

## Supporting Information

### **Tuning Graphene oxide selectivity under normal reaction conditions using dopants and nucleophiles towards cyclic/polycarbonate formation- A DFT study**

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**Table S1.** The computed activation energy in kcal/mol for the ring-closure step of **GO-27**, using different functionals.

Functional	$\Delta G^\ddagger$ for cyclisation (kcal/mol)
B3LYP-D3	+14.3
B3P86	+13.2
M062X	+16.2
TPSSH	+11.0
$\omega$ B97XD	+13.1

**Table S2.** The binding energies of oxirane at different HBD functional groups of the catalyst models, **GO-27**, **NGO**, and **BGO**.

Catalyst models	HBD group	Binding energy of oxirane (kcal/mol)	O3-H distance in Å
<b>GO-27</b>	-OH	-11.4	1.53
	-COOH	-4.8	1.54
<b>NGO</b>	-OH	-3.0	1.68
	-COOH	-8.3	1.80
	-NH <sub>2</sub>	-7.9	2.08
	Pyrrole	-23.9	1.83
<b>BGO</b>	-OH	-29.8	1.69
	-COOH	-3.6	1.55
	-BOH	-3.2	1.62
	-B(OH) <sub>2</sub>	-19.3	1.82, 1.86

**Table S3.** The activation ( $\Delta G^\ddagger$ ) of the key reaction steps involved in the cyclic/polycarbonate formation, mediated by the -COOH groups of **GO-27**, **GO-56** and **GO-118** models.

Catalyst models	$\Delta G^\ddagger$ for ring-closure step (kcal/mol)	$\Delta G^\ddagger$ for chain-initiation step(kcal/mol)
GO-27	+14.3	+12.2
GO-56	+14.1	+12.2

GO-118	+16.3	+13.3
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**Table S4.** The activation ( $\Delta G^\ddagger$ ) and reaction free energies ( $\Delta G_{R,E}$ ) of the key reaction steps involved in the cyclic/polycarbonate formation, mediated by the -NH<sub>2</sub>, -OH, and -COOH groups of NGO.

HBD groups of NGO	Key reaction steps for cyclic/polycarbonate formation	$\Delta G^\ddagger$ (kcal/mol)	$\Delta G_{R,E}$ (kcal/mol)
<b>-NH<sub>2</sub></b>	Ring-opening	+7.7	-16.3
	CO <sub>2</sub> -addition	+4.7	-13.9
	Ring-closure	+10.1	-19.6
	Chain-initiation	+14.0	-30.6
<b>Pyrrolic-site</b>	Ring-opening	+23.9	-19.1
<b>-OH</b>	Ring-opening	+9.8	-19.5
	CO <sub>2</sub> -addition	+15.1	-4.2
	Ring-closure	+12.2	-19.4
<b>-COOH</b>	Ring-opening	+4.1	-28.7
	CO <sub>2</sub> -addition	+9.0	-19.0
	Ring-closure	+14.8	-35.1

**Table S5.** The activation ( $\Delta G^\ddagger$ ) and reaction free energies ( $\Delta G_{R,E}$ ) of the key reaction steps involved in the cyclic/polycarbonate formation, mediated by the -BOH, -B(OH)<sub>2</sub>, and -COOH groups of **BGO**.

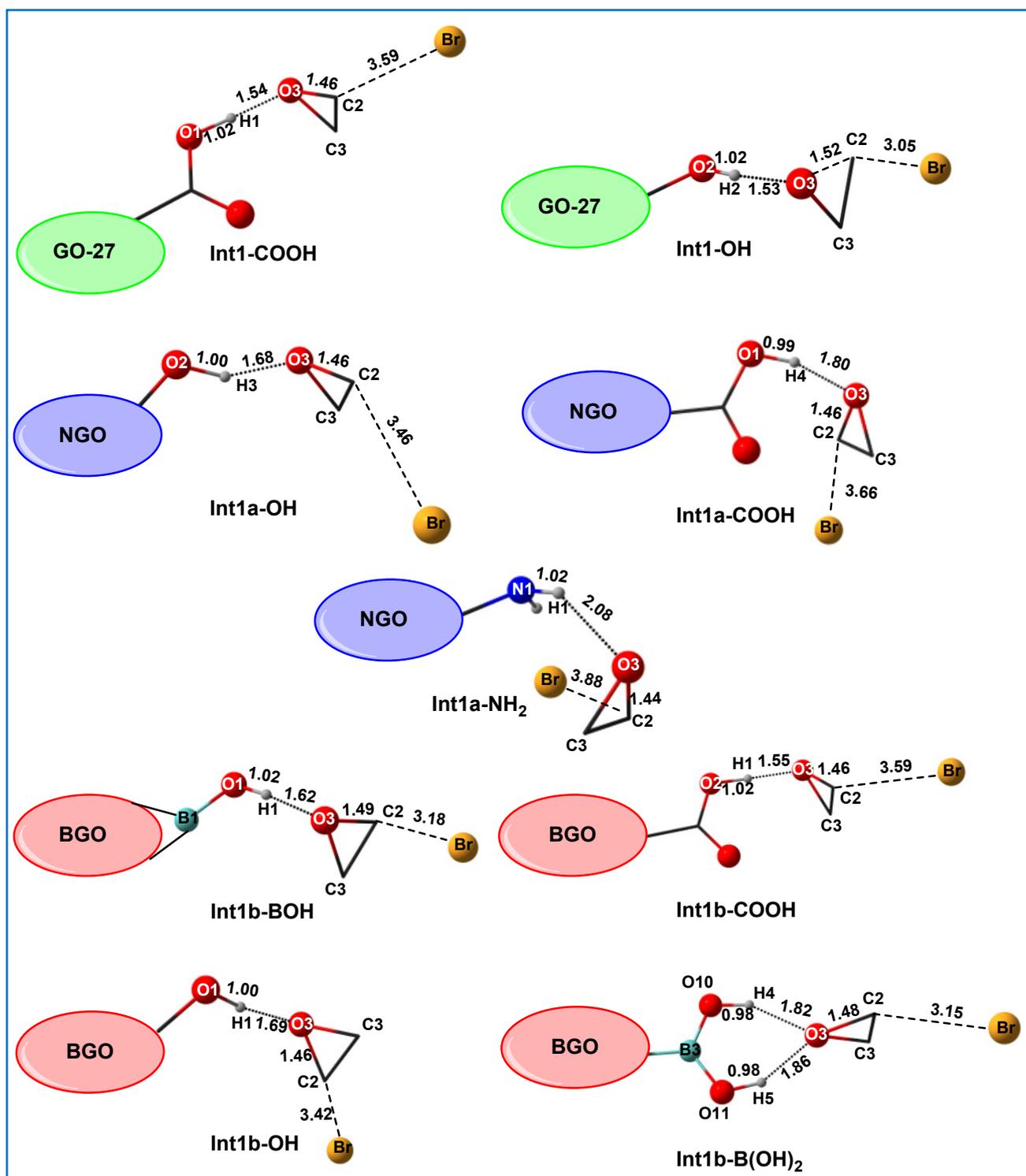
HBD groups of BGO	Key reaction steps for cyclic/polycarbonate formation	$\Delta G^\ddagger$ (kcal/mol)	$\Delta G_{R,E}$ (kcal/mol)
<b>-BOH</b>	Ring-opening	+8.0	-13.7
	CO <sub>2</sub> -addition	+8.8	-3.1
	Ring-closure	+10.2	-37.2
	Chain-initiation	+4.5	-57.0
<b>-B(OH)<sub>2</sub></b>	Ring-opening	+5.1	-29.1
	CO <sub>2</sub> -addition	+3.9	-31.2
	Ring-closure	+12.4	-30.3
<b>-COOH</b>	Ring-opening	+6.0	-20.0
	CO <sub>2</sub> -addition	+11.3	-7.5
	Ring-closure	+13.3	-32.8

**Table S6.** The energy gap between the donor-acceptor orbitals obtained from the NBO analysis for the key transition states.

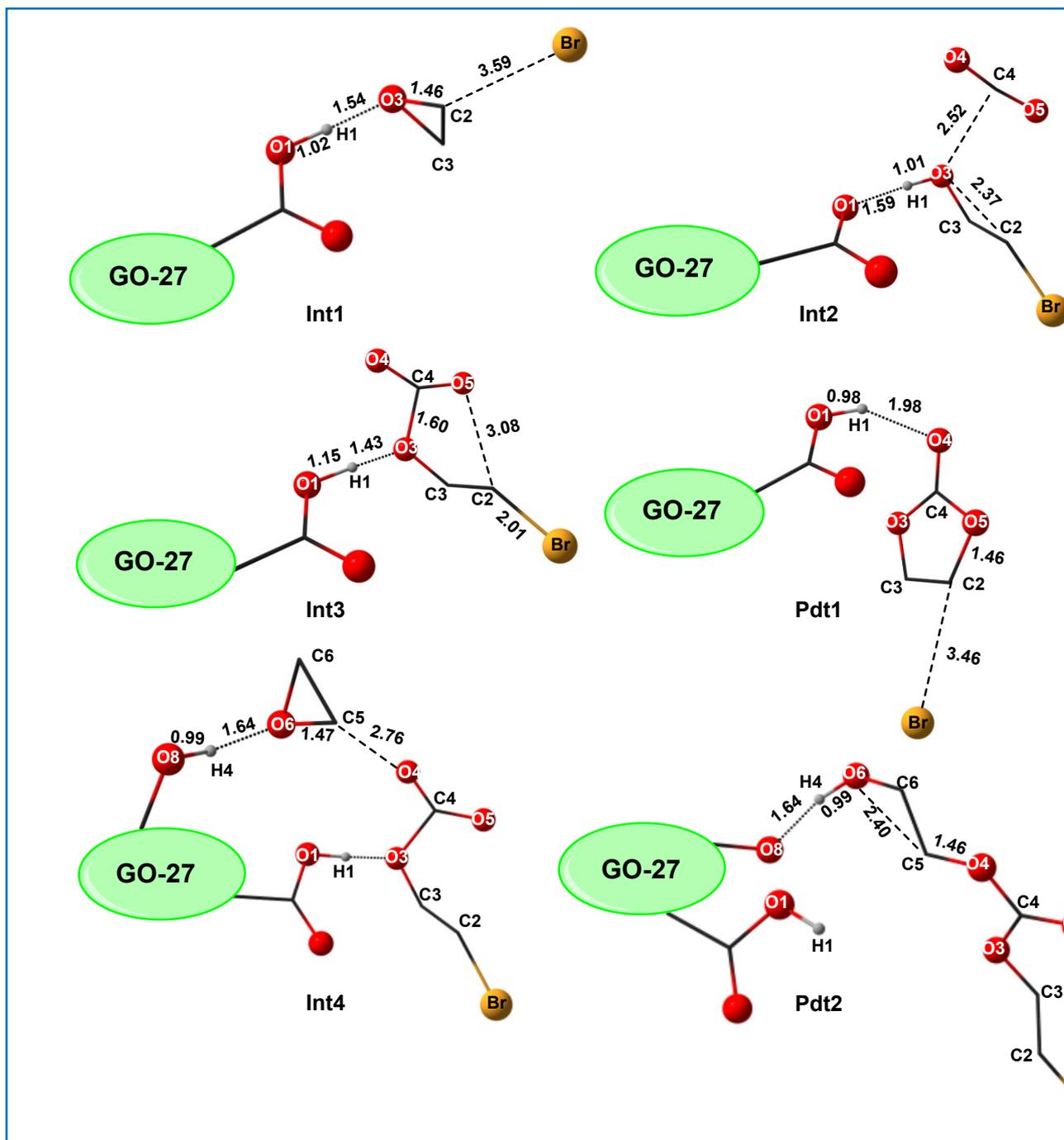
Catalyst models	Energy gap obtained from NBO for ring-closure (eV)	Energy gap obtained from NBO for chain-initiation (eV)
<b>GO-27</b>	6.25	3.81
<b>NGO</b>	5.98	4.35
<b>BGO</b>	6.50	2.99

**Table S7.** The activation energy ( $\Delta G^\ddagger$ ) of the ring-closure step involved in the cyclic carbonate formation, mediated by **GO-27** and orbitals interacting in C2-Nu bond for the studied nucleophiles, obtained from the NBO analysis.

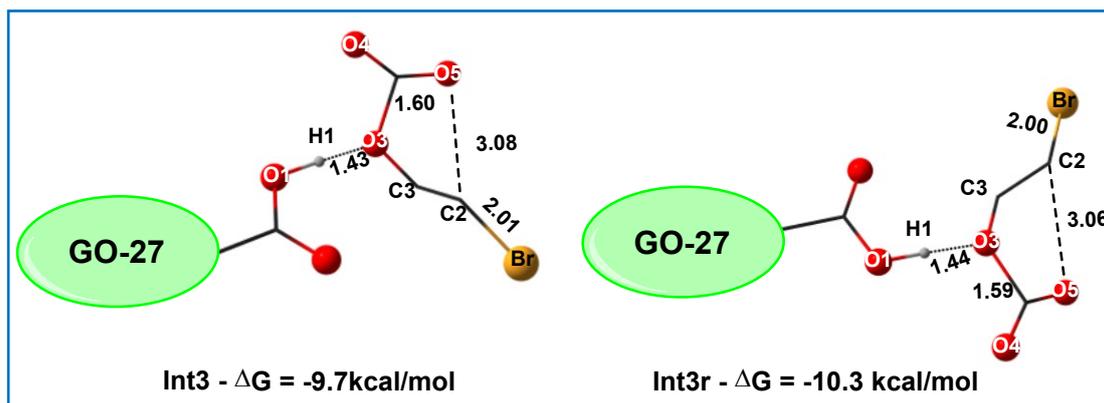
Nucleophile	$\Delta G^\ddagger$ (kcal/mol)	Interacting orbitals
CN <sup>-</sup>	+51.5	2pz-2s
N <sub>3</sub> <sup>-</sup>	+25.8	2pz-2pz
Cl <sup>-</sup>	+17.0	2pz-3pz
Br <sup>-</sup>	+14.3	2pz-4pz
I <sup>-</sup>	+10.6	2pz-5pz



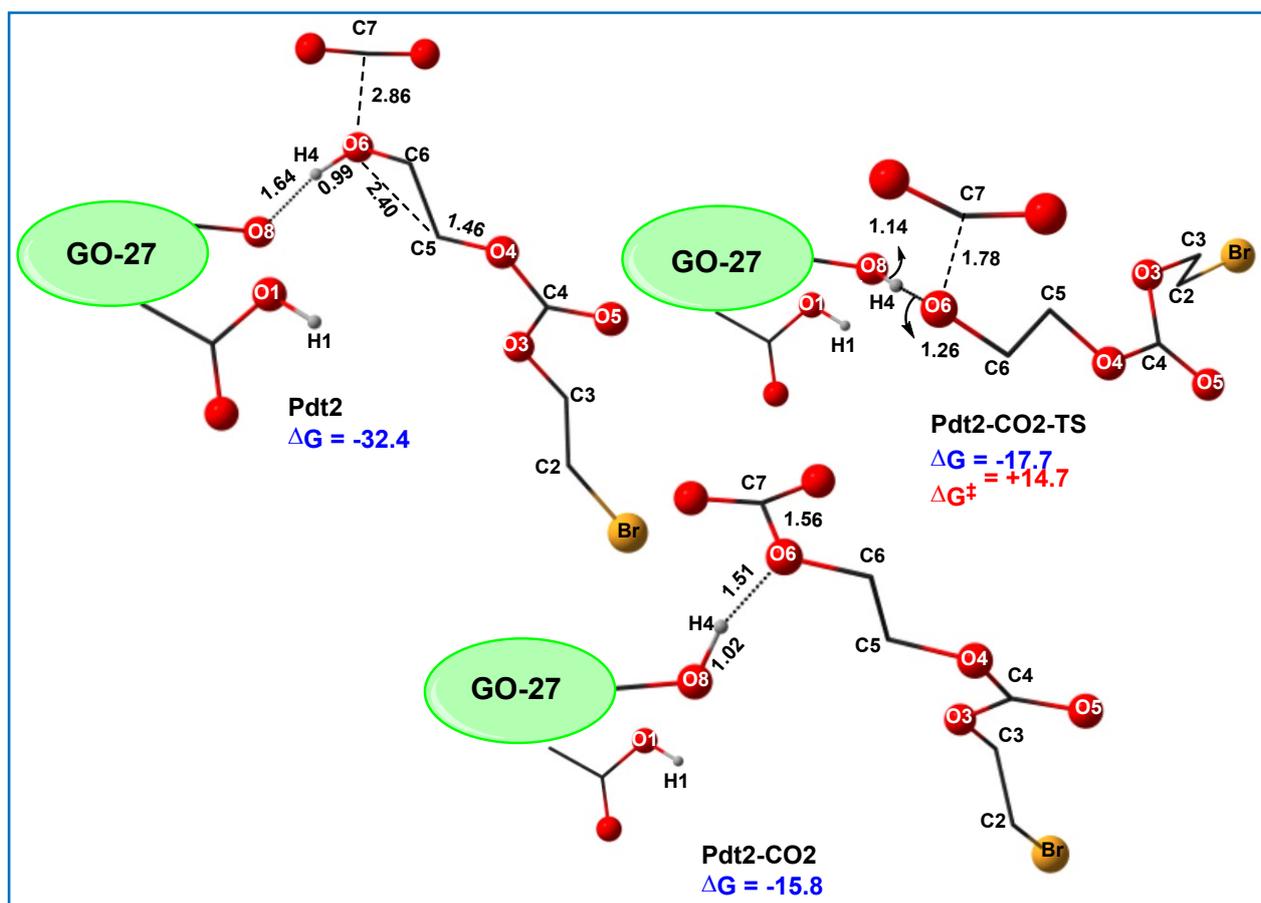
**Figure S1.** The optimised geometries of epoxide stabilised intermediates at different HBD groups at GO-27, NGO, and BGO. Selected bond distances are shown in Å.



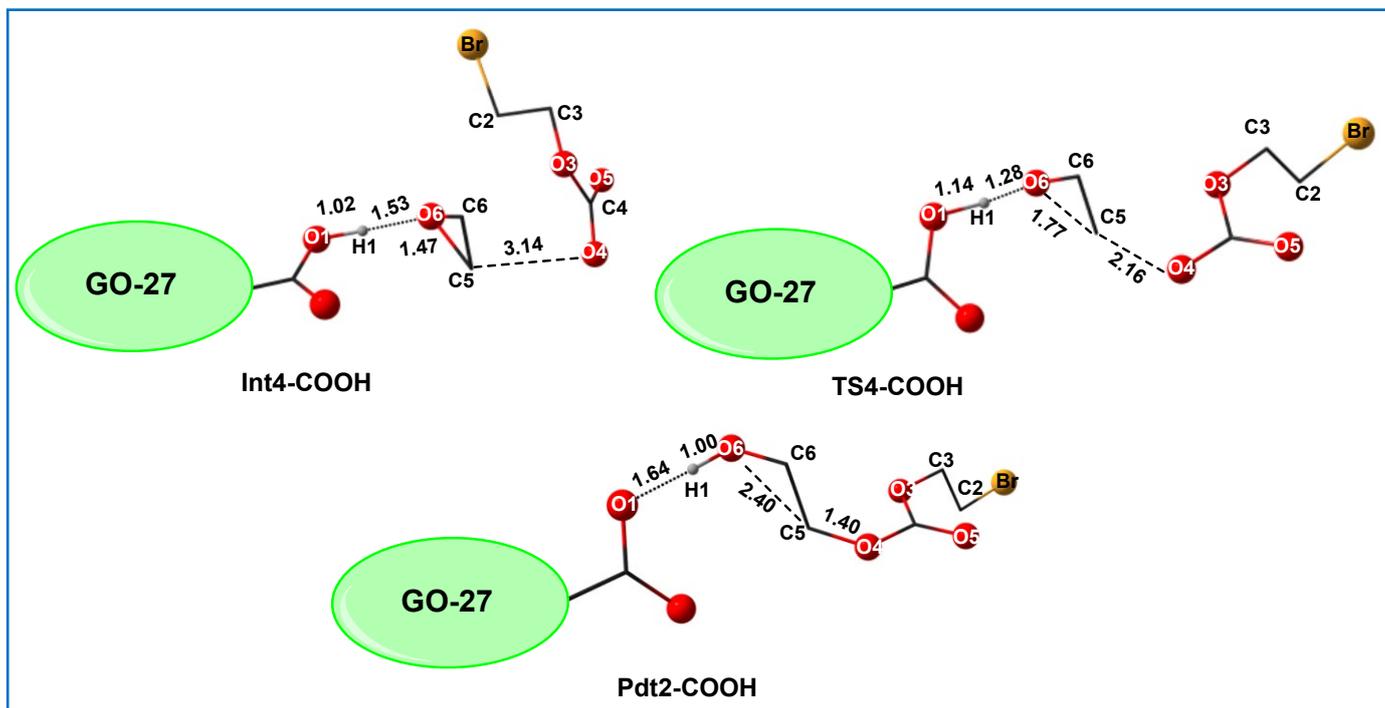
**Figure S2.** The optimized intermediate for the formation of cyclic/poly carbonate from oxirane and CO<sub>2</sub>, mediated at the COOH edge of the GO-27. Selected bond distances are shown in Å.



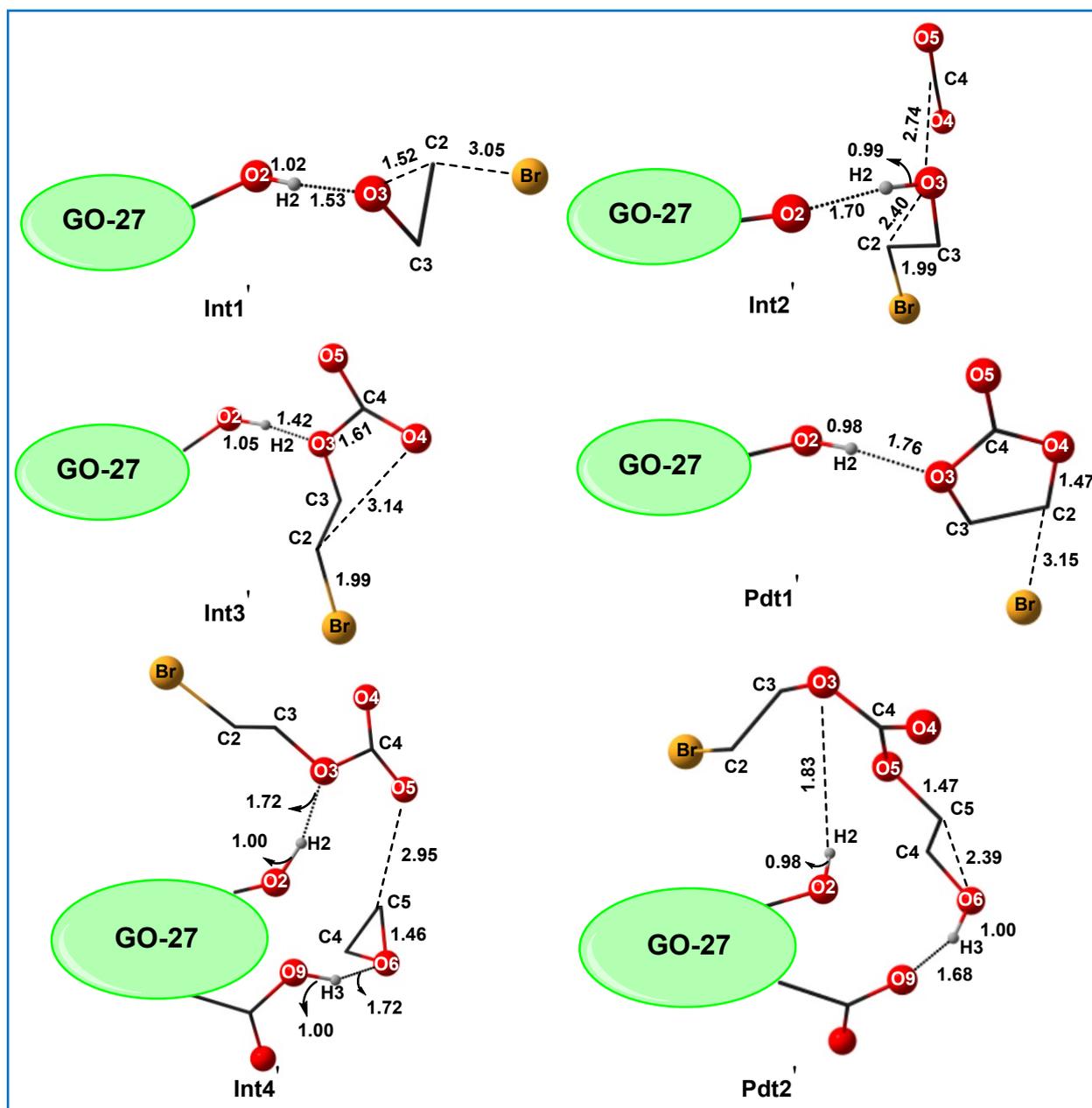
**Figure S3.** The geometry and energetic comparison of Int3 and Int3r with a change in the orientation of H1. The selected bond lengths are given in Å.



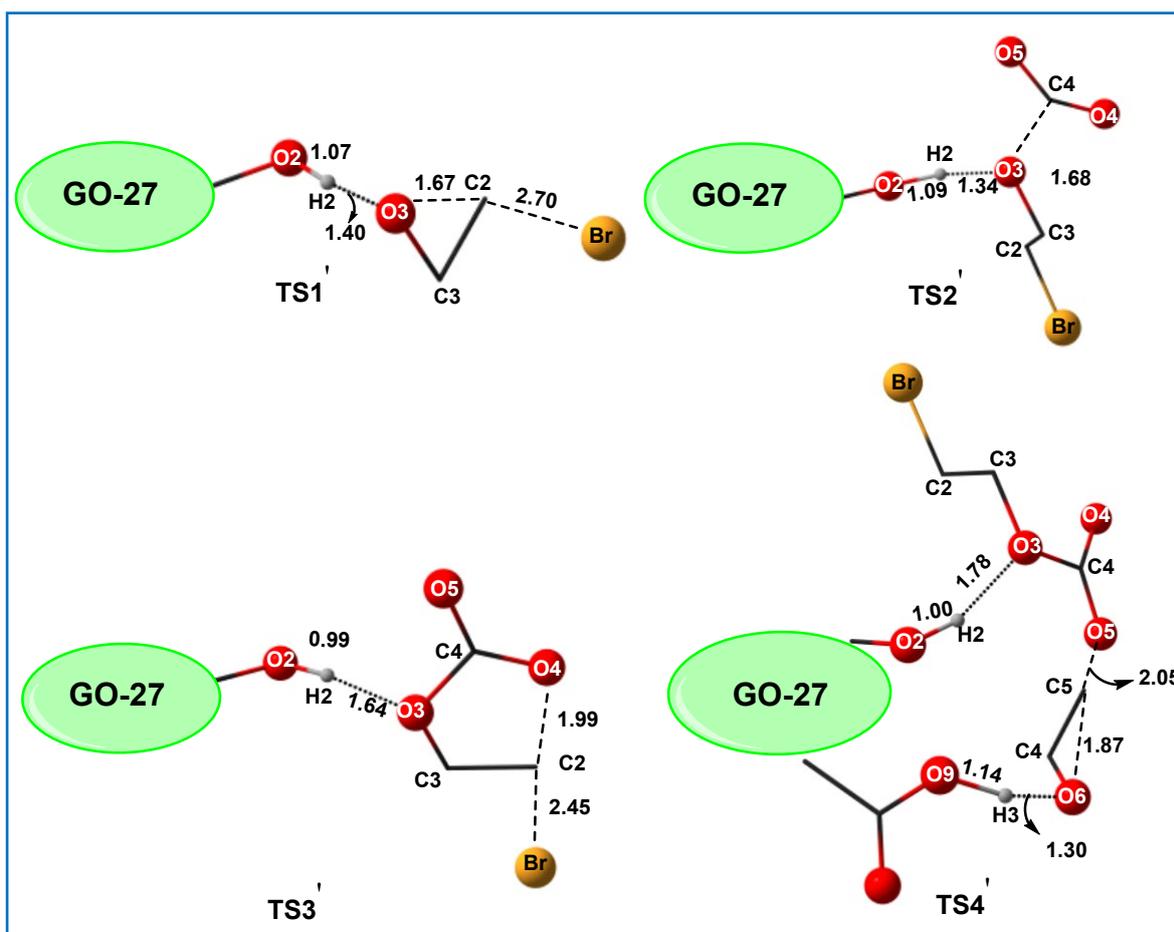
**Figure S4.** The optimized geometries of intermediates and transition states for the second CO<sub>2</sub> insertion step mediated by GO-27. The selected bond lengths are in Å and the energies are in kcal/mol.



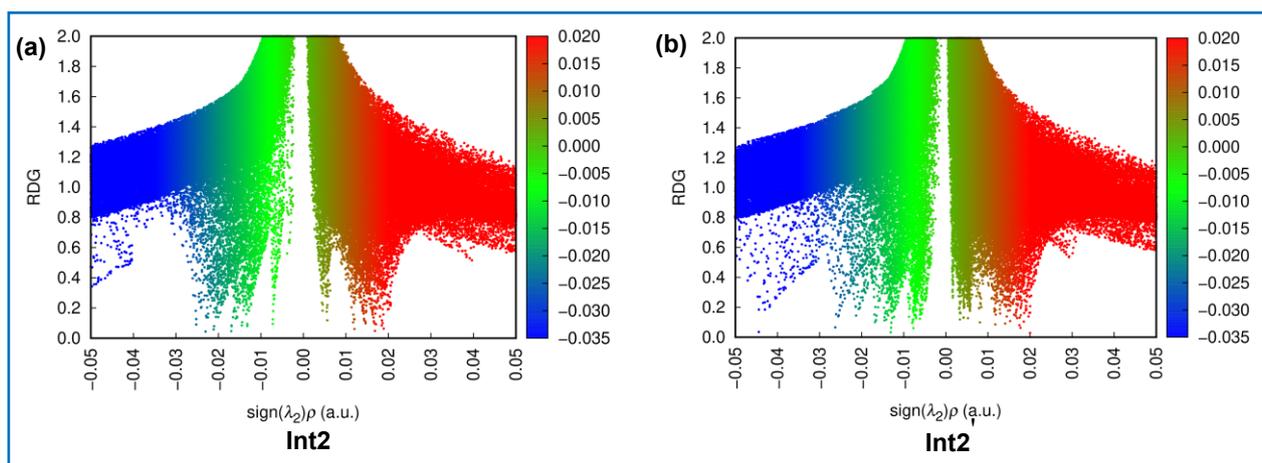
**Figure S5.** The optimised intermediate, transition state and product for the formation of polycarbonate from oxirane and CO<sub>2</sub>, mediated at the COOH edge of the GO-27, without the assistance of adjacent hydrogen bond donors. Selected bond distances are shown in Å.



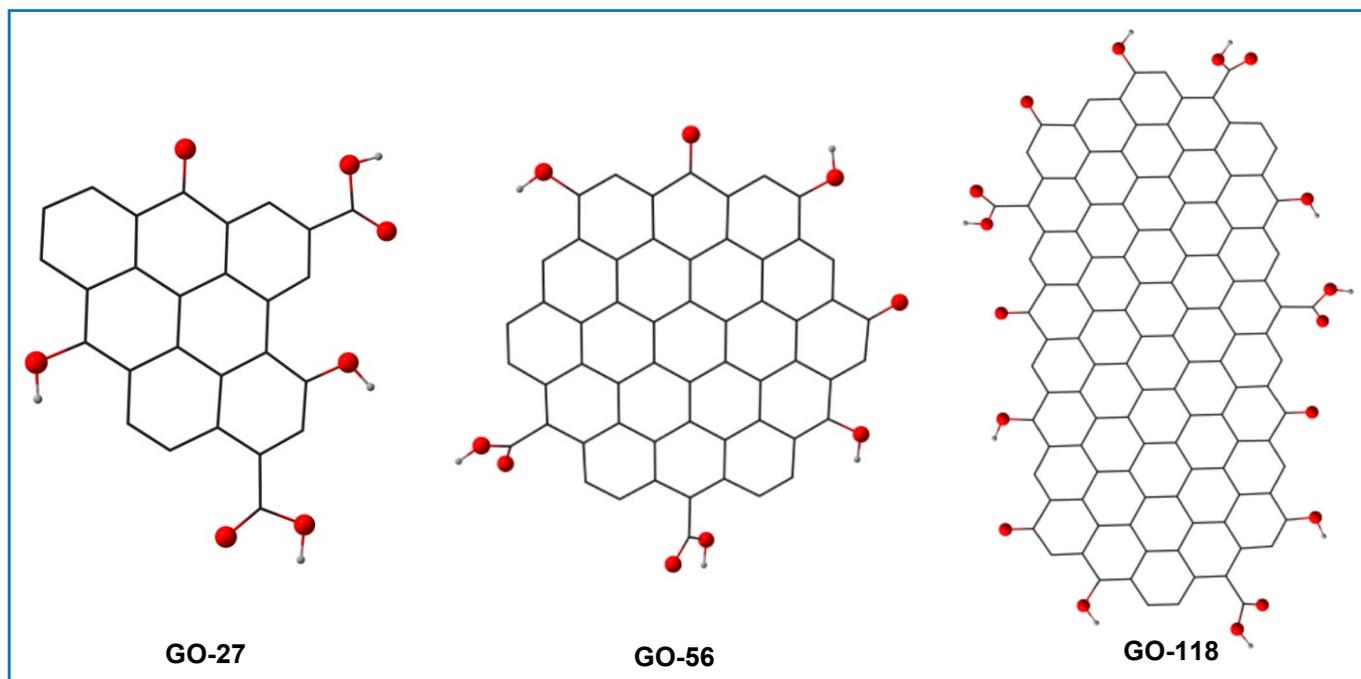
**Figure S6.** The optimised intermediates for the formation of cyclic/poly carbonate from oxirane and CO<sub>2</sub>, mediated at the -OH edge of the GO-27. Selected bond distances are shown in Å



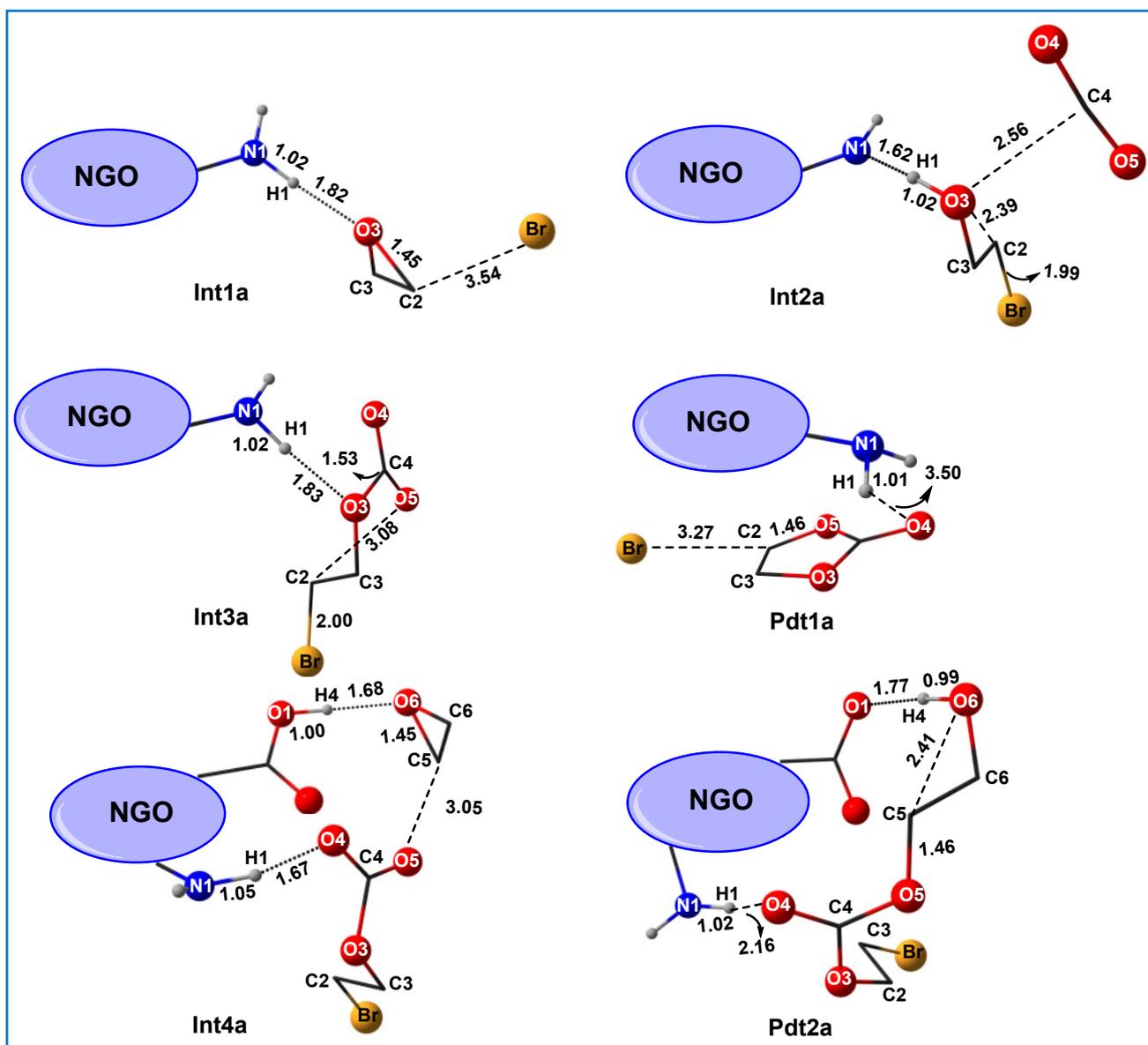
**Figure S7.** The optimised transition states for the formation of cyclic/poly carbonate from oxirane and  $\text{CO}_2$ , mediated at the -OH edge of the **GO-27**. Selected bond distances are shown in Å.



