3.914477000	-1.954742000	-1.032921000

H	-4.948632000	2.125123000	-0.171509000
H	-7.348414000	1.591745000	-0.498157000
H	-8.025414000	-0.713766000	-1.090086000
H	-6.323020000	-2.488966000	-1.357064000
C	-2.190314000	-0.462052000	2.933546000
H	-3.192164000	-0.891635000	2.981382000
H	-1.782442000	-0.340417000	3.938760000
H	-1.540017000	-1.109576000	2.335827000
O	-1.094633000	1.445469000	2.299079000
O	-2.358995000	0.799200000	2.315776000

Zero-point correction= 0.280797
(Hartree/Particle)

Thermal correction to Energy=	0.305435
Thermal correction to Enthalpy=	0.306379
Thermal correction to Gibbs Free Energy=	0.219101
Sum of electronic and zero-point Energies=	-1324.187693
Sum of electronic and thermal Energies=	-1324.163055
Sum of electronic and thermal Enthalpies=	-1324.162111
Sum of electronic and thermal Free Energies=	-1324.249389

P-4-N8-H +$CH_3OO^{\bullet}$

C	-5.153275000	0.453113000	-0.212358000
C	-4.040340000	1.188496000	-0.576971000
C	-2.754803000	0.670066000	-0.570164000
C	-2.574668000	-0.657760000	-0.186773000
C	-3.673398000	-1.439068000	0.168915000
C	-4.930994000	-0.863964000	0.155482000
H	-6.145502000	0.883109000	-0.216988000
H	-1.926376000	1.296636000	-0.873606000
H	-3.538839000	-2.475894000	0.450295000
C	-1.224118000	-1.310611000	-0.164947000
O	-1.098317000	-2.509382000	-0.092757000
N	-0.159477000	-0.387428000	-0.205588000
H	-0.231979000	1.362017000	0.637449000
N	0.991257000	-0.987301000	-0.269892000
C	2.053865000	-0.186880000	-0.281729000
C	3.351802000	-0.727313000	-0.278815000
C	4.514367000	0.144971000	-0.212714000
C	5.807141000	-0.427588000	-0.270233000
C	5.940249000	-1.849323000	-0.373253000
C	4.862027000	-2.675913000	-0.405201000
C	3.549282000	-2.140033000	-0.348933000
H	1.887078000	0.886322000	-0.273411000
C	5.544172000	2.331385000	-0.018474000
C	4.411729000	1.545204000	-0.074316000
C	6.948611000	0.395413000	-0.213478000
C	6.823465000	1.760364000	-0.092497000
H	5.439068000	3.404453000	0.087013000
H	3.445379000	2.028612000	0.001476000
H	7.928317000	-0.067017000	-0.263169000
H	7.703242000	2.390051000	-0.049028000
H	4.958676000	-3.751666000	-0.473368000
H	6.940564000	-2.267021000	-0.418346000
O	2.565375000	-3.007087000	-0.379780000
H	1.689435000	-2.530295000	-0.332792000
N	-6.099603000	-1.689838000	0.544005000
O	-7.186391000	-1.160001000	0.507715000
O	-5.883628000	-2.833615000	0.870557000
N	-4.237466000	2.593853000	-1.005567000
O	-3.280993000	3.168162000	-1.470570000
O	-5.342848000	3.063841000	-0.862215000

C	1.610049000	1.719942000	2.530131000
H	2.682785000	1.896274000	2.631233000
H	1.409819000	0.642476000	2.509906000
H	1.071267000	2.182951000	3.358661000
O	-0.162878000	2.183298000	1.164906000
O	1.243819000	2.323656000	1.304885000

Zero-point correction= 0.333129
(Hartree/Particle)
Thermal correction to Energy= 0.361183
Thermal correction to Enthalpy= 0.362127
Thermal correction to Gibbs Free Energy= 0.267231
Sum of electronic and zero-point Energies= -1552.996104
Sum of electronic and thermal Energies= -1552.968050
Sum of electronic and thermal Enthalpies= -1552.967106
Sum of electronic and thermal Free Energies= -1553.062002