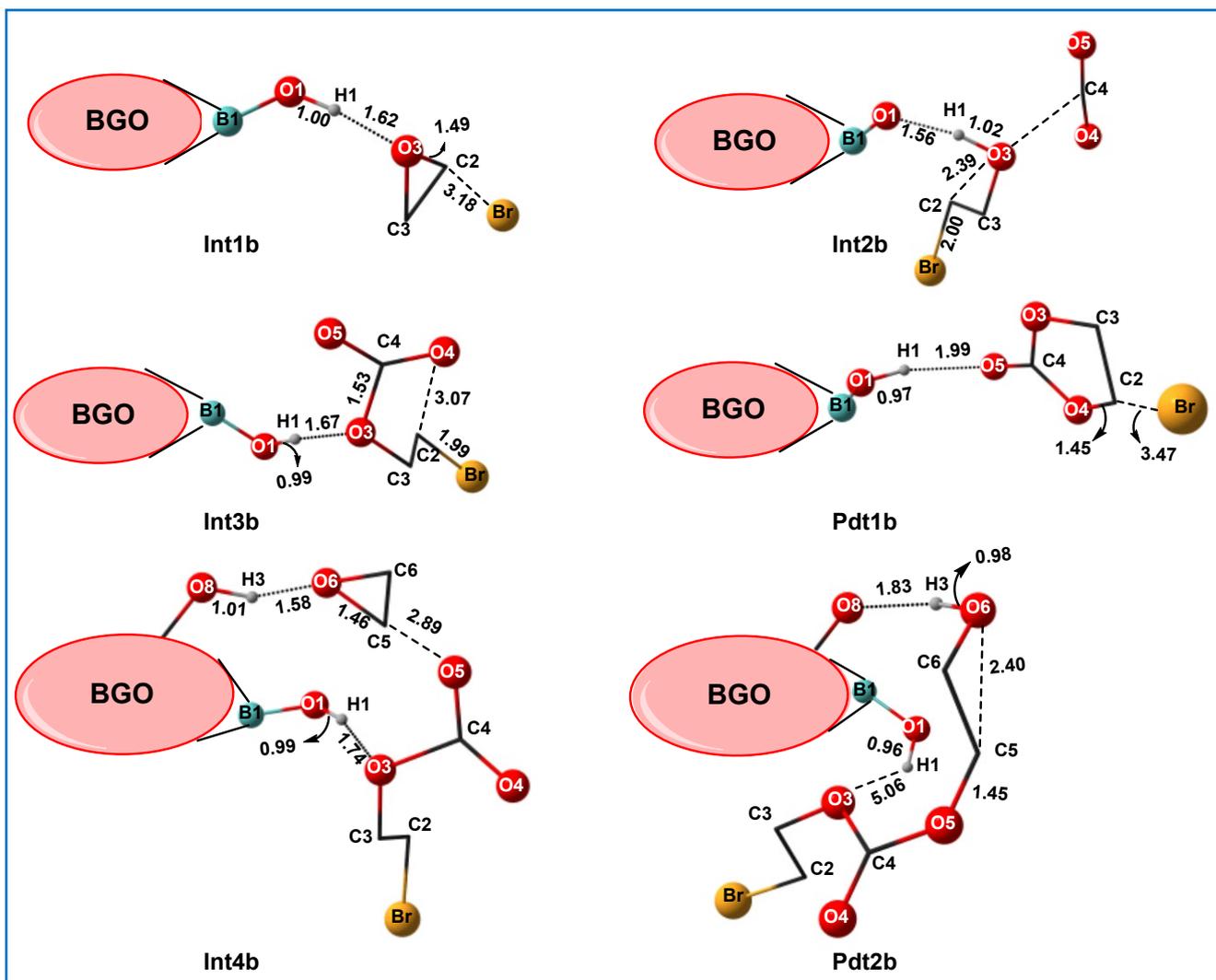
**Figure S8.** The RDG Scatter plot highlighting the NCI energy in **Int2** (left) and **Int2'** (right), with Vander Waals (green), H-bonding (blue), and steric interactions (red).



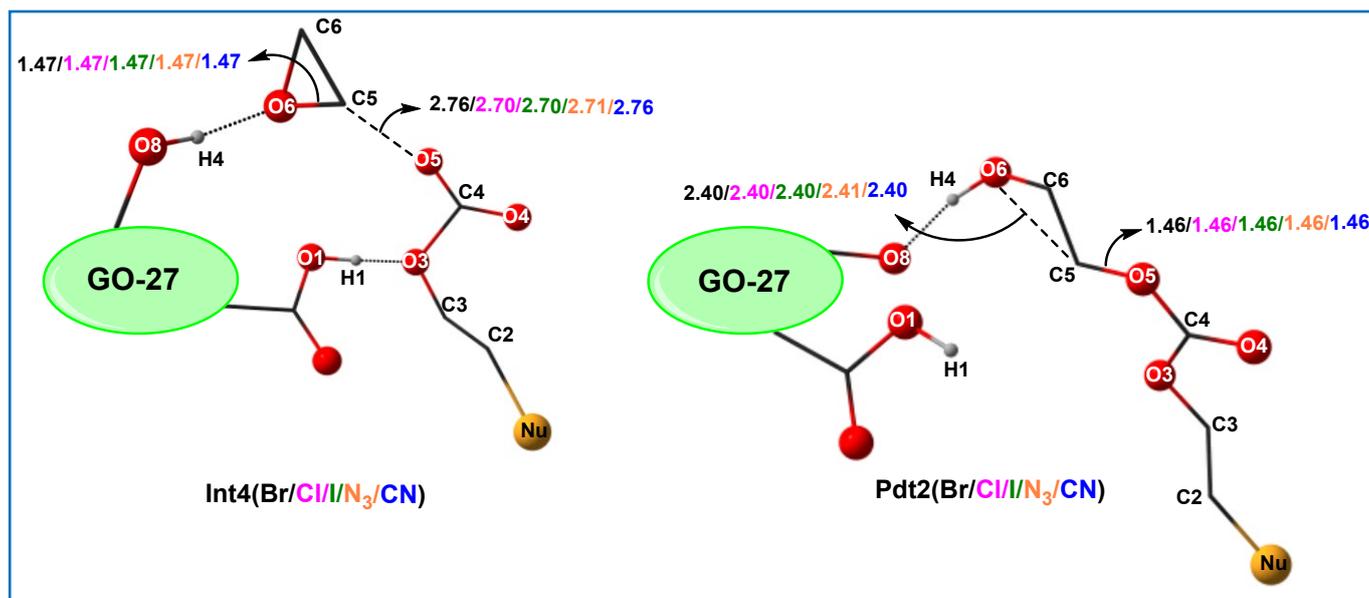
**Figure S9.** The optimised geometries of models **GO-27**, **GO-56**, and **GO-118**.



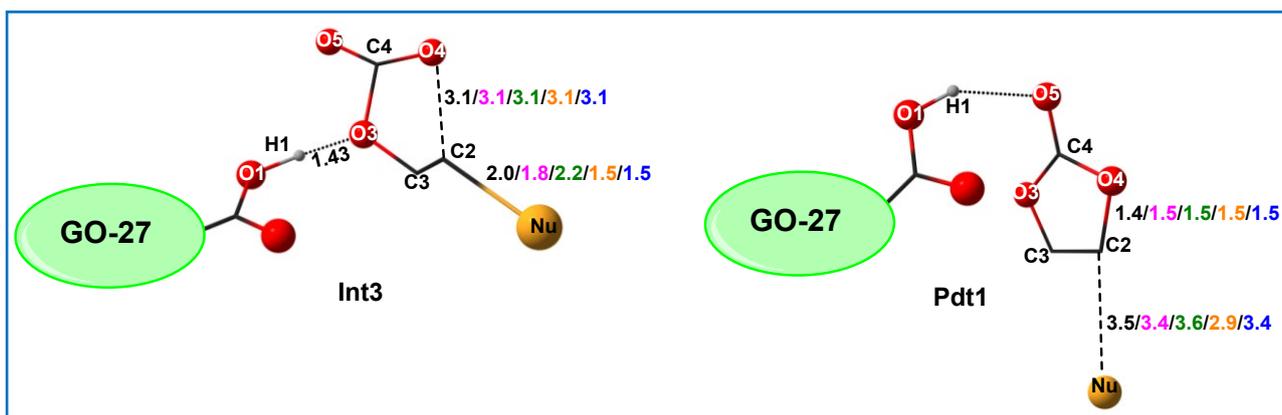
**Figure S10.** The optimised intermediates for the formation of cyclic/poly carbonate from oxirane and CO<sub>2</sub>, mediated at the -NH<sub>2</sub> edge of the NGO. Selected bond distances are shown in Å



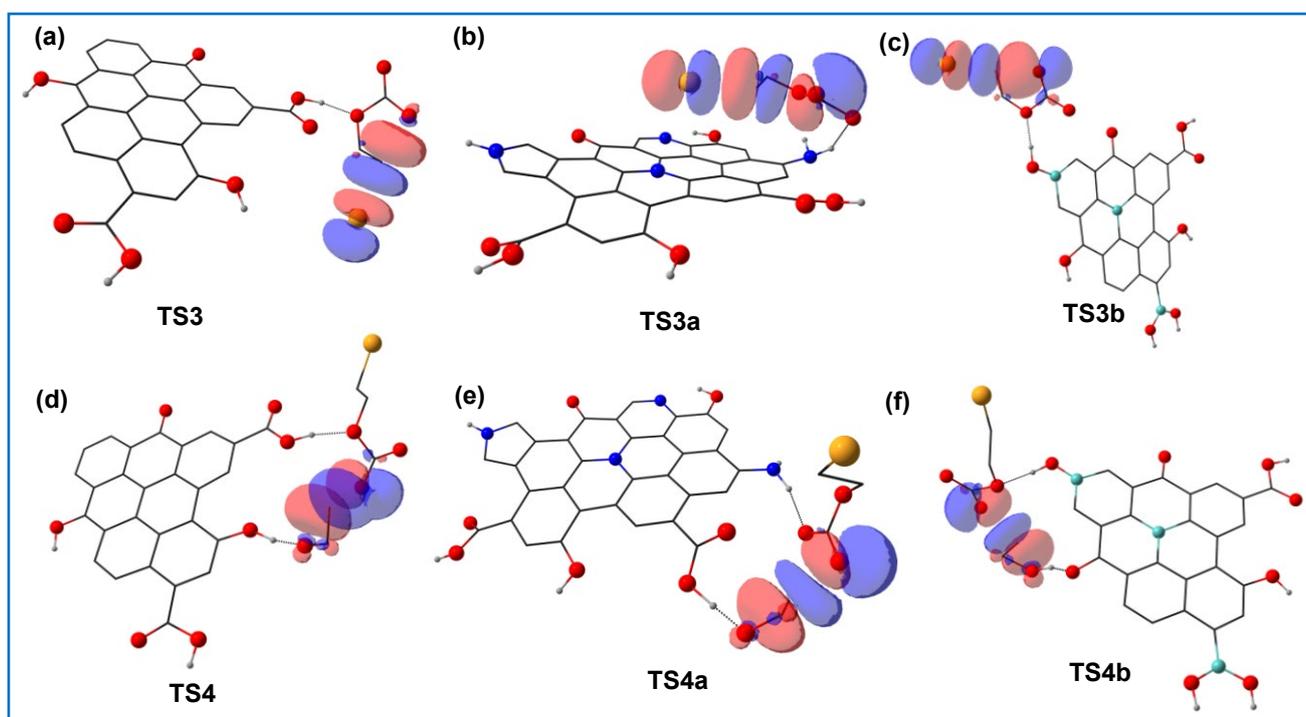
**Figure S11.** The optimized intermediates of the formation of cyclic/poly carbonate from oxirane and CO<sub>2</sub>, mediated at the -BOH edge of the BGO. Selected bond distances are shown in Å.



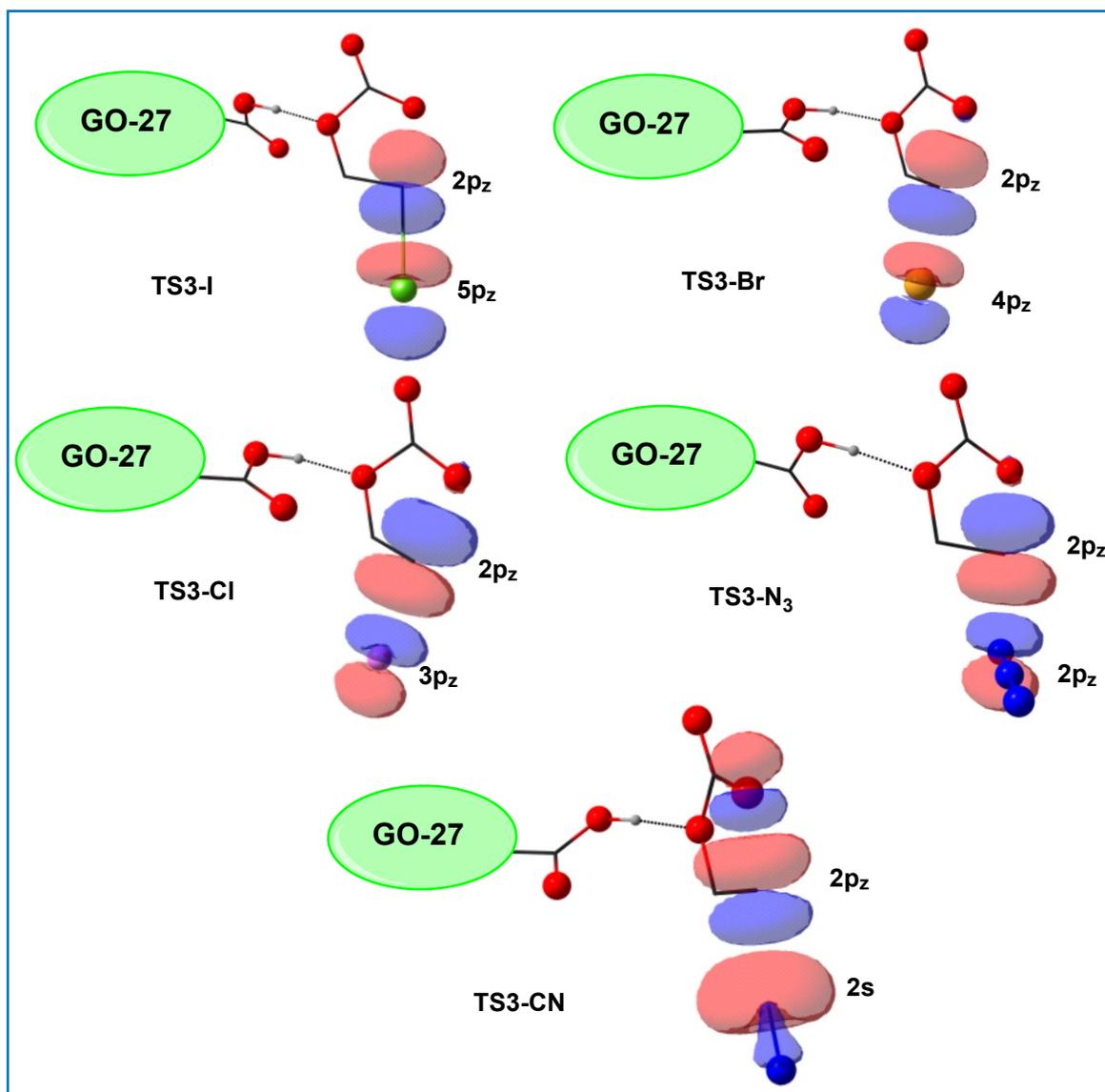
**Figure S12.** The optimised intermediates for the formation of polycarbonate from oxirane and  $\text{CO}_2$ , mediated at the  $-\text{COOH}$  edge of the **GO-27** with different nucleophiles. Selected bond distances of Br-(black), Cl-(Pink), I-(green),  $\text{N}_3$ -(orange), and CN-(blue) are shown in Å.



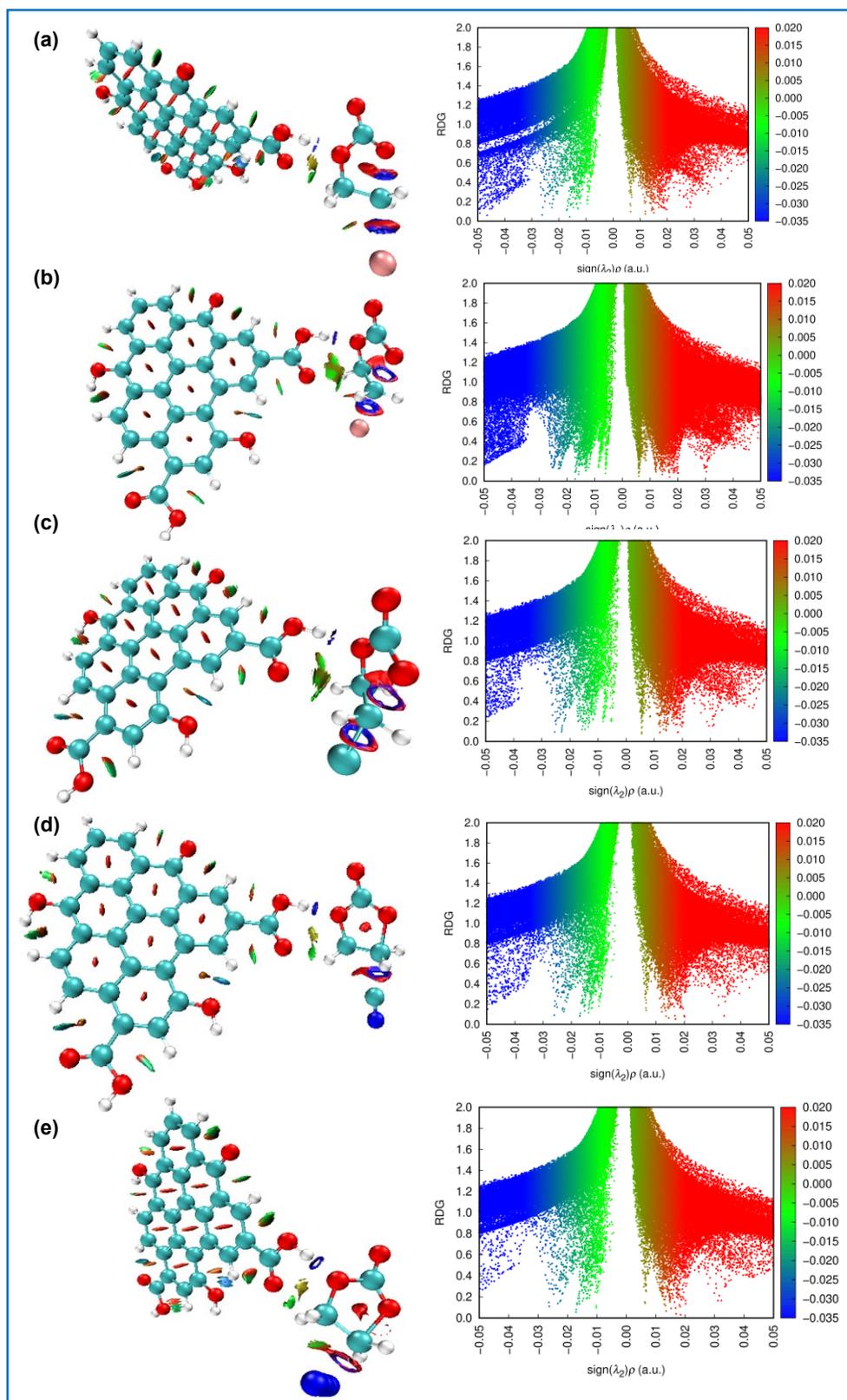
**Figure S13.** The optimised intermediates for the formation of cyclic carbonate from oxirane and CO<sub>2</sub>, mediated at the -COOH edge of the **GO-27** with different nucleophiles. Selected bond distances of Br<sup>-</sup>(black), Cl<sup>-</sup>(Pink), I<sup>-</sup>(green), N<sub>3</sub><sup>-</sup>(orange), and CN<sup>-</sup>(blue) are shown in Å.



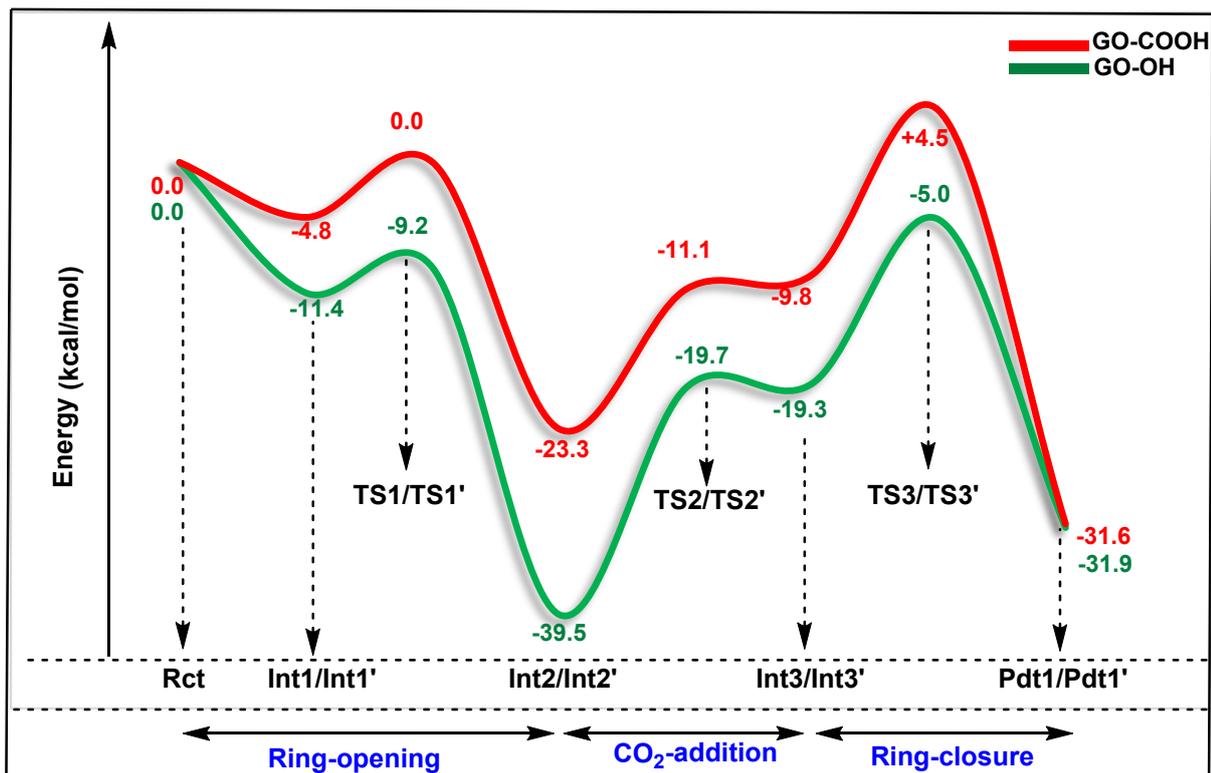
**Figure S14.** The NBO orbitals involved in the key transition states.



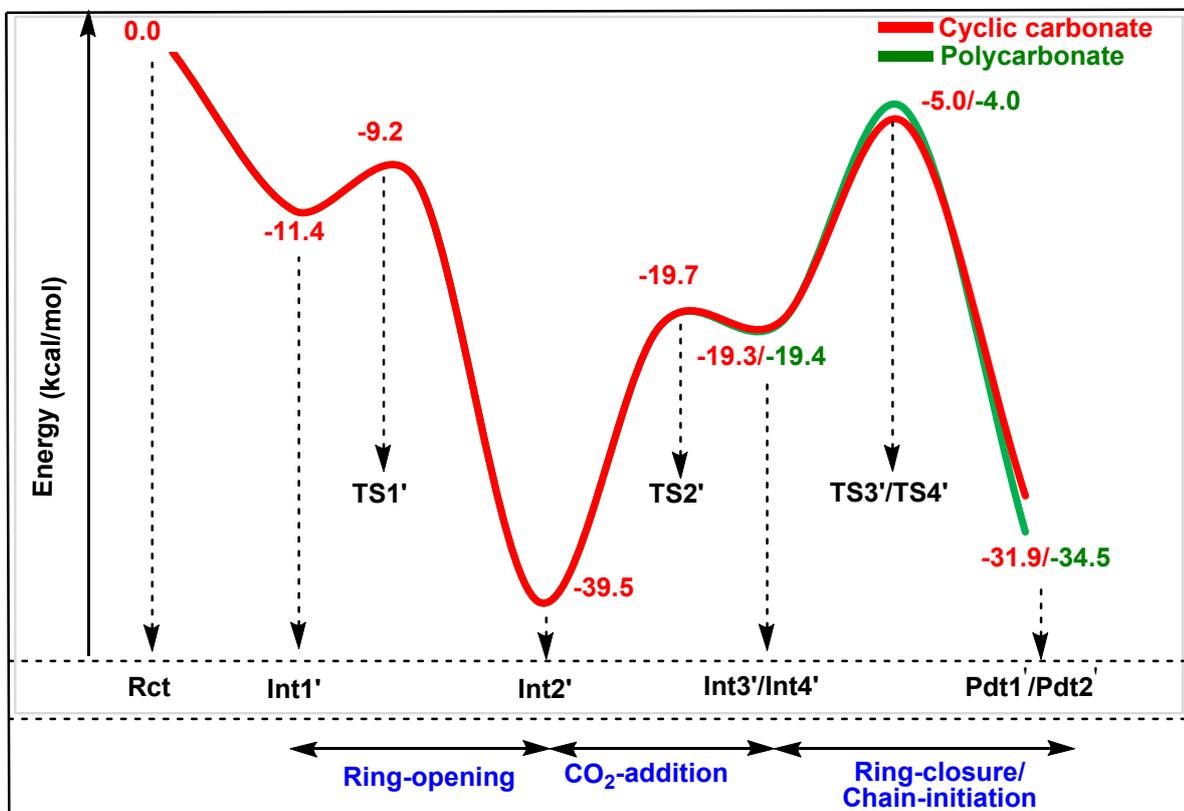
**Figure S15.** The interacting orbitals of C2-Nu in the TS3, wherein the isosurface is 0.05.



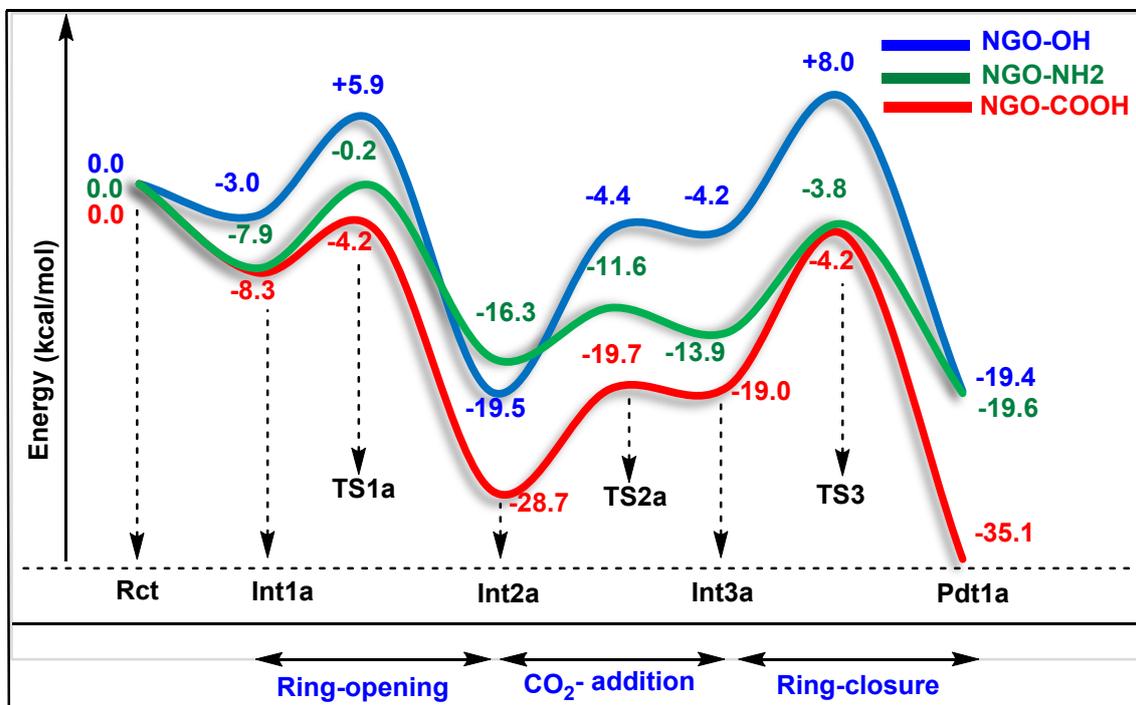
**Figure S16.** The NCI-RDG plot (left) and its corresponding scatter graph (right) for TS3 using I (a), Br (b), Cl (c), CN (d), and N<sub>3</sub><sup>-</sup> (e) as the nucleophiles, representing the Vander Waals (green colour), H-bonding (blue colour) and steric interactions (red colour).



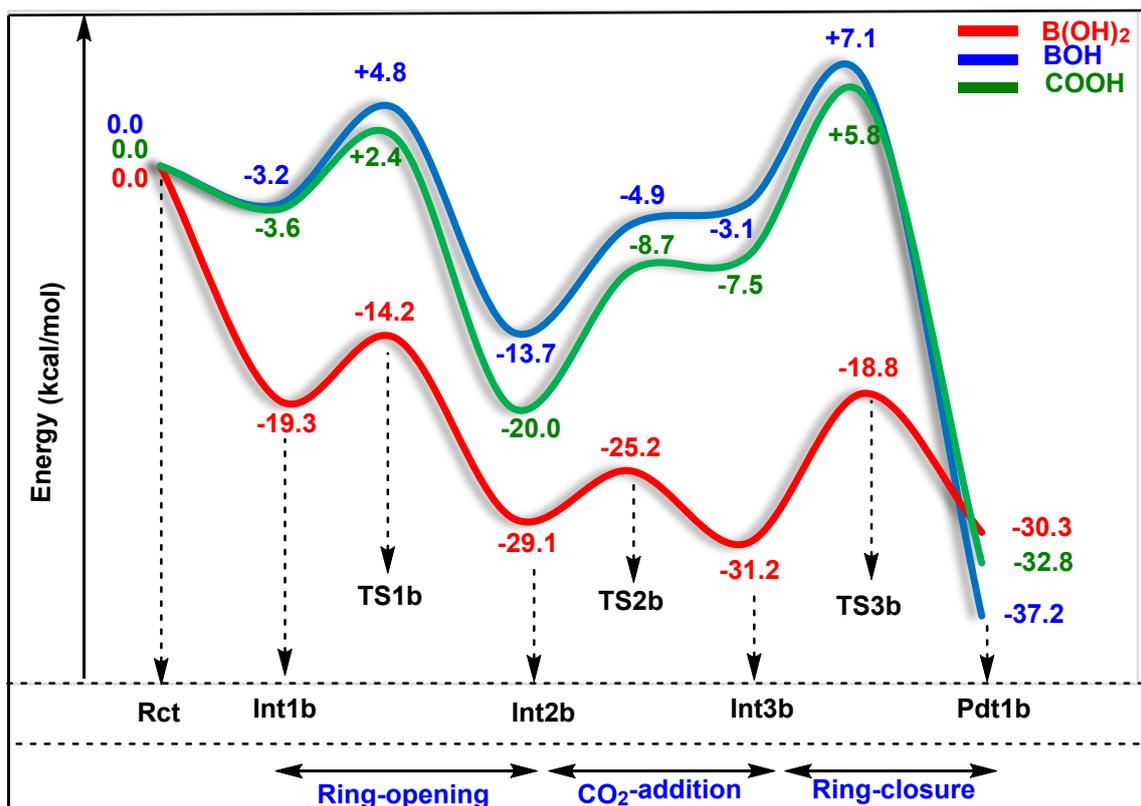
**Scheme S1.** The computed free-energy profile for GO-27 catalysed cyclic carbonate formation from oxirane and CO<sub>2</sub> at the -COOH (red) and -OH (green) edges.



**Scheme S2.** The computed free-energy profile for **GO-27** catalysed cyclic (red)/poly (green) carbonate formation from oxirane and CO<sub>2</sub> at the -OH edge.



**Scheme S3.** The computed free-energy profile for **NGO** catalysed cyclic carbonate formation from oxirane and CO<sub>2</sub> at the -COOH (red), -OH (blue), and -NH<sub>2</sub> (green) edges.



**Scheme S4.** The computed free-energy profile for **BGO** catalyzed cyclic carbonate formation from oxirane and CO<sub>2</sub> at the -COOH (green), -BOH (blue), and -B(OH)<sub>2</sub> (red) edges.

## Coordinates of optimised geometries

### Oxirane

SCF Energy (B3LYP-D3/B2) = -153.837848922

Enthalpy 0K = 0.328199

Enthalpy 298 K = 0.353026

Free Energy 298 K = 0.272211

C	0.00000000	0.73507500	-0.37114000
C	0.00000000	-0.73507500	-0.37114000
O	0.00000000	0.00000000	0.85607000
H	0.92032500	1.27451600	-0.59872100
H	-0.92032500	1.27451600	-0.59872100
H	0.92032500	-1.27451600	-0.59872100
H	-0.92032500	-1.27451600	-0.59872100

### Br<sup>-</sup>

SCF Energy (B3LYP-D3/B2) = -2574.23783781

Enthalpy 0K = 0.000000

Enthalpy 298 K = 0.001416

Free Energy 298 K = -0.016176

Br	0.00000000	0.00000000	0.00000000
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### CO<sub>2</sub>

SCF Energy (B3LYP-D3/B2) = -188.646790599

Enthalpy 0K = 0.011616

Enthalpy 298 K = 0.014257

Free Energy 298 K = -0.009101

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16966500
O	0.00000000	0.00000000	-1.16966500

### GO-27

SCF Energy (B3LYP-D3/B2) = -1563.25171263

Enthalpy 0K = 0.328199

Enthalpy 298 K = 0.353026

Free Energy 298 K = 0.272211

C	2.01989000	2.30958500	0.04967300
C	1.06328100	1.26039800	0.01704200
C	3.38262400	2.04852500	0.04087100
C	1.57870200	-0.07882900	-0.00440300
C	3.89583600	0.75353600	0.00376100
C	2.99352800	-0.34086000	-0.01740100
H	4.06997400	2.88723800	0.06390400
C	3.45527900	-1.70235700	-0.05646200
C	2.58748600	-2.74186600	-0.05938800
C	1.17078100	-2.54284600	-0.02281700
C	0.65805900	-1.19661200	-0.00961400
C	0.28445600	-3.62615100	-0.00325700
C	-0.73669700	-0.98187600	0.00271900
C	-1.12053900	-3.43255200	0.00648600
C	-1.62762300	-2.09872100	0.00513000
C	-0.38566200	1.48328200	0.00756500
C	-0.96968400	2.76667700	-0.00805700

C	-1.26479500	0.35702300	0.00574200
C	-2.35056000	2.95370800	-0.01592400
C	-2.67282900	0.56736500	0.00272400
C	-3.20550100	1.85036700	-0.00696800
H	-0.35836500	3.65222700	-0.01587000
H	-4.28282000	1.96458800	-0.00957400
C	-3.62957100	-0.56690700	0.00808700
C	-3.04093900	-1.92495000	0.01130300
C	-3.89058000	-3.02172300	0.01965200
C	-3.37946800	-4.33058400	0.02399600
C	-2.01446900	-4.53338900	0.01821700
H	4.51964000	-1.87858100	-0.08494900
H	3.00479200	-3.74539800	-0.10548600
H	-1.60323200	-5.53607600	0.02178100
H	-4.05718600	-5.17849000	0.03210500
H	-4.95905000	-2.83181700	0.02347000
O	0.69807500	-4.91971800	0.00451700
H	1.65919600	-4.96739800	0.07037800
O	1.61194600	3.61129200	0.09383400
H	2.38659600	4.18746500	0.11305900
C	-2.85424200	4.35264800	-0.03403700
O	-2.15293600	5.34629100	-0.04505800
O	-4.20854600	4.42342200	-0.03755100
H	-4.42730600	5.36923200	-0.04973300
C	5.37798800	0.59664800	-0.00713500
O	6.01635100	-0.44081000	-0.03227900
O	6.02409700	1.79540600	0.01502000
H	6.96993200	1.57736600	0.00612200
O	-4.84782100	-0.38808200	0.01023600

### Int1

SCF Energy (B3LYP-D3/B2) = -4291.36383651

Enthalpy 0K = 0.387375

Enthalpy 298 K = 0.418858

Free Energy 298 K = 0.318710

C	-1.18332300	2.82489400	-0.14686200
C	-1.62973900	1.47568300	-0.06204700
C	-2.07304900	3.88668800	-0.11317500
C	-3.04962700	1.27589400	0.00747700
C	-3.45471600	3.70640400	-0.00740600
C	-3.96723100	2.38364300	0.04791800
H	-1.67632400	4.89438000	-0.17305800
C	-5.37719500	2.12154400	0.15254900
C	-5.86317400	0.85667100	0.16966500
C	-5.00169700	-0.28279400	0.08305000
C	-3.57576200	-0.07238000	0.03053500
C	-5.51606600	-1.58236100	0.05406800
C	-2.70901400	-1.18457000	-0.00789300
C	-4.66438500	-2.71395000	0.01882000
C	-3.25151600	-2.50548500	-0.00255400
C	-0.72837900	0.32273300	-0.05107700
C	0.67977200	0.44010800	-0.03546900
C	-1.28021800	-0.99396600	-0.03712500
C	1.52026300	-0.66801900	-0.02988800
C	-0.40758500	-2.11837600	-0.04232300
C	0.97482800	-1.95224500	-0.04192700
H	1.15823400	1.40393600	-0.02437300
H	1.61106600	-2.82903000	-0.04524800
C	-0.93213500	-3.50333200	-0.04528400
C	-2.40858200	-3.65289800	-0.02845800
C	-2.95027100	-4.92916600	-0.03641300

C	-4.342807000	-5.122672000	-0.022486000
C	-5.187604000	-4.032041000	0.003538000
H	-6.046656000	2.965632000	0.220324000
H	-6.937836000	0.727745000	0.281568000
H	-6.263567000	-4.162960000	0.014257000
H	-4.751083000	-6.128888000	-0.032428000
H	-2.261461000	-5.767638000	-0.055177000
O	-6.854620000	-1.845296000	0.063581000
H	-7.348509000	-1.028206000	-0.073188000
O	0.147037000	3.097078000	-0.272408000
H	0.275782000	4.053041000	-0.313849000
C	3.003005000	-0.422828000	-0.010768000
O	3.470029000	0.709916000	0.011581000
O	3.715668000	-1.536292000	-0.020430000
H	4.717213000	-1.310532000	-0.007583000
C	-4.309875000	4.918042000	0.030907000
O	-5.527344000	4.977803000	0.110540000
O	-3.582421000	6.072534000	-0.034731000
H	-4.241321000	6.783894000	-0.001937000
O	-0.190381000	-4.486605000	-0.061727000
C	6.587280000	0.223567000	-0.700463000
H	5.752967000	0.688708000	-1.221813000
C	6.575424000	0.202035000	0.760564000
H	5.732748000	0.651887000	1.281849000
H	7.545033000	0.141377000	1.252164000
O	6.222370000	-1.000828000	0.009349000
Br	10.088758000	0.497943000	0.057301000
H	7.564752000	0.177209000	-1.177916000

## TS1

SCF Energy (B3LYP-D3/B2) = -4291.35377598  
 Enthalpy 0K = 0.383932  
 Enthalpy 298 K = 0.414899  
 Free Energy 298 K = 0.316283

C	-0.939956000	2.803060000	0.222312000
C	-1.408846000	1.459394000	0.207745000
C	-1.816130000	3.875880000	0.154215000
C	-2.821621000	1.276849000	0.037926000
C	-3.198534000	3.709733000	0.047316000
C	-3.725475000	2.394941000	-0.024618000
H	-1.405735000	4.879342000	0.183600000
C	-5.137065000	2.146905000	-0.151752000
C	-5.626318000	0.889184000	-0.270258000
C	-4.768622000	-0.257396000	-0.277150000
C	-3.352164000	-0.063988000	-0.085941000
C	-5.277759000	-1.545420000	-0.460242000
C	-2.496208000	-1.183013000	-0.038165000
C	-4.436947000	-2.685199000	-0.416289000
C	-3.039271000	-2.495110000	-0.191859000
C	-0.530841000	0.295951000	0.336870000
C	0.848114000	0.395332000	0.632308000
C	-1.082390000	-1.011061000	0.186236000
C	1.672263000	-0.719330000	0.729953000
C	-0.225969000	-2.144137000	0.276455000
C	1.134690000	-1.991883000	0.533627000
H	1.319366000	1.348779000	0.798675000
H	1.766331000	-2.870235000	0.591881000
C	-0.747803000	-3.518566000	0.107496000
C	-2.208115000	-3.649567000	-0.136917000
C	-2.745866000	-4.916228000	-0.304494000
C	-4.121907000	-5.091848000	-0.534822000

C	-4.955448000	-3.993783000	-0.590505000
H	-5.804607000	2.995157000	-0.149478000
H	-6.705955000	0.767891000	-0.331988000
H	-6.018547000	-4.111240000	-0.766685000
H	-4.526500000	-6.090848000	-0.668243000
H	-2.066944000	-5.761328000	-0.252303000
O	-6.602222000	-1.789847000	-0.685404000
H	-7.057020000	-0.961407000	-0.877825000
O	0.395888000	3.055748000	0.294205000
H	0.547260000	4.009042000	0.271745000
C	3.134602000	-0.500070000	1.055059000
O	3.544804000	0.630029000	1.314707000
O	3.841868000	-1.596388000	1.021758000
H	4.915602000	-1.430361000	1.285984000
C	-4.040616000	4.932828000	0.001303000
O	-5.255588000	5.005674000	-0.090619000
O	-3.301582000	6.077929000	0.076529000
H	-3.951258000	6.797460000	0.036980000
O	-0.022616000	-4.512318000	0.166368000
C	7.087490000	-0.766337000	0.194385000
H	6.409389000	-0.823496000	-0.642773000
C	6.712940000	-0.013713000	1.373824000
H	5.947672000	0.755329000	1.264961000
H	7.509578000	0.263250000	2.068064000
O	6.199752000	-1.339706000	1.581627000
Br	8.554679000	0.901154000	-1.374678000
H	7.987795000	-1.357138000	0.183655000

## Int2

SCF Energy (B3LYP-D3/B2) = -4480.05083777  
 Enthalpy 0K = 0.400213  
 Enthalpy 298 K = 0.435533  
 Free Energy 298 K = 0.324206

C	1.331543000	2.735286000	0.511354000
C	1.811353000	1.415551000	0.267885000
C	2.188979000	3.823571000	0.549861000
C	3.233821000	1.272213000	0.130694000
C	3.569636000	3.700540000	0.372627000
C	4.117053000	2.408530000	0.167584000
H	1.765659000	4.806167000	0.728099000
C	5.529419000	2.203666000	-0.015193000
C	6.050419000	0.962890000	-0.170832000
C	5.227097000	-0.208465000	-0.161429000
C	3.797377000	-0.049002000	-0.042942000
C	5.780656000	-1.485404000	-0.271057000
C	2.963702000	-1.184782000	-0.086511000
C	4.963840000	-2.641619000	-0.320434000
C	3.546586000	-2.480731000	-0.238414000
C	0.941297000	0.244502000	0.165559000
C	-0.473145000	0.320127000	0.197278000
C	1.531261000	-1.045145000	0.003677000
C	-1.287218000	-0.800927000	0.102229000
C	0.688853000	-2.190203000	-0.080137000
C	-0.698314000	-2.059240000	-0.026690000
H	-0.989289000	1.259862000	0.293264000
H	-1.328774000	-2.938475000	-0.092805000
C	1.252827000	-3.547513000	-0.229507000
C	2.736433000	-3.649234000	-0.301193000
C	3.313375000	-4.902515000	-0.433117000
C	4.710075000	-5.051054000	-0.504264000
C	5.523948000	-3.938456000	-0.447673000
H	6.171315000	3.071455000	-0.028413000
H	7.122396000	0.878833000	-0.339035000

H	6.602435000	-4.034535000	-0.501039000
H	5.146183000	-6.041009000	-0.603538000
H	2.647842000	-5.758688000	-0.477414000
O	7.129697000	-1.701328000	-0.344855000
H	7.597264000	-0.891907000	-0.107823000
O	0.003637000	2.949596000	0.723201000
H	-0.152177000	3.893429000	0.852711000
C	-2.813265000	-0.630436000	0.140329000
O	-3.238877000	0.539430000	0.254913000
O	-3.466727000	-1.713553000	0.045959000
H	-5.046851000	-1.660110000	0.227257000
C	4.386095000	4.937724000	0.422272000
O	5.596906000	5.049105000	0.305142000
O	3.629083000	6.057390000	0.627390000
H	4.268307000	6.787005000	0.639513000
O	0.550437000	-4.558105000	-0.292646000
C	-6.354954000	0.664064000	-0.256526000
H	-5.310499000	0.917614000	-0.064088000
C	-6.481516000	-0.766538000	-0.771923000
H	-5.885660000	-0.874764000	-1.690474000
H	-7.527966000	-0.985091000	-1.019895000
O	-6.058150000	-1.652639000	0.233835000
Br	-7.023999000	1.971009000	-1.628590000
H	-6.982732000	0.824802000	0.618752000
C	-7.329497000	-1.651134000	2.409865000
O	-8.223611000	-1.030084000	1.971292000
O	-6.522885000	-2.274500000	2.983936000

## TS2

SCF Energy (B3LYP-D3/B2) = -4480.03608969

Enthalpy 0K = 0.397786

Enthalpy 298 K = 0.431634

Free Energy 298 K = 0.325121

C	1.304463000	2.757405000	0.425880000
C	1.794040000	1.435996000	0.220902000
C	2.157002000	3.850404000	0.453273000
C	3.217260000	1.295616000	0.095937000
C	3.539209000	3.729153000	0.296184000
C	4.094926000	2.436355000	0.120024000
H	1.727572000	4.834772000	0.604725000
C	5.509841000	2.235381000	-0.045652000
C	6.037298000	0.994829000	-0.178167000
C	5.218914000	-0.179693000	-0.159574000
C	3.788258000	-0.026160000	-0.052130000
C	5.778998000	-1.456117000	-0.249864000
C	2.961235000	-1.167259000	-0.082828000
C	4.968004000	-2.617161000	-0.287208000
C	3.550025000	-2.462614000	-0.212890000
C	0.931827000	0.255973000	0.143021000
C	-0.480634000	0.322981000	0.181700000
C	1.527966000	-1.033025000	0.002859000
C	-1.285240000	-0.807253000	0.111505000
C	0.693171000	-2.184319000	-0.060771000
C	-0.693880000	-2.065937000	-0.001522000
H	-0.997052000	1.263421000	0.265122000
H	-1.308882000	-2.956856000	-0.049194000
C	1.264656000	-3.542361000	-0.196360000
C	2.747071000	-3.636814000	-0.261921000
C	3.331183000	-4.888839000	-0.374317000
C	4.728766000	-5.030507000	-0.438676000
C	5.535826000	-3.912440000	-0.394651000

H	6.148150000	3.105604000	-0.065109000
H	7.111453000	0.913868000	-0.332678000
H	6.614926000	-4.003294000	-0.442788000
H	5.170644000	-6.019107000	-0.522462000
H	2.671088000	-5.749631000	-0.408651000
O	7.126999000	-1.667673000	-0.314882000
H	7.593718000	-0.850362000	-0.104588000
O	-0.028157000	2.971050000	0.608483000
H	-0.190151000	3.915650000	0.724629000
C	-2.791470000	-0.622670000	0.157136000
O	-3.256507000	0.516989000	0.239644000
O	-3.449346000	-1.738253000	0.092793000
H	-4.587272000	-1.621849000	0.167923000
C	4.350847000	4.972129000	0.333399000
O	5.562020000	5.083895000	0.228419000
O	3.586265000	6.089931000	0.509371000
H	4.219358000	6.825066000	0.517304000
O	0.563284000	-4.552795000	-0.253547000
C	-6.461886000	0.738135000	0.041901000
H	-5.455439000	1.070873000	0.286566000
C	-6.432471000	-0.600995000	-0.684931000
H	-5.833046000	-0.515849000	-1.601674000
H	-7.451635000	-0.899901000	-0.954799000
O	-5.858232000	-1.565179000	0.161840000
Br	-7.254083000	2.161594000	-1.129400000
H	-7.107635000	0.684380000	0.915903000
C	-6.844208000	-2.160855000	1.485672000
O	-7.954752000	-1.695701000	1.364105000
O	-6.126433000	-2.870844000	2.138921000

## Int3

SCF Energy (B3LYP-D3/B2) = -4480.03668124

Enthalpy 0K = 0.400678

Enthalpy 298 K = 0.434835

Free Energy 298 K = 0.327799

C	1.212910000	2.755741000	-0.016551000
C	1.745244000	1.435773000	0.009288000
C	2.034128000	3.869893000	0.066992000
C	3.174857000	1.324476000	0.067026000
C	3.423396000	3.772495000	0.165653000
C	4.020022000	2.485867000	0.159216000
H	1.573570000	4.851705000	0.052636000
C	5.444837000	2.309562000	0.251794000
C	6.009425000	1.079107000	0.207262000
C	5.222622000	-0.108431000	0.064548000
C	3.785697000	0.012786000	0.024155000
C	5.819217000	-1.368333000	-0.029097000
C	2.991128000	-1.148007000	-0.068162000
C	5.041151000	-2.549024000	-0.119911000
C	3.617972000	-2.430353000	-0.129533000
C	0.918389000	0.228601000	-0.028873000
C	-0.494552000	0.256115000	0.003969000
C	1.552649000	-1.048461000	-0.082875000
C	-1.264981000	-0.899547000	-0.036549000
C	0.751642000	-2.223750000	-0.139487000
C	-0.638956000	-2.144087000	-0.117855000
H	-1.036196000	1.183981000	0.065859000
H	-1.224805000	-3.054868000	-0.157753000
C	1.363843000	-3.569138000	-0.221928000
C	2.849045000	-3.625278000	-0.212725000

C	3.470061000	-4.862472000	-0.285205000
C	4.872279000	-4.967744000	-0.281504000
C	5.646910000	-3.828921000	-0.201443000
H	6.060116000	3.189658000	0.360993000
H	7.090467000	1.013335000	0.313282000
H	6.729035000	-3.891832000	-0.197918000
H	5.343160000	-5.944521000	-0.341749000
H	2.835138000	-5.740571000	-0.345794000
O	7.172825000	-1.545635000	-0.033763000
H	7.612404000	-0.693254000	-0.135079000
O	-0.130348000	2.947095000	-0.134409000
H	-0.324051000	3.892910000	-0.130319000
C	-2.768783000	-0.748849000	0.005571000
O	-3.278293000	0.366761000	0.078539000
O	-3.400487000	-1.892927000	-0.051590000
H	-4.453690000	-1.770680000	-0.006783000
C	4.199945000	5.035378000	0.260985000
O	5.410545000	5.169428000	0.340714000
O	3.399838000	6.141438000	0.252812000
H	4.011212000	6.891948000	0.318574000
O	0.690681000	-4.596971000	-0.297037000
C	-6.488547000	0.664329000	0.323994000
H	-5.495819000	0.931033000	0.678650000
C	-6.418766000	-0.472736000	-0.685841000
H	-5.765144000	-0.192105000	-1.520147000
H	-7.421478000	-0.698792000	-1.062322000
O	-5.869457000	-1.608401000	-0.052831000
Br	-7.227721000	2.321959000	-0.529342000
H	-7.173774000	0.413234000	1.130418000
C	-6.821477000	-2.429553000	0.945661000
O	-7.957472000	-1.970147000	0.960939000
O	-6.165049000	-3.320942000	1.450750000

### Int3r

SCF Energy (B3LYP-D3/B2) = -4480.01768218

Enthalpy 0K = 0.400929

Enthalpy 298 K = 0.435071

Free Energy 298 K = 0.328192

C	-1.614209000	2.741795000	0.131758000
C	-2.028255000	1.381607000	0.050138000
C	-2.529565000	3.781626000	0.058951000
C	-3.440286000	1.146134000	-0.042113000
C	-3.901921000	3.564255000	-0.078097000
C	-4.383007000	2.230671000	-0.120900000
H	-2.158082000	4.798886000	0.114108000
C	-5.784384000	1.931441000	-0.249631000
C	-6.238447000	0.655134000	-0.249423000
C	-5.351800000	-0.461908000	-0.120715000
C	-3.932477000	-0.215097000	-0.048221000
C	-5.835046000	-1.771764000	-0.070322000
C	-3.039380000	-1.303446000	0.028521000
C	-4.956603000	-2.881115000	0.004484000
C	-3.549800000	-2.637362000	0.043122000
C	-1.098357000	0.251243000	0.066994000
C	0.307458000	0.408400000	0.054820000
C	-1.616230000	-1.077434000	0.073489000
C	1.176829000	-0.676125000	0.080455000
C	-0.713949000	-2.178686000	0.111934000
C	0.662654000	-1.971774000	0.120879000
H	0.753107000	1.386147000	0.022950000

H	1.335680000	-2.821222000	0.151795000
C	-1.204316000	-3.574490000	0.140200000
C	-2.678467000	-3.761519000	0.106743000
C	-3.188261000	-5.050345000	0.135210000
C	-4.575355000	-5.279066000	0.105170000
C	-5.446990000	-4.211391000	0.041732000
H	-6.473169000	2.756545000	-0.349353000
H	-7.306929000	0.496601000	-0.381429000
H	-6.519083000	-4.369712000	0.017744000
H	-4.958508000	-6.294951000	-0.131833000
H	-2.478861000	-5.870326000	0.182571000
O	-7.167906000	-2.067845000	-0.095602000
H	-7.681840000	-1.260893000	0.026257000
O	-0.298239000	3.039530000	0.294483000
H	-0.169729000	3.996383000	0.313025000
C	2.673160000	-0.465925000	0.072631000
O	3.442369000	-1.419345000	0.130778000
O	2.999038000	0.802539000	0.000948000
H	4.036050000	0.971564000	0.003801000
C	-4.785840000	4.756204000	-0.159401000
O	-6.001364000	4.784096000	-0.268496000
O	-4.088278000	5.927175000	-0.099112000
H	-4.761312000	6.623274000	-0.160722000
O	-0.442639000	-4.541221000	0.188820000
C	7.450964000	0.186634000	-0.683834000
H	8.017236000	1.115323000	-0.674480000
C	6.359602000	0.226559000	0.376129000
H	6.810390000	0.431955000	1.352933000
H	5.802935000	-0.714999000	0.408068000
O	5.453764000	1.251569000	0.011084000
Br	8.767630000	-1.274018000	-0.311932000
H	7.045942000	-0.025876000	-1.672961000
C	5.848216000	2.739362000	0.396121000
O	6.998100000	2.816558000	0.818637000
O	4.895591000	3.465722000	0.164780000

### TS3

SCF Energy (B3LYP-D3/B2) = -4480.01680201

Enthalpy 0K = 0.401980

Enthalpy 298 K = 0.435357

Free Energy 298 K = 0.330663

C	0.777671000	2.608796000	0.198136000
C	1.426469000	1.342556000	0.182393000
C	1.501940000	3.788905000	0.287647000
C	2.859664000	1.353977000	0.171620000
C	2.897004000	3.808619000	0.344214000
C	3.604043000	2.580820000	0.273611000
H	0.958157000	4.726723000	0.312627000
C	5.041443000	2.524546000	0.305972000
C	5.706336000	1.350454000	0.182900000
C	5.017931000	0.106367000	0.011016000
C	3.576371000	0.103312000	0.039633000
C	5.712978000	-1.090771000	-0.180408000
C	2.879196000	-1.116249000	-0.081842000
C	5.033485000	-2.328063000	-0.307600000
C	3.606624000	-2.333761000	-0.246721000
C	0.706372000	0.069304000	0.152435000
C	-0.693261000	-0.028451000	0.308350000
C	1.439422000	-1.142522000	-0.014667000
C	-1.365425000	-1.243468000	0.240371000

C	0.737662000	-2.378034000	-0.095676000
C	-0.650407000	-2.420270000	0.015661000
H	-1.299210000	0.843310000	0.486811000
H	-1.157606000	-3.374941000	-0.058175000
C	1.454264000	-3.657655000	-0.297391000
C	2.936912000	-3.584638000	-0.365167000
C	3.655717000	-4.756986000	-0.540692000
C	5.060204000	-4.739564000	-0.607539000
C	5.739508000	-3.544013000	-0.493328000
H	5.583838000	3.449263000	0.432108000
H	6.792545000	1.373737000	0.244720000
H	6.821937000	-3.513081000	-0.542196000
H	5.608071000	-5.666616000	-0.748325000
H	3.095390000	-5.682653000	-0.624499000
O	7.074565000	-1.149239000	-0.254239000
H	7.435181000	-0.257493000	-0.324694000
O	-0.577201000	2.672568000	0.112638000
H	-0.869006000	3.593009000	0.100866000
C	-2.859215000	-1.213707000	0.411047000
O	-3.443598000	-0.195330000	0.746375000
O	-3.436237000	-2.378191000	0.147169000
H	-4.438047000	-2.273594000	0.250831000
C	3.565657000	5.131174000	0.461089000
O	4.762262000	5.364066000	0.520558000
O	2.674840000	6.163191000	0.502593000
H	3.219524000	6.962534000	0.578476000
O	0.864393000	-4.733535000	-0.402607000
C	-6.529473000	0.498457000	0.239837000
H	-5.707418000	0.879177000	0.823371000
C	-6.303395000	-0.754928000	-0.582421000
H	-5.453420000	-0.609622000	-1.247720000
H	-7.193115000	-0.973566000	-1.183334000
O	-5.989056000	-1.889523000	0.239783000
Br	-6.133436000	2.102298000	-1.547959000
H	-7.503576000	0.936158000	0.353471000
C	-6.497619000	-1.794899000	1.592506000
O	-7.086368000	-0.692473000	1.803876000
O	-6.275029000	-2.765112000	2.295640000

### Pdt1

SCF Energy (B3LYP-D3/B2) = -4480.08110177

Enthalpy 0K = 0.404701

Enthalpy 298 K = 0.437661

Free Energy 298 K = 0.337500

C	-0.868684000	1.679966000	0.432423000
C	0.320375000	0.892115000	0.418589000
C	-0.793950000	3.075321000	0.331491000
C	1.569189000	1.571116000	0.259669000
C	0.423137000	3.743675000	0.237023000
C	1.637163000	3.003519000	0.203201000
H	-1.731068000	3.620035000	0.312129000
C	2.926721000	3.634703000	0.137797000
C	4.070608000	2.910874000	0.045263000
C	4.049355000	1.478887000	-0.018133000
C	2.785709000	0.799558000	0.120328000
C	5.216414000	0.736586000	-0.220748000
C	2.745355000	-0.611744000	0.081529000
C	5.197425000	-0.679399000	-0.271853000
C	3.946179000	-1.352560000	-0.116809000
C	0.299721000	-0.568424000	0.489836000

C	-0.867576000	-1.300574000	0.776502000
C	1.495306000	-1.307036000	0.254876000
C	-0.914955000	-2.689594000	0.684881000
C	1.444409000	-2.729563000	0.204308000
C	0.237235000	-3.408484000	0.368985000
H	-1.773243000	-0.787369000	1.046312000
H	0.225628000	-4.487968000	0.272409000
C	2.665437000	-3.531518000	-0.033610000
C	3.936066000	-2.776405000	-0.180831000
C	5.112689000	-3.481291000	-0.385617000
C	6.339078000	-2.809964000	-0.536820000
C	6.381070000	-1.431203000	-0.483117000
H	2.966084000	4.713825000	0.156964000
H	5.017064000	3.448174000	0.038811000
H	7.318057000	-0.899086000	-0.603024000
H	7.251328000	-3.376864000	-0.699028000
H	5.050272000	-4.564019000	-0.427606000
O	6.438929000	1.325246000	-0.389457000
H	6.318460000	2.271792000	-0.532023000
O	-2.063743000	1.096581000	0.537015000
H	-2.845351000	1.710951000	0.279087000
C	-2.260535000	-3.302616000	0.872199000
O	-3.162813000	-2.747460000	1.477523000
O	-2.404440000	-4.485250000	0.251521000
H	-3.370012000	-4.655863000	0.184705000
C	0.387845000	5.231160000	0.149040000
O	1.308420000	5.981616000	-0.138938000
O	-0.840274000	5.736692000	0.428136000
H	-0.761635000	6.694353000	0.294894000
O	2.640181000	-4.763181000	-0.100284000
C	-5.229435000	-0.694476000	0.104111000
H	-4.675237000	-0.536838000	1.030860000
C	-4.305808000	-0.788277000	-1.112926000
H	-3.329950000	-0.339412000	-0.945657000
H	-4.753158000	-0.374191000	-2.019462000
O	-4.142786000	-2.222909000	-1.282234000
Br	-4.476620000	2.640697000	-0.449320000
H	-6.008771000	0.056295000	-0.001074000
C	-5.049667000	-2.872346000	-0.526913000
O	-5.826692000	-2.020776000	0.157082000
O	-5.145785000	-4.081838000	-0.486631000

### Int4

SCF Energy (B3LYP-D3/B2) = -4633.90753700

Enthalpy 0K = 0.461312

Enthalpy 298 K = 0.499399

Free Energy 298 K = 0.384199

C	-1.634434000	2.496659000	0.445503000
C	-2.068805000	1.153648000	0.252306000
C	-2.528710000	3.554669000	0.303440000
C	-3.471762000	0.931383000	0.084591000
C	-3.888265000	3.354513000	0.052442000
C	-4.394135000	2.028233000	-0.019697000
H	-2.142084000	4.559884000	0.417080000
C	-5.792750000	1.741940000	-0.198860000
C	-6.259793000	0.468699000	-0.221979000
C	-5.386891000	-0.660095000	-0.087843000
C	-3.969329000	-0.425908000	0.022027000
C	-5.876868000	-1.969062000	-0.071831000
C	-3.083212000	-1.522535000	0.077451000

C	-5.005486000	-3.085776000	-0.017067000	C	-3.370362000	1.032650000	-0.110277000
C	-3.596916000	-2.851907000	0.036169000	C	-3.560510000	3.479255000	-0.245727000
C	-1.146129000	0.019773000	0.202520000	C	-4.194438000	2.203956000	-0.229170000
C	0.253195000	0.182653000	0.143997000	H	-1.689849000	4.531760000	-0.074651000
C	-1.659682000	-1.305115000	0.132664000	C	-5.617758000	2.040390000	-0.332501000
C	1.128088000	-0.892033000	0.048563000	C	-6.202943000	0.816686000	-0.271704000
C	-0.754375000	-2.404517000	0.090103000	C	-5.431285000	-0.379735000	-0.104083000
C	0.622643000	-2.193507000	0.051051000	C	-3.994493000	-0.273894000	-0.059565000
H	0.676050000	1.168396000	0.177145000	C	-6.037442000	-1.634104000	0.013851000
H	1.295594000	-3.042596000	0.007780000	C	-3.214069000	-1.446683000	0.050045000
C	-1.250327000	-3.799454000	0.073217000	C	-5.273480000	-2.822469000	0.124791000
C	-2.726968000	-3.979964000	0.054474000	C	-3.848033000	-2.720377000	0.128183000
C	-3.242916000	-5.266617000	0.039470000	C	-1.146303000	-0.090941000	-0.015176000
C	-4.631782000	-5.487342000	0.007395000	C	0.257156000	-0.065687000	-0.107291000
C	-5.500082000	-4.415037000	-0.021945000	C	-1.776462000	-1.363690000	0.054372000
H	-6.471158000	2.573901000	-0.314044000	C	1.035085000	-1.217840000	-0.065450000
H	-7.325265000	0.320285000	-0.386631000	C	-0.974405000	-2.541379000	0.110075000
H	-6.572727000	-4.569221000	-0.052724000	C	0.417839000	-2.463207000	0.066770000
H	-5.019116000	-6.502041000	0.001691000	H	0.746217000	0.883563000	-0.203761000
H	-2.538039000	-6.091801000	0.052101000	H	1.005510000	-3.372671000	0.124283000
O	-7.212384000	-2.254284000	-0.120107000	C	-1.598185000	-3.879734000	0.213037000
H	-7.718492000	-1.447474000	0.033031000	C	-3.085251000	-3.920743000	0.221756000
O	-0.363228000	2.742989000	0.809198000	C	-3.718772000	-5.150670000	0.316370000
H	0.015787000	3.603263000	0.470604000	C	-5.122445000	-5.240795000	0.324570000
C	2.608977000	-0.647979000	-0.061938000	C	-5.888248000	-4.096119000	0.230646000
O	3.416758000	-1.568650000	-0.064345000	H	-6.222474000	2.925258000	-0.464325000
O	2.902034000	0.636609000	-0.167779000	H	-7.283336000	0.760980000	-0.390807000
H	3.919770000	0.810801000	-0.246834000	H	-6.971107000	-4.150259000	0.234390000
C	-4.749147000	4.557818000	-0.096230000	H	-5.602538000	-6.211991000	0.403903000
O	-5.955041000	4.598551000	-0.286466000	H	-3.093662000	-6.035307000	0.384261000
O	-4.043785000	5.720273000	-0.002867000	O	-7.396343000	-1.792371000	0.023708000
H	-4.703431000	6.422743000	-0.115192000	H	-7.814318000	-0.930457000	0.138152000
O	-0.490527000	-4.769240000	0.071970000	O	-0.066018000	2.576462000	0.255361000
C	6.582630000	-0.739359000	0.391208000	H	0.522754000	3.524324000	0.037474000
H	5.689125000	-1.251305000	0.743149000	C	2.525272000	-1.088066000	-0.123846000
C	6.277016000	0.126535000	-0.821862000	O	3.298884000	-2.015263000	0.061079000
H	5.804490000	-0.476088000	-1.604350000	O	2.894772000	0.165329000	-0.398273000
H	7.196423000	0.580986000	-1.200519000	H	3.872257000	0.349513000	-0.306989000
O	5.358078000	1.140283000	-0.447084000	C	-4.319163000	4.750461000	-0.395536000
Br	7.882439000	-2.177170000	-0.093369000	O	-5.525143000	4.894976000	-0.531586000
H	7.063163000	-0.147249000	1.167039000	O	-3.514143000	5.850661000	-0.372687000
C	5.918320000	2.342175000	0.340509000	H	-4.119419000	6.600947000	-0.481261000
O	7.136748000	2.308005000	0.484290000	O	-0.930743000	-4.914088000	0.286108000
O	4.991454000	3.085229000	0.658585000	C	6.542255000	-0.897425000	0.154785000
C	1.867187000	3.801388000	-1.205800000	H	5.636124000	-1.503297000	0.182708000
C	2.457734000	4.018100000	0.110309000	C	6.390650000	0.317784000	-0.749340000
O	1.136027000	4.577802000	-0.217528000	H	6.125049000	0.011770000	-1.765825000
H	2.207695000	4.381622000	-2.061230000	H	7.316279000	0.896988000	-0.765390000
H	1.444982000	2.824438000	-1.433656000	O	5.313305000	1.131592000	-0.276924000
H	3.243244000	4.751923000	0.244578000	Br	7.982988000	-2.076381000	-0.550353000
H	2.457386000	3.198083000	0.819808000	H	6.855924000	-0.590266000	1.150025000

## TS4

SCF Energy (B3LYP-D3/B2) = -4633.88769566

Enthalpy 0K = 0.458487

Enthalpy 298 K = 0.496576

Free Energy 298 K = 0.383687

C	-1.354840000	2.435724000	0.041683000
C	-1.948273000	1.129804000	-0.032787000
C	-2.177154000	3.565216000	-0.098980000

H	1.812874000	3.728332000	1.898962000
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## Pdt2

SCF Energy (B3LYP-D3/B2) = -4633.94012845  
 Enthalpy 0K = 0.465666  
 Enthalpy 298 K = 0.502805  
 Free Energy 298 K = 0.391248

C	-1.290483000	2.433561000	-0.447255000
C	-1.909220000	1.117942000	-0.354040000
C	-2.158680000	3.561409000	-0.341265000
C	-3.320735000	1.020029000	-0.161697000
C	-3.530014000	3.469844000	-0.177608000
C	-4.156778000	2.187412000	-0.089823000
H	-1.672545000	4.527836000	-0.391755000
C	-5.572421000	2.024284000	0.027456000
C	-6.151738000	0.797586000	0.136439000
C	-5.360781000	-0.395646000	0.156202000
C	-3.933092000	-0.286986000	-0.023734000
C	-5.939845000	-1.653991000	0.349405000
C	-3.146663000	-1.463076000	-0.046723000
C	-5.171074000	-2.841876000	0.330489000
C	-3.759779000	-2.738643000	0.123315000
C	-1.115145000	-0.100106000	-0.425929000
C	0.273385000	-0.070215000	-0.665329000
C	-1.724606000	-1.376423000	-0.246267000
C	1.052815000	-1.227216000	-0.659084000
C	-0.919879000	-2.553741000	-0.266793000
C	0.458717000	-2.474004000	-0.447694000
H	0.724370000	0.893053000	-0.836914000
H	1.050977000	-3.381826000	-0.428829000
C	-1.521048000	-3.894720000	-0.088784000
C	-2.992079000	-3.939287000	0.110006000
C	-3.604339000	-5.171444000	0.290349000
C	-4.992354000	-5.262600000	0.495562000
C	-5.762875000	-4.116920000	0.518489000
H	-6.188906000	2.911447000	0.029527000
H	-7.237862000	0.739793000	0.169027000
H	-6.833725000	-4.170709000	0.680634000
H	-5.456845000	-6.234241000	0.639424000
H	-2.974169000	-6.054877000	0.271525000
O	-7.284701000	-1.807185000	0.569318000
H	-7.657829000	-0.947341000	0.799310000
O	-0.037725000	2.627391000	-0.613469000
H	0.886562000	4.010606000	-0.579867000
C	2.523724000	-1.117635000	-0.799362000
O	3.326415000	-2.005072000	-0.550933000
O	2.908804000	0.111726000	-1.215326000
H	3.860808000	0.225691000	-1.057722000
C	-4.300434000	4.739188000	-0.073668000
O	-5.465144000	4.885796000	0.268274000
O	-3.561798000	5.837793000	-0.403762000
H	-4.163931000	6.585301000	-0.262876000
O	-0.842905000	-4.926448000	-0.103264000
C	6.324681000	-0.880941000	0.338005000
H	5.473615000	-1.433861000	-0.061687000
C	6.474603000	0.499644000	-0.284762000
H	6.584440000	0.432394000	-1.368824000
H	7.328365000	1.028017000	0.143497000
O	5.271556000	1.283203000	-0.083189000
Br	7.947910000	-1.930826000	-0.094384000
H	6.275791000	-0.815384000	1.422397000
C	5.138132000	1.822470000	1.174481000
O	5.907771000	1.589374000	2.078782000
O	4.095412000	2.623924000	1.296186000

C	3.266645000	3.035667000	0.162390000
C	2.352567000	4.154744000	0.663950000
O	1.601300000	4.676940000	-0.399368000
H	3.907790000	3.395753000	-0.646944000
H	2.680281000	2.186536000	-0.187862000
H	2.972176000	4.955706000	1.089053000
H	1.724660000	3.755605000	1.476024000

### Pdt2-CO<sub>2</sub>-TS

SCF Energy (B3LYP-D3/B2) = -4822.57922090  
 Enthalpy 0K = 0.515186  
 Enthalpy 298 K = 0.502805  
 Free Energy 298 K = 0.397940

C	-1.215378000	2.108845000	0.003370000
C	-1.931003000	0.869420000	-0.097247000
C	-1.938589000	3.318698000	-0.022626000
C	-3.357502000	0.897721000	-0.074793000
C	-3.327280000	3.351995000	-0.080883000
C	-4.075868000	2.139090000	-0.083941000
H	-1.360339000	4.235070000	-0.034242000
C	-5.510558000	2.108040000	-0.080460000
C	-6.201108000	0.939030000	-0.027045000
C	-5.530809000	-0.327130000	0.032783000
C	-4.090739000	-0.349578000	-0.021269000
C	-6.235702000	-1.530016000	0.148460000
C	-3.411625000	-1.590033000	0.004140000
C	-5.574107000	-2.783082000	0.177974000
C	-4.147249000	-2.805566000	0.095195000
C	-1.245114000	-0.415024000	-0.183759000
C	0.141629000	-0.504771000	-0.388252000
C	-1.975927000	-1.631324000	-0.088223000
C	0.819811000	-1.722143000	-0.387252000
C	-1.276904000	-2.874637000	-0.098705000
C	0.111999000	-2.914453000	-0.216936000
H	0.696848000	0.403277000	-0.529687000
H	0.620577000	-3.871692000	-0.189153000
C	-2.007451000	-4.157032000	0.022210000
C	-3.488493000	-4.069965000	0.115801000
C	-4.221496000	-5.242870000	0.220542000
C	-5.624738000	-5.211042000	0.309697000
C	-6.290708000	-4.001694000	-0.289259000
H	-6.039874000	3.048173000	-0.136783000
H	-7.288068000	0.986370000	-0.060118000
H	-7.372136000	-3.962478000	0.357071000
H	-6.183533000	-6.138734000	0.394373000
H	-3.674215000	-6.180069000	0.231943000
O	-7.599631000	-1.572247000	0.240428000
H	-7.935270000	-0.677430000	0.372203000
O	0.091500000	2.124624000	0.115638000
H	0.657424000	3.096678000	0.326766000
C	2.302238000	-1.703811000	-0.480606000
O	3.041738000	-2.641288000	-0.226221000
O	2.756927000	-0.487203000	-0.854551000
H	3.706601000	-0.395805000	-0.668139000
C	-3.982042000	4.689224000	-0.145824000
O	-5.134984000	4.937164000	-0.466415000
O	-3.139655000	5.698340000	0.195364000
H	-3.648780000	6.512877000	0.059109000
O	-1.425826000	-5.244979000	0.041563000
C	6.243009000	-1.560450000	0.255753000

H	5.313107000	-2.093023000	0.049120000
C	6.314374000	-0.208701000	-0.440458000
H	6.189611000	-0.312431000	-1.519904000
H	7.256806000	0.294660000	-0.219797000
O	5.208109000	0.629769000	-0.017809000
Br	7.711556000	-2.693506000	-0.434963000
H	6.407615000	-1.453800000	1.325715000
C	5.375591000	1.233656000	1.206783000
O	6.328617000	1.021220000	1.921093000
O	4.401004000	2.064612000	1.526350000
C	3.302452000	2.421883000	0.627034000
C	2.598485000	3.601116000	1.305137000
O	1.463576000	4.024509000	0.591458000
H	3.697201000	2.719526000	-0.346096000
H	2.637130000	1.564473000	0.513915000
H	3.311403000	4.430106000	1.381048000
H	2.305992000	3.302233000	2.322075000
C	1.763986000	4.956417000	-0.898114000
O	2.949843000	5.159662000	-0.983785000
O	0.673574000	5.107550000	-1.382137000

### Pdt2-CO<sub>2</sub>

SCF Energy (B3LYP-D3/B2) = -4822.58082797

Enthalpy 0K = 0.479445

Enthalpy 298 K = 0.519231

Free Energy 298 K = 0.402435

C	-1.254491000	2.113867000	0.105903000
C	-1.949659000	0.875980000	-0.024644000
C	-1.951451000	3.326073000	-0.001378000
C	-3.375312000	0.905061000	-0.077134000
C	-3.336245000	3.357391000	-0.144019000
C	-4.086253000	2.147370000	-0.149417000
H	-1.360769000	4.236564000	-0.022694000
C	-5.521563000	2.118231000	-0.207487000
C	-6.214164000	0.951166000	-0.154563000
C	-5.550217000	-0.315337000	-0.040428000
C	-4.109948000	-0.340499000	-0.033839000
C	-6.260927000	-1.515475000	0.069292000
C	-3.432888000	-1.579641000	0.040012000
C	-5.601425000	-2.768347000	0.147148000
C	-4.172626000	-2.792994000	0.118999000
C	-1.259159000	-0.409204000	-0.080231000
C	0.130143000	-0.500385000	-0.258010000
C	-1.994579000	-1.622945000	-0.001429000
C	0.806651000	-1.718184000	-0.245843000
C	-1.296794000	-2.866589000	0.013891000
C	0.094033000	-2.908297000	-0.079668000
H	0.695581000	0.401590000	-0.395319000
H	0.601202000	-3.865881000	-0.039277000
C	-2.032511000	-4.146867000	0.131269000
C	-3.515881000	-4.057315000	0.178935000
C	-4.253688000	-5.227829000	0.274106000
C	-5.659259000	-5.193771000	0.313548000
C	-6.322982000	-3.984712000	0.250415000
H	-6.046006000	3.057283000	-0.309539000
H	-7.298986000	0.999104000	-0.230195000
H	-7.406120000	-3.944361000	0.277089000
H	-6.221577000	-6.119810000	0.391598000
H	-3.708634000	-6.165452000	0.316243000
O	-7.626238000	-1.557309000	0.107042000

H	-7.970158000	-0.660217000	0.194286000
O	0.055260000	2.105796000	0.334579000
H	0.525134000	3.008208000	0.452879000
C	2.290837000	-1.701743000	-0.336248000
O	3.026834000	-2.644836000	-0.094547000
O	2.743320000	-0.482623000	-0.697815000
H	3.698945000	-0.390841000	-0.539287000
C	-3.982976000	4.692557000	-0.292189000
O	-5.107358000	4.926145000	-0.709501000
O	-3.168446000	5.705873000	0.090996000
H	-3.652484000	6.521356000	-0.113907000
O	-1.452979000	-5.234396000	0.182522000
C	6.274375000	-1.571565000	0.180890000
H	5.327450000	-2.099924000	0.057117000
C	6.307409000	-0.242263000	-0.560030000
H	6.101297000	-0.376250000	-1.623452000
H	7.268323000	0.256226000	-0.424930000
O	5.244028000	0.621688000	-0.081925000
Br	7.678305000	-2.742268000	-0.577561000
H	6.516365000	-1.434359000	1.232545000
C	5.509053000	1.265005000	1.105927000
O	6.507440000	1.058402000	1.757040000
O	4.571726000	2.121518000	1.464680000
C	3.425522000	2.480009000	0.625622000
C	2.781040000	3.679997000	1.321352000
O	1.575998000	4.062626000	0.692292000
H	3.761905000	2.760058000	-0.373732000
H	2.741273000	1.631179000	0.570605000
H	3.490092000	4.513798000	1.310636000
H	2.552359000	3.413920000	2.360928000
C	1.704709000	4.849362000	-0.652538000
O	2.866097000	5.107249000	-0.951175000
O	0.578255000	5.015934000	-1.107472000

### Int4-COOH

SCF Energy (B3LYP-D3/B2) = -4633.88219295

Enthalpy 0K = 0.461945

Enthalpy 298 K = 0.500305

Free Energy 298 K = 0.381385

C	1.531318000	2.455967000	0.368508000
C	2.337320000	1.294849000	0.204056000
C	2.091574000	3.722735000	0.442752000
C	3.755944000	1.504538000	0.141082000
C	3.467294000	3.939768000	0.365363000
C	4.328243000	2.823161000	0.213307000
H	1.429248000	4.572612000	0.565973000
C	5.755594000	2.974684000	0.118556000
C	6.573613000	1.902518000	-0.005040000
C	6.064490000	0.565269000	-0.046077000
C	4.637318000	0.364012000	0.004465000
C	6.921059000	-0.535281000	-0.140369000
C	4.115495000	-0.943624000	-0.075088000
C	6.418631000	-1.857503000	-0.228534000
C	5.004713000	-2.054608000	-0.201948000
C	1.794755000	-0.062097000	0.101118000
C	0.408951000	-0.343658000	0.121699000
C	2.691639000	-1.163314000	-0.035455000
C	-0.086820000	-1.639265000	0.019861000
C	2.167850000	-2.483910000	-0.135484000
C	0.796548000	-2.711193000	-0.107141000