P-5-N8-H +$CH_3OO^{\bullet}$

C	-3.211328000	0.696120000	-0.621572000
C	-1.884835000	0.300679000	-0.621478000
C	-1.577875000	-0.999680000	-0.233569000
C	-2.598131000	-1.894759000	0.085660000
C	-3.906989000	-1.447834000	0.052839000
C	-4.251161000	-0.145090000	-0.275883000
H	-1.122859000	1.014162000	-0.904087000
H	-2.366215000	-2.914580000	0.366159000
H	-5.278437000	0.192476000	-0.260376000
N	-4.993719000	-2.390852000	0.405522000
O	-6.127357000	-1.969874000	0.360365000
O	-4.673048000	-3.515718000	0.712245000
N	-3.515810000	2.100520000	-0.962498000
O	-4.592454000	2.532924000	-0.615359000
O	-2.666792000	2.724403000	-1.556830000
C	-0.158284000	-1.469858000	-0.121571000
O	0.136173000	-2.636321000	-0.106810000
N	0.751968000	-0.391756000	0.045534000
N	1.990065000	-0.761746000	-0.069637000
C	2.855388000	0.218751000	0.150618000
H	2.491782000	1.215505000	0.410200000
C	6.513985000	0.859188000	0.202492000
C	7.010513000	-0.408556000	-0.122822000
C	6.136570000	-1.480451000	-0.361535000
C	4.779649000	-1.285497000	-0.276124000
C	4.257188000	-0.011733000	0.051466000
C	5.150575000	1.050804000	0.287967000
H	7.199509000	1.679792000	0.384949000
H	6.559140000	-2.445787000	-0.609229000
H	4.088134000	-2.099652000	-0.454518000
H	0.217312000	1.387733000	0.672180000
H	4.757461000	2.029560000	0.539943000
O	8.326931000	-0.664733000	-0.222415000
H	8.843917000	0.126203000	-0.040543000
C	-1.525722000	3.850450000	1.153597000
H	-0.891051000	4.399321000	1.854046000
H	-2.572023000	3.932893000	1.451640000
H	-1.395842000	4.229908000	0.137510000
O	0.123189000	2.354763000	0.776962000
O	-1.238595000	2.470068000	1.204239000

Zero-point correction= 0.285625
(Hartree/Particle)
Thermal correction to Energy= 0.311321
Thermal correction to Enthalpy= 0.312266

Thermal correction to Gibbs Free Energy= 0.223832
Sum of electronic and zero-point Energies= -1399.413094
Sum of electronic and thermal Energies= -1399.387397
Sum of electronic and thermal Enthalpies= -1399.386453
Sum of electronic and thermal Free Energies= -1399.474886

P-5-O4′-H +$CH_3OO^{\bullet}$

C	-4.624948000	1.335917000	-0.028232000
C	-3.319426000	0.942688000	-0.281949000
C	-3.000898000	-0.409733000	-0.206787000
C	-3.991457000	-1.343970000	0.094659000
C	-5.274788000	-0.894421000	0.344735000
C	-5.630870000	0.443685000	0.291377000
H	-2.597625000	1.699321000	-0.562643000
H	-3.756080000	-2.400598000	0.125329000
H	-6.643499000	0.771441000	0.484208000
N	-6.326629000	-1.886310000	0.681848000
O	-7.440480000	-1.459584000	0.878398000
O	-5.991568000	-3.045581000	0.736893000
N	-4.956634000	2.778532000	-0.111182000
O	-6.107053000	3.092417000	0.077211000
O	-4.046964000	3.538436000	-0.358315000
C	-1.626092000	-0.951295000	-0.496775000
O	-1.458052000	-2.065733000	-0.910884000
N	-0.597935000	-0.062621000	-0.233845000
N	0.672792000	-0.417276000	-0.496967000
C	1.594099000	0.403047000	-0.135414000
H	1.357454000	1.345086000	0.370847000
C	5.295455000	0.796090000	-0.186506000
C	5.721116000	-0.424893000	-0.857608000
C	4.682513000	-1.359835000	-1.271244000
C	3.369689000	-1.097828000	-1.042518000
C	2.983346000	0.107898000	-0.387412000
C	3.970075000	1.036036000	0.028553000
H	6.065610000	1.484809000	0.138414000
H	5.010755000	-2.264737000	-1.768107000
H	2.593311000	-1.788735000	-1.348006000
H	-0.785786000	0.795751000	0.275597000
H	3.657290000	1.946705000	0.528736000
O	6.918121000	-0.665961000	-1.078076000
H	8.149974000	0.502146000	-0.356072000
C	8.627981000	-0.464047000	2.024967000
H	8.107297000	-0.761712000	2.936312000
H	9.641031000	-0.131755000	2.262217000
H	8.661986000	-1.303651000	1.323649000
O	8.548689000	1.067715000	0.334349000
O	7.870101000	0.601243000	1.491859000

Zero-point correction= 0.285332
(Hartree/Particle)
Thermal correction to Energy= 0.311109
Thermal correction to Enthalpy= 0.312053
Thermal correction to Gibbs Free Energy= 0.221296
Sum of electronic and zero-point Energies= -1399.414821
Sum of electronic and thermal Energies= -1399.389045
Sum of electronic and thermal Enthalpies= -1399.388101
Sum of electronic and thermal Free Energies= -1399.478857