H	-0.308694000	0.450501000	0.216869000
H	0.418216000	-3.724106000	-0.185242000
C	3.057338000	-3.660311000	-0.273961000
C	4.516235000	-3.388572000	-0.296272000
C	5.392220000	-4.457351000	-0.409641000
C	6.782783000	-4.251945000	-0.430250000
C	7.289098000	-2.971709000	-0.339365000
H	6.163662000	3.973558000	0.144894000
H	7.641286000	2.089398000	-0.100528000
H	8.358447000	-2.795219000	-0.352275000
H	7.455598000	-5.099900000	-0.516409000
H	4.965001000	-5.452554000	-0.479259000
O	8.278835000	-0.414713000	-0.160550000
H	8.531362000	0.493350000	0.043822000
O	0.177042000	2.342119000	0.460683000
H	-0.217054000	3.217779000	0.562750000
C	-1.564505000	-1.909764000	0.043937000
O	-2.015814000	-3.044175000	-0.046903000
O	-2.290957000	-0.810596000	0.170296000
H	-3.288238000	-1.043798000	0.185302000
C	3.951638000	5.343704000	0.453476000
O	5.104318000	5.741857000	0.420212000
O	2.930683000	6.237236000	0.586753000
H	3.359344000	7.106423000	0.635195000
O	2.619406000	-4.807452000	-0.364267000
C	-7.365502000	0.889841000	-0.171525000
H	-6.317456000	0.596024000	-0.201698000
C	-8.270870000	-0.219337000	-0.693642000
H	-8.049817000	-0.422921000	-1.749299000
H	-9.318503000	0.083411000	-0.590432000
O	-7.990859000	-1.390909000	0.037816000
Br	-7.515988000	2.547031000	-1.296023000
H	-7.671444000	1.178744000	0.831565000
C	-8.542318000	-1.431567000	1.422402000
O	-9.308348000	-0.502746000	1.712053000
O	-8.101520000	-2.412629000	2.038097000
C	-5.167389000	-2.554034000	0.934986000
C	-5.189493000	-2.522041000	-0.529230000
O	-4.792494000	-1.334426000	0.212465000
H	-6.116867000	-2.482455000	1.471514000
H	-4.316369000	-3.036725000	1.412885000
H	-6.156592000	-2.412045000	-1.009901000
H	-4.372456000	-2.986463000	-1.077459000

## TS4-COOH

SCF Energy (B3LYP-D3/B2) = -4633.86534337

Enthalpy 0K = 0.458530

Enthalpy 298 K = 0.496205

Free Energy 298 K = 0.379366

C	-2.935833000	2.842692000	-0.283445000
C	-3.367833000	1.491303000	-0.165341000
C	-3.821875000	3.901240000	-0.155810000
C	-4.775048000	1.287084000	0.032579000
C	-5.185567000	3.714982000	0.078890000
C	-5.687682000	2.391864000	0.169295000
H	-3.435140000	4.910675000	-0.244682000
C	-7.081783000	2.124219000	0.403164000
C	-7.560356000	0.857995000	0.450814000
C	-6.708861000	-0.278585000	0.270476000
C	-5.293960000	-0.062869000	0.089268000

C	-7.221650000	-1.578154000	0.273592000
C	-4.431751000	-1.170323000	-0.041941000
C	-6.374223000	-2.706631000	0.146143000
C	-4.969941000	-2.493393000	-0.002683000
C	-2.465256000	0.341663000	-0.244281000
C	-1.058546000	0.466132000	-0.346870000
C	-3.011657000	-0.975243000	-0.196912000
C	-0.217228000	-0.637353000	-0.423551000
C	-2.139148000	-2.096544000	-0.291962000
C	-0.763468000	-1.921048000	-0.405319000
H	-0.588793000	1.432999000	-0.365116000
H	-0.112262000	-2.785216000	-0.473104000
C	-2.659842000	-3.481932000	-0.270998000
C	-4.130236000	-3.636754000	-0.120182000
C	-4.667057000	-4.914564000	-0.093871000
C	-6.052002000	-5.113131000	0.046197000
C	-6.893713000	-4.026292000	0.163300000
H	-7.744463000	2.964598000	0.543429000
H	-8.619539000	0.724057000	0.661468000
H	-7.963748000	-4.161137000	0.271876000
H	-6.456859000	-6.120737000	0.062085000
H	-3.980436000	-5.749957000	-0.186163000
O	-8.553883000	-1.846037000	0.403690000
H	-9.060179000	-1.029638000	-0.318866000
O	-1.626012000	3.122706000	-0.536516000
H	-1.506201000	4.079641000	-0.581046000
C	1.284644000	-0.468685000	-0.529904000
O	2.006528000	-1.462203000	-0.601324000
O	1.670577000	0.777292000	-0.532748000
H	2.801522000	0.901230000	-0.656798000
C	-6.036356000	4.925605000	0.209554000
O	-7.240473000	4.981406000	0.401166000
O	-5.319985000	6.081819000	0.090475000
H	-5.973799000	6.791504000	0.191824000
O	-1.925517000	-4.464761000	-0.373510000
C	10.086864000	-0.098963000	-0.326725000
H	9.823308000	0.019019000	-1.377671000
C	9.075395000	0.579875000	0.588247000
H	9.037214000	1.655240000	0.382250000
H	9.363258000	0.415050000	1.631342000
O	7.787819000	0.060042000	0.317749000
Br	11.895344000	0.725639000	-0.122535000
H	10.192562000	-1.147287000	-0.057921000
C	7.511586000	-1.248482000	0.883317000
O	8.423845000	-1.792854000	1.510995000
O	6.342555000	-1.627339000	0.622697000
C	5.039631000	-0.284553000	-0.458602000
C	4.711942000	0.784247000	0.461025000
O	4.049545000	1.153426000	-0.753874000
H	5.858043000	-0.141407000	-1.143120000
H	4.349975000	-1.108633000	-0.570183000
H	5.520890000	1.454947000	0.755366000
H	4.042487000	0.537319000	1.290826000

## Pdt2-COOH

SCF Energy (B3LYP-D3/B2) = -4633.91603260

Enthalpy 0K = 0.465059

Enthalpy 298 K = 0.502562

Free Energy 298 K = 0.386749

C	-3.191794000	2.860069000	-0.275113000
C	-3.491504000	1.472251000	-0.151536000

C	-4.178039000	3.827704000	-0.166287000
C	-4.877648000	1.134120000	0.011879000
C	-5.522570000	3.511119000	0.047113000
C	-5.895650000	2.145378000	0.128315000
H	-3.889208000	4.869456000	-0.254798000
C	-7.261736000	1.742552000	0.332973000
C	-7.617373000	0.435642000	0.363550000
C	-6.656814000	-0.612625000	0.194182000
C	-5.264575000	-0.259251000	0.052219000
C	-7.042473000	-1.954140000	0.170980000
C	-4.295218000	-1.276458000	-0.059691000
C	-6.087247000	-2.994401000	0.060918000
C	-4.705701000	-2.645193000	-0.042525000
C	-2.478245000	0.419028000	-0.196463000
C	-1.085757000	0.679803000	-0.241567000
C	-2.896147000	-0.945297000	-0.169807000
C	-0.134793000	-0.331211000	-0.290983000
C	-1.914616000	-1.974975000	-0.237744000
C	-0.557988000	-1.660796000	-0.301786000
H	-0.697498000	1.683586000	-0.234755000
H	0.182234000	-2.451373000	-0.351857000
C	-2.299338000	-3.401261000	-0.239239000
C	-3.754718000	-3.699728000	-0.139279000
C	-4.165628000	-5.023411000	-0.138482000
C	-5.528813000	-5.356688000	-0.045673000
C	-6.476128000	-4.358356000	0.051584000
H	-8.004828000	2.514361000	0.464894000
H	-8.661748000	0.196964000	0.555440000
H	-7.531045000	-4.597315000	0.124177000
H	-5.834100000	-6.399208000	-0.050346000
H	-3.397797000	-5.786824000	-0.213124000
O	-8.349902000	-2.347981000	0.258762000
H	-8.923989000	-1.583846000	0.130314000
O	-1.913233000	3.261644000	-0.517311000
H	-1.883323000	4.225474000	-0.562273000
C	1.362553000	0.015273000	-0.337899000
O	2.148181000	-0.954239000	-0.404198000
O	1.620735000	1.256664000	-0.301676000
H	3.153296000	1.777897000	-0.569963000
C	-6.487114000	4.631597000	0.162512000
O	-7.694868000	4.574014000	0.336553000
O	-5.885931000	5.854515000	0.051924000
H	-6.610527000	6.493065000	0.143078000
O	-1.475385000	-4.314202000	-0.319164000
C	9.978546000	-0.415104000	-0.314758000
H	9.718363000	-0.632981000	-1.350198000
C	9.158463000	0.741008000	0.239413000
H	9.309876000	1.647101000	-0.350106000
H	9.422320000	0.925878000	1.283453000
O	7.764557000	0.434484000	0.121235000
Br	11.901371000	0.065193000	-0.304630000
H	9.872790000	-1.299594000	0.309594000
C	7.270617000	-0.421589000	1.070815000
O	7.961205000	-0.926445000	1.932939000
O	5.980379000	-0.652657000	0.935491000
C	5.170366000	0.047604000	-0.073879000
C	4.807149000	1.461428000	0.386329000
O	4.094029000	2.117346000	-0.624453000
H	5.715090000	0.087461000	-1.019132000
H	4.262989000	-0.551810000	-0.178548000
H	5.729129000	2.023741000	0.594867000
H	4.241462000	1.386515000	1.330082000

## Int1'

SCF Energy (B3LYP-D3/B2) = -4291.37237400  
 Enthalpy 0K = 0.387071  
 Enthalpy 298 K = 0.418635  
 Free Energy 298 K = 0.316815

C	-3.409041000	2.642188000	0.260036000
C	-2.712242000	1.419418000	0.076564000
C	-2.764245000	3.864426000	0.164679000
C	-1.300202000	1.511478000	-0.171414000
C	-1.400688000	3.973609000	-0.108136000
C	-0.636019000	2.786595000	-0.275472000
H	-3.346875000	4.768722000	0.306254000
C	0.772742000	2.820615000	-0.542305000
C	1.500085000	1.681823000	-0.671735000
C	0.897967000	0.391943000	-0.549485000
C	-0.518238000	0.300327000	-0.316927000
C	1.676488000	-0.782121000	-0.665792000
C	-1.142299000	-0.967723000	-0.229321000
C	1.049736000	-2.066844000	-0.578243000
C	-0.356640000	-2.152815000	-0.367174000
C	-3.358042000	0.104505000	0.132329000
C	-4.743955000	-0.067827000	0.309816000
C	-2.554904000	-1.071461000	-0.014665000
C	-5.337262000	-1.330636000	0.360256000
C	-3.177639000	-2.354000000	0.048012000
C	-4.548145000	-2.475935000	0.234570000
H	-5.396494000	0.781884000	0.410941000
H	-4.975984000	-3.470476000	0.274741000
C	-2.395008000	-3.606614000	-0.085693000
C	-0.941864000	-3.449984000	-0.293793000
C	-0.156258000	-4.589884000	-0.417901000
C	1.228479000	-4.492812000	-0.615021000
C	1.822404000	-3.246452000	-0.693668000
H	1.253550000	3.781709000	-0.638166000
H	2.561649000	1.764583000	-0.868489000
H	2.891207000	-3.146019000	-0.841993000
H	1.832135000	-5.390915000	-0.703125000
H	-0.654098000	-5.552248000	-0.353598000
O	2.983667000	-0.802267000	-0.878996000
H	3.525117000	0.053684000	-0.747842000
O	-4.751386000	2.641214000	0.541971000
H	-5.044757000	3.555199000	0.642407000
C	-6.805041000	-1.394578000	0.548261000
O	-7.547359000	-0.434653000	0.658069000
O	-7.281632000	-2.668590000	0.589922000
H	-8.239945000	-2.580982000	0.714945000
C	-0.826385000	5.339231000	-0.204592000
O	0.319200000	5.657292000	-0.472687000
O	-1.753587000	6.315459000	0.046407000
H	-1.262579000	7.146755000	-0.049641000
O	-2.932629000	-4.716632000	-0.026106000
C	5.973635000	0.452202000	-0.462572000
H	6.762861000	1.093697000	-0.831126000
H	5.985685000	-0.575524000	-0.802922000
C	5.293849000	0.782602000	0.770660000
H	5.607545000	1.654109000	1.339703000
H	4.839326000	-0.016868000	1.352632000
O	4.603810000	1.099642000	-0.481023000
Br	8.507239000	-0.706477000	0.775063000

## TS1'

SCF Energy (B3LYP-D3/B2) = -4291.36850202

Enthalpy 0K = 0.385269

Enthalpy 298 K = 0.416182

Free Energy 298 K = 0.316360

C	-3.304114000	2.658057000	0.325006000
C	-2.626488000	1.432289000	0.095406000
C	-2.656432000	3.876552000	0.208210000
C	-1.227079000	1.516407000	-0.219477000
C	-1.307281000	3.979597000	-0.131475000
C	-0.559436000	2.788350000	-0.345552000
H	-3.225077000	4.783330000	0.386543000
C	0.834110000	2.814559000	-0.679115000
C	1.545663000	1.670403000	-0.851456000
C	0.941309000	0.384909000	-0.710745000
C	-0.461271000	0.300976000	-0.410990000
C	1.712285000	-0.794603000	-0.874613000
C	-1.091553000	-0.963809000	-0.301618000
C	1.073062000	-2.076498000	-0.761642000
C	-0.321743000	-2.153558000	-0.483680000
C	-3.279388000	0.121808000	0.169355000
C	-4.657044000	-0.041686000	0.405450000
C	-2.491581000	-1.050973000	-0.022616000
C	-5.257872000	-1.300771000	0.473193000
C	-3.121395000	-2.338020000	0.059950000
C	-4.483143000	-2.450745000	0.306159000
H	-5.298054000	0.812141000	0.540273000
H	-4.916051000	-3.442527000	0.358956000
C	-2.355513000	-3.595061000	-0.116476000
C	-0.912726000	-3.447054000	-0.390324000
C	-0.142037000	-4.592242000	-0.557504000
C	1.231767000	-4.503924000	-0.819210000
C	1.829286000	-3.259948000	-0.919712000
H	1.317459000	3.772741000	-0.790108000
H	2.598364000	1.743064000	-1.096545000
H	2.890296000	-3.163135000	-1.118263000
H	1.824462000	-5.405656000	-0.940013000
H	-0.643973000	-5.551127000	-0.474838000
O	2.997190000	-0.819160000	-1.151169000
H	3.609652000	0.045439000	-1.041839000
O	-4.631254000	2.663855000	0.675064000
H	-4.910324000	3.579168000	0.800500000
C	-6.715659000	-1.355511000	0.723444000
O	-7.447096000	-0.391789000	0.870712000
O	-7.200408000	-2.626758000	0.778243000
H	-8.151512000	-2.530966000	0.944918000
C	-0.729935000	5.341083000	-0.245893000
O	0.402321000	5.655922000	-0.570370000
O	-1.636290000	6.322419000	0.060951000
H	-1.143199000	7.149987000	-0.053914000
O	-2.898114000	-4.702257000	-0.039078000
C	6.030151000	0.238709000	-0.455598000
H	6.837492000	0.796357000	-0.901317000
H	5.926348000	-0.810370000	-0.684754000
C	5.137472000	0.864980000	0.491934000
H	5.443967000	1.801364000	0.957669000
H	4.560452000	0.218930000	1.156075000
O	4.601134000	1.012324000	-0.841652000
Br	8.113696000	-0.715778000	1.140931000

## Int2'

SCF Energy (B3LYP-D3/B2) = -4480.08079444

Enthalpy 0K = 0.401711

Enthalpy 298 K = 0.436654

Free Energy 298 K = 0.328749

C	-1.532187000	3.313750000	-0.236137000
C	-1.491427000	1.943950000	0.134266000
C	-0.431367000	4.140051000	-0.082963000
C	-0.242337000	1.453230000	0.647467000
C	0.780334000	3.691626000	0.446515000
C	0.893713000	2.324708000	0.839239000
H	-0.516500000	5.176365000	-0.394927000
C	2.083998000	1.796975000	1.427097000
C	2.192147000	0.468245000	1.717697000
C	1.137889000	-0.439490000	1.457733000
C	-0.105086000	0.048043000	0.968281000
C	1.369761000	-1.852555000	1.683695000
C	-1.200434000	-0.843657000	0.781064000
C	0.221999000	-2.744224000	1.513865000
C	-1.034305000	-2.235749000	1.075639000
C	-2.634590000	1.032854000	0.010454000
C	-3.913416000	1.453485000	-0.386749000
C	-2.454492000	-0.359599000	0.326838000
C	-4.992006000	0.567233000	-0.503013000
C	-3.565512000	-1.254219000	0.187658000
C	-4.807597000	-0.789489000	-0.222155000
H	-4.106479000	2.487770000	-0.614339000
H	-5.617800000	-1.503756000	-0.309741000
C	-3.438966000	-2.699581000	0.480564000
C	-2.109685000	-3.158783000	0.926605000
C	-1.923431000	-4.513627000	1.201590000
C	-0.683003000	-4.998927000	1.623284000
C	0.378543000	-4.114365000	1.772814000
H	2.902061000	2.468042000	1.636516000
H	3.102489000	0.083002000	2.158292000
H	1.360116000	-4.448886000	2.093389000
H	-0.549847000	-6.057352000	1.829776000
H	-2.778255000	-5.170315000	1.071816000
O	2.505062000	-2.314627000	1.991635000
H	3.870086000	-1.712702000	1.173603000
O	-2.676253000	3.853624000	-0.777476000
H	-2.503220000	4.780233000	-0.983587000
C	-6.293452000	1.118186000	-0.923643000
O	-6.529000000	2.289432000	-1.175188000
O	-7.275112000	0.173336000	-1.016836000
H	-8.064186000	0.662539000	-1.297978000
C	1.895064000	4.654470000	0.537204000
O	3.047758000	4.450765000	0.888169000
O	1.532844000	5.924836000	0.156411000
H	2.351289000	6.437588000	0.244819000
O	-4.394998000	-3.478034000	0.357652000
C	4.318337000	-1.972042000	-0.710586000
H	4.104990000	-3.049084000	-0.644651000
H	5.214350000	-1.845205000	-1.328159000
C	3.143596000	-1.264163000	-1.383955000
H	2.202941000	-1.426824000	-0.862161000
H	3.330971000	-0.198517000	-1.496142000
O	4.578693000	-1.404596000	0.553583000
Br	2.870252000	-1.983639000	-3.222632000
C	5.237116000	1.255920000	0.494438000
O	5.367301000	1.302541000	1.655589000
O	5.149074000	1.279089000	-0.672692000

## TS2'

SCF Energy (B3LYP-D3/B2) = -4480.05396688

Enthalpy 0K = 0.399740

Enthalpy 298 K = 0.433031

Free Energy 298 K = 0.329311

C	-3.632365000	2.521315000	0.540044000
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C	-2.907983000	1.352787000	0.191871000
C	-3.050143000	3.776642000	0.482496000
C	-1.530069000	1.532008000	-0.173387000
C	-1.726702000	3.974772000	0.087718000
C	-0.930020000	2.842581000	-0.246238000
H	-3.652439000	4.637840000	0.753212000
C	0.436386000	2.963855000	-0.660422000
C	1.202516000	1.871669000	-0.923745000
C	0.670593000	0.552350000	-0.801556000
C	-0.713751000	0.374692000	-0.472519000
C	1.503292000	-0.573253000	-1.033584000
C	-1.277089000	-0.927471000	-0.437964000
C	0.925478000	-1.889631000	-1.034249000
C	-0.458858000	-2.058047000	-0.739463000
C	-3.493457000	0.007657000	0.190522000
C	-4.850105000	-0.242898000	0.463776000
C	-2.658898000	-1.114333000	-0.124584000
C	-5.389343000	-1.532582000	0.448476000
C	-3.225647000	-2.425927000	-0.129382000
C	-4.570144000	-2.625024000	0.155048000
H	-5.523567000	0.564845000	0.692778000
H	-4.954815000	-3.637740000	0.137970000
C	-2.410576000	-3.623846000	-0.441098000
C	-0.985904000	-3.382527000	-0.742754000
C	-0.167151000	-4.470129000	-1.027508000
C	1.193501000	-4.292557000	-1.311606000
C	1.730270000	-3.016485000	-1.310185000
H	0.860126000	3.950725000	-0.763109000
H	2.225503000	2.016253000	-1.253504000
H	2.779869000	-2.849185000	-1.523510000
H	1.823290000	-5.150704000	-1.527264000
H	-0.621590000	-5.455909000	-1.017274000
O	2.790248000	-0.486218000	-1.275046000
H	3.346012000	0.317796000	-0.786561000
O	-4.940985000	2.434333000	0.950851000
H	-5.256336000	3.324736000	1.148311000
C	-6.829903000	-1.680407000	0.747980000
O	-7.600713000	-0.771317000	1.004848000
O	-7.254060000	-2.975174000	0.713138000
H	-8.200594000	-2.937327000	0.922987000
C	-1.225527000	5.369478000	0.047200000
O	-0.127001000	5.768324000	-0.297402000
O	-2.168103000	6.279036000	0.459332000
H	-1.719347000	7.135664000	0.382861000
O	-2.898456000	-4.759870000	-0.444779000
C	4.840251000	0.377195000	0.952031000
H	4.110049000	-0.070152000	1.638051000
H	5.490754000	1.054408000	1.513094000
C	5.680394000	-0.707854000	0.288235000
H	5.063270000	-1.389413000	-0.296287000
H	6.463481000	-0.261893000	-0.321720000
O	4.147450000	1.099932000	-0.044624000
Br	6.600695000	-1.831120000	1.653681000
C	5.050943000	2.199338000	-0.937639000
O	4.318374000	2.617307000	-1.809014000
O	6.176006000	2.283529000	-0.490299000

### Int3'

SCF Energy (B3LYP-D3/B2) = -4480.05499711  
 Enthalpy 0K = 0.401353  
 Enthalpy 298 K = 0.435115

### Free Energy 298 K = 0.330897

C	-1.834514000	3.199472000	0.053739000
C	-1.715742000	1.812128000	-0.212202000
C	-0.793949000	4.076140000	-0.208501000
C	-0.442260000	1.353552000	-0.691584000
C	0.425226000	3.656553000	-0.741074000
C	0.631883000	2.270247000	-0.985050000
H	-0.940308000	5.130615000	0.002244000
C	1.865274000	1.758719000	-1.510038000
C	2.075905000	0.424623000	-1.661656000
C	1.069277000	-0.525351000	-1.305848000
C	-0.219523000	-0.063917000	-0.877258000
C	1.336990000	-1.912727000	-1.395773000
C	-1.261004000	-0.992913000	-0.629257000
C	0.275445000	-2.853699000	-1.182653000
C	-1.019364000	-2.387860000	-0.809852000
C	-2.809145000	0.853523000	-0.018680000
C	-4.115863000	1.236373000	0.333505000
C	-2.556699000	-0.541235000	-0.225270000
C	-5.144788000	0.305828000	0.504206000
C	-3.616071000	-1.479290000	-0.034336000
C	-4.888349000	-1.055759000	0.327149000
H	-4.364896000	2.273599000	0.479273000
H	-5.661638000	-1.803075000	0.458851000
C	-3.407072000	-2.935539000	-0.218782000
C	-2.045548000	-3.355925000	-0.606899000
C	-1.781166000	-4.711331000	-0.768359000
C	-0.500866000	-5.158522000	-1.124427000
C	0.514158000	-4.239031000	-1.323261000
H	2.641598000	2.455584000	-1.786094000
H	3.021858000	0.084931000	-2.069357000
H	1.515812000	-4.554463000	-1.592658000
H	-0.306569000	-6.220962000	-1.239052000
H	-2.599498000	-5.405211000	-0.603307000
O	2.524300000	-2.406238000	-1.689935000
H	3.339436000	-1.861025000	-1.306012000
O	-2.993677000	3.708362000	0.586371000
H	-2.875799000	4.656773000	0.720579000
C	-6.483440000	0.818657000	0.869906000
O	-6.777056000	1.991168000	1.027683000
O	-7.410702000	-0.167801000	1.023576000
H	-8.232657000	0.290858000	1.259111000
C	1.445495000	4.696753000	-1.022893000
O	2.504519000	4.571456000	-1.610433000
O	1.081648000	5.930411000	-0.545990000
H	1.816588000	6.510626000	-0.800063000
O	-4.321805000	-3.749848000	-0.052605000
C	4.365876000	-1.502250000	0.864996000
H	5.382131000	-1.570214000	1.264661000
H	3.829778000	-2.436240000	1.072933000
C	3.644769000	-0.319341000	1.500391000
H	4.213611000	0.595612000	1.347807000
H	2.626594000	-0.211289000	1.129178000
O	4.404072000	-1.313498000	-0.533474000
Br	3.486545000	-0.567630000	3.472052000
C	5.464086000	-0.251737000	-1.107903000
O	5.233788000	-0.103568000	-2.297341000
O	6.216256000	0.148819000	-0.234593000

### TS3'

SCF Energy (B3LYP-D3/B2) = -4480.03176775  
 Enthalpy 0K = 0.402455  
 Enthalpy 298 K = 0.435764  
 Free Energy 298 K = 0.330457

C	-3.295884000	2.799910000	0.587969000
C	-2.792692000	1.528182000	0.213193000
C	-2.532259000	3.947717000	0.450427000
C	-1.436800000	1.483491000	-0.257555000
C	-1.232359000	3.928709000	-0.055429000
C	-0.651187000	2.682037000	-0.417036000
H	-2.967976000	4.896712000	0.745314000
C	0.680572000	2.580898000	-0.942269000
C	1.249208000	1.380385000	-1.224383000
C	0.535514000	0.159755000	-1.010045000
C	-0.833333000	0.206881000	-0.574450000
C	1.155158000	-1.083872000	-1.248492000
C	-1.580859000	-0.989750000	-0.453027000
C	0.403487000	-2.295221000	-1.150395000
C	-0.967360000	-2.240643000	-0.762050000
C	-3.578967000	0.292372000	0.287947000
C	-4.939494000	0.264545000	0.647344000
C	-2.953104000	-0.951823000	-0.042221000
C	-5.670368000	-0.924234000	0.705512000
C	-3.712129000	-2.157748000	0.032550000
C	-5.050313000	-2.138587000	0.403360000
H	-5.464127000	1.173267000	0.887485000
H	-5.587157000	-3.078702000	0.444743000
C	-3.111121000	-3.475941000	-0.285055000
C	-1.687796000	-3.467486000	-0.679432000
C	-1.064109000	-4.675489000	-0.966585000
C	0.288483000	-4.718282000	-1.336117000
C	1.012009000	-3.543252000	-1.422644000
H	1.238557000	3.487905000	-1.116265000
H	2.249719000	1.368921000	-1.647109000
H	2.059691000	-3.550735000	-1.699904000
H	0.765792000	-5.670181000	-1.548765000
H	-1.659849000	-5.579496000	-0.888932000
O	2.432756000	-1.221147000	-1.600717000
H	3.040339000	-0.487437000	-1.299619000
O	-4.561096000	2.922025000	1.105920000
H	-4.718541000	3.851747000	1.311603000
C	-7.097298000	-0.837061000	1.091637000
O	-7.698410000	0.188856000	1.357847000
O	-7.715289000	-2.049641000	1.126937000
H	-8.630848000	-1.863038000	1.388739000
C	-0.525130000	5.228899000	-0.178369000
O	0.581813000	5.443080000	-0.637964000
O	-1.269392000	6.276363000	0.299898000
H	-0.705968000	7.053996000	0.161379000
O	-3.766299000	-4.520760000	-0.219590000
C	5.105402000	-0.429491000	0.326217000
H	5.117065000	-1.478832000	0.018741000
H	4.647586000	-0.361889000	1.313088000
C	6.526337000	0.108673000	0.374278000
H	7.318833000	-0.347808000	-0.190671000
H	6.760812000	0.981971000	0.959300000
O	4.270938000	0.316118000	-0.582514000
Br	7.176727000	-1.321790000	2.252724000
C	4.969546000	1.188864000	-1.471946000
O	4.278666000	1.711209000	-2.336528000
O	6.205277000	1.277851000	-1.206046000

**Pdt1'**

SCF Energy (B3LYP-D3/B2) = -4480.08238263

Enthalpy 0K = 0.405251  
 Enthalpy 298 K = 0.437985  
 Free Energy 298 K = 0.338267

C	0.709097000	-3.069024000	-0.173631000
C	1.284763000	-1.775941000	-0.229445000
C	-0.661167000	-3.258164000	-0.314329000
C	0.383939000	-0.685013000	-0.468347000
C	-1.541331000	-2.210304000	-0.546586000
C	-1.021337000	-0.900917000	-0.681886000
H	-1.082117000	-4.257622000	-0.233555000
C	-1.841384000	0.212747000	-1.083342000
C	-1.362572000	1.478809000	-1.093266000
C	-0.019812000	1.762382000	-0.689028000
C	0.886122000	0.670907000	-0.461872000
C	0.415831000	3.086162000	-0.538060000
C	2.251380000	0.934825000	-0.213720000
C	1.791169000	3.368946000	-0.301453000
C	2.710700000	2.283835000	-0.160758000
C	2.717344000	-1.505343000	-0.050923000
C	3.681692000	-2.519789000	0.093232000
C	3.175511000	-0.149680000	-0.029900000
C	5.039099000	-2.236836000	0.269683000
C	4.560774000	0.122129000	0.164013000
C	5.477472000	-0.912174000	0.312063000
H	3.394316000	-3.557411000	0.068298000
H	6.521593000	-0.661282000	0.454549000
C	5.080591000	1.510977000	0.214165000
C	4.083894000	2.593309000	0.060192000
C	4.507207000	3.913727000	0.138761000
C	3.592953000	4.972458000	0.014595000
C	2.253922000	4.702705000	-0.196690000
H	-2.856876000	0.017230000	-1.389849000
H	-1.997856000	2.288894000	-1.425983000
H	1.528259000	5.502824000	-0.289094000
H	3.937622000	5.999742000	0.088941000
H	5.564385000	4.094380000	0.305764000
O	-0.417327000	4.141156000	-0.640708000
H	-1.314397000	3.936590000	-0.284660000
O	1.494837000	-4.168560000	0.053126000
H	0.925811000	-4.948409000	0.074511000
C	5.969105000	-3.382046000	0.406821000
O	5.655053000	-4.558308000	0.371999000
O	7.264273000	-2.999593000	0.582505000
H	7.766478000	-3.826436000	0.658540000
C	-3.003610000	-2.607550000	-0.559394000
O	-3.345093000	-3.767276000	-0.719960000
O	-3.826453000	-1.596520000	-0.314773000
H	-4.813508000	-1.845351000	-0.195445000
O	6.280296000	1.749620000	0.382452000
C	-5.230744000	1.412520000	-0.092625000
H	-5.132404000	0.607303000	-0.814364000
H	-6.236024000	1.833073000	-0.149775000
C	-4.824195000	0.992789000	1.324535000
H	-4.258271000	0.063147000	1.333288000
H	-5.659807000	0.927312000	2.016755000
O	-4.271452000	2.467182000	-0.412489000
Br	-6.816063000	-1.483667000	0.311395000
C	-3.581155000	2.801308000	0.686733000
O	-2.727389000	3.669161000	0.710065000
O	-3.936312000	2.076618000	1.748536000

### Int4'

SCF Energy (B3LYP-D3/B2) = -4633.91672831

Enthalpy 0K = 0.463026

Enthalpy 298 K = 0.500610

Free Energy 298 K = 0.388654

C	-1.322340000	3.343136000	0.216175000
C	-1.579697000	2.006813000	-0.176969000
C	-0.058029000	3.902268000	0.081045000
C	-0.468044000	1.261520000	-0.691512000
C	1.003181000	3.218601000	-0.502114000
C	0.813195000	1.877286000	-0.921571000
H	0.128208000	4.906800000	0.453355000
C	1.856742000	1.097557000	-1.530248000
C	1.714043000	-0.228301000	-1.763822000
C	0.513319000	-0.911231000	-1.401304000
C	-0.616242000	-0.154553000	-0.942981000
C	0.443553000	-2.313527000	-1.483117000
C	-1.849002000	-0.804992000	-0.706963000
C	-0.800368000	-2.980251000	-1.265347000
C	-1.950184000	-2.213850000	-0.900960000
C	-2.890723000	1.357151000	-0.055736000
C	-4.068126000	2.054355000	0.266957000
C	-2.997031000	-0.049610000	-0.298366000
C	-5.303548000	1.410308000	0.388415000
C	-4.258249000	-0.695895000	-0.145043000
C	-5.393448000	0.029756000	0.196042000
H	-4.048930000	3.119595000	0.427400000
H	-6.333150000	-0.499521000	0.298303000
C	-4.409019000	-2.158367000	-0.345264000
C	-3.183802000	-2.901927000	-0.712269000
C	-3.254138000	-4.280532000	-0.870104000
C	-2.114094000	-5.026701000	-1.207946000
C	-0.904072000	-4.384440000	-1.398273000
H	2.776572000	1.582558000	-1.810027000
H	2.539355000	-0.760633000	-2.219859000
H	-0.008709000	-4.938592000	-1.656847000
H	-2.182709000	-6.105156000	-1.317046000
H	-4.217936000	-4.755913000	-0.717195000
O	1.502963000	-3.074765000	-1.775866000
H	2.374722000	-2.669342000	-1.471632000
O	-2.318430000	4.101318000	0.778247000
H	-1.946118000	4.957956000	1.022134000
C	-6.482785000	2.239990000	0.723719000
O	-6.477523000	3.446937000	0.891246000
O	-7.631838000	1.516430000	0.834622000
H	-8.319979000	2.164501000	1.053679000
C	2.316115000	3.948586000	-0.476883000
O	2.562466000	4.802694000	0.359965000
O	3.183787000	3.587288000	-1.430200000
H	4.115809000	3.800614000	-1.147959000
O	-5.498383000	-2.723814000	-0.206246000
C	3.475418000	-2.642565000	0.789945000
H	4.440746000	-2.791388000	1.280043000
H	2.909711000	-3.580217000	0.793534000
C	2.696826000	-1.547434000	1.508645000
H	3.282929000	-0.632350000	1.548216000
H	1.722229000	-1.368906000	1.056921000
O	3.662156000	-2.271383000	-0.569159000
Br	2.337866000	-2.077750000	3.392788000
C	4.707488000	-1.209332000	-0.836937000
O	4.692107000	-0.881523000	-2.026281000
O	5.345031000	-0.865267000	0.161906000
C	5.334704000	2.353607000	0.516981000
C	5.893124000	1.895714000	-0.747143000

O	5.641414000	3.321163000	-0.521541000
H	4.274550000	2.203572000	0.710827000
H	5.964095000	2.425783000	1.401469000
H	5.257141000	1.393971000	-1.471791000
H	6.947529000	1.636456000	-0.796952000

### TS4'

SCF Energy (B3LYP-D3/B2) = -4633.89322768

Enthalpy 0K = 0.460478

Enthalpy 298 K = 0.496753

Free Energy 298 K = 0.389662

C	-1.219377000	3.319267000	-0.045071000
C	-1.504439000	1.965675000	-0.343626000
C	0.060551000	3.839091000	-0.200980000
C	-0.408838000	1.173383000	-0.820223000
C	1.115403000	3.102478000	-0.724229000
C	0.881336000	1.751703000	-1.086030000
H	0.274025000	4.855676000	0.121171000
C	1.893157000	0.928407000	-1.696921000
C	1.727221000	-0.405492000	-1.860691000
C	0.527746000	-1.052770000	-1.423851000
C	-0.583438000	-0.251506000	-0.989662000
C	0.435137000	-2.452152000	-1.406111000
C	-1.819621000	-0.869085000	-0.694926000
C	-0.807036000	-3.089794000	-1.123763000
C	-1.942324000	-2.285561000	-0.794723000
C	-2.822246000	1.344516000	-0.163647000
C	-3.984691000	2.076728000	0.137102000
C	-2.952336000	-0.072178000	-0.315006000
C	-5.225660000	1.458528000	0.320416000
C	-4.218006000	-0.690118000	-0.100388000
C	-5.338107000	0.070632000	0.214853000
H	-3.947238000	3.149384000	0.232022000
H	-6.282600000	-0.437800000	0.366088000
C	-4.390748000	-2.159923000	-0.204962000
C	-3.180794000	-2.943279000	-0.541204000
C	-3.270849000	-4.327776000	-0.604218000
C	-2.144657000	-5.110184000	-0.907433000
C	-0.930151000	-4.499360000	-1.158663000
H	2.794254000	1.414562000	-2.034424000
H	2.516965000	-0.981736000	-2.326422000
H	-0.047082000	-5.083339000	-1.392616000
H	-2.228408000	-6.192563000	-0.942405000
H	-4.237733000	-4.779122000	-0.405208000
O	1.487752000	-3.253386000	-1.665364000
H	2.342800000	-2.837503000	-1.396759000
O	-2.200520000	4.137921000	0.454040000
H	-1.806362000	5.000273000	0.636665000
C	-6.387968000	2.323622000	0.626452000
O	-6.364277000	3.538034000	0.720222000
O	-7.543799000	1.623930000	0.802494000
H	-8.219146000	2.293741000	0.994347000
C	2.469269000	3.803535000	-0.690702000
O	2.619073000	4.767769000	0.055623000
O	3.405422000	3.295081000	-1.453981000
H	4.444958000	3.353692000	-0.991764000
O	-5.484240000	-2.701170000	-0.013666000
C	3.439524000	-2.431344000	1.051165000
H	4.378427000	-2.431190000	1.608730000
H	2.920277000	-3.381398000	1.203659000

C	2.564283000	-1.267719000	1.498936000
H	3.080569000	-0.320055000	1.369689000
H	1.600489000	-1.254477000	0.994429000
O	3.698337000	-2.347764000	-0.354452000
Br	2.170555000	-1.445077000	3.435517000
C	4.638757000	-1.362927000	-0.804364000
O	4.730428000	-1.283292000	-2.024225000
O	5.202893000	-0.708513000	0.125261000
C	5.149584000	2.078171000	0.567105000
C	5.598939000	1.199089000	-0.503769000
O	5.546972000	3.060519000	-0.376688000
H	4.077230000	2.055997000	0.792761000
H	5.740694000	2.079032000	1.488092000
H	4.969230000	1.044222000	-1.366579000
H	6.657161000	1.015301000	-0.613895000

### Pdt2'

SCF Energy (B3LYP-D3/B2) = -4633.94709087

Enthalpy 0K = 0.466851

Enthalpy 298 K = 0.503227

Free Energy 298 K = 0.394831

C	-0.292639000	3.189870000	-0.708235000
C	-0.734312000	1.853879000	-0.853547000
C	1.036742000	3.544422000	-0.923419000
C	0.259468000	0.900054000	-1.254276000
C	2.006698000	2.639080000	-1.325503000
C	1.607185000	1.298808000	-1.545419000
H	1.368127000	4.570228000	-0.770583000
C	2.521052000	0.321619000	-2.080502000
C	2.210623000	-0.996432000	-2.114652000
C	0.944896000	-1.464426000	-1.627403000
C	-0.075542000	-0.503719000	-1.299385000
C	0.697790000	-2.831987000	-1.455900000
C	-1.368794000	-0.948864000	-0.942859000
C	-0.600897000	-3.298261000	-1.112927000
C	-1.643680000	-2.345953000	-0.883832000
C	-2.107483000	1.403427000	-0.600487000
C	-3.172784000	2.284040000	-0.337772000
C	-2.399721000	0.003445000	-0.625756000
C	-4.469286000	1.826952000	-0.080895000
C	-3.719534000	-0.448111000	-0.338363000
C	-4.740274000	0.457552000	-0.069945000
H	-3.010879000	3.349332000	-0.329650000
H	-5.731080000	0.073744000	0.140175000
C	-4.055842000	-1.892365000	-0.305525000
C	-2.941783000	-2.834801000	-0.556530000
C	-3.178499000	-4.199524000	-0.460052000
C	-2.143002000	-5.126666000	-0.666594000
C	-0.872945000	-4.681828000	-0.981647000
H	3.477866000	0.690880000	-2.422610000
H	2.920596000	-1.716004000	-2.503496000
H	-0.056863000	-5.378049000	-1.139014000
H	-2.340840000	-6.190828000	-0.574449000
H	-4.185430000	-4.519814000	-0.211709000
O	1.667723000	-3.765689000	-1.621289000
H	2.515650000	-3.443576000	-1.241144000
O	-1.169389000	4.167592000	-0.312724000
H	-0.674091000	4.993680000	-0.240819000
C	-5.518971000	2.839629000	0.177098000
O	-5.358718000	4.047075000	0.171771000

O	-6.740530000	2.291237000	0.432224000
H	-7.330158000	3.047052000	0.582562000
C	3.462341000	3.184474000	-1.392746000
O	3.581518000	4.418469000	-1.324212000
O	4.384212000	2.306511000	-1.460777000
H	5.656941000	2.168140000	-0.368826000
O	-5.200402000	-2.289619000	-0.065462000
C	1.788716000	-1.795693000	2.451979000
H	2.562402000	-1.343775000	3.074346000
H	1.217133000	-2.514553000	3.041048000
C	0.875799000	-0.741615000	1.850100000
H	1.423735000	-0.024018000	1.242271000
H	0.072392000	-1.188878000	1.270759000
O	2.381961000	-2.580578000	1.389926000
Br	0.014518000	0.283192000	3.299597000
C	3.431401000	-2.093969000	0.702190000
O	3.867953000	-2.702458000	-0.261656000
O	3.893036000	-0.954270000	1.188098000
C	5.183906000	1.077075000	1.128320000
C	4.963059000	-0.273676000	0.451775000
O	6.147378000	1.804516000	0.417131000
H	4.213163000	1.594074000	1.179741000
H	5.536118000	0.922854000	2.157871000
H	4.638262000	-0.123458000	-0.576364000
H	5.858775000	-0.899652000	0.475984000

### GO-56

SCF Energy (B3LYP-D3/B2) = -2821.70692462

Enthalpy 0K = 0.560118

Enthalpy 298 K = 0.602027

Free Energy 298 K = 0.489504

C	3.377497000	0.776434000	0.004807000
C	2.146864000	1.492316000	0.005444000
C	0.906885000	0.783100000	0.001107000
C	0.906341000	-0.648910000	-0.005556000
C	2.131243000	-1.363983000	-0.008929000
C	3.372636000	-0.655343000	-0.004158000
C	-0.316300000	1.494328000	0.007354000
C	-0.328860000	-1.357984000	-0.011946000
C	-1.557881000	-0.646405000	-0.005975000
C	-1.559064000	0.785659000	0.003371000
C	-2.787210000	-1.358971000	-0.010431000
C	-2.787929000	-2.783839000	-0.021280000
C	-1.568347000	-3.489650000	-0.029210000
C	-0.335941000	-2.785586000	-0.023375000
C	0.895401000	-3.499959000	-0.030338000
C	2.124386000	-2.796022000	-0.016800000
C	2.150592000	2.915866000	0.012924000
C	0.918183000	3.624194000	0.024883000
C	-0.315105000	2.921820000	0.017811000
C	-1.549525000	3.635838000	0.022707000
C	-2.782999000	2.926312000	0.020002000
C	-2.778463000	1.490936000	0.011382000
C	-4.018938000	-0.645961000	-0.001902000
C	-4.015345000	0.776146000	0.008953000
C	-5.252024000	1.461540000	0.017716000
C	-5.249488000	-1.366691000	-0.004646000
C	-6.455692000	0.756977000	0.015351000
C	-6.466669000	-0.636570000	0.004324000
C	4.614376000	1.493280000	0.018984000
C	4.602477000	-1.373902000	-0.013262000
C	5.816573000	-0.628121000	-0.002000000

C	5.823015000	0.739111000	0.014383000
C	3.377063000	-3.513008000	-0.006590000
C	4.581182000	-2.803598000	0.004773000
C	-4.041596000	-3.485524000	-0.023506000
C	-5.226166000	-2.788365000	-0.015382000
C	0.882248000	-4.946459000	-0.049782000
C	-1.594253000	-4.942920000	-0.037033000
C	3.325497000	-4.954997000	-0.062511000
C	-4.073952000	-4.978788000	-0.032776000
C	2.148402000	-5.625178000	-0.083330000
C	-0.326640000	-5.630805000	-0.042983000
C	-2.782991000	-5.641944000	-0.037307000
C	-5.296431000	2.950173000	0.028579000
C	4.600588000	2.918002000	0.001120000
C	-3.993847000	3.651603000	0.028559000
C	3.397006000	3.635115000	0.006114000
C	-3.985424000	5.052939000	0.024892000
C	-1.541288000	5.068631000	0.031605000
C	0.907254000	5.060957000	0.051349000
C	3.345840000	5.078615000	0.053422000
C	-2.793665000	5.756396000	0.019075000
C	-0.299689000	5.742938000	0.058369000
C	2.167889000	5.750171000	0.076102000
O	-6.370031000	3.556204000	0.035890000
O	-5.140035000	-5.607132000	-0.034053000
O	-7.616982000	-1.353209000	0.001684000
H	-8.374728000	-0.753354000	0.008624000
C	5.916269000	3.634953000	0.013124000
O	6.815683000	3.437265000	0.803541000
O	6.032546000	4.538715000	-0.992596000
H	6.912766000	4.940156000	-0.889030000

## GO-56-Int1'

SCF Energy (B3LYP-D3/B2) = -5549.83300034

Enthalpy 0K = 0.619093

Enthalpy 298 K = 0.667765

Free Energy 298 K = 0.533482

C	1.231441000	-3.429636000	-0.071420000
C	0.321297000	-2.335020000	-0.110844000
C	0.812046000	-0.994284000	-0.081420000
C	2.220988000	-0.753728000	-0.010758000
C	3.130710000	-1.842721000	0.030991000
C	2.640561000	-3.185197000	0.001584000
C	-0.093348000	0.094814000	-0.125371000
C	2.713901000	0.583873000	0.021739000
C	1.808097000	1.675982000	-0.020349000
C	0.398629000	1.437012000	-0.094089000
C	2.306641000	3.008477000	0.011449000
C	3.708654000	3.246360000	0.083442000
C	4.609047000	2.161820000	0.126600000
C	4.119384000	0.828741000	0.095456000
C	5.026115000	-0.265333000	0.140587000
C	4.539487000	-1.595015000	0.103015000
C	-1.080321000	-2.576053000	-0.182157000
C	-1.981951000	-1.478008000	-0.234859000
C	-1.498528000	-0.143249000	-0.202323000
C	-2.410758000	0.953000000	-0.246357000
C	-1.911818000	2.283871000	-0.214172000
C	-0.503931000	2.520932000	-0.138197000
C	1.398972000	4.103015000	-0.032485000
C	-0.001630000	3.863286000	-0.107309000
C	-0.879073000	4.966805000	-0.151227000
C	1.904470000	5.437071000	-0.002159000

C	-0.386243000	6.272447000	-0.120607000
C	0.982305000	6.514516000	-0.046944000
C	0.730727000	-4.769227000	-0.109286000
C	3.554428000	-4.277858000	0.050336000
C	3.022252000	-5.598474000	0.011684000
C	1.677407000	-5.833638000	-0.064434000
C	5.455607000	-2.708792000	0.134317000
C	4.958251000	-4.015536000	0.097004000
C	4.192697000	4.600231000	0.110125000
C	3.308375000	5.651124000	0.069006000
C	6.446651000	-0.006117000	0.222697000
C	6.034335000	2.433546000	0.190863000
C	6.862798000	-2.414531000	0.265442000
C	5.660139000	4.884037000	0.178486000
C	7.324341000	-1.140793000	0.308391000
C	6.918371000	1.300650000	0.227499000
C	6.523990000	3.727678000	0.212569000
C	-2.353766000	4.763512000	-0.232531000
C	-0.676578000	-4.994145000	-0.149780000
C	-2.833507000	3.359132000	-0.261065000
C	-1.585078000	-3.924559000	-0.196723000
C	-4.202064000	3.121999000	-0.331412000
C	-3.822051000	0.703016000	-0.325338000
C	-3.395166000	-1.704444000	-0.325596000
C	-3.013081000	-4.111486000	-0.309670000
C	-4.726744000	1.821034000	-0.358700000
C	-4.275665000	-0.633160000	-0.372632000
C	-3.867823000	-3.058841000	-0.369921000
O	-3.123651000	5.723608000	-0.273680000
O	6.091262000	6.047806000	0.200957000
O	1.494857000	7.772472000	-0.015780000
H	0.771666000	8.412230000	-0.051362000
C	-1.162245000	-6.408140000	-0.170023000
O	-0.768015000	-7.282975000	-0.916319000
O	-2.100465000	-6.660297000	0.779798000
H	-2.348899000	-7.593210000	0.662197000
C	5.890269000	-5.184189000	0.138747000
O	5.816786000	-6.123565000	0.905630000
O	6.857414000	-5.127192000	-0.816274000
H	7.394550000	-5.927970000	-0.688672000
H	-4.887613000	3.960848000	-0.361416000
H	-1.104541000	7.087637000	-0.156658000
H	3.708056000	6.658937000	0.090590000
H	7.566318000	-3.233037000	0.333962000
H	3.696617000	-6.442765000	0.059412000
H	1.327035000	-6.855713000	-0.106400000
H	-3.408919000	-5.117265000	-0.337962000
O	-6.046955000	1.727711000	-0.424954000
H	-6.474785000	0.808269000	-0.358104000
H	-5.336096000	-0.846864000	-0.443454000
O	8.244473000	1.611351000	0.274703000
H	8.774990000	0.815698000	0.151185000
H	8.394458000	-0.995060000	0.440374000
H	7.589489000	3.913375000	0.256929000
H	-4.938440000	-3.224242000	-0.452700000
C	-8.283330000	-0.373500000	0.928502000
H	-8.187684000	0.529502000	1.527934000
H	-8.404037000	-1.296553000	1.489687000
C	-8.836903000	-0.278776000	-0.403219000
H	-9.111887000	0.691078000	-0.798758000
H	-9.324018000	-1.138692000	-0.842777000
O	-7.345988000	-0.465763000	-0.194369000
Br	-11.730420000	-0.162647000	0.511582000

## GO-56-TS1'

SCF Energy (B3LYP-D3/B2) = -5549.82732242  
 Enthalpy 0K = 0.617503  
 Enthalpy 298 K = 0.665442  
 Free Energy 298 K = 0.534285

C	1.303853000	-3.424278000	-0.148410000
C	0.357316000	-2.364634000	-0.245677000
C	0.794364000	-1.006190000	-0.186525000
C	2.185346000	-0.712668000	-0.028163000
C	3.131468000	-1.767028000	0.071895000
C	2.695466000	-3.126859000	0.013155000
C	-0.147306000	0.048522000	-0.288228000
C	2.624222000	0.643024000	0.033404000
C	1.682164000	1.699995000	-0.066814000
C	0.290614000	1.407960000	-0.227941000
C	2.127300000	3.051136000	-0.006250000
C	3.511858000	3.341650000	0.152310000
C	4.448690000	2.291351000	0.253755000
C	4.012257000	0.940807000	0.194377000
C	4.954662000	-0.118405000	0.298118000
C	4.522373000	-1.466048000	0.232026000
C	-1.027128000	-2.658195000	-0.405166000
C	-1.964712000	-1.594470000	-0.515590000
C	-1.534908000	-0.242180000	-0.453027000
C	-2.483480000	0.818852000	-0.554773000
C	-2.037478000	2.167436000	-0.493558000
C	-0.648897000	2.457341000	-0.330373000
C	1.183295000	4.110506000	-0.108803000
C	-0.200264000	3.818500000	-0.270753000
C	-1.114035000	4.887745000	-0.372032000
C	1.635707000	5.462826000	-0.049435000
C	-0.672568000	6.211934000	-0.312794000
C	0.677399000	6.504821000	-0.153579000
C	0.857321000	-4.782082000	-0.217213000
C	3.645568000	-4.184515000	0.120525000
C	3.166528000	-5.524437000	0.049015000
C	1.839433000	-5.810112000	-0.111766000
C	5.476190000	-2.543796000	0.322823000
C	5.031970000	-3.869403000	0.255142000
C	3.942322000	4.712579000	0.206152000
C	3.022721000	5.729513000	0.108315000
C	6.355569000	0.195161000	0.468713000
C	5.855185000	2.617578000	0.405232000
C	6.859163000	-2.195887000	0.544610000
C	5.391065000	5.052460000	0.364047000
C	7.268037000	-0.905022000	0.614446000
C	6.776205000	1.519601000	0.498643000
C	6.293039000	3.930912000	0.453889000
C	-2.570710000	4.630034000	-0.547197000
C	-0.534557000	-5.059718000	-0.346102000
C	-2.995758000	3.208182000	-0.600713000
C	-1.478576000	-4.024367000	-0.450995000
C	-4.346187000	2.920366000	-0.753507000
C	-3.876276000	0.516004000	-0.722854000
C	-3.358936000	-1.873396000	-0.697861000
C	-2.887863000	-4.264461000	-0.655305000
C	-4.825005000	1.598465000	-0.810567000
C	-4.274546000	-0.834849000	-0.802992000
C	-3.775817000	-3.243964000	-0.771803000
O	-3.372028000	5.560916000	-0.642841000
O	5.773630000	6.233478000	0.409687000
O	1.139864000	7.782115000	-0.092099000
H	0.395353000	8.392658000	-0.171756000
C	-0.964660000	-6.490126000	-0.394510000
O	-0.491935000	-7.351351000	-1.111003000
O	-1.952770000	-6.778273000	0.493522000

H	-2.155535000	-7.720158000	0.361441000
C	6.003557000	-5.001048000	0.354045000
O	5.917991000	-5.948416000	1.110263000
O	7.029033000	-4.901455000	-0.535185000
H	7.586906000	-5.681471000	-0.373140000
H	-5.059352000	3.733226000	-0.825606000
H	-1.417400000	6.999459000	-0.395562000
H	3.382524000	6.751454000	0.152768000
H	7.587545000	-2.986729000	0.661756000
H	3.868041000	-6.342694000	0.139895000
H	1.531273000	-6.844628000	-0.174915000
H	-3.243096000	-5.284394000	-0.707646000
O	-6.125314000	1.450334000	-0.958813000
H	-6.561524000	0.497910000	-0.859824000
H	-5.321530000	-1.082621000	-0.944773000
O	8.086173000	1.878062000	0.626544000
H	8.650418000	1.103295000	0.521536000
H	8.320466000	-0.718066000	0.817896000
H	7.346167000	4.156145000	0.563230000
H	-4.832003000	-3.449459000	-0.922957000
C	-7.840060000	-0.738997000	0.684127000
H	-7.452428000	0.029575000	1.356699000
H	-7.860482000	-1.730346000	1.139198000
C	-8.921723000	-0.371824000	-0.202363000
H	-9.111764000	0.666804000	-0.423562000
H	-9.531019000	-1.130355000	-0.665756000
O	-7.315250000	-0.706478000	-0.654983000
Br	-11.093783000	-0.139682000	1.463417000

## GO-56-Int2'

SCF Energy (B3LYP-D3/B2) = -5738.54297965  
 Enthalpy 0K = 0.633980  
 Enthalpy 298 K = 0.685988  
 Free Energy 298 K = 0.545223

C	0.932080000	3.450087000	-0.305913000
C	0.099659000	2.307873000	-0.480919000
C	0.660814000	0.995905000	-0.409886000
C	2.057379000	0.830045000	-0.169265000
C	2.892261000	1.968316000	0.004057000
C	2.333828000	3.280908000	-0.063004000
C	-0.169839000	-0.144330000	-0.576809000
C	2.619429000	-0.481722000	-0.107895000
C	1.789217000	-1.619632000	-0.280999000
C	0.389599000	-1.455548000	-0.514657000
C	2.360091000	-2.926837000	-0.220883000
C	3.752777000	-3.086901000	0.015144000
C	4.580431000	-1.953946000	0.188026000
C	4.019025000	-0.650278000	0.128414000
C	4.847944000	0.491259000	0.298888000
C	4.292902000	1.794417000	0.243984000
C	-1.294946000	2.473351000	-0.726361000
C	-2.125341000	1.325282000	-0.879017000
C	-1.568078000	0.018131000	-0.805975000
C	-2.403399000	-1.125569000	-0.964720000
C	-1.833983000	-2.427487000	-0.908393000
C	-0.446496000	-2.590116000	-0.685293000
C	1.529310000	-4.068858000	-0.394922000
C	0.132652000	-3.910143000	-0.627032000
C	-0.661293000	-5.058725000	-0.795452000
C	2.108410000	-5.372988000	-0.332908000
C	-0.094789000	-6.338513000	-0.737415000
C	1.263563000	-6.501177000	-0.510188000
C	0.360257000	4.762706000	-0.371403000

C	3.175372000	4.421874000	0.105199000
C	2.572010000	5.712098000	0.038507000
C	1.235481000	5.876093000	-0.188594000
C	5.130157000	2.952346000	0.427853000
C	4.563000000	4.233653000	0.369048000
C	4.310804000	-4.411634000	0.077506000
C	3.501558000	-5.509323000	-0.094315000
C	6.260653000	0.304273000	0.530744000
C	5.994204000	-2.153846000	0.441450000
C	6.544719000	2.732239000	0.599961000
C	5.772982000	-4.619745000	0.334559000
C	7.072974000	1.482914000	0.644975000
C	6.792290000	-0.978665000	0.621271000
C	6.549451000	-3.426256000	0.512171000
C	-2.124076000	-4.942981000	-1.039515000
C	-1.025384000	4.913057000	-0.656349000
C	-2.693160000	-3.562719000	-1.082871000
C	-1.862649000	3.789825000	-0.825337000
C	-4.043970000	-3.414063000	-1.285494000
C	-3.806544000	-0.952148000	-1.178598000
C	-3.529635000	1.473544000	-1.110378000
C	-3.282226000	3.895455000	-1.045493000
C	-4.685688000	-2.120491000	-1.324743000
C	-4.334766000	0.339857000	-1.251247000
C	-4.070593000	2.794921000	-1.185052000
O	-2.824003000	-5.943227000	-1.196687000
O	6.251658000	-5.768321000	0.388263000
O	1.848019000	-7.730476000	-0.446018000
H	1.169805000	-8.405686000	-0.576487000
C	-1.577980000	6.294830000	-0.752980000
O	-1.400202000	7.197257000	0.044115000
O	-2.311210000	6.502296000	-1.882680000
H	-2.621704000	7.421363000	-1.818337000
C	5.414733000	5.446465000	0.555667000
O	5.461729000	6.409128000	-0.185679000
O	6.154629000	5.407938000	1.698509000
H	6.661831000	6.237600000	1.701516000
H	-4.669422000	-4.291460000	-1.406623000
H	-0.753481000	-7.192242000	-0.874671000
C	3.956660000	-6.491877000	-0.040540000
H	7.203027000	3.586062000	0.688402000
H	3.191767000	6.591177000	0.154333000
H	0.828457000	6.877223000	-0.216258000
H	-3.730512000	4.877062000	-1.112927000
O	-5.933006000	-2.032217000	-1.472722000
H	-7.017792000	-0.883534000	-0.892971000
H	-5.400813000	0.462214000	-1.407997000
O	8.117794000	-1.207659000	0.875828000
H	8.525114000	-0.400065000	1.209464000
H	8.153504000	1.391223000	0.734477000
H	7.606970000	-3.550401000	0.706999000
H	-5.135615000	2.905679000	-1.363989000
C	-7.571577000	-0.836167000	0.971758000
H	-7.645395000	-1.931796000	0.975357000
H	-8.426012000	-0.431709000	1.523181000
C	-6.277207000	-0.408084000	1.658119000
H	-5.397287000	-0.820469000	1.167306000
H	-6.199942000	0.676799000	1.718069000
O	-7.610787000	-0.314672000	-0.341431000
Br	-6.225630000	-1.073351000	3.530423000
C	-7.861773000	2.275943000	-0.344458000
O	-7.545556000	2.394402000	-1.465595000
O	-8.184296000	2.261484000	0.780530000

Enthalpy 0K = 0.631054  
 Enthalpy 298 K = 0.681395  
 Free Energy 298 K = 0.546433

C	1.036745000	3.443496000	-0.335802000
C	0.148173000	2.346475000	-0.519503000
C	0.640734000	1.007534000	-0.445851000
C	2.027067000	0.770180000	-0.193230000
C	2.916146000	1.862463000	-0.009250000
C	2.425138000	3.202887000	-0.079114000
C	-0.244557000	-0.085439000	-0.622481000
C	2.521362000	-0.567332000	-0.131012000
C	1.636678000	-1.661412000	-0.315627000
C	0.246996000	-1.426155000	-0.559290000
C	2.138096000	-2.993730000	-0.257824000
C	3.519965000	-3.226880000	-0.011377000
C	4.400458000	-2.139468000	0.174757000
C	3.907840000	-0.807935000	0.116390000
C	4.792974000	0.288784000	0.299689000
C	4.304117000	1.617729000	0.243862000
C	-1.232482000	2.583133000	-0.778906000
C	-2.116875000	1.481694000	-0.942959000
C	-1.629661000	0.148951000	-0.863104000
C	-2.521752000	-0.950122000	-1.024853000
C	-2.024542000	-2.280141000	-0.971396000
C	-0.638195000	-2.513367000	-0.740200000
C	1.251488000	-4.090465000	-0.445677000
C	-0.131714000	-3.855990000	-0.687143000
C	-0.988082000	-4.959464000	-0.871020000
C	1.759854000	-5.422778000	-0.387737000
C	-0.491002000	-6.264549000	-0.817331000
C	0.858135000	-6.501871000	-0.579364000
C	0.533114000	4.781823000	-0.406796000
C	3.320492000	4.298409000	0.099728000
C	2.785589000	5.617448000	0.027678000
C	1.460390000	5.848735000	-0.213976000
C	5.196386000	2.732620000	0.441084000
C	4.695965000	4.039067000	0.378753000
C	4.006886000	-4.579392000	0.046927000
C	3.143833000	-5.632497000	-0.138332000
C	6.194017000	0.031731000	0.544667000
C	5.802436000	-2.408920000	0.438065000
C	6.596690000	2.441945000	0.632724000
C	5.453655000	-4.860111000	0.313529000
C	7.062187000	1.168866000	0.678312000
C	6.660492000	-1.275069000	0.630534000
C	6.291545000	-3.704717000	0.505126000
C	-2.444169000	-4.760770000	-1.126299000
C	-0.842459000	5.002573000	-0.705597000
C	-2.934266000	-3.357015000	-1.158010000
C	-1.734134000	3.928405000	-0.884552000
C	-4.289272000	-3.124317000	-1.348243000
C	-3.912900000	-0.704171000	-1.248611000
C	-3.507728000	1.703004000	-1.208022000
C	-3.146748000	4.107543000	-1.122554000
C	-4.828130000	-1.815906000	-1.356973000
C	-4.367681000	0.622408000	-1.370560000
C	-3.988366000	3.052257000	-1.284511000
O	-3.192758000	-5.723135000	-1.299552000
O	5.881179000	-6.026346000	0.364732000
O	1.372944000	-7.760202000	-0.519410000
H	0.661426000	-8.398637000	-0.658447000
C	-1.322369000	6.413714000	-0.802138000
O	-1.114786000	7.295171000	0.010013000
O	-2.015704000	6.663834000	-1.945070000
H	-2.290625000	7.594383000	-1.882081000

## GO-56-TS2'

SCF Energy (B3LYP-D3/B2) = -5738.51890351

C	5.606330000	5.208278000	0.573982000	C	-1.489500000	-4.762740000	-0.149102000
O	5.712658000	6.161411000	-0.172558000	C	-4.221122000	-3.954428000	0.227604000
O	6.324279000	5.136782000	1.728239000	C	-3.840448000	-5.327206000	0.190506000
H	6.872370000	5.940069000	1.739714000	C	-2.541260000	-5.712862000	0.010549000
H	-4.965020000	-3.964402000	-1.459629000	C	-5.916493000	-2.178451000	0.471434000
H	-1.192194000	-7.081906000	-0.966001000	C	-5.568680000	-3.533967000	-0.442606000
H	3.545475000	-6.638394000	-0.087485000	C	-3.869785000	4.940872000	0.070119000
H	7.294038000	3.262184000	0.737331000	C	-2.882739000	5.884164000	-0.084722000
H	3.447675000	6.464010000	0.150826000	C	-6.599267000	0.620328000	0.506346000
H	1.104798000	6.869327000	-0.244726000	C	-5.921972000	2.997350000	0.396582000
H	-3.544243000	5.111465000	-1.178754000	C	-7.280974000	-1.725959000	0.599435000
O	-6.119751000	-1.668571000	-1.467356000	C	-5.284101000	5.389837000	0.268574000
H	-6.590643000	-0.794810000	-0.915860000	C	-7.598009000	-0.407623000	0.612886000
H	-5.405681000	0.820562000	-1.605393000	C	-6.914801000	1.972717000	0.558335000
O	7.966904000	-1.577559000	0.892256000	C	-6.259636000	4.340568000	0.430589000
H	8.428864000	-0.788042000	1.196942000	C	2.605023000	4.355204000	-0.809329000
H	8.135197000	1.025025000	0.787252000	C	-0.136537000	-5.144792000	-0.383001000
H	7.339510000	-3.886123000	0.706664000	C	2.925838000	2.906034000	-0.810536000
H	-5.051467000	3.201968000	-1.453083000	C	0.881167000	-4.185052000	-0.529745000
C	-7.186463000	-0.506553000	1.213868000	C	4.254710000	2.510897000	-0.944915000
H	-7.274138000	-1.599196000	1.170689000	C	3.598219000	0.155050000	-0.836004000
H	-8.044364000	-0.101780000	1.759153000	C	2.911817000	-2.184825000	-0.785051000
C	-5.895848000	-0.104826000	1.920062000	C	2.272951000	-4.530065000	-0.703318000
H	-5.013550000	-0.489021000	1.409132000	C	4.622536000	1.156694000	-0.929697000
H	-5.836834000	0.977251000	2.024833000	C	3.902445000	-1.220222000	-0.916736000
O	-7.165735000	0.007369000	-0.100023000	C	3.238850000	-3.582170000	-0.831398000
Br	-5.834554000	-0.853673000	3.761813000	O	3.468773000	5.222082000	-0.951822000
C	-7.507705000	1.713302000	-0.273668000	O	-5.577791000	6.596778000	0.292108000
O	-7.238359000	1.991487000	-1.419615000	O	-0.859678000	7.785940000	-0.403250000
O	-7.898427000	2.131017000	0.785895000	H	-0.073869000	8.336064000	-0.518038000

### GO-56-Int3'

SCF Energy (B3LYP-D3/B2) = -5738.54297965

Enthalpy 0K = 0.634938

Enthalpy 298 K = 0.685473

Free Energy 298 K = 0.549944

C	-1.837469000	-3.374936000	-0.111683000	H	1.626317000	6.808138000	-0.726287000
C	-0.820153000	-2.390980000	-0.263740000	H	-3.165922000	6.930625000	-0.060818000
C	-1.156166000	-1.003058000	-0.223364000	H	-8.071905000	-2.459191000	0.682002000
C	-2.516291000	-0.603769000	-0.036230000	H	-4.600865000	-6.090041000	0.290548000
C	-3.533120000	-1.582933000	0.116485000	H	-2.305147000	-6.768065000	0.004121000
C	-3.198265000	-2.972303000	0.080005000	H	2.551473000	-5.574327000	-0.738479000
C	-0.143055000	-0.023243000	-0.368599000	O	5.914860000	0.873531000	-1.026191000
C	-2.854585000	0.782102000	-0.007287000	H	6.200172000	-0.028074000	-0.635831000
C	-1.841837000	1.764104000	-0.160742000	H	4.915394000	-1.568268000	-1.103368000
C	-0.478494000	1.366636000	-0.339136000	O	-8.186197000	2.429678000	0.755756000
C	-2.186614000	3.145178000	-0.136622000	H	-8.756522000	1.701599000	1.028223000
C	-3.542037000	3.540440000	0.045124000	H	-8.650891000	-0.140468000	0.675756000
C	-4.549421000	2.565023000	0.200082000	H	-7.287201000	4.645482000	0.581989000
C	-4.213163000	1.184675000	0.174900000	H	4.286019000	-3.846919000	-0.956221000
C	-5.227232000	0.200494000	0.327206000	C	7.677763000	-0.551987000	1.226090000
C	-4.893351000	-1.176349000	0.304643000	H	8.027218000	-1.327904000	1.911462000
C	0.533375000	-2.788957000	-0.457376000	H	7.086969000	0.187868000	1.777406000
C	1.545619000	-1.800169000	-0.589163000	C	8.865587000	0.112103000	0.543905000
C	1.214792000	-0.419267000	-0.543213000	H	9.483568000	-0.636386000	0.052324000
C	2.235848000	0.565657000	-0.675216000	H	8.546226000	0.887360000	-0.152501000
C	1.894594000	1.945413000	-0.656309000	O	6.839057000	-1.121272000	0.231972000
C	0.531812000	2.340945000	-0.488891000	Br	10.027386000	1.019296000	1.882652000
C	-1.171085000	4.129248000	-0.293149000	C	7.291969000	-2.485641000	-0.354149000
C	0.184213000	3.731935000	-0.469598000	O	6.480255000	-2.841652000	-1.210857000
C	1.171886000	4.726201000	-0.623296000	O	8.327260000	-2.909569000	0.139865000
C	-1.522525000	5.512011000	-0.269406000				
C	0.828591000	6.079858000	-0.603060000				
C	-0.493730000	6.476104000	-0.429010000				

### GO-56-TS3'

SCF Energy (B3LYP-D3/B2) = -5738.49623703  
 Enthalpy 0K = 0.635176  
 Enthalpy 298 K = 0.685448  
 Free Energy 298 K = 0.548924

C	-1.482142000	-3.410795000	-0.209468000
C	-0.581624000	-2.324226000	-0.396724000
C	-1.057287000	-0.979686000	-0.316754000
C	-2.440733000	-0.727350000	-0.053982000
C	-3.340558000	-1.808856000	0.134408000
C	-2.865496000	-3.155128000	0.057903000
C	-0.160790000	0.101564000	-0.497747000
C	-2.919217000	0.614420000	0.015008000
C	-2.023468000	1.698880000	-0.174149000
C	-0.637151000	1.448450000	-0.428660000
C	-2.507968000	3.035324000	-0.109712000
C	-3.886059000	3.284745000	0.147561000
C	-4.776443000	2.207784000	0.337900000
C	-4.300639000	0.870658000	0.272993000
C	-5.197793000	-0.215843000	0.461157000
C	-4.723979000	-1.549475000	0.398718000
C	0.793862000	-2.576241000	-0.664943000
C	1.690097000	-1.486102000	-0.832362000
C	1.220569000	-0.148403000	-0.747897000
C	2.124714000	0.939991000	-0.916990000
C	1.643361000	2.276344000	-0.858529000
C	0.255674000	2.524761000	-0.614363000
C	-1.610049000	4.122021000	-0.301836000
C	-0.232456000	3.870316000	-0.554329000
C	0.637441000	4.964733000	-0.742682000
C	-2.101246000	5.460001000	-0.237052000
C	0.157439000	6.274148000	-0.681947000
C	-1.188269000	6.528288000	-0.432748000
C	-0.995235000	-4.753841000	-0.287323000
C	-3.771120000	-4.240340000	0.241150000
C	-3.253147000	-5.565202000	0.161524000
C	-1.931871000	-5.810654000	-0.090712000
C	-5.627093000	-2.655432000	0.601602000
C	-5.142611000	-3.966054000	0.532178000
C	-4.355503000	4.642689000	0.211949000
C	-3.481183000	5.685766000	0.022892000
C	-6.595171000	0.055128000	0.717564000
C	-6.174808000	2.491127000	0.610738000
C	-7.022670000	-2.350256000	0.808983000
C	-5.796074000	4.938409000	0.488454000
C	-7.474145000	-1.073035000	0.860677000
C	-7.047016000	1.365896000	0.806295000
C	-6.648426000	3.789749000	0.683188000
C	2.089021000	4.747526000	-1.010374000
C	0.376655000	-4.989583000	-0.594878000
C	2.557086000	3.340870000	-1.049989000
C	1.278992000	-3.928065000	-0.776813000
C	3.912775000	3.088133000	-1.259125000
C	3.512603000	0.676898000	-1.154788000
C	3.078181000	-1.724488000	-1.103379000
C	2.688365000	-4.124781000	-1.026172000
C	4.414426000	1.783218000	-1.286719000
C	3.952645000	-0.659407000	-1.270434000
C	3.543226000	-3.081503000	-1.187948000
O	2.848876000	5.701084000	-1.187158000
O	-6.214741000	6.105830000	0.545962000
O	-1.686094000	7.791400000	-0.365794000
H	-0.969267000	8.423287000	-0.508422000
C	0.840217000	-6.407684000	-0.693326000
O	0.639009000	-7.278984000	0.130483000
O	1.505926000	-6.668911000	-1.848118000

H	1.775550000	-7.601443000	-1.789785000
C	-6.064653000	-5.126497000	0.729930000
O	-6.187948000	-6.072343000	-0.022579000
O	-6.769200000	-5.053353000	1.891562000
H	-7.326135000	-5.850585000	1.906510000
H	4.597284000	3.919817000	-1.378441000
H	0.867619000	7.083102000	-0.834088000
H	-3.869437000	6.696749000	0.078468000
H	-7.726771000	-3.163420000	0.922233000
H	-3.923957000	-6.404393000	0.287250000
H	-1.587922000	-6.835199000	-0.126619000
H	3.071136000	-5.133999000	-1.091561000
O	5.731029000	1.646695000	-1.464166000
H	6.107024000	0.783683000	-1.151471000
H	4.983512000	-0.895993000	-1.515439000
O	-8.345246000	1.686767000	1.074446000
H	-8.828458000	0.899154000	1.349946000
H	-8.543935000	-0.919046000	0.985800000
H	-7.692764000	3.984498000	0.891125000
H	4.603217000	-3.239986000	-1.368237000
C	7.852118000	0.168269000	0.783867000
H	7.211251000	0.308317000	1.656936000
H	8.233955000	1.140295000	0.471267000
C	9.001637000	-0.763859000	1.129539000
H	8.920623000	-1.474757000	1.932454000
H	9.934121000	-0.711542000	0.593810000
O	7.042912000	-0.348320000	-0.297809000
Br	9.936775000	0.816215000	2.782722000
C	7.377982000	-1.652331000	-0.729305000
O	6.678061000	-2.114587000	-1.627602000
O	8.365808000	-2.148026000	-0.109120000

### GO-56-Pdt1'

SCF Energy (B3LYP-D3/B2) = -5738.51825630  
 Enthalpy 0K = 0.637401  
 Enthalpy 298 K = 0.688205  
 Free Energy 298 K = 0.549411

C	-1.536934000	-3.406476000	-0.189708000
C	-0.634200000	-2.321383000	-0.377568000
C	-1.107774000	-0.975808000	-0.300624000
C	-2.491902000	-0.721363000	-0.041155000
C	-3.393570000	-1.801423000	0.147815000
C	-2.920750000	-3.148460000	0.074905000
C	-0.209393000	0.103421000	-0.482313000
C	-2.967860000	0.620722000	0.024154000
C	-2.069897000	1.703855000	-0.165649000
C	-0.683655000	1.451134000	-0.416789000
C	-2.551868000	3.041272000	-0.104843000
C	-3.930472000	3.293976000	0.148838000
C	-4.822800000	2.217833000	0.339323000
C	-4.349275000	0.880090000	0.278428000
C	-5.248851000	-0.204906000	0.467101000
C	-4.777090000	-1.539920000	0.408777000
C	0.741427000	-2.575963000	-0.643106000
C	1.640554000	-1.487372000	-0.810507000
C	1.173116000	-0.149264000	-0.729173000
C	2.078556000	0.938401000	-0.900165000
C	1.599543000	2.276451000	-0.845206000
C	0.210106000	2.526267000	-0.603458000
C	-1.651587000	4.126235000	-0.297208000
C	-0.273931000	3.871399000	-0.546616000
C	0.599905000	4.964423000	-0.735695000
C	-2.140827000	5.465255000	-0.235669000
C	0.120498000	6.275175000	-0.677591000

C	-1.224217000	6.531942000	-0.431370000
C	-1.052808000	-4.750288000	-0.263858000
C	-3.828182000	-4.232183000	0.259044000
C	-3.311628000	-5.558094000	0.183398000
C	-1.990480000	-5.805707000	-0.066338000
C	-5.682353000	-2.643908000	0.612623000
C	-5.200121000	-3.956210000	0.547692000
C	-4.397384000	4.651829000	0.209291000
C	-3.519551000	5.693754000	0.020317000
C	-6.645960000	0.068399000	0.719380000
C	-6.220752000	2.503790000	0.607551000
C	-7.077741000	-2.335734000	0.815815000
C	-5.836815000	4.950809000	0.480879000
C	-7.526900000	-1.057430000	0.863477000
C	-7.095918000	1.380811000	0.803102000
C	-6.692077000	3.803538000	0.675768000
C	2.048708000	4.745402000	-1.000803000
C	0.319019000	-4.988403000	-0.568890000
C	2.512338000	3.339763000	-1.036864000
C	1.221859000	-3.928902000	-0.752114000
C	3.871309000	3.083231000	-1.244258000
C	3.466944000	0.674668000	-1.135212000
C	3.030174000	-1.728772000	-1.076711000
C	2.630805000	-4.129400000	-1.001364000
C	4.364340000	1.782318000	-1.273156000
C	3.904374000	-0.663403000	-1.241107000
C	3.487608000	-3.088469000	-1.161166000
O	2.812780000	5.697421000	-1.179537000
O	-6.255769000	6.118455000	0.534900000
O	-1.720859000	7.795914000	-0.367026000
H	-1.002393000	8.426366000	-0.507855000
C	0.781587000	-6.407429000	-0.662762000
O	0.584384000	-7.274179000	0.166299000
O	1.442246000	-6.674259000	-1.819593000
H	1.707630000	-7.607972000	-1.759751000
C	-6.123035000	-5.114877000	0.747841000
O	-6.239288000	-6.068344000	0.003445000
O	-6.838268000	-5.032461000	1.902556000
H	-7.395140000	-5.829683000	1.918517000
H	4.555893000	3.914863000	-1.363635000
H	0.832682000	7.082401000	-0.829748000
H	-3.906214000	6.705473000	0.073048000
H	-7.783607000	-3.147121000	0.929559000
H	-3.983674000	-6.395965000	0.310209000
H	-1.647819000	-6.830850000	-0.099367000
H	3.010800000	-5.139602000	-1.069177000
O	5.689103000	1.637353000	-1.461974000
H	6.036567000	0.776044000	-1.158585000
H	4.935633000	-0.893725000	-1.479746000
O	-8.393476000	1.704347000	1.066389000
H	-8.882091000	0.916781000	1.332492000
H	-8.596698000	-0.901803000	0.986981000
H	-7.736647000	4.001025000	0.880204000
H	4.544378000	-3.258777000	-1.343730000
C	8.175115000	0.029206000	0.618567000
H	7.684190000	0.344325000	1.535863000
H	8.696954000	0.876797000	0.178654000
C	9.066584000	-1.209136000	0.798733000
H	9.020594000	-1.622724000	1.804414000
H	10.105729000	-1.026973000	0.536227000
O	7.152283000	-0.437957000	-0.329712000
Br	10.350979000	0.959991000	2.739558000
C	7.421264000	-1.704938000	-0.737832000
O	6.742147000	-2.295784000	-1.545324000
O	8.506703000	-2.188886000	-0.137290000