P-6-N8-H +$CH_3OO^{\bullet}$

C	-4.170172000	1.020911000	-0.711693000
C	-2.828138000	0.679342000	-0.647852000
C	-2.485875000	-0.623353000	-0.291471000

C	-3.485210000	-1.555520000	-0.016822000
C	-4.808056000	-1.155884000	-0.085153000
C	-5.190139000	0.130236000	-0.429942000
H	-2.075022000	1.417513000	-0.887677000
H	-3.223064000	-2.573305000	0.243274000
H	-6.230159000	0.421690000	-0.478816000
N	-5.870956000	-2.143768000	0.217573000
O	-7.017442000	-1.764912000	0.137654000
O	-5.519136000	-3.259268000	0.524199000
N	-4.534533000	2.401675000	-1.107890000
O	-5.705420000	2.701595000	-1.054514000
O	-3.636689000	3.132047000	-1.458698000
C	-1.055961000	-1.089409000	-0.215583000
O	-0.787618000	-2.265406000	-0.164417000
N	-0.139723000	-0.025521000	-0.158484000
N	1.095652000	-0.424569000	-0.249020000
C	1.983970000	0.549239000	-0.098802000
H	1.649719000	1.567605000	0.102189000
C	5.657164000	1.085466000	-0.069311000
C	6.153966000	-0.220731000	-0.331966000
C	5.209283000	-1.272055000	-0.512889000
C	3.864386000	-1.029287000	-0.437666000
C	3.369056000	0.273456000	-0.180292000
C	4.306820000	1.314667000	0.002253000
H	6.339744000	1.909657000	0.079172000
H	5.549404000	-2.278403000	-0.711124000
H	3.151285000	-1.833331000	-0.573273000
H	-0.480501000	1.565783000	0.800080000
H	3.944246000	2.315882000	0.208952000
N	7.486292000	-0.459998000	-0.406629000
C	7.977751000	-1.803965000	-0.672035000
C	8.437334000	0.624532000	-0.216132000
H	7.660022000	-2.501676000	0.107816000
H	7.621341000	-2.170479000	-1.638733000
H	9.064149000	-1.785432000	-0.692612000
H	9.446027000	0.232947000	-0.317080000
H	8.296164000	1.408666000	-0.965318000
H	8.337521000	1.066704000	0.779255000
C	-0.210214000	0.728783000	3.271806000
H	0.536080000	0.275438000	3.925593000
H	-0.753781000	-0.055545000	2.733712000
H	-0.907115000	1.333575000	3.856252000
O	-0.420270000	2.204287000	1.542024000
O	0.519202000	1.540332000	2.376350000

Zero-point correction= 0.355414
(Hartree/Particle)

Thermal correction to Energy=	0.384288
Thermal correction to Enthalpy=	0.385233
Thermal correction to Gibbs Free Energy=	0.288353
Sum of electronic and zero-point Energies=	-1458.068628
Sum of electronic and thermal Energies=	-1458.039753
Sum of electronic and thermal Enthalpies=	-1458.038809
Sum of electronic and thermal Free Energies=	-1458.135688

P-BHA +$CH_3OO^{\bullet}$

C	0.628727000	-2.070735000	-0.207188000
C	1.871031000	-1.451378000	0.022555000
C	1.975695000	-0.041456000	0.110840000
C	0.893744000	0.785275000	-0.025499000
C	-0.413302000	0.163150000	-0.275839000
C	-0.479712000	-1.280457000	-0.349511000

H	0.539362000	-3.146834000	-0.267772000
H	2.969470000	0.345989000	0.292953000
H	-1.461716000	-1.711450000	-0.507652000
O	-1.454506000	0.841469000	-0.427181000
H	-2.978115000	0.048168000	-0.936051000
O	3.024034000	-2.113220000	0.176304000
C	3.013828000	-3.531276000	0.101323000
H	4.044371000	-3.842747000	0.248405000
H	2.384436000	-3.956021000	0.887006000
H	2.663877000	-3.864800000	-0.878517000
C	1.007025000	2.302466000	0.068072000
C	0.554654000	2.937129000	-1.261080000
C	0.124584000	2.815455000	1.222232000
C	2.449004000	2.745122000	0.339520000
H	1.171095000	2.575062000	-2.088384000
H	-0.488649000	2.710885000	-1.473199000
H	0.672502000	4.022551000	-1.200421000
H	0.236894000	3.899831000	1.307080000
H	-0.925332000	2.586048000	1.049217000
H	0.434374000	2.367470000	2.170377000
H	2.824758000	2.348511000	1.286533000
H	3.125960000	2.439670000	-0.462750000
H	2.479166000	3.835045000	0.401145000
C	-4.443990000	-0.695641000	1.129935000
H	-4.390042000	-1.351600000	2.000241000
H	-5.480660000	-0.593335000	0.800539000
H	-4.031575000	0.287371000	1.377649000
O	-3.759891000	-0.534131000	-1.040631000
O	-3.669376000	-1.327336000	0.134190000

Zero-point correction= 0.296988
(Hartree/Particle)
Thermal correction to Energy= 0.315660
Thermal correction to Enthalpy= 0.316604
Thermal correction to Gibbs Free Energy= 0.246686
Sum of electronic and zero-point Energies= -769.065556
Sum of electronic and thermal Energies= -769.046884
Sum of electronic and thermal Enthalpies= -769.045940
Sum of electronic and thermal Free Energies= -769.115858