### GO-56-Int3

SCF Energy (B3LYP-D3/B2) = -5738.51175559  
 Enthalpy 0K = 0.633461  
 Enthalpy 298 K = 0.684312  
 Free Energy 298 K = 0.548002

C	0.543056000	2.644380000	0.084459000
C	-0.877545000	2.561857000	0.051242000
C	-1.518889000	1.284796000	0.042485000
C	-0.728428000	0.093010000	0.057867000
C	0.686400000	0.174475000	0.094311000
C	1.327886000	1.449385000	0.110468000
C	-2.931934000	1.201143000	0.015342000
C	-1.364194000	-1.181363000	0.033713000
C	-2.779919000	-1.268623000	0.000483000
C	-3.574447000	-0.075680000	-0.003467000
C	-3.408732000	-2.542413000	-0.026648000
C	-2.619172000	-3.728553000	-0.023652000
C	-1.212839000	-3.640317000	0.009652000
C	-0.578250000	-2.373184000	0.039756000
C	0.844256000	-2.286424000	0.077795000
C	1.476044000	-1.019839000	0.112510000
C	-1.661885000	3.749781000	0.023620000
C	-3.081581000	3.659150000	0.011940000
C	-3.720423000	2.390396000	0.009993000
C	-5.143582000	2.301647000	-0.004634000
C	-5.779921000	1.027456000	-0.027479000
C	-4.979639000	-0.163811000	-0.031393000
C	-4.829659000	-2.630432000	-0.057822000
C	-5.614519000	-1.442692000	-0.057669000
C	-7.023563000	-1.553790000	-0.085507000
C	-5.454125000	-3.911499000	-0.086195000
C	-7.633482000	-2.810534000	-0.113938000
C	-6.871851000	-3.974671000	-0.115192000
C	1.181651000	3.925022000	0.093856000
C	2.750627000	1.525305000	0.140614000
C	3.356176000	2.817079000	0.140498000
C	2.608613000	3.961786000	0.120840000
C	2.913999000	-0.924654000	0.171933000
C	3.526263000	0.332656000	0.197369000
C	-3.273873000	-5.006911000	-0.053626000
C	-4.645524000	-5.082734000	-0.084000000
C	1.640675000	-3.493050000	0.081851000
C	-0.423424000	-4.863336000	0.013811000
C	3.681627000	-2.147729000	0.166360000
C	-2.469126000	-6.266939000	-0.051065000
C	3.071429000	-3.356677000	0.118814000
C	1.011674000	-4.731975000	0.050557000
C	-1.028603000	-6.103197000	-0.015493000
C	-7.885012000	-0.340692000	-0.082010000
C	0.382959000	5.100535000	0.030722000
C	-7.190202000	0.959481000	-0.050256000
C	-1.018944000	5.035381000	-0.000209000
C	-7.957248000	2.137574000	-0.018074000
C	-5.928930000	3.499950000	0.001032000
C	-3.885253000	4.849084000	-0.009176000
C	-1.859187000	6.209104000	-0.013249000
C	-7.353078000	3.377513000	0.018994000
C	-5.270759000	4.749085000	-0.018944000
C	-3.213891000	6.118894000	-0.020781000
O	-9.118300000	-0.433415000	-0.103145000
O	-3.009732000	-7.381729000	-0.073710000
O	-7.437266000	-5.211767000	-0.142773000
H	-8.398784000	-5.120019000	-0.160551000
C	1.079432000	6.425681000	0.027656000
O	1.898794000	6.795360000	0.843151000
O	0.722850000	7.207025000	-1.026461000

H	1.234408000	8.028292000	-0.926221000	C	-7.073457000	-3.732375000	-0.165121000
C	5.036899000	0.418033000	0.213069000	C	1.347375000	3.770461000	0.157481000
O	5.650524000	1.027863000	-0.652658000	C	2.796200000	1.299416000	0.237818000
O	5.570519000	-0.235226000	1.222222000	C	3.464410000	2.559244000	0.247480000
H	6.535757000	-0.545497000	0.971558000	C	2.773450000	3.738885000	0.210951000
H	-9.038389000	2.060270000	-0.010252000	C	2.840733000	-1.157256000	0.267418000
H	-8.720013000	-2.844893000	-0.134518000	C	3.508392000	0.068694000	0.310481000
H	-5.106399000	-6.064119000	-0.105814000	C	-3.530895000	-4.936668000	-0.048456000
H	4.765126000	-2.130982000	0.211160000	C	-4.904110000	-4.946243000	-0.098618000
H	4.436486000	2.882844000	0.135940000	C	1.448426000	-3.660839000	0.150537000
H	3.113888000	4.918352000	0.138118000	C	-0.678478000	-4.930201000	0.057193000
H	-1.393320000	7.185685000	-0.027330000	C	3.552978000	-2.414301000	0.260533000
O	-8.167770000	4.476682000	0.058728000	C	-2.788151000	-6.233966000	-0.032581000
H	-7.666072000	5.237699000	0.375646000	C	2.884788000	-3.591951000	0.199102000
H	-5.842950000	5.672344000	-0.077974000	C	0.761178000	-4.867904000	0.110879000
O	1.690667000	-5.905563000	0.053439000	C	-1.341793000	-6.139663000	0.021380000
H	2.641593000	-5.737739000	0.088120000	C	-7.910053000	-0.053310000	-0.155958000
H	3.725384000	-4.226270000	0.110977000	C	0.607523000	4.983516000	0.078602000
H	-0.434297000	-7.008245000	-0.012271000	C	-7.153546000	1.212714000	-0.117143000
H	-3.818841000	7.022027000	-0.0311330000	C	-0.794445000	4.985671000	0.022962000
C	8.698051000	-0.291025000	-0.188400000	C	-7.863321000	2.425727000	-0.101710000
H	8.358133000	0.741300000	-0.060673000	C	-5.772218000	3.689086000	-0.053455000
H	8.742266000	-0.521390000	-1.256375000	C	-3.665753000	4.938033000	-0.033864000
C	10.061479000	-0.521485000	0.444440000	C	-1.576693000	6.198968000	-0.007691000
H	10.050688000	-0.320197000	1.515566000	C	-7.200569000	3.635903000	-0.058871000
H	10.403180000	-1.533069000	0.236113000	C	-5.053664000	4.905002000	-0.065685000
O	7.769345000	-1.138562000	0.470338000	C	-2.933599000	6.174169000	-0.037740000
Br	11.425875000	0.711902000	-0.330418000	O	-9.145310000	-0.086029000	-0.195743000
C	7.643907000	-2.593739000	-0.077918000	O	-3.381159000	-7.321406000	-0.063597000
O	6.613410000	-3.103426000	0.357120000	O	-7.696994000	-4.940303000	-0.198624000
O	8.581674000	-2.912615000	-0.798004000	H	-8.652812000	-4.803694000	-0.231684000

## GO-56-TS3

SCF Energy (B3LYP-D3/B2) = -5738.49074606

Enthalpy 0K = 0.634257

Enthalpy 298 K = 0.684568

Free Energy 298 K = 0.549490

C	0.647749000	2.522602000	0.138388000	C	1.367887000	6.273622000	0.089269000
C	-0.774304000	2.508302000	0.081220000	O	2.186726000	6.601750000	0.922430000
C	-1.476278000	1.263721000	0.064651000	O	1.071434000	7.069402000	-0.971781000
C	-0.744715000	0.034901000	0.094911000	H	1.621415000	7.864575000	-0.863988000
C	0.671496000	0.048161000	0.154230000	C	5.015119000	0.087926000	0.376838000
C	1.373002000	1.291105000	0.179934000	O	5.699310000	0.626689000	-0.477707000
C	-2.890740000	1.248176000	0.015052000	O	5.478105000	-0.540406000	1.447946000
C	-1.440494000	-1.207287000	0.062223000	H	6.450282000	-0.761274000	1.296722000
C	-2.858193000	-1.226256000	0.007560000	H	-8.946902000	2.400921000	-0.111826000
C	-3.593831000	0.003529000	-0.011035000	H	-8.864432000	-2.514503000	-0.215147000
C	-3.547110000	-2.468349000	-0.027140000	H	-5.411475000	-5.904300000	-0.125544000
C	-2.815905000	-3.691263000	-0.010907000	H	4.637720000	-2.433213000	0.294277000
C	-1.407637000	-3.670973000	0.041926000	H	4.546720000	2.575547000	0.264361000
C	-0.713246000	-2.435700000	0.080774000	H	3.324323000	4.669711000	0.235492000
C	0.710547000	-2.417505000	0.138506000	H	-1.063755000	7.151682000	-0.016904000
C	1.401364000	-1.183147000	0.184517000	O	-7.963126000	4.771030000	-0.036295000
C	-1.499384000	3.732500000	0.038222000	H	-7.429484000	5.513750000	0.271574000
C	-2.921146000	3.710436000	0.003190000	H	-5.578990000	5.855040000	-0.134652000
C	-3.620514000	2.474236000	-0.005967000	O	1.380445000	-6.074589000	0.120890000
C	-5.045817000	2.454273000	-0.043137000	H	2.337894000	-5.956881000	0.166610000
C	-5.742340000	1.212251000	-0.072441000	H	3.487404000	-4.497525000	0.178787000
C	-5.000972000	-0.016624000	-0.060585000	H	-0.792231000	-7.072444000	0.032973000
C	-4.969823000	-2.487765000	-0.079445000	H	-3.493926000	7.105343000	-0.061009000
C	-5.696242000	-1.263669000	-0.093785000	C	8.828694000	-0.343729000	0.284944000
C	-7.108369000	-1.307021000	-0.143072000	H	9.322563000	0.072349000	1.160685000
C	-5.654953000	-3.737391000	-0.114842000	H	8.290728000	0.445875000	-0.246364000
C	-7.777978000	-2.532445000	-0.177995000	C	9.834726000	-1.013218000	-0.629731000
				H	10.529551000	-1.735067000	-0.232368000
				H	9.868644000	-0.802077000	-1.682692000
				O	7.873227000	-1.309378000	0.777777000
				Br	11.564732000	0.746218000	-0.387366000
				C	7.640142000	-2.377313000	-0.138595000
				O	6.649513000	-3.066750000	0.075817000
				O	8.527640000	-2.446616000	-1.041501000

## GO-56-Pdt1

SCF Energy (B3LYP-D3/B2) = -5738.51577576

Enthalpy 0K = 0.637146

Enthalpy 298 K = 0.687822

Free Energy 298 K = 0.551080

C	0.788403000	2.367292000	0.183133000
C	-0.631341000	2.439113000	0.109179000
C	-1.407710000	1.239373000	0.084461000
C	-0.753421000	-0.031689000	0.122846000
C	0.661396000	-0.104704000	0.197336000
C	1.437252000	1.093349000	0.231263000
C	-2.820193000	1.310044000	0.019119000
C	-1.524017000	-1.228814000	0.083118000
C	-2.939972000	-1.160911000	0.013115000
C	-3.597838000	0.110767000	-0.014300000
C	-3.704508000	-2.359019000	-0.028235000
C	-3.050869000	-3.624841000	-0.002559000
C	-1.643074000	-3.691057000	0.065163000
C	-0.874335000	-2.500083000	0.110090000
C	0.546442000	-2.568918000	0.181244000
C	1.312465000	-1.378649000	0.234331000
C	-1.279800000	3.705399000	0.058394000
C	-2.700138000	3.769903000	0.006930000
C	-3.473487000	2.578612000	-0.010068000
C	-4.896926000	2.645828000	-0.063085000
C	-5.667893000	1.448685000	-0.100032000
C	-5.003876000	0.177403000	-0.079527000
C	-5.125002000	-2.290470000	-0.096173000
C	-5.774807000	-1.023874000	-0.119696000
C	-7.186653000	-0.979259000	-0.184712000
C	-5.885515000	-3.496297000	-0.137833000
C	-7.930023000	-2.163112000	-0.226113000
C	-7.301735000	-3.402590000	-0.204188000
C	1.561544000	3.570739000	0.213246000
C	2.858011000	1.016366000	0.306343000
C	3.600047000	2.234295000	0.330339000
C	2.982275000	3.452927000	0.286786000
C	2.749194000	-1.440992000	0.330320000
C	3.489624000	-0.257119000	0.383476000
C	-3.840062000	-4.823449000	-0.045782000
C	-5.212348000	-4.747388000	-0.111397000
C	1.202853000	-3.855948000	0.200101000
C	-0.996722000	-4.991891000	0.091130000
C	3.378820000	-2.740696000	0.318157000
C	-3.181737000	-6.164220000	-0.018850000
C	2.640302000	-3.875657000	0.252052000
C	0.441520000	-5.018984000	0.159745000
C	-1.735314000	-6.159518000	0.051292000
C	-7.908916000	0.318653000	-0.207523000
C	0.898665000	4.826665000	0.125902000
C	-7.076353000	1.535230000	-0.160663000
C	-0.500149000	4.913524000	0.052170000
C	-7.710315000	2.790120000	-0.152607000
C	-5.546369000	3.922636000	-0.081448000
C	-3.367894000	5.040222000	-0.038671000
C	-1.206691000	6.171963000	0.012647000
C	-6.975539000	3.956963000	-0.102204000
C	-4.755091000	5.091952000	-0.086385000
C	-2.562221000	6.229271000	-0.033855000
O	-9.144570000	0.363610000	-0.261087000
O	-3.843046000	-7.213172000	-0.053926000
O	-7.997794000	-4.571065000	-0.243535000
H	-8.942662000	-4.374708000	-0.287612000
C	1.736127000	6.067474000	0.148287000
O	2.566692000	6.342032000	0.989537000

O	1.499023000	6.884370000	-0.911802000
H	2.095602000	7.643834000	-0.794796000
C	4.987419000	-0.321482000	0.480701000
O	5.738810000	0.179359000	-0.337680000
O	5.397740000	-0.983561000	1.567834000
H	6.366884000	-1.145774000	1.469704000
H	-8.793259000	2.831017000	-0.174205000
H	-9.012809000	-2.077848000	-0.275496000
H	-5.776957000	-5.672648000	-0.142324000
H	4.458757000	-2.816048000	0.345823000
H	4.681070000	2.190104000	0.364890000
H	3.588049000	4.348541000	0.321642000
H	-0.636874000	7.091734000	0.010091000
O	-7.666148000	5.138215000	-0.087715000
H	-7.093042000	5.843249000	0.237401000
H	-5.220908000	6.072038000	-0.162407000
O	0.985712000	-6.263030000	0.181623000
H	1.946057000	-6.205182000	0.257723000
H	3.181022000	-4.819305000	0.223262000
H	-1.244715000	-7.124434000	-0.071744000
H	-3.064678000	7.192780000	-0.063616000
C	8.865172000	-0.646584000	0.278328000
H	9.629977000	-0.485025000	1.032185000
H	8.303322000	0.268321000	0.086980000
C	9.406076000	-1.289944000	-0.997947000
H	10.351991000	-1.809862000	-0.840516000
H	9.514426000	-0.589761000	-1.821352000
O	7.914438000	-1.656840000	0.752885000
Br	11.699343000	0.941000000	-0.366420000
C	7.575373000	-2.474656000	-0.288153000
O	6.670459000	-3.270515000	-0.235369000
O	8.375054000	-2.270374000	-1.336618000

## GO-56-Int4

SCF Energy (B3LYP-D3/B2) = -5892.37305936

Enthalpy 0K = 0.694618

Enthalpy 298 K = 0.749383

Free Energy 298 K = 0.604331

C	0.068002000	3.024878000	-0.009314000
C	-1.331568000	2.764266000	0.013653000
C	-1.807985000	1.416726000	-0.015377000
C	-0.875770000	0.334788000	-0.061186000
C	0.518316000	0.593052000	-0.081697000
C	0.995754000	1.937441000	-0.049263000
C	-3.200081000	1.155922000	0.005289000
C	-1.345815000	-1.009547000	-0.086430000
C	-2.740059000	-1.274153000	-0.063440000
C	-3.677376000	-0.190695000	-0.021269000
C	-3.204430000	-2.616811000	-0.084439000
C	-2.272710000	-3.693831000	-0.124164000
C	-0.887996000	-3.428670000	-0.148912000
C	-0.418449000	-2.093564000	-0.132669000
C	0.984647000	-1.831866000	-0.168533000
C	1.448639000	-0.493511000	-0.141439000
C	-2.258569000	3.843746000	0.073327000
C	-3.656343000	3.574485000	0.088934000
C	-4.131140000	2.235923000	0.048957000
C	-5.532131000	1.968799000	0.059460000
C	-6.004344000	0.624800000	0.035438000
C	-5.060833000	-0.455370000	-0.000842000
C	-4.603493000	-2.883026000	-0.061232000
C	-5.530552000	-1.803291000	-0.022076000
C	-6.915087000	-2.090344000	-0.002202000
C	-5.062873000	-4.232307000	-0.079069000

C	-7.362704000	-3.414445000	-0.020115000
C	-6.462114000	-4.473082000	-0.057163000
C	0.540319000	4.376353000	0.010637000
C	2.399988000	2.190001000	-0.046644000
C	2.839547000	3.547048000	-0.000343000
C	1.953930000	4.586875000	0.025714000
C	2.862313000	-0.218753000	-0.158566000
C	3.312773000	1.103146000	-0.063831000
C	-2.762186000	-5.043484000	-0.137246000
C	-4.114172000	-5.291888000	-0.115775000
C	1.929013000	-2.921662000	-0.228209000
C	0.050906000	-4.540133000	-0.179311000
C	3.768348000	-1.325213000	-0.321117000
C	-1.804841000	-6.189494000	-0.170344000
C	3.324478000	-2.605620000	-0.349099000
C	1.472854000	-4.241194000	-0.199619000
C	-0.392605000	-5.843528000	-0.183716000
C	-7.921797000	-0.995865000	0.035348000
C	-0.398950000	5.441954000	0.064471000
C	-7.395335000	0.379213000	0.052920000
C	-1.783137000	5.199159000	0.122309000
C	-8.303627000	1.454363000	0.061437000
C	-6.461305000	3.059074000	0.096654000
C	-4.602207000	4.651976000	0.153860000
C	-2.762506000	6.256765000	0.192137000
C	-7.859539000	2.759457000	0.071593000
C	-5.965234000	4.378455000	0.163329000
C	-4.095018000	5.993894000	0.210767000
O	-9.134522000	-1.244991000	0.048823000
O	-2.195037000	-7.364704000	-0.183102000
O	-6.868263000	-5.772170000	-0.074645000
H	-7.833657000	-5.800729000	-0.054763000
C	0.073340000	6.861984000	0.078096000
O	-0.255140000	7.712946000	0.881472000
O	0.912083000	7.147728000	-0.951145000
H	1.162900000	8.079983000	-0.833976000
C	4.796512000	1.353325000	0.008993000
O	5.396720000	2.057523000	-0.791891000
O	5.345194000	0.712803000	1.029657000
H	6.329176000	0.547576000	0.880573000
H	-9.366610000	1.242610000	0.047680000
H	-8.436551000	-3.584288000	-0.003982000
H	-4.448872000	-6.323357000	-0.126323000
H	4.825966000	-1.155476000	-0.458715000
H	3.903341000	3.748795000	-0.008136000
H	2.339019000	5.597579000	0.048981000
H	-2.420514000	7.281300000	0.250713000
O	-8.803900000	3.752028000	0.071071000
H	-8.401484000	4.575279000	-0.231813000
H	-6.648348000	5.219422000	0.259912000
O	2.267010000	-5.311959000	-0.210423000
H	3.221570000	-5.140018000	-0.008990000
H	4.054082000	-3.395466000	-0.475471000
H	0.313536000	-6.664141000	-0.198874000
H	-4.808249000	6.812357000	0.268875000
C	8.015813000	0.094884000	-1.001032000
H	7.149683000	0.064219000	-1.676935000
H	8.764004000	-0.599574000	-1.396782000
C	8.528312000	1.517080000	-0.995946000
H	8.752408000	1.853930000	-2.008791000
H	7.814529000	2.192985000	-0.530213000
O	7.643489000	-0.281260000	0.316749000
Br	10.235704000	1.719115000	0.012204000
C	7.093128000	-1.665193000	0.446278000
O	6.890736000	-1.954682000	1.622810000
O	6.897264000	-2.234005000	-0.645557000
C	6.208854000	-5.204774000	0.171411000

C	5.709175000	-4.851905000	1.504084000
O	4.809289000	-5.398076000	0.505737000
H	6.427600000	-4.377354000	-0.502891000
H	6.749368000	-6.139018000	0.022079000
H	5.604034000	-3.792010000	1.728874000
H	5.883544000	-5.522781000	2.344577000

## GO-56-TS4

SCF Energy (B3LYP-D3/B2) = -5892.35587867

Enthalpy 0K = 0.692452

Enthalpy 298 K = 0.745659

Free Energy 298 K = 0.606600

C	0.120297000	3.018319000	-0.069044000
C	-1.281810000	2.766801000	-0.034561000
C	-1.769955000	1.423079000	-0.081974000
C	-0.849044000	0.339082000	-0.170476000
C	0.547115000	0.591132000	-0.226847000
C	1.040310000	1.926672000	-0.158948000
C	-3.164947000	1.170678000	-0.033543000
C	-1.330111000	-1.003042000	-0.194518000
C	-2.724724000	-1.260516000	-0.131159000
C	-3.652510000	-0.171173000	-0.061643000
C	-3.196868000	-2.601566000	-0.139487000
C	-2.273092000	-3.684641000	-0.192632000
C	-0.887259000	-3.424874000	-0.257561000
C	-0.417067000	-2.093296000	-0.274077000
C	0.988045000	-1.835037000	-0.385695000
C	1.463600000	-0.498129000	-0.358886000
C	-2.200985000	3.850913000	0.064129000
C	-3.601987000	3.590629000	0.094887000
C	-4.087116000	2.255080000	0.042644000
C	-5.489952000	1.996333000	0.076580000
C	-5.973112000	0.655320000	0.050464000
C	-5.037110000	-0.428568000	-0.010871000
C	-4.596976000	-2.859231000	-0.081369000
C	-5.515788000	-1.772770000	-0.024915000
C	-6.902363000	-2.049785000	0.024720000
C	-5.063987000	-4.206493000	-0.081598000
C	-7.357321000	-3.373948000	0.019473000
C	-6.466291000	-4.437146000	-0.030467000
C	0.602496000	4.365137000	-0.006135000
C	2.452266000	2.164354000	-0.149454000
C	2.899318000	3.518432000	-0.037389000
C	2.020573000	4.560740000	0.022551000
C	2.876222000	-0.240346000	-0.415255000
C	3.350530000	1.071269000	-0.223182000
C	-2.767659000	-5.030807000	-0.175862000
C	-4.123086000	-5.270685000	-0.125417000
C	1.913009000	-2.913340000	-0.502124000
C	0.047391000	-4.541908000	-0.276358000
C	3.751075000	-1.335572000	-0.726146000
C	-1.816005000	-6.179661000	-0.205518000
C	3.278335000	-2.611399000	-0.771837000
C	1.497788000	-4.259716000	-0.314906000
C	-0.395223000	-5.836571000	-0.239642000
C	-7.901437000	-0.950870000	0.081769000
C	-0.326415000	5.434026000	0.081170000
C	-7.365861000	0.416379000	0.094515000
C	-1.715108000	5.200556000	0.139272000
C	-8.265586000	1.502439000	0.123814000
C	-6.410649000	3.093161000	0.142642000
C	-4.538687000	4.671449000	0.192779000
C	-2.685378000	6.262015000	0.238419000
C	-7.812285000	2.801603000	0.136464000

C	-5.905893000	4.406808000	0.219579000	C	2.438763000	-3.696712000	0.119056000
C	-4.020550000	6.007299000	0.266085000	C	1.045398000	-3.479085000	0.220174000
O	-9.117340000	-1.196238000	0.116360000	C	0.532750000	-2.165041000	0.255607000
O	-2.201357000	-7.354756000	-0.194482000	C	-0.886019000	-1.946121000	0.396311000
O	-6.880115000	-5.735883000	-0.033196000	C	-1.399971000	-0.618246000	0.389630000
H	-7.845041000	-5.755662000	0.007213000	C	2.140187000	3.839301000	0.014729000
C	0.157056000	6.848542000	0.131708000	C	3.546941000	3.619047000	-0.052286000
O	-0.165421000	7.683896000	0.954126000	C	4.068837000	2.295636000	-0.044682000
O	1.002728000	7.154009000	-0.887624000	C	5.477935000	2.078223000	-0.114350000
H	1.258359000	8.081202000	-0.744231000	C	5.999722000	0.751674000	-0.130816000
C	4.826126000	1.266593000	-0.041635000	C	5.095678000	-0.357602000	-0.074309000
O	5.512573000	2.075474000	-0.649918000	C	4.732666000	-2.799589000	-0.036698000
O	5.299657000	0.436483000	0.893816000	C	5.616968000	-1.685389000	-0.096062000
H	6.284045000	0.333296000	0.825922000	C	7.010546000	-1.918408000	-0.179997000
H	-9.330175000	1.297957000	0.125297000	C	5.241064000	-4.132279000	-0.064245000
H	-8.432054000	-3.535243000	0.057857000	C	7.504825000	-3.231288000	-0.206321000
H	-4.465232000	-6.299786000	-0.116722000	C	6.650111000	-4.319132000	-0.151759000
H	4.798893000	-1.167026000	-0.935443000	C	-0.670848000	4.276924000	0.153003000
H	3.964299000	3.712881000	-0.029233000	C	-2.467140000	2.025496000	0.261570000
H	2.413234000	5.567038000	0.086519000	C	-2.945653000	3.374109000	0.186553000
H	-2.336686000	7.283349000	0.312567000	C	-2.093894000	4.436824000	0.146542000
O	-8.745288000	3.809345000	0.160776000	C	-2.814183000	-0.403675000	0.475513000
H	-8.347815000	4.612193000	-0.198930000	C	-3.334074000	0.908237000	0.305928000
H	-6.583221000	5.248452000	0.344519000	C	2.974631000	-5.025448000	0.082886000
O	2.325193000	-5.230355000	-0.170977000	C	4.336958000	-5.223038000	-0.005445000
H	3.423572000	-5.069679000	0.540435000	C	-1.772354000	-3.037800000	0.532738000
H	3.945217000	-3.423421000	-1.035671000	C	0.154604000	-4.628874000	0.269496000
H	0.316935000	-6.653747000	-0.240118000	C	-3.643981000	-1.520415000	0.789041000
H	-4.726824000	6.830038000	0.346861000	C	2.065593000	-6.203308000	0.139039000
C	8.062308000	-0.027232000	-1.042949000	C	-3.132425000	-2.790208000	0.809102000
H	7.177337000	0.048866000	-1.688463000	C	-1.323190000	-4.410177000	0.361413000
H	8.778108000	-0.690007000	-1.538596000	C	0.633552000	-5.903795000	0.225025000
C	8.619115000	1.366267000	-0.868163000	C	7.975005000	-0.794079000	-0.238102000
H	8.831504000	1.819231000	-1.836949000	C	0.224825000	5.371150000	0.078800000
H	7.934825000	2.000779000	-0.308814000	C	7.398519000	0.552862000	-0.209523000
O	7.708147000	-0.552021000	0.235452000	C	1.618746000	5.177194000	-0.013557000
Br	10.348700000	1.384387000	0.115639000	C	8.265794000	1.667840000	-0.229134000
C	7.142900000	-1.880485000	0.206551000	C	6.366574000	3.202441000	-0.172243000
O	6.992715000	-2.349626000	1.353969000	C	4.451190000	4.726796000	-0.141780000
O	6.859037000	-2.336624000	-0.915633000	C	2.555992000	6.266504000	-0.103870000
C	5.621664000	-4.180174000	1.098428000	C	7.776310000	2.951089000	-0.201351000
C	4.517917000	-3.831194000	1.966364000	C	5.825503000	4.501591000	-0.205503000
O	4.245475000	-5.108339000	1.306874000	C	3.896982000	6.048591000	-0.167810000
H	5.676033000	-3.833096000	0.075426000	O	9.199046000	-1.003027000	-0.305069000
H	6.436138000	-4.774186000	1.485402000	O	2.482359000	-7.366530000	0.113434000
H	3.870550000	-3.013225000	1.662641000	O	7.100805000	-5.607911000	-0.176699000
H	4.633929000	-3.942285000	3.042211000	H	8.064622000	-5.595663000	-0.238357000

## GO-56-Pdt2

SCF Energy (B3LYP-D3/B2) = -5892.42484287

Enthalpy 0K = 0.699251

Enthalpy 298 K = 0.752924

Free Energy 298 K = 0.611080

C	-0.155467000	2.940485000	0.171610000	H	8.583155000	-3.356854000	-0.271113000
C	1.251973000	2.727281000	0.102979000	H	4.710263000	-6.240905000	-0.029087000
C	1.776309000	1.395570000	0.104772000	H	-4.688121000	-1.364602000	1.025806000
C	0.887116000	0.285356000	0.182942000	H	-4.013869000	3.545143000	0.191411000
C	-0.515269000	0.499537000	0.267506000	H	-2.511956000	5.434597000	0.113361000
C	-1.045948000	1.822965000	0.247110000	H	2.178644000	7.279638000	-0.142481000
C	3.178438000	1.184629000	0.022992000	O	8.676254000	3.992895000	-0.220676000
C	1.408716000	-1.045518000	0.173152000	H	8.272849000	4.755918000	0.212192000
C	2.810339000	-1.259475000	0.077761000	H	6.477765000	5.363275000	-0.325800000
C	3.705181000	-0.142530000	0.010494000	O	-2.118446000	-5.363637000	0.274164000
C	3.325714000	-2.585496000	0.055620000	H	-3.872576000	-5.211122000	-0.619886000

H	-3.762329000	-3.641442000	1.039323000
H	-0.055430000	-6.740915000	0.255223000
H	4.579459000	6.891934000	-0.241834000
C	-8.266890000	0.315087000	1.013937000
H	-7.429786000	0.512806000	1.690969000
H	-9.080217000	-0.153258000	1.573390000
C	-8.682311000	1.617800000	0.378505000
H	-8.965189000	2.332424000	1.151387000
H	-7.879208000	2.035252000	-0.225316000
O	-7.828715000	-0.581549000	-0.031150000
Br	-10.267837000	1.418043000	-0.793129000
C	-7.336690000	-1.763724000	0.421635000
O	-6.950182000	-2.478240000	-0.630948000
O	-7.261173000	-2.067425000	1.592497000
C	-6.333638000	-3.765527000	-0.345432000
C	-5.269561000	-4.046639000	-1.405858000
O	-4.687989000	-5.307542000	-1.147209000
H	-5.900244000	-3.743742000	0.655233000
H	-7.113417000	-4.532705000	-0.368242000
H	-4.545000000	-3.223389000	-1.414166000
H	-5.743443000	-4.078808000	-2.394964000

## GO-118

SCF Energy (B3LYP-D3/B2) = -5792.19064784

Enthalpy 0K = 1.067921

Enthalpy 298 K = 1.150775

Free Energy 298 K = 0.956792

C	-9.702598000	-0.851032000	-0.002387000
C	-8.455793000	-1.530792000	-0.015581000
C	-7.238826000	-0.784565000	-0.016561000
C	-7.271279000	0.642263000	-0.007801000
C	-8.519165000	1.323849000	-0.006104000
C	-9.733772000	0.576564000	-0.003147000
C	-5.993435000	-1.459921000	-0.024408000
C	-6.060975000	1.385424000	-0.008332000
C	-4.811631000	0.706518000	-0.011413000
C	-4.775322000	-0.720638000	-0.021110000
C	-3.597549000	1.445326000	-0.011482000
C	-3.637480000	2.877227000	-0.004860000
C	-4.881783000	3.554560000	0.002518000
C	-6.101630000	2.817869000	-0.002899000
C	-7.343296000	3.493257000	-0.006138000
C	-8.552301000	2.749713000	-0.007047000
C	-8.421369000	-2.955991000	-0.038919000
C	-7.172393000	-3.629273000	-0.048442000
C	-5.957958000	-2.884434000	-0.041811000
C	-4.713621000	-3.559631000	-0.042454000
C	-3.493637000	-2.832225000	-0.025993000
C	-3.528821000	-1.400895000	-0.018014000
C	-2.350625000	0.766988000	-0.011038000
C	-2.313884000	-0.661412000	-0.012834000
C	-1.067288000	-1.342346000	-0.003444000
C	-1.134054000	1.508213000	-0.010451000
C	0.147613000	-0.602043000	0.000743000
C	0.113741000	0.824667000	-0.006251000
C	-10.930651000	-1.589438000	0.012970000
C	-10.972233000	1.276591000	-0.004999000
C	-12.179405000	0.510838000	-0.007632000
C	-12.154055000	-0.864295000	-0.002138000
C	-9.815146000	3.416618000	-0.006973000
C	-10.987040000	2.684389000	-0.006266000
C	-2.414348000	3.610234000	-0.008506000
C	-1.172198000	2.933774000	-0.011775000
C	-7.400597000	4.949196000	-0.013929000

C	-4.924122000	4.996735000	0.020924000
C	-9.893234000	4.901867000	-0.007668000
C	-2.473816000	5.044019000	-0.009027000
C	-8.629043000	5.600133000	-0.017007000
C	-6.155265000	5.664819000	0.016470000
C	-3.678523000	5.697147000	0.003621000
C	-1.032267000	-2.773632000	0.006243000
C	-10.879614000	-3.016830000	-0.008651000
C	-2.244975000	-3.514073000	-0.009159000
C	-9.653793000	-3.702500000	-0.060143000
C	-2.213363000	-4.955010000	0.006439000
C	-4.669925000	-4.995319000	-0.051934000
C	-7.133360000	-5.064007000	-0.087991000
C	-9.566692000	-5.143411000	-0.100875000
C	-3.442419000	-5.648207000	0.008562000
C	-5.906610000	-5.719927000	-0.107659000
C	-8.371938000	-5.787072000	-0.119866000
H	-13.094068000	-1.401578000	0.009872000
C	8.721055000	1.755144000	0.006321000
C	7.507757000	1.006899000	0.005921000
C	6.255505000	1.682511000	0.000019000
C	7.546229000	-0.415497000	0.012314000
C	6.329583000	-1.157741000	0.019058000
C	5.080631000	-0.485108000	0.012128000
C	5.042060000	0.939395000	0.002708000
C	9.970500000	1.080164000	0.015082000
C	8.801909000	-1.090489000	0.016618000
C	3.863053000	-1.229433000	0.017297000
C	3.795388000	1.619639000	-0.003446000
C	2.574744000	0.880145000	-0.001221000
C	2.610032000	-0.546926000	0.008947000
C	10.015363000	-0.340723000	0.012322000
C	1.331767000	1.560664000	-0.006794000
C	1.396423000	-1.283498000	0.010945000
C	12.431201000	1.121050000	0.069779000
C	12.476448000	-0.234391000	0.056225000
C	11.276929000	-1.035676000	-0.001937000
C	11.193098000	1.846008000	0.024692000
C	1.431218000	-2.713407000	0.029595000
C	3.897208000	-2.647749000	0.031490000
C	6.368028000	-2.586430000	0.031521000
C	8.844370000	-2.513694000	0.030108000
C	11.304433000	-2.440182000	-0.012551000
C	0.214623000	-3.455586000	0.033356000
C	2.682068000	-3.385058000	0.040209000
C	7.626660000	-3.259283000	0.040313000
C	10.096339000	-3.204099000	0.037353000
C	5.158978000	-3.331009000	0.038750000
C	10.090524000	-4.628369000	0.057191000
C	7.648119000	-4.683008000	0.056007000
C	5.220124000	-4.753977000	0.051165000
C	2.694663000	-4.817300000	0.058416000
C	0.249201000	-4.894376000	0.073475000
C	8.918286000	-5.341707000	0.070199000
C	6.441991000	-5.403966000	0.060930000
C	3.982093000	-5.569033000	0.051226000
C	1.525509000	-5.533261000	0.079149000
C	-0.958328000	-5.623025000	0.056856000
C	1.298222000	2.992729000	-0.013482000
C	3.763719000	3.042485000	-0.011232000
C	6.219557000	3.107934000	-0.006434000
C	8.678082000	3.176660000	0.000720000
C	11.144844000	3.238511000	0.001963000
C	0.056110000	3.677712000	-0.015563000
C	2.517607000	3.728212000	-0.016117000
C	4.972661000	3.785704000	-0.012904000
C	7.440325000	3.845903000	-0.007418000

C	9.898782000	3.959458000	-0.004359000	C	-5.811641000	0.093212000	-0.239784000
C	9.875026000	5.343719000	-0.016853000	C	-5.715258000	1.515459000	-0.198671000
C	7.391336000	5.281131000	-0.016763000	C	-6.895110000	2.310790000	-0.206771000
C	4.947492000	5.222971000	-0.020574000	C	-8.172650000	1.681134000	-0.254197000
C	2.479893000	5.156588000	-0.023173000	C	-4.637288000	-0.698468000	-0.224051000
C	0.049294000	5.103992000	-0.021695000	C	-4.439001000	2.139750000	-0.156487000
C	8.641177000	6.095476000	-0.021734000	C	-3.260390000	1.346793000	-0.145495000
C	6.179209000	5.926851000	-0.023004000	C	-3.356895000	-0.078479000	-0.183464000
C	3.701921000	5.885199000	-0.025753000	C	-1.982045000	1.966955000	-0.106277000
C	1.233202000	5.816165000	-0.026198000	C	-1.888516000	3.395206000	-0.069169000
C	-1.230805000	5.858782000	-0.022276000	C	-3.065231000	4.186191000	-0.071415000
O	-5.923805000	-7.076849000	-0.168240000	C	-4.347518000	3.569345000	-0.117338000
H	-5.067488000	-7.408579000	-0.466828000	C	-5.521580000	4.357229000	-0.128496000
O	12.251576000	4.019126000	-0.011645000	C	-6.796751000	3.734777000	-0.170020000
H	13.048945000	3.481897000	-0.091455000	C	-7.193655000	-1.958245000	-0.319170000
C	12.601886000	-3.181216000	-0.064909000	C	-6.022879000	-2.745658000	-0.298036000
O	12.904278000	-4.133043000	0.629031000	C	-4.738857000	-2.119609000	-0.262892000
O	13.443425000	-2.716284000	-1.024447000	C	-3.566481000	-2.908591000	-0.242994000
H	14.242281000	-3.268007000	-0.963622000	C	-2.282422000	-2.300827000	-0.194533000
C	-6.198219000	7.163763000	0.003378000	C	-2.181450000	-0.873954000	-0.163305000
O	-6.754120000	7.833808000	-0.839112000	C	-0.804852000	1.173869000	-0.093017000
O	-5.552515000	7.708870000	1.062383000	C	-0.901835000	-0.252165000	-0.122115000
H	-5.619752000	8.673890000	0.955970000	C	0.273213000	-1.047545000	-0.099417000
C	-12.141930000	-3.819741000	-0.009167000	C	0.474796000	1.796916000	-0.054312000
O	-12.403608000	-4.728390000	-0.771610000	C	1.552711000	-0.424397000	-0.059158000
O	-13.003503000	-3.457857000	0.978491000	C	1.652616000	0.998493000	-0.039400000
H	-13.772751000	-4.045532000	0.882410000	C	-9.551844000	-0.360005000	-0.372017000
O	8.602607000	7.336135000	-0.030820000	C	-9.350566000	2.488250000	-0.257844000
O	3.586292000	7.226076000	-0.032907000	C	-10.635301000	1.837859000	-0.312049000
H	4.455126000	7.649708000	-0.033794000	C	-10.696603000	0.446561000	-0.357433000
O	-1.255762000	7.087788000	-0.031229000	C	-7.992737000	4.514406000	-0.176957000
O	8.884678000	-6.699211000	0.097120000	C	-9.230986000	3.887071000	-0.218981000
H	9.787344000	-7.043328000	0.125923000	C	-0.603212000	4.010693000	-0.033005000
O	4.010485000	-6.797917000	0.042525000	C	0.570618000	3.219793000	-0.026842000
C	-0.884648000	-7.116769000	0.142325000	C	-5.442121000	5.809858000	-0.102165000
O	-0.236593000	-7.734295000	0.959152000	C	-2.972025000	5.624882000	-0.020538000
O	-1.612482000	-7.749290000	-0.818448000	C	-7.932675000	5.997096000	-0.141296000
H	-1.462644000	-8.700039000	-0.673528000	C	-0.527491000	5.444507000	-0.002359000
H	-10.479278000	-5.721045000	-0.139722000	C	-6.604654000	6.572849000	-0.110885000
H	-8.335258000	-6.869336000	-0.158057000	C	-4.136364000	6.404234000	-0.033254000
H	-3.411878000	-6.727442000	0.069094000	C	-1.667547000	6.206602000	0.002859000
H	1.606074000	-6.611779000	0.109566000	C	0.172488000	-2.476400000	-0.113961000
H	6.452447000	-6.487479000	0.072103000	C	-9.642038000	-1.792324000	-0.417594000
H	11.031697000	-5.161865000	0.094579000	C	-1.103872000	-3.098875000	-0.162552000
H	13.437266000	-0.727391000	0.093261000	C	-8.497761000	-2.582991000	-0.366949000
H	13.376928000	1.653967000	0.139647000	C	-1.211337000	-4.536936000	-0.166474000
H	10.796100000	5.912467000	-0.022994000	C	-3.662014000	-4.343288000	-0.265543000
H	6.236582000	7.014439000	-0.030248000	C	-6.122071000	-4.182033000	-0.347447000
H	1.183099000	6.898581000	-0.031505000	C	-8.554676000	-4.026387000	-0.400924000
H	-3.652927000	6.779175000	0.010906000	C	-2.505439000	-5.109158000	-0.187522000
H	-8.691200000	6.679835000	-0.043049000	C	-4.964117000	-4.945371000	-0.348088000
O	-10.981517000	5.497717000	0.001937000	C	-7.429257000	-4.783823000	-0.400908000
O	-13.335917000	1.219973000	-0.018969000	H	-11.679231000	0.016681000	-0.434247000
H	-14.088947000	0.614590000	-0.014487000	C	10.308867000	1.119746000	0.141945000
H	-11.926390000	3.225700000	-0.007071000	C	9.030541000	0.488409000	0.106846000

### GO-118-Int3

SCF Energy (B3LYP-D3/B2) = -8709.01687922

Enthalpy 0K = 1.142425

Enthalpy 298 K = 1.233827

Free Energy 298 K = 1.017434

C	-8.260194000	0.260519000	-0.303695000	C	11.400053000	-1.088084000	0.129973000
C	-7.090671000	-0.533631000	-0.285686000				



C	0.249142000	-1.048380000	-0.178685000	C	7.353296000	-5.775545000	-0.011001000
C	0.440790000	1.795778000	-0.094831000	C	4.889539000	-5.715223000	-0.100697000
C	1.525688000	-0.422024000	-0.111172000	C	2.445744000	-5.456883000	-0.143883000
C	1.620725000	1.000893000	-0.072165000	C	-0.037115000	-5.320537000	-0.241003000
C	-9.570002000	-0.386208000	-0.624715000	C	2.995651000	3.052143000	0.032837000
C	-9.381346000	2.459393000	-0.447096000	C	5.453626000	2.877183000	0.114363000
C	-10.659181000	1.804377000	-0.536998000	C	7.904504000	2.719856000	0.197102000
C	-10.719015000	0.421218000	-0.634968000	C	10.358569000	2.565127000	0.281300000
C	-8.032936000	4.487584000	-0.306521000	C	12.814729000	2.404487000	0.355939000
C	-9.267776000	3.858519000	-0.376984000	C	1.820011000	3.847387000	0.015191000
C	-0.644390000	4.005751000	-0.060642000	C	4.275194000	3.673068000	0.094163000
C	0.531537000	3.218527000	-0.047421000	C	6.724738000	3.507031000	0.175264000
C	-5.487694000	5.790726000	-0.173164000	C	9.186280000	3.343603000	0.257634000
C	-3.018471000	5.612432000	-0.059697000	C	11.642277000	3.235538000	0.337120000
C	-7.977743000	5.969978000	-0.243962000	C	11.741691000	4.618932000	0.368275000
C	-0.573876000	5.439094000	-0.009436000	C	9.267455000	4.777267000	0.294014000
C	-6.652479000	6.549849000	-0.185329000	C	6.829139000	4.940313000	0.215474000
C	-4.184933000	6.388331000	-0.076546000	C	4.366707000	5.099322000	0.135589000
C	-1.716162000	6.197657000	-0.009771000	C	1.941912000	5.268433000	0.059838000
C	0.153270000	-2.477234000	-0.211686000	C	10.584505000	5.477179000	0.352092000
C	-9.654409000	-1.815741000	-0.676956000	C	8.117844000	5.529339000	0.273048000
C	-1.120226000	-3.102993000	-0.286948000	C	5.648127000	5.712098000	0.195606000
C	-8.509355000	-2.606145000	-0.607086000	C	3.184978000	5.868910000	0.117489000
C	-1.222740000	-4.541041000	-0.308455000	C	0.736051000	6.136580000	0.046917000
C	-3.672166000	-4.354334000	-0.442543000	O	-5.101032000	-6.314575000	-0.629858000
C	-6.131605000	-4.198725000	-0.558592000	H	-4.280124000	-6.701806000	-0.959352000
C	-8.563304000	-4.048940000	-0.645666000	O	13.993120000	3.079450000	0.397726000
C	-2.513927000	-5.117244000	-0.355808000	H	14.733394000	2.470118000	0.293217000
C	-4.971073000	-4.959963000	-0.549156000	C	13.690824000	-4.118237000	0.121707000
C	-7.435814000	-4.803710000	-0.632881000	O	13.886483000	-5.122279000	0.781101000
H	-11.693733000	-0.014791000	-0.761457000	O	14.607418000	-3.695025000	-0.789810000
C	10.272664000	1.144977000	0.240992000	H	15.348484000	-4.321033000	-0.721065000
C	8.997066000	0.510415000	0.178766000	C	-4.090885000	7.884156000	-0.029699000
C	7.811458000	1.296847000	0.156892000	O	-4.535485000	8.635187000	-0.869856000
C	8.907077000	-0.909087000	0.139164000	O	-3.455091000	8.326668000	1.082599000
C	7.628405000	-1.537468000	0.084031000	H	-3.431419000	9.296964000	1.013262000
C	6.446714000	-0.754559000	0.060731000	C	-11.027613000	-2.436465000	-0.692075000
C	6.537073000	0.667495000	0.097368000	O	-11.426160000	-3.197193000	0.168999000
C	11.453438000	0.359615000	0.265950000	O	-11.762949000	-2.015420000	-1.730070000
C	10.095725000	-1.695649000	0.159887000	H	-12.719717000	-2.061529000	-1.490335000
C	5.166665000	-1.385273000	0.003525000	O	10.651014000	6.718758000	0.381824000
C	5.356707000	1.457995000	0.075134000	O	5.657499000	7.058853000	0.231764000
C	4.075125000	0.832476000	0.014025000	H	6.563230000	7.393757000	0.274216000
C	3.981078000	-0.591531000	-0.021797000	O	0.823198000	7.363315000	0.082764000
C	11.370898000	-1.059272000	0.217733000	O	9.669252000	-7.290824000	0.055879000
C	2.899620000	1.623206000	-0.008381000	H	10.538155000	-7.710927000	0.102004000
C	2.706904000	-1.214557000	-0.082144000	O	4.810588000	-6.941841000	-0.149336000
C	13.902371000	0.176970000	0.403591000	C	-0.100525000	-6.814945000	-0.201611000
C	13.826804000	-1.176505000	0.347074000	O	0.473432000	-7.517494000	-0.603483000
C	12.564071000	-1.864893000	0.220162000	O	-0.863677000	-7.351979000	-1.193806000
C	12.737631000	1.013248000	0.338208000	H	-0.808498000	-8.315100000	-1.066606000
C	2.611597000	-2.642161000	-0.107746000	H	-9.534976000	-4.526533000	-0.673866000
C	5.072500000	-2.799518000	-0.027437000	H	-7.497437000	-5.884897000	-0.668704000
C	7.537031000	-2.963334000	0.050638000	H	-2.587721000	-6.194802000	-0.310035000
C	10.009027000	-3.117225000	0.128097000	H	2.427151000	-6.538561000	-0.145137000
C	12.465372000	-3.266228000	0.163569000	H	7.264757000	-6.855217000	-0.035408000
C	1.332129000	-3.270703000	-0.164393000	H	11.942836000	-5.955502000	0.170578000
C	3.794717000	-3.424434000	-0.079881000	H	14.737859000	-1.754933000	0.404204000
C	8.728572000	-3.748570000	0.075927000	H	14.888193000	0.619858000	0.529507000
C	11.192302000	-3.918558000	0.151220000	H	12.710615000	5.100088000	0.406746000
C	6.265678000	-3.593800000	-0.003799000	H	8.274150000	6.607008000	0.302993000
C	11.055748000	-5.336792000	0.122569000	H	3.232457000	6.950997000	0.149393000
C	8.620041000	-5.168268000	0.044831000	H	-1.594391000	7.272215000	0.040355000
C	6.196720000	-5.016804000	-0.036435000	H	-6.617332000	7.631274000	-0.166584000
C	3.676987000	-4.850661000	-0.107213000	O	-9.001084000	6.671631000	-0.241087000
C	1.234172000	-4.705570000	-0.166622000	O	-11.759023000	2.552319000	-0.527828000
C	9.824225000	-5.939195000	0.075671000	H	-12.571269000	1.970389000	-0.609151000

H	-10.159953000	4.475461000	-0.381283000
C	-14.800747000	-2.336042000	0.329995000
H	-14.009404000	-2.996219000	0.686354000
H	-15.537261000	-2.915985000	-0.224430000
C	-15.460131000	-1.603681000	1.485314000
H	-14.960167000	-1.500363000	2.432745000
H	-16.486001000	-1.282774000	1.421434000
O	-14.196163000	-1.401055000	-0.612431000
Br	-16.368505000	-3.766868000	2.403336000
C	-14.230758000	-0.079113000	-0.192318000
O	-13.676566000	0.748018000	-0.934471000
O	-14.824986000	0.110971000	0.910308000

C	-8.523819000	-2.482394000	-0.630286000
C	-1.260045000	-4.494564000	-0.321445000
C	-3.706763000	-4.280952000	-0.456673000
C	-6.163322000	-4.098672000	-0.578482000
C	-8.592408000	-3.923663000	-0.675327000
C	-2.554732000	-5.056760000	-0.371225000
C	-5.009668000	-4.873180000	-0.567305000
C	-7.472097000	-4.689878000	-0.659739000
H	-11.689759000	0.142466000	-0.775485000
C	10.291511000	1.073651000	0.245742000
C	9.009601000	0.451977000	0.181914000
C	7.832116000	1.250236000	0.161307000
C	8.905467000	-0.966802000	0.139243000
C	7.621152000	-1.581987000	0.082559000
C	6.446846000	-0.786968000	0.060560000
C	6.551476000	0.633805000	0.100266000
C	11.464500000	0.276107000	0.269573000
C	10.086553000	-1.765524000	0.158754000
C	5.160723000	-1.404405000	0.001727000
C	5.378775000	1.436120000	0.079307000
C	4.091757000	0.823996000	0.016678000
C	3.983162000	-0.598847000	-0.022205000
C	11.367958000	-1.142041000	0.218341000
C	2.923576000	1.626809000	-0.004311000
C	2.702434000	-1.208828000	-0.084385000
C	13.910477000	0.069183000	0.409348000
C	13.821814000	-1.283668000	-0.350074000
C	12.552951000	-1.959237000	0.219849000
C	12.754351000	0.916754000	0.343703000
C	2.592833000	-2.635149000	-0.113099000
C	5.052016000	-2.818023000	-0.032398000
C	7.515374000	-3.006924000	0.045988000
C	9.985774000	-3.185872000	0.123966000
C	12.440412000	-3.360116000	0.159888000
C	1.307683000	-3.250407000	-0.171855000
C	3.769043000	-3.429257000	-0.086576000
C	8.698980000	-3.804201000	0.069943000
C	11.161279000	-3.999233000	0.145769000
C	6.237857000	-3.624538000	-0.010230000
C	11.010022000	-5.416263000	0.113699000
C	8.576153000	-5.222770000	0.035499000
C	6.154743000	-5.046300000	-0.046258000
C	3.636828000	-4.854350000	-0.117390000
C	1.195199000	-4.684965000	-0.177173000
C	9.772781000	-6.005835000	0.064965000
C	7.303784000	-5.817033000	-0.022231000
C	4.840801000	-5.731260000	-0.112757000
C	2.400182000	-5.448163000	-0.155937000
C	-0.080632000	-5.287400000	-0.254308000
C	3.033945000	3.054270000	0.039864000
C	5.489849000	2.854620000	0.121466000
C	7.939431000	2.672475000	0.204487000
C	10.391869000	2.492467000	0.289044000
C	12.845013000	2.307857000	0.363442000
C	1.866122000	3.860990000	0.023731000
C	4.319748000	3.662124000	0.102572000
C	6.767242000	3.471548000	0.183860000
C	9.226904000	3.283247000	0.266517000
C	11.681679000	3.150039000	0.346173000
C	11.794255000	4.533256000	0.379752000
C	9.322497000	4.715676000	0.305620000
C	6.885945000	4.903450000	0.226881000
C	4.425635000	5.087692000	0.146782000
C	2.002236000	5.281541000	0.071047000
C	10.646298000	5.402512000	0.365104000
C	8.180140000	5.479382000	0.285820000
C	5.712062000	5.687079000	0.208194000

## GO-118-Pdt1

SCF Energy (B3LYP-D3/B2) = -8709.01193085

Enthalpy 0K = 1.145071

Enthalpy 298 K = 1.236837

Free Energy 298 K = 1.017868

C	-8.276748000	0.356374000	-0.528718000
C	-7.110233000	-0.447233000	-0.495839000
C	-5.827919000	0.170108000	-0.412594000
C	-5.721605000	1.591483000	-0.346254000
C	-6.895829000	2.395565000	-0.360054000
C	-8.177069000	1.776098000	-0.445949000
C	-4.659580000	-0.629883000	-0.386741000
C	-4.443707000	2.206112000	-0.267904000
C	-3.269689000	1.403639000	-0.250673000
C	-3.375340000	-0.019335000	-0.311936000
C	-1.988444000	2.014049000	-0.178849000
C	-1.885268000	3.441619000	-0.116503000
C	-3.056071000	4.241558000	-0.121719000
C	-4.342764000	3.633888000	-0.200016000
C	-5.510708000	4.430597000	-0.212896000
C	-6.788763000	3.815937000	-0.288386000
C	-7.221271000	-1.868087000	-0.549218000
C	-6.053317000	-2.666365000	-0.513848000
C	-4.769304000	-2.049962000	-0.445471000
C	-3.601997000	-2.848723000	-0.414728000
C	-2.315350000	-2.250572000	-0.335837000
C	-2.205476000	-0.823942000	-0.283794000
C	-0.817012000	1.212007000	-0.159753000
C	-0.923415000	-0.212351000	-0.211354000
C	0.246742000	-1.017226000	-0.181752000
C	0.466943000	1.825211000	-0.090744000
C	1.529084000	-0.404267000	-0.111926000
C	1.638853000	1.018020000	-0.069833000
C	-9.566761000	-0.251764000	-0.644347000
C	-9.346955000	2.591036000	-0.445599000
C	-10.627422000	1.947929000	-0.536006000
C	-10.712005000	0.574788000	-0.649635000
C	-7.980413000	4.603513000	-0.292580000
C	-9.220323000	3.989757000	-0.364937000
C	-0.596413000	4.046373000	-0.050944000
C	0.572554000	3.246244000	-0.040052000
C	-5.422552000	5.882843000	-0.153141000
C	-2.954510000	5.677808000	-0.041732000
C	-7.910049000	6.086005000	-0.220183000
C	-0.511686000	5.477271000	0.003568000
C	-6.581989000	6.652202000	-0.159393000
C	-4.114853000	6.466554000	-0.053240000
C	-1.646640000	6.248190000	0.006697000
C	0.136737000	-2.444482000	-0.217935000
C	-9.661839000	-1.676193000	-0.702579000
C	-1.143360000	-3.057342000	-0.296100000

C	3.250763000	5.869070000	0.129866000	C	5.478222000	0.506476000	-0.106552000
C	0.805145000	6.161554000	0.059634000	C	5.316185000	1.923209000	-0.122419000
O	-5.156271000	-6.224820000	-0.653295000	C	6.459245000	2.768437000	-0.142756000
H	-4.331526000	-6.624254000	-0.957614000	C	7.763806000	2.193071000	-0.153383000
O	14.031166000	2.970012000	0.406161000	C	4.338122000	-0.334079000	-0.090347000
H	14.763850000	2.352889000	0.294378000	C	4.013766000	2.492633000	-0.110946000
C	13.657122000	-4.223803000	0.115119000	C	2.870697000	1.649694000	-0.093654000
O	13.842520000	-5.233840000	0.768644000	C	3.030979000	0.230035000	-0.079210000
O	14.579780000	-3.804832000	-0.792628000	C	1.566405000	2.214144000	-0.080820000
H	15.314107000	-4.438829000	-0.725344000	C	1.409857000	3.637418000	-0.093175000
C	-4.006372000	7.959797000	0.005259000	C	2.550171000	4.478713000	-0.117576000
O	-4.460585000	8.725493000	-0.817193000	C	3.859084000	3.917077000	-0.124041000
O	-3.345292000	8.388266000	1.109424000	C	4.997161000	4.754990000	-0.139374000
H	-3.312269000	9.358452000	1.044054000	C	6.298008000	4.186495000	-0.151175000
C	-11.029433000	-2.295292000	-0.745832000	C	6.949356000	-1.481767000	-0.100147000
O	-11.460123000	-3.063007000	0.092976000	C	5.810551000	-2.319541000	-0.083375000
O	-11.745042000	-1.875172000	-1.805577000	C	4.501195000	-1.749486000	-0.070713000
H	-12.689277000	-2.061026000	-1.629073000	C	3.363180000	-2.588153000	-0.057990000
O	10.724303000	6.643869000	0.397075000	C	2.053791000	-2.036546000	-0.058894000
O	5.736267000	7.034274000	0.246992000	C	1.890663000	-0.615042000	-0.069803000
H	6.645998000	7.357886000	0.290310000	C	0.424757000	1.370969000	-0.066590000
O	0.904447000	7.387572000	0.096606000	C	0.584549000	-0.049356000	-0.060582000
O	9.604102000	-7.356108000	0.041966000	C	-0.555317000	-0.894825000	-0.055537000
H	10.469000000	-7.784437000	0.087401000	C	-0.881348000	1.937922000	-0.054196000
O	4.749314000	-6.956936000	-0.164718000	C	-1.861086000	-0.328103000	-0.045965000
C	-0.158899000	-6.780485000	-0.219411000	C	-2.023222000	1.089210000	-0.042432000
O	0.413307000	-7.492971000	0.578512000	C	9.243290000	0.213630000	-0.131670000
O	-0.934913000	-7.307876000	-1.207852000	C	8.900353000	3.050720000	-0.177032000
H	-0.886581000	-8.271618000	-1.082940000	C	10.211880000	2.461344000	-0.195338000
H	-9.567105000	-4.394399000	-0.710582000	C	10.356399000	1.082044000	-0.189069000
H	-7.545220000	-5.770244000	-0.699713000	C	7.458167000	5.017459000	-0.172573000
H	-2.638792000	-6.133730000	-0.329112000	C	8.721120000	4.444749000	-0.185449000
H	2.370940000	-6.529510000	-0.160145000	C	0.098290000	4.196618000	-0.077605000
H	7.204288000	-6.895668000	-0.049266000	C	-1.039592000	3.355426000	-0.057493000
H	11.890815000	-6.043984000	0.160611000	C	4.855086000	6.203368000	-0.139901000
H	14.727136000	-1.870963000	0.407883000	C	2.393775000	5.912409000	-0.142842000
H	14.900270000	0.502210000	0.538645000	C	7.334107000	6.496974000	-0.182530000
H	12.768010000	5.004511000	0.419075000	C	-0.040016000	5.625662000	-0.083522000
H	8.347467000	6.555325000	0.317782000	C	5.983811000	7.015782000	-0.158224000
H	3.309250000	6.950563000	0.163766000	C	3.523569000	6.741590000	-0.156492000
H	-1.512772000	7.320977000	0.058650000	C	1.065390000	6.436810000	-0.113863000
H	-6.536328000	7.732882000	-0.133857000	C	-0.392489000	-2.317972000	-0.062821000
O	-8.930558000	6.793274000	-0.211631000	C	9.395619000	-1.208126000	-0.093483000
O	-11.719887000	2.728445000	-0.510851000	C	0.910344000	-2.884377000	-0.062212000
H	-12.527008000	2.172959000	-0.546173000	C	8.278437000	-2.047703000	-0.097305000
H	-10.104218000	4.618045000	-0.362696000	C	1.079613000	-4.316037000	-0.078165000
C	-14.790648000	-2.324009000	0.395053000	C	3.521000000	-4.017355000	-0.049636000
H	-13.947841000	-2.923222000	0.739144000	C	5.972666000	-3.748879000	-0.041498000
H	-15.542582000	-2.960365000	-0.062954000	C	8.395382000	-3.488135000	-0.056030000
C	-15.366675000	-1.388152000	1.464238000	C	2.396337000	-4.832330000	-0.099936000
H	-15.033717000	-1.624039000	2.471317000	C	4.848628000	-4.563026000	-0.008762000
H	-16.454858000	-1.339741000	1.446874000	C	7.303654000	-4.292902000	-0.022375000
O	-14.279889000	-1.385027000	-0.616928000	H	11.351832000	0.665705000	-0.204680000
Br	-16.577997000	-4.250637000	2.320516000	C	-10.677643000	0.832678000	0.053350000
C	-14.281593000	-0.129769000	-0.119158000	C	-9.372734000	0.257612000	0.038931000
O	-13.822630000	0.822720000	-0.718374000	C	-8.224814000	1.098315000	0.026929000
O	-14.834194000	-0.074490000	1.088495000	C	-9.215840000	-1.156590000	0.035576000

#### GO-118-Int4

SCF Energy (B3LYP-D3/B2) = -8862.86209160

Enthalpy 0K = 1.200490

Enthalpy 298 K = 1.296872

Free Energy 298 K = 1.068066

C	7.923123000	0.777516000	-0.135068000
C	6.784789000	-0.064833000	-0.116021000

C	5.478222000	0.506476000	-0.106552000
C	5.316185000	1.923209000	-0.122419000
C	6.459245000	2.768437000	-0.142756000
C	7.763806000	2.193071000	-0.153383000
C	4.338122000	-0.334079000	-0.090347000
C	4.013766000	2.492633000	-0.110946000
C	2.870697000	1.649694000	-0.093654000
C	3.030979000	0.230035000	-0.079210000
C	1.566405000	2.214144000	-0.080820000
C	1.409857000	3.637418000	-0.093175000
C	2.550171000	4.478713000	-0.117576000
C	3.859084000	3.917077000	-0.124041000
C	4.997161000	4.754990000	-0.139374000
C	6.298008000	4.186495000	-0.151175000
C	6.949356000	-1.481767000	-0.100147000
C	5.810551000	-2.319541000	-0.083375000
C	4.501195000	-1.749486000	-0.070713000
C	3.363180000	-2.588153000	-0.057990000
C	2.053791000	-2.036546000	-0.058894000
C	1.890663000	-0.615042000	-0.069803000
C	0.424757000	1.370969000	-0.066590000
C	0.584549000	-0.049356000	-0.060582000
C	-0.555317000	-0.894825000	-0.055537000
C	-0.881348000	1.937922000	-0.054196000
C	-1.861086000	-0.328103000	-0.045965000
C	-2.023222000	1.089210000	-0.042432000
C	9.243290000	0.213630000	-0.131670000
C	8.900353000	3.050720000	-0.177032000
C	10.211880000	2.461344000	-0.195338000
C	10.356399000	1.082044000	-0.189069000
C	7.458167000	5.017459000	-0.172573000
C	8.721120000	4.444749000	-0.185449000
C	0.098290000	4.196618000	-0.077605000
C	-1.039592000	3.355426000	-0.057493000
C	4.855086000	6.203368000	-0.139901000
C	2.393775000	5.912409000	-0.142842000
C	7.334107000	6.496974000	-0.182530000
C	-0.040016000	5.625662000	-0.083522000
C	5.983811000	7.015782000	-0.158224000
C	3.523569000	6.741590000	-0.156492000
C	1.065390000	6.436810000	-0.113863000
C	-0.392489000	-2.317972000	-0.062821000
C	9.395619000	-1.208126000	-0.093483000
C	0.910344000	-2.884377000	-0.062212000
C	8.278437000	-2.047703000	-0.097305000
C	1.079613000	-4.316037000	-0.078165000
C	3.521000000	-4.017355000	-0.049636000
C	5.972666000	-3.748879000	-0.041498000
C	8.395382000	-3.488135000	-0.056030000
C	2.396337000	-4.832330000	-0.099936000
C	4.848628000	-4.563026000	-0.008762000
C	7.303654000	-4.292902000	-0.022375000
H	11.351832000	0.665705000	-0.204680000
C	-10.677643000	0.832678000	0.053350000
C	-9.372734000	0.257612000	0.038931000
C	-8.224814000	1.098315000	0.026929000
C	-9.215840000	-1.156590000	0.035576000
C	-7.908456000	-1.725147000	0.014146000
C	-6.764234000	-0.888158000	0.003559000
C	-6.921515000	0.528496000	0.009966000
C	-11.820932000	-0.006649000	0.062140000
C	-10.366737000	-1.997607000	0.048903000
C	-5.455260000	-1.459002000	-0.015846000
C	-5.778983000	1.373044000	-0.001418000
C	-4.468613000	0.807366000	-0.017355000
C	-4.307599000	-0.611066000	-0.024516000
C	-11.671121000	-1.420839000	0.067843000



C	6.954670000	-1.475778000	-0.199364000	C	-10.206298000	-3.414925000	0.040314000
C	5.818234000	-2.312815000	-0.179006000	C	-12.651369000	-3.680247000	0.130701000
C	4.507584000	-1.743816000	-0.156355000	C	-1.528141000	-3.162379000	-0.134649000
C	3.370407000	-2.583021000	-0.143076000	C	-3.982113000	-3.430950000	-0.095449000
C	2.060179000	-2.032342000	-0.131095000	C	-8.897148000	-3.985523000	-0.000922000
C	1.896457000	-0.611202000	-0.126839000	C	-11.350957000	-4.270745000	0.049173000
C	0.429918000	1.374094000	-0.090343000	C	-6.443261000	-3.715532000	-0.046865000
C	0.590107000	-0.046328000	-0.101732000	C	-11.147714000	-5.680943000	0.014872000
C	-0.549227000	-0.892360000	-0.097180000	C	-8.721781000	-5.398578000	-0.031356000
C	-0.876312000	1.940346000	-0.061031000	C	-6.307116000	-5.133906000	-0.073612000
C	-1.855341000	-0.326099000	-0.071437000	C	-3.797552000	-4.849670000	-0.128910000
C	-2.017849000	1.090901000	-0.050106000	C	-1.364239000	-4.589872000	-0.189341000
C	9.249317000	0.226610000	-0.264518000	C	-9.889107000	-6.224669000	-0.027854000
C	8.904589000	3.059683000	-0.289007000	C	-7.427184000	-5.945874000	-0.067063000
C	10.230231000	2.481099000	-0.358573000	C	-4.967470000	-5.770551000	-0.106270000
C	10.354083000	1.083979000	-0.383587000	C	-2.539104000	-5.396992000	-0.178371000
C	7.460504000	5.025900000	-0.232744000	C	-0.063067000	-5.145320000	-0.200202000
C	8.724215000	4.450945000	-0.276877000	C	-3.489217000	3.076232000	0.001493000
C	0.102697000	4.199507000	-0.065541000	C	-5.937164000	2.786672000	0.045832000
C	-1.034979000	3.357539000	-0.046120000	C	-8.379158000	2.515184000	0.088612000
C	4.858010000	6.208834000	-0.150512000	C	-10.824549000	2.246127000	0.130029000
C	2.396903000	5.916717000	-0.130398000	C	-13.270440000	1.971001000	0.181508000
C	7.337102000	6.504769000	-0.222342000	C	-2.351989000	3.925766000	-0.012595000
C	-0.036142000	5.628603000	-0.053105000	C	-4.797257000	3.636860000	0.034321000
C	5.986560000	7.021924000	-0.173667000	C	-7.237374000	3.356592000	0.078387000
C	3.526520000	6.746321000	-0.145209000	C	-9.689595000	3.078522000	0.121566000
C	1.068890000	6.440404000	-0.083232000	C	-12.138521000	2.856071000	0.169879000
C	-0.386080000	-2.315146000	-0.121161000	C	-12.302637000	4.233729000	0.198828000
C	9.397800000	-1.199229000	-0.188276000	C	-9.838422000	4.507022000	0.146384000
C	0.917155000	-2.881133000	-0.135076000	C	-7.409465000	4.783715000	0.101117000
C	8.286364000	-2.042140000	-0.191103000	C	-4.956253000	5.057772000	0.055386000
C	1.086625000	-4.312752000	-0.165841000	C	-2.541142000	5.340186000	0.007346000
C	3.527765000	-4.012151000	-0.146750000	C	-11.187356000	5.144989000	0.186517000
C	5.978965000	-3.743445000	-0.138794000	C	-8.724951000	5.311985000	0.135803000
C	8.402475000	-3.483015000	-0.138760000	C	-6.265649000	5.609931000	0.088859000
C	2.404485000	-4.827432000	-0.199531000	C	-3.811757000	5.881885000	0.041227000
C	4.856543000	-4.557401000	-0.110572000	C	-1.377514000	6.264060000	-0.009299000
C	7.310567000	-4.286990000	-0.112547000	O	5.049607000	-5.906922000	-0.058244000
H	11.346730000	0.673929000	-0.479643000	H	4.270453000	-6.330448000	0.324341000
C	-10.671358000	0.831109000	0.109605000	O	-14.479818000	2.589347000	0.230188000
C	-9.366410000	0.256618000	0.078258000	H	-15.183035000	1.941184000	0.354779000
C	-8.218768000	1.097668000	0.067343000	C	-13.832014000	-4.590881000	0.205078000
C	-9.209288000	-1.157447000	0.056979000	O	-14.017667000	-5.579304000	-0.480518000
C	-7.901990000	-1.725334000	0.018799000	O	-14.716031000	-4.245035000	1.179525000
C	-6.758050000	-0.888035000	0.009209000	H	-15.429898000	-4.903244000	1.125761000
C	-6.915548000	0.528431000	0.033541000	C	3.361374000	8.236349000	-0.120328000
C	-11.814177000	-0.008537000	0.117174000	O	3.816103000	8.972716000	0.727348000
C	-10.359867000	-1.998898000	0.069223000	O	2.645260000	8.694150000	-1.176669000
C	-5.449081000	-1.458304000	-0.026894000	H	2.580402000	9.658190000	-1.061735000
C	-5.773172000	1.373282000	0.023308000	C	10.777427000	-1.794623000	-0.050827000
C	-4.462904000	0.808103000	-0.009418000	O	11.215418000	-2.669316000	-0.781178000
C	-4.301580000	-0.609967000	-0.034521000	O	11.436243000	-1.280080000	0.984389000
C	-11.664130000	-1.422704000	0.104941000	H	12.385672000	-1.622369000	1.011590000
C	-3.325480000	1.653042000	-0.019605000	O	-11.311350000	6.382625000	0.209142000
C	-2.998640000	-1.172871000	-0.066768000	O	-6.339450000	6.955266000	0.107554000
C	-14.255743000	-0.302934000	0.103372000	H	-7.260925000	7.246405000	0.128443000
C	-14.115247000	-1.652489000	0.102341000	O	-1.522760000	7.485837000	0.010098000
C	-12.817302000	-2.283948000	0.134711000	O	-9.671516000	-7.567481000	-0.069417000
C	-13.128844000	0.585301000	0.139783000	H	-10.521767000	-8.026174000	-0.084675000
C	-2.836555000	-2.594342000	-0.100499000	O	-4.829967000	-6.993096000	-0.111028000
C	-5.288500000	-2.866435000	-0.056037000	C	0.067464000	-6.632613000	-0.293340000
C	-7.743420000	-3.145370000	-0.008708000	O	-0.513108000	-7.336801000	-1.092534000

O	0.903704000	-7.163988000	0.641581000	C	5.879509000	-2.254838000	-0.266751000
H	0.887292000	-8.123898000	0.483337000	C	4.565094000	-1.690181000	-0.232081000
H	9.392351000	-3.919507000	-0.141488000	C	3.430937000	-2.532346000	-0.234108000
H	7.423334000	-5.364096000	-0.076595000	C	2.117797000	-1.986553000	-0.207217000
H	2.528195000	-5.898171000	-0.281333000	C	1.950440000	-0.567048000	-0.173201000
H	-2.470493000	-6.475891000	-0.218882000	C	0.478323000	1.412790000	-0.089885000
H	-7.287833000	-7.020205000	-0.089665000	C	0.642221000	-0.006906000	-0.131472000
H	-12.006649000	-6.339497000	-0.009704000	C	-0.494689000	-0.856523000	-0.139202000
H	-15.000660000	-2.271308000	0.070688000	C	-0.829964000	1.974565000	-0.042932000
H	-15.266232000	0.096634000	0.046948000	C	-1.802938000	-0.294295000	-0.095650000
H	-13.293335000	4.668740000	0.231754000	C	-1.969235000	1.121168000	-0.043566000
H	-8.932194000	6.381273000	0.156932000	C	9.309774000	0.294727000	-0.308889000
H	-3.910501000	6.960879000	0.056084000	C	8.946929000	3.133131000	-0.324682000
H	0.895474000	7.509051000	-0.081167000	C	10.302942000	2.570305000	-0.431611000
H	5.900535000	8.100246000	-0.141375000	C	10.402572000	1.136972000	-0.443585000
O	8.326863000	7.253449000	-0.255996000	C	7.494844000	5.091185000	-0.220776000
O	11.256992000	3.287807000	-0.394802000	C	8.763247000	4.515153000	-0.295701000
H	12.235551000	2.772580000	-0.477477000	C	0.143873000	4.236178000	-0.006630000
H	9.588390000	5.105520000	-0.305834000	C	-0.992730000	3.389484000	0.002128000
C	14.112205000	-3.444114000	0.774818000	C	4.894085000	6.261666000	-0.089268000
H	13.201436000	-3.774631000	0.270295000	C	2.433190000	5.959615000	-0.052902000
H	14.251781000	-3.980061000	1.716581000	C	7.372493000	6.568937000	-0.184604000
C	15.325610000	-3.635347000	-0.121077000	C	0.001494000	5.663516000	0.035050000
H	15.210450000	-3.110429000	-1.069201000	C	6.023327000	7.078366000	-0.112051000
H	16.235422000	-3.331918000	0.392410000	C	3.563356000	6.792864000	-0.061314000
O	13.939874000	-2.043332000	1.019832000	C	1.105910000	6.478677000	0.013523000
Br	15.543719000	-5.556702000	-0.570902000	C	-0.328092000	-2.277383000	-0.193851000
C	14.850933000	-1.433250000	2.012134000	C	9.449774000	-1.140886000	-0.236917000
O	14.645847000	-0.196407000	2.106493000	C	0.977140000	-2.839474000	-0.224753000
O	15.636964000	-2.188397000	2.564723000	C	8.346053000	-1.985553000	-0.265347000
C	13.749629000	0.828250000	0.537802000	C	1.149687000	-4.270202000	-0.285706000
C	14.299030000	2.174005000	0.453985000	C	3.589710000	-3.960586000	-0.268483000
O	13.399726000	2.161273000	-0.646972000	C	6.039782000	-3.688022000	-0.250449000
H	14.093623000	0.065829000	-0.141209000	C	8.463125000	-3.427649000	-0.230948000
H	12.806078000	0.692088000	1.038642000	C	2.471036000	-4.778120000	-0.336726000
H	15.350499000	2.274850000	0.169514000	C	4.921033000	-4.503265000	-0.242027000
H	14.038565000	2.858300000	1.268529000	C	7.371940000	-4.231480000	-0.225421000

## GO-118-Pdt2

SCF Energy (B3LYP-D3/B2) = -8862.89721877

Enthalpy 0K = 1.205719

Enthalpy 298 K = 1.301101

Free Energy 298 K = 1.074813

C	7.975365000	0.853902000	-0.274406000	C	-11.761514000	-0.005583000	0.154721000
C	6.847729000	0.005864000	-0.254298000	C	-10.303204000	-1.991256000	0.056951000
C	5.535554000	0.570698000	-0.216834000	C	-5.394143000	-1.436450000	-0.055518000
C	5.368644000	1.985611000	-0.195071000	C	-5.724407000	1.392466000	0.055524000
C	6.508442000	2.836553000	-0.217670000	C	-4.413474000	0.831139000	0.003948000
C	7.815324000	2.269200000	-0.273618000	C	-4.248481000	-0.585139000	-0.051828000
C	4.398410000	-0.275277000	-0.211598000	C	-11.608462000	-1.418993000	0.111958000
C	4.063257000	2.548528000	-0.148391000	C	-3.277727000	1.679233000	0.005159000
C	2.924004000	1.701405000	-0.139695000	C	-2.943913000	-1.143993000	-0.102643000
C	3.088563000	0.283017000	-0.170344000	C	-14.201549000	-0.304433000	0.145588000
C	1.616216000	2.260114000	-0.092862000	C	-14.058390000	-1.653655000	0.115187000
C	1.455145000	3.682086000	-0.058260000	C	-12.759321000	-2.283278000	0.129602000
C	2.593216000	4.528367000	-0.074419000	C	-13.076703000	0.585431000	0.197279000
C	3.904021000	3.973511000	-0.118691000	C	-2.778575000	-2.564240000	-0.167194000
C	5.036950000	4.815683000	-0.132079000	C	-5.230352000	-2.842828000	-0.114883000
C	6.342785000	4.255234000	-0.188739000	C	-7.684219000	-3.128883000	-0.059462000
C	7.010848000	-1.417430000	-0.271285000	C	-10.146253000	-3.406059000	-0.002369000

C	-12.590084000	-3.679408000	0.095877000	H	0.975896000	-8.093069000	0.270685000
C	-1.468545000	-3.128336000	-0.219898000	H	9.452610000	-3.865803000	-0.232609000
C	-3.922183000	-3.403365000	-0.173247000	H	7.484326000	-5.309238000	-0.206782000
C	-8.835664000	-3.972233000	-0.062598000	H	2.598361000	-5.846008000	-0.444220000
C	-11.288755000	-4.264836000	-0.004986000	H	-2.402745000	-6.439887000	-0.366949000
C	-6.382641000	-3.694434000	-0.116697000	H	-7.218215000	-6.999982000	-0.222578000
C	-11.081336000	-5.673670000	-0.069044000	H	-11.938580000	-6.334116000	-0.102222000
C	-8.656479000	-5.384001000	-0.122998000	H	-14.942850000	-2.273236000	0.072415000
C	-6.242606000	-5.111753000	-0.173322000	H	-15.212906000	0.094442000	0.099067000
C	-3.734060000	-4.819424000	-0.236856000	H	-13.250204000	4.666421000	0.379237000
C	-1.301290000	-4.553225000	-0.305181000	H	-8.894659000	6.388955000	0.312898000
C	-9.821672000	-6.212683000	-0.129805000	H	-3.874261000	6.982968000	0.193659000
C	-7.360378000	-5.926758000	-0.177163000	H	0.929660000	7.546697000	0.037268000
C	-4.901075000	-5.743637000	-0.226432000	H	5.932127000	8.155713000	-0.061053000
C	-2.473588000	-5.362378000	-0.304254000	O	8.364842000	7.316975000	-0.215762000
C	0.003598000	-5.105505000	-0.332571000	O	11.319595000	3.308206000	-0.502351000
C	-3.444980000	3.101072000	0.056864000	H	12.741923000	2.534558000	-1.106164000
C	-5.891607000	2.804803000	0.108503000	H	9.628962000	5.168001000	-0.334812000
C	-8.333102000	2.526850000	0.159465000	C	14.086522000	-3.403008000	1.515700000
C	-10.777927000	2.250988000	0.209468000	H	13.143863000	-3.570078000	2.039989000
C	-13.220814000	1.969806000	0.270846000	H	14.927909000	-3.653469000	2.161620000
C	-2.309249000	3.953458000	0.054107000	C	14.123057000	-4.164392000	0.202114000
C	-4.753949000	3.657645000	0.108374000	H	13.281009000	-3.886687000	-0.430792000
C	-7.193267000	3.370713000	0.160289000	H	15.073164000	-4.021205000	-0.312199000
C	-9.644516000	3.086171000	0.211988000	O	14.115838000	-1.986767000	1.206626000
C	-12.092175000	2.857601000	0.270738000	Br	13.963474000	-6.096622000	0.579294000
C	-12.258513000	4.235170000	0.330414000	C	15.351226000	-1.383203000	1.191614000
C	-9.796678000	4.513457000	0.268019000	O	15.300132000	-0.136678000	0.739908000
C	-7.368475000	4.796591000	0.213840000	O	16.365332000	-1.923646000	1.556565000
C	-4.916172000	5.077909000	0.159772000	C	14.103673000	0.374970000	0.086192000
C	-2.501459000	5.367571000	0.104137000	C	14.463331000	1.676392000	-0.631658000
C	-11.146622000	5.148246000	0.330359000	O	13.446957000	1.997894000	-1.545027000
C	-8.684525000	5.320888000	0.267654000	H	13.753318000	-0.348436000	-0.655426000
C	-6.225973000	5.625466000	0.212000000	H	13.320065000	0.534751000	0.831415000
C	-3.773123000	5.904716000	0.156146000	H	15.397253000	1.512723000	-1.184963000
C	-1.340308000	6.294495000	0.099864000	H	14.654453000	2.471452000	0.104439000
O	5.113869000	-5.854615000	-0.213513000				
H	4.328912000	-6.281334000	0.153810000				
O	-14.433435000	2.582813000	0.341349000				
H	-15.130314000	1.928786000	0.470219000				
C	-13.767644000	-4.593713000	0.159541000				
O	-13.954711000	-5.572215000	-0.540384000				
O	-14.650059000	-4.266475000	1.142667000				
H	-15.361839000	-4.925892000	1.078472000				
C	3.391778000	8.280936000	-0.007318000	C	-1.480283000	2.815536000	0.239271000
O	3.841185000	9.004443000	0.854340000	C	-1.945791000	1.477063000	0.146888000
O	2.673337000	8.756311000	-1.055210000	C	-2.357887000	3.885538000	0.262630000
H	2.604509000	9.717353000	-0.919963000	C	-3.363704000	1.298614000	0.068291000
C	10.818413000	-1.717979000	-0.053277000	C	-3.738577000	3.720880000	0.195696000
O	11.325670000	-2.587876000	-0.742832000	C	-4.265601000	2.413094000	0.095605000
O	11.439631000	-1.183400000	1.014383000	H	-1.953190000	4.889792000	0.335757000
H	12.365252000	-1.503022000	1.032300000	C	-5.677512000	2.177221000	0.024734000
O	-11.270503000	6.386008000	0.380403000	C	-6.177311000	0.924904000	-0.080225000
O	-6.304635000	6.970428000	0.258926000	C	-5.328819000	-0.222014000	-0.126665000
H	-7.227691000	7.255610000	0.289775000	C	-3.905014000	-0.034166000	-0.042853000
O	-1.488795000	7.515755000	0.145439000	C	-5.854554000	-1.508178000	-0.248807000
O	-9.601587000	-7.554895000	-0.199952000	C	-3.052293000	-1.151957000	-0.072845000
H	-10.451860000	-8.013210000	-0.220304000	C	-5.016259000	-2.645884000	-0.278763000
O	-4.761002000	-6.965942000	-0.256603000	C	-3.608532000	-2.458154000	-0.187519000
C	0.137125000	-6.588467000	-0.455190000	C	-1.061936000	0.316774000	0.127951000
O	-0.457569000	-7.284398000	-1.252288000	C	0.341999000	0.411871000	0.219803000
O	0.995901000	-7.137391000	0.451521000	C	-1.627312000	-0.984491000	0.015440000

### Int3-B3P86

SCF Energy (B3P86/B2) = -4485.72027691

Enthalpy 0K = 0.402582

Enthalpy 298 K = 0.436801

Free Energy 298 K = 0.328495

C	-1.480283000	2.815536000	0.239271000
C	-1.945791000	1.477063000	0.146888000
C	-2.357887000	3.885538000	0.262630000
C	-3.363704000	1.298614000	0.068291000
C	-3.738577000	3.720880000	0.195696000
C	-4.265601000	2.413094000	0.095605000
H	-1.953190000	4.889792000	0.335757000
C	-5.677512000	2.177221000	0.024734000
C	-6.177311000	0.924904000	-0.080225000
C	-5.328819000	-0.222014000	-0.126665000
C	-3.905014000	-0.034166000	-0.042853000
C	-5.854554000	-1.508178000	-0.248807000
C	-3.052293000	-1.151957000	-0.072845000
C	-5.016259000	-2.645884000	-0.278763000
C	-3.608532000	-2.458154000	-0.187519000
C	-1.061936000	0.316774000	0.127951000
C	0.341999000	0.411871000	0.219803000
C	-1.627312000	-0.984491000	0.015440000

C	1.166535000	-0.702584000	0.200437000
C	-0.771111000	-2.116353000	-0.006717000
C	0.608221000	-1.972713000	0.085367000
H	0.839726000	1.363320000	0.310542000
H	1.236862000	-2.856283000	0.067774000
C	-1.309487000	-3.484296000	-0.128668000
C	-2.781706000	-3.610434000	-0.218290000
C	-3.332709000	-4.873627000	-0.333245000
C	-4.721471000	-5.047396000	-0.423579000
C	-5.551781000	-3.949082000	-0.397484000
H	-6.333881000	3.035035000	0.059285000
H	-7.260208000	0.819428000	-0.117932000
H	-6.627891000	-4.061326000	-0.466690000
H	-5.139683000	-6.045203000	-0.514123000
H	-2.647762000	-5.715785000	-0.350784000
O	-7.184623000	-1.751711000	-0.344277000
H	-7.663592000	-0.916212000	-0.362033000
O	-0.151690000	3.070886000	0.305102000
H	-0.014022000	4.023110000	0.363099000
C	2.651648000	-0.475732000	0.304264000
O	3.097521000	0.661365000	0.403145000
O	3.337396000	-1.583711000	0.271758000
H	4.378303000	-1.424294000	0.349042000
C	-4.577620000	4.938407000	0.231427000
O	-5.792791000	5.015114000	0.184052000
O	-3.838957000	6.072538000	0.329468000
H	-4.492058000	6.787868000	0.343664000
O	-0.587015000	-4.476544000	-0.157282000
C	7.222770000	0.261121000	-0.762100000
H	6.677488000	0.118664000	-1.694595000
C	6.328773000	0.086400000	0.450253000
H	5.489283000	0.787667000	0.431771000
H	6.923083000	0.226925000	1.358443000
O	5.796641000	-1.217433000	0.411933000
Br	7.958144000	2.093592000	-0.849347000
H	8.078437000	-0.407574000	-0.694868000
C	6.714091000	-2.365946000	0.940195000
O	7.841071000	-1.963755000	1.211212000
O	6.084129000	-3.407667000	0.948121000

### TS3-B3P86

SCF Energy (B3P86/B2) = -4485.70202475

Enthalpy 0K = 0.403603

Enthalpy 298 K = 0.437163

Free Energy 298 K = 0.331280

C	-1.445980000	2.789993000	0.274523000
C	-1.946444000	1.466017000	0.166213000
C	-2.296161000	3.881990000	0.311979000
C	-3.367245000	1.325142000	0.071898000
C	-3.680016000	3.753233000	0.239982000
C	-4.240416000	2.461577000	0.114064000
H	-1.866246000	4.874416000	0.400281000
C	-5.657436000	2.263193000	0.030900000
C	-6.188022000	1.026658000	-0.105511000
C	-5.368012000	-0.139757000	-0.174511000
C	-3.941202000	0.009335000	-0.073091000
C	-5.924391000	-1.408861000	-0.335888000
C	-3.116983000	-1.129165000	-0.121849000
C	-5.114734000	-2.566602000	-0.386685000
C	-3.703945000	-2.417575000	-0.274954000

C	-1.093314000	0.282654000	0.142754000
C	0.308936000	0.338165000	0.272561000
C	-1.690056000	-1.000373000	-0.009591000
C	1.103377000	-0.798419000	0.244467000
C	-0.863794000	-2.153728000	-0.044041000
C	0.515896000	-2.049636000	0.080918000
H	0.826590000	1.274424000	0.401902000
H	1.117254000	-2.951367000	0.053312000
C	-1.433853000	-3.503992000	-0.212919000
C	-2.906500000	-3.589992000	-0.325226000
C	-3.488326000	-4.835222000	-0.479379000
C	-4.879721000	-4.970561000	-0.590748000
C	-5.681798000	-3.851990000	-0.545558000
H	-6.292116000	3.136394000	0.081514000
H	-7.272948000	0.948997000	-0.149789000
H	-6.759491000	-3.934570000	-0.629996000
H	-5.322253000	-5.954443000	-0.712113000
H	-2.825490000	-5.694481000	-0.510249000
O	-7.258319000	-1.615837000	-0.452273000
H	-7.716062000	-0.768305000	-0.460878000
O	-0.111305000	3.008551000	0.340212000
H	0.054529000	3.955847000	0.406043000
C	2.584642000	-0.610755000	0.392777000
O	3.073149000	0.496375000	0.549006000
O	3.249781000	-1.744099000	0.327677000
H	4.243262000	-1.578193000	0.452900000
C	-4.488453000	4.991642000	0.295741000
O	-5.701072000	5.098379000	0.248438000
O	-3.721224000	6.103700000	0.414154000
H	-4.354262000	6.836571000	0.440245000
O	-0.733624000	-4.511762000	-0.260306000
C	7.724057000	0.160921000	0.306084000
H	8.495876000	-0.553036000	0.067203000
C	6.293587000	-0.111031000	-0.099363000
H	6.234093000	-0.274839000	-1.174785000
H	5.650946000	0.733908000	0.164350000
O	5.796922000	-1.300642000	0.520402000
Br	8.309773000	1.503232000	-1.567163000
H	7.983796000	0.985099000	0.945018000
C	6.380136000	-1.567210000	1.799831000
O	7.391623000	-0.837254000	2.018275000
O	5.838754000	-2.437842000	2.454849000

### Pdt1-B3P86

SCF Energy (B3P86/B2) = -4485.73081385

Enthalpy 0K = 0.406459

Enthalpy 298 K = 0.440401

Free Energy 298 K = 0.332691

C	-1.245439000	2.718744000	0.292069000
C	-1.829761000	1.429726000	0.193245000
C	-2.026290000	3.860846000	0.355322000
C	-3.256853000	1.376430000	0.113295000
C	-3.416362000	3.816450000	0.314457000
C	-4.058115000	2.563195000	0.184673000
H	-1.534842000	4.824596000	0.439396000
C	-5.485554000	2.451337000	0.125938000
C	-6.091510000	1.251768000	-0.029090000
C	-5.343653000	0.041300000	-0.143633000
C	-3.910560000	0.101185000	-0.051931000
C	-5.976007000	-1.187076000	-0.340931000

C	-3.157352000	-1.084308000	-0.135985000
C	-5.238762000	-2.390208000	-0.428336000
C	-3.821049000	-2.330821000	-0.318356000
C	-1.052350000	0.195334000	0.157326000
C	0.346844000	0.161075000	0.310158000
C	-1.726064000	-1.045148000	-0.024939000
C	1.069699000	-1.022757000	0.255233000
C	-0.972297000	-2.246240000	-0.086496000
C	0.410260000	-2.230268000	0.044799000
H	0.915447000	1.061145000	0.477375000
H	0.951760000	-3.167881000	-0.010748000
C	-1.623074000	-3.555162000	-0.288755000
C	-3.096496000	-3.548055000	-0.402353000
C	-3.754276000	-4.751329000	-0.589115000
C	-5.150861000	-4.797647000	-0.701028000
C	-5.883345000	-3.633540000	-0.622117000
H	-6.065966000	3.359060000	0.209761000
H	-7.179785000	1.237555000	-0.046908000
H	-6.964112000	-3.647842000	-0.706045000
H	-5.653068000	-5.748632000	-0.849284000
H	-3.145870000	-5.648678000	-0.645019000
O	-7.320161000	-1.307964000	-0.459370000
H	-7.721655000	-0.432385000	-0.475453000
O	0.101431000	2.851683000	0.320791000
H	0.332448000	3.786764000	0.362231000
C	2.550266000	-0.927255000	0.429989000
O	3.111059000	0.122847000	0.683982000
O	3.165089000	-2.093036000	0.275138000
H	4.138980000	-1.954794000	0.402505000
C	-4.147085000	5.101297000	0.402324000
O	-5.351882000	5.279673000	0.387241000
O	-3.311304000	6.162863000	0.511623000
H	-3.896350000	6.933543000	0.560008000
O	-0.982269000	-4.601330000	-0.358776000
C	7.593840000	-0.125374000	0.789952000
H	8.520773000	-0.447839000	0.315206000
C	6.369069000	-0.388733000	-0.075212000
H	6.621865000	-0.568717000	-1.116343000
H	5.604712000	0.384555000	-0.001358000
O	5.825109000	-1.609855000	0.518753000
Br	8.110608000	1.760147000	-1.705724000
H	7.694352000	0.915203000	1.084759000
C	6.374771000	-1.812089000	1.746861000
O	7.355961000	-0.939589000	1.972927000
O	6.006998000	-2.671151000	2.502202000

### Int3-M062X

SCF Energy (M062X-D3/B2) = -4479.29558270

Enthalpy 0K = 0.406812

Enthalpy 298 K = 0.440588

Free Energy 298 K = 0.334422

C	-1.616153000	2.732623000	-0.191608000
C	-2.028069000	1.381099000	-0.074701000
C	-2.528793000	3.770937000	-0.109447000
C	-3.429615000	1.145128000	0.045077000
C	-3.890582000	3.545681000	0.065556000
C	-4.368420000	2.221830000	0.133799000
H	-2.165335000	4.789545000	-0.189043000
C	-5.770761000	1.923107000	0.304997000
C	-6.220586000	0.653117000	0.314623000

C	-5.331964000	-0.464296000	0.156046000
C	-3.918664000	-0.218093000	0.062497000
C	-5.813010000	-1.765653000	0.102437000
C	-3.029085000	-1.296142000	-0.031661000
C	-4.934317000	-2.871664000	0.011695000
C	-3.537508000	-2.628025000	-0.042476000
C	-1.091823000	0.254120000	-0.088809000
C	0.310280000	0.415792000	-0.067772000
C	-1.603673000	-1.067793000	-0.091925000
C	1.173461000	-0.667216000	-0.094100000
C	-0.705263000	-2.164290000	-0.134217000
C	0.666599000	-1.962517000	-0.143120000
H	0.763671000	1.390662000	-0.025053000
H	1.341081000	-2.811837000	-0.176571000
C	-1.196355000	-3.561523000	-0.165148000
C	-2.670358000	-3.750748000	-0.119149000
C	-3.174278000	-5.033540000	-0.146681000
C	-4.562193000	-5.262755000	-0.102534000
C	-5.428243000	-4.199176000	-0.025274000
H	-6.457587000	2.745869000	0.430177000
H	-7.281812000	0.491099000	0.485695000
H	-6.500865000	-4.351418000	0.010802000
H	-4.944809000	-6.277600000	-0.128891000
H	-2.464070000	-5.852017000	-0.204101000
O	-7.138108000	-2.064076000	0.140591000
H	-7.655076000	-1.267628000	-0.016683000
O	-0.312711000	3.021245000	-0.401896000
H	-0.178469000	3.974918000	-0.437365000
C	2.667007000	-0.449932000	-0.077030000
O	3.436003000	-1.393585000	-0.133705000
O	2.984571000	0.812440000	0.000411000
H	4.018856000	0.976017000	0.001126000
C	-4.775340000	4.740597000	0.151674000
O	-5.982046000	4.765711000	0.259601000
O	-4.079440000	5.898550000	0.094348000
H	-4.742801000	6.600809000	0.155636000
O	-0.441057000	-4.518709000	-0.224630000
C	7.448536000	0.189635000	0.692798000
H	7.044650000	-0.023483000	1.681226000
C	6.355272000	0.219194000	-0.361812000
H	5.809541000	-0.728325000	-0.390861000
H	6.801847000	0.434097000	-1.336913000
O	5.435702000	1.225032000	-0.005431000
Br	8.740513000	-1.241156000	0.310853000
H	8.003026000	1.124705000	0.678803000
C	5.812006000	2.663874000	-0.346242000
O	6.966331000	2.767115000	-0.748312000
O	4.860947000	3.394239000	-0.128826000

### TS3-M062X

SCF Energy (M062X-D3/B2) = -4479.27006588

Enthalpy 0K = 0.407177

Enthalpy 298 K = 0.440570

Free Energy 298 K = 0.334810

C	1.783462000	2.771569000	0.117080000
C	2.142654000	1.404735000	0.017279000
C	2.734802000	3.772981000	0.019775000
C	3.534222000	1.112837000	-0.095626000
C	4.086319000	3.493175000	-0.155607000
C	4.513109000	2.151065000	-0.204296000

H	2.411384000	4.806003000	0.085976000
C	5.902628000	1.795787000	-0.372273000
C	6.303491000	0.509523000	-0.355862000
C	5.373734000	-0.569434000	-0.169614000
C	3.971207000	-0.267852000	-0.080919000
C	5.805186000	-1.886652000	-0.082815000
C	3.041724000	-1.308394000	0.043623000
C	4.885355000	-2.955675000	0.040743000
C	3.499026000	-2.657858000	0.091632000
C	1.163920000	0.314930000	0.049152000
C	-0.230794000	0.528350000	0.004173000
C	1.626145000	-1.024300000	0.094682000
C	-1.132079000	-0.522224000	0.059751000
C	0.687819000	-2.084886000	0.168077000
C	-0.674581000	-1.833071000	0.163211000
H	-0.642224000	1.519329000	-0.078879000
H	-1.379423000	-2.655790000	0.224886000
C	1.125851000	-3.498798000	0.246521000
C	2.590814000	-3.744565000	0.202916000
C	3.045965000	-5.044018000	0.265860000
C	4.423965000	-5.326928000	0.224147000
C	5.329051000	-4.299355000	0.114037000
H	6.619873000	2.588981000	-0.515954000
H	7.357389000	0.303835000	-0.525067000
H	6.394970000	-4.493063000	0.079151000
H	4.768095000	-6.354275000	0.278286000
H	2.305732000	-5.833409000	0.348791000
O	7.116855000	-2.236341000	-0.115792000
H	7.665778000	-1.456432000	0.013777000
O	0.491072000	3.113860000	0.325872000
H	0.406335000	4.071754000	0.388311000
C	-2.613587000	-0.266255000	0.024183000
O	-3.420544000	-1.161232000	0.168683000
O	-2.901750000	1.002356000	-0.176561000
H	-3.899493000	1.137489000	-0.152236000
C	5.015973000	4.652197000	-0.262663000
O	6.220986000	4.628442000	-0.385311000
O	4.366139000	5.836664000	-0.207618000
H	5.055088000	6.512471000	-0.283378000
O	0.333643000	-4.422111000	0.339643000
C	-7.788020000	0.684875000	0.292022000
H	-8.288525000	1.379734000	-0.363710000
C	-6.389556000	0.198503000	-0.049202000
H	-6.374899000	-0.262139000	-1.033965000
H	-6.051575000	-0.536248000	0.686780000
O	-5.484524000	1.299190000	-0.095551000
Br	-8.961993000	-1.136296000	-0.686053000
H	-8.260860000	0.439101000	1.225445000
C	-5.828483000	2.355935000	0.788764000
O	-6.991483000	2.210546000	1.263142000
O	-4.979621000	3.211857000	0.938634000

**Pdt1-M062X**

SCF Energy (M062X-D3/B2) = -4479.30724075

Enthalpy 0K = 0.410685

Enthalpy 298 K = 0.444210

Free Energy 298 K = 0.338624

C	-1.992308000	-2.862072000	0.136753000
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C	-2.235183000	-1.471239000	0.026561000
C	-3.016126000	-3.784208000	0.003860000
C	-3.593073000	-1.069791000	-0.150047000
C	-4.332726000	-3.398835000	-0.224356000
C	-4.646890000	-2.027182000	-0.296384000
H	-2.779793000	-4.839808000	0.082895000
C	-5.995232000	-1.564700000	-0.525971000
C	-6.291601000	-0.250595000	-0.537003000
C	-5.287141000	0.752334000	-0.319638000
C	-3.918800000	0.341475000	-0.164103000
C	-5.615101000	2.101226000	-0.266321000
C	-2.915840000	1.306519000	-0.005416000
C	-4.619151000	3.095218000	-0.110402000
C	-3.265257000	2.689073000	0.009409000
C	-1.176089000	-0.461458000	0.106141000
C	0.197365000	-0.784460000	0.145058000
C	-1.532062000	0.910978000	0.117625000
C	1.173884000	0.193638000	0.241042000
C	-0.517828000	1.895260000	0.231810000
C	0.818080000	1.538706000	0.303062000
H	0.528796000	-1.806821000	0.097696000
H	1.580422000	2.305563000	0.394457000
C	-0.844519000	3.341657000	0.274379000
C	-2.280237000	3.702118000	0.154713000
C	-2.632561000	5.034466000	0.182570000
C	-3.979955000	5.424978000	0.070935000
C	-4.957612000	4.470626000	-0.072179000
H	-6.767142000	-2.299649000	-0.693609000
H	-7.318027000	0.035626000	-0.751588000
H	-6.001851000	4.747520000	-0.160186000
H	-4.243166000	6.476935000	0.097703000
H	-1.836712000	5.764000000	0.293776000
O	-6.889947000	2.554769000	-0.364214000
H	-7.507742000	1.823175000	-0.267162000
O	-0.739635000	-3.315017000	0.389772000
H	-0.752276000	-4.275623000	0.463790000
C	2.626462000	-0.168010000	0.292128000
O	3.498661000	0.655542000	0.457288000
O	2.840276000	-1.469163000	0.127931000
H	3.804679000	-1.629184000	0.251907000
C	-5.347841000	-4.480851000	-0.361777000
O	-6.541860000	-4.361404000	-0.525419000
O	-4.796110000	-5.712819000	-0.282054000
H	-5.533392000	-6.332667000	-0.379352000
O	0.015007000	4.197708000	0.399080000
C	7.278048000	-0.046708000	0.945438000
H	8.221387000	-0.559105000	1.133512000
C	6.446667000	-0.735641000	-0.132988000
H	7.038031000	-1.392068000	-0.762842000
H	5.878356000	-0.028305000	-0.738553000
O	5.509720000	-1.517347000	0.656895000
Br	9.094501000	0.255053000	-1.641972000
H	7.476173000	0.997645000	0.726817000
C	5.463763000	-1.025815000	1.924615000
O	6.435347000	-0.142818000	2.122229000
O	4.648280000	-1.378741000	2.728826000

**Int3-TPSSH**

SCF Energy (TPSSH/B2) = -4479.92271122

Enthalpy 0K = 0.397523

Enthalpy 298 K = 0.432255

Free Energy 298 K = 0.322713

C	-1.521085000	2.832600000	0.265835000
C	-1.974062000	1.485935000	0.156629000
C	-2.407614000	3.900843000	0.290918000
C	-3.396015000	1.297489000	0.069082000
C	-3.791562000	3.726211000	0.210092000
C	-4.310023000	2.409531000	0.096288000
H	-2.009081000	4.907036000	0.376314000
C	-5.722582000	2.163418000	0.008559000
C	-6.214550000	0.902380000	-0.103272000
C	-5.355753000	-0.241266000	-0.139509000
C	-3.928342000	-0.042553000	-0.050181000
C	-5.871466000	-1.537628000	-0.258685000
C	-3.063740000	-1.158956000	-0.081112000
C	-5.024069000	-2.673482000	-0.291792000
C	-3.611988000	-2.473711000	-0.201374000
C	-1.078273000	0.329878000	0.130492000
C	0.330248000	0.435631000	0.220356000
C	-1.636331000	-0.980481000	0.009948000
C	1.166276000	-0.676848000	0.194665000
C	-0.767907000	-2.109778000	-0.018164000
C	0.615638000	-1.955199000	0.074559000
H	0.820572000	1.390915000	0.313994000
H	1.250614000	-2.834118000	0.052912000
C	-1.298261000	-3.484252000	-0.147337000
C	-2.773336000	-3.623109000	-0.236068000
C	-3.317049000	-4.895506000	-0.353963000
C	-4.708528000	-5.080381000	-0.442101000
C	-5.551142000	-3.984835000	-0.411729000
H	-6.385964000	3.016458000	0.034483000
H	-7.296290000	0.787369000	-0.163149000
H	-6.626689000	-4.106183000	-0.478599000
H	-5.119348000	-6.081569000	-0.533771000
H	-2.626504000	-5.733194000	-0.374866000
O	-7.208724000	-1.795157000	-0.350052000
H	-7.695632000	-0.959141000	-0.327777000
O	-0.186174000	3.098279000	0.348018000
H	-0.061423000	4.056302000	0.416008000
C	2.653999000	-0.436631000	0.297663000
O	3.092618000	0.710483000	0.396271000
O	3.350140000	-1.546868000	0.264552000
H	4.401816000	-1.381608000	0.346056000
C	-4.642270000	4.938889000	0.247472000
O	-5.863486000	5.012778000	0.190911000
O	-3.903690000	6.085116000	0.360405000
H	-4.566728000	6.797244000	0.374267000
O	-0.563721000	-4.476955000	-0.182292000
C	7.274264000	0.233769000	-0.771567000
H	6.744878000	0.074759000	-1.710250000
C	6.354036000	0.114705000	0.435141000
H	5.521954000	0.822522000	0.379255000
H	6.932660000	0.271150000	1.350955000
O	5.816270000	-1.197446000	0.412279000
Br	8.050299000	2.067527000	-0.915939000
H	8.124947000	-0.436585000	-0.670013000
C	6.739128000	-2.353789000	1.063207000
O	7.847367000	-1.916586000	1.362429000
O	6.097388000	-3.390149000	1.083442000

TS3-TPSSH

SCF Energy (TPSSH/B2) = -4479.90858583

Enthalpy 0K = 0.398920

Enthalpy 298 K = 0.432870

Free Energy 298 K = 0.326069

C	-1.515754000	2.815174000	0.276235000
C	-1.994026000	1.478078000	0.165253000
C	-2.383099000	3.899347000	0.307311000
C	-3.417833000	1.315983000	0.062717000
C	-3.769510000	3.749578000	0.225721000
C	-4.311746000	2.443828000	0.097100000
H	-1.966707000	4.897775000	0.397661000
C	-5.728149000	2.223866000	0.001774000
C	-6.241526000	0.973782000	-0.134279000
C	-5.402108000	-0.183468000	-0.189845000
C	-3.972837000	-0.012321000	-0.082222000
C	-5.938676000	-1.467739000	-0.345393000
C	-3.128123000	-1.143646000	-0.124328000
C	-5.111123000	-2.617913000	-0.391317000
C	-3.697241000	-2.445869000	-0.276793000
C	-1.120260000	0.304720000	0.147139000
C	0.285649000	0.381482000	0.282428000
C	-1.699890000	-0.992693000	-0.006392000
C	1.099825000	-0.747788000	0.258962000
C	-0.852842000	-2.137811000	-0.036232000
C	0.529906000	-2.012407000	0.094341000
H	0.788477000	1.325937000	0.412403000
H	1.144446000	-2.905349000	0.070331000
C	-1.404480000	-3.499822000	-0.205748000
C	-2.879132000	-3.609885000	-0.322040000
C	-3.444089000	-4.869448000	-0.474444000
C	-4.837011000	-5.026692000	-0.587912000
C	-5.659861000	-3.916487000	-0.547080000
H	-6.376729000	3.087675000	0.041459000
H	-7.325016000	0.877899000	-0.194531000
H	-6.736245000	-4.016587000	-0.632618000
H	-5.264504000	-6.017894000	-0.706904000
H	-2.769111000	-5.719514000	-0.501713000
O	-7.278012000	-1.698982000	-0.462080000
H	-7.749624000	-0.853970000	-0.449704000
O	-0.175908000	3.054926000	0.351456000
H	-0.030353000	4.010102000	0.418913000
C	2.581363000	-0.535379000	0.413922000
O	3.055846000	0.584844000	0.568840000
O	3.264833000	-1.668132000	0.355888000
H	4.260672000	-1.489466000	0.485316000
C	-4.599084000	4.977542000	0.274666000
O	-5.818631000	5.071922000	0.219468000
O	-3.840034000	6.108236000	0.397829000
H	-4.488570000	6.833474000	0.418871000
O	-0.684584000	-4.503117000	-0.250229000
C	7.804951000	0.170434000	0.298303000
H	8.511345000	-0.610333000	0.066097000
C	6.340638000	-0.018631000	-0.044639000
H	6.213985000	-0.149709000	-1.118444000
H	5.752823000	0.842860000	0.284316000
O	5.823155000	-1.218381000	0.564807000
Br	8.436400000	1.429506000	-1.618774000
H	8.137044000	0.979574000	0.922424000
C	6.405865000	-1.490700000	1.862722000
O	7.434392000	-0.773892000	2.075543000
O	5.842103000	-2.351909000	2.521432000

## Pdt1-TPSSH

SCF Energy (TPSSH/B2) = -4479.93435091

Enthalpy 0K = 0.401689

Enthalpy 298 K = 0.436068

Free Energy 298 K = 0.327280

C	-1.290313000	2.738921000	0.297606000
C	-1.863770000	1.440511000	0.191955000
C	-2.079149000	3.880880000	0.357775000
C	-3.296221000	1.378108000	0.104982000
C	-3.473765000	3.827976000	0.307593000
C	-4.109187000	2.564809000	0.172109000
H	-1.592472000	4.847135000	0.446397000
C	-5.538090000	2.443312000	0.102941000
C	-6.137482000	1.233770000	-0.054374000
C	-5.379638000	0.025296000	-0.159872000
C	-3.942442000	0.095159000	-0.061719000
C	-6.002968000	-1.214668000	-0.355093000
C	-3.178130000	-1.091759000	-0.139711000
C	-5.258215000	-2.417971000	-0.437131000
C	-3.835155000	-2.348337000	-0.321917000
C	-1.075298000	0.207980000	0.157688000
C	0.328980000	0.183039000	0.309730000
C	-1.744487000	-1.042668000	-0.023772000
C	1.061493000	-1.002061000	0.259509000
C	-0.980079000	-2.244274000	-0.080642000
C	0.407335000	-2.218855000	0.053745000
H	0.891529000	1.087844000	0.472480000
H	0.953541000	-3.154056000	0.003129000
C	-1.624277000	-3.560894000	-0.281011000
C	-3.099666000	-3.564870000	-0.399990000
C	-3.752640000	-4.778946000	-0.586378000
C	-5.151662000	-4.834143000	-0.703011000
C	-5.896049000	-3.670104000	-0.629756000
H	-6.126131000	3.347021000	0.179585000
H	-7.226179000	1.210312000	-0.084358000
H	-6.976640000	-3.692563000	-0.717129000
H	-5.647790000	-5.789034000	-0.850112000
H	-3.139035000	-5.673150000	-0.637676000
O	-7.355817000	-1.347197000	-0.477278000
H	-7.761677000	-0.468599000	-0.482826000
O	0.065270000	2.882492000	0.336662000
H	0.281783000	3.825226000	0.387305000
C	2.544319000	-0.895490000	0.433685000
O	3.108343000	0.164869000	0.667758000
O	3.166498000	-2.072154000	0.301881000
H	4.141326000	-1.926741000	0.432782000
C	-4.215049000	5.109392000	0.392043000
O	-5.426248000	5.287282000	0.368432000
O	-3.377170000	6.183358000	0.510526000
H	-3.973041000	6.951399000	0.555616000
O	-0.970854000	-4.609709000	-0.345697000
C	7.651222000	-0.108232000	0.808994000
H	8.576117000	-0.476066000	0.364873000
C	6.426243000	-0.378433000	-0.064000000
H	6.682155000	-0.601899000	-1.095441000
H	5.670312000	0.404495000	-0.015359000
O	5.854582000	-1.584400000	0.561847000
Br	8.249142000	1.702269000	-1.749216000
H	7.769007000	0.937599000	1.076268000

C	6.383842000	-1.751126000	1.814167000
O	7.378794000	-0.877678000	2.029067000
O	5.991476000	-2.582648000	2.595572000

## Int3-ωB97XD

SCF Energy (TPSSH/B2) = -4479.35506842

Enthalpy 0K = 0.407779

Enthalpy 298 K = 0.441529

Free Energy 298 K = 0.335228

C	-1.616153000	2.732623000	-0.191608000
C	-2.028069000	1.381099000	-0.074701000
C	-2.528793000	3.770937000	-0.109447000
C	-3.429615000	1.145128000	0.045077000
C	-3.890582000	3.545681000	0.065556000
C	-4.368420000	2.221830000	0.133799000
H	-2.165335000	4.789545000	-0.189043000
C	-5.770761000	1.923107000	0.304997000
C	-6.220586000	0.653117000	0.314623000
C	-5.331964000	-0.464296000	0.156046000
C	-3.918664000	-0.218093000	0.062497000
C	-5.813010000	-1.765653000	0.102437000
C	-3.029085000	-1.296142000	-0.031661000
C	-4.934317000	-2.871664000	0.011695000
C	-3.537508000	-2.628025000	-0.042476000
C	-1.091823000	0.254120000	-0.088809000
C	0.310280000	0.415792000	-0.067772000
C	-1.603673000	-1.067793000	-0.091925000
C	1.173461000	-0.667216000	-0.094100000
C	-0.705263000	-2.164290000	-0.134217000
C	0.666599000	-1.962517000	-0.143120000
H	0.763671000	1.390662000	-0.025053000
H	1.341081000	-2.811837000	-0.176571000
C	-1.196355000	-3.561523000	-0.165148000
C	-2.670358000	-3.750748000	-0.119149000
C	-3.174278000	-5.033540000	-0.146681000
C	-4.562193000	-5.262755000	-0.102534000
C	-5.428243000	-4.199176000	-0.025274000
H	-6.457587000	2.745869000	0.430177000
H	-7.281812000	0.491099000	0.485695000
H	-6.500865000	-4.351418000	0.010802000
H	-4.944809000	-6.277600000	-0.128891000
H	-2.464070000	-5.852017000	-0.204101000
O	-7.138108000	-2.064076000	0.140591000
H	-7.655076000	-1.267628000	-0.016683000
O	-0.312711000	3.021245000	-0.401896000
H	-0.178469000	3.974918000	-0.437365000
C	2.667007000	-0.449932000	-0.077030000
O	3.436003000	-1.393585000	-0.133705000
O	2.984571000	0.812440000	0.000411000
H	4.018856000	0.976017000	0.001126000
C	-4.775340000	4.740597000	0.151674000
O	-5.982046000	4.765711000	0.259601000
O	-4.079440000	5.898550000	0.094348000
H	-4.742801000	6.600809000	0.155636000
O	-0.441057000	-4.518709000	-0.224630000
C	7.448536000	0.189635000	0.692798000
H	7.044650000	-0.023483000	1.681226000
C	6.355272000	0.219194000	-0.361812000
H	5.809541000	-0.728325000	-0.390861000
H	6.801847000	0.434097000	-1.336913000

O	5.435702000	1.225032000	-0.005431000
Br	8.740513000	-1.241156000	0.310853000
H	8.003026000	1.124705000	0.678803000
C	5.812006000	2.663874000	-0.346242000
O	6.966331000	2.767115000	-0.748312000
O	4.860947000	3.394239000	-0.128826000

### TS3- $\omega$ B97XD

SCF Energy (TPSSH/B2) = -4479.33009974

Enthalpy 0K = 0.408351

Enthalpy 298 K = 0.441583

Free Energy 298 K = 0.336500

C	1.725731000	2.758331000	0.106823000
C	2.117950000	1.400182000	0.018873000
C	2.650379000	3.780644000	-0.015583000
C	3.513358000	1.141481000	-0.114481000
C	4.005963000	3.535303000	-0.207390000
C	4.462733000	2.202641000	-0.247109000
H	2.303422000	4.806542000	0.041250000
C	5.858514000	1.881082000	-0.421166000
C	6.291925000	0.607460000	-0.402757000
C	5.392825000	-0.495962000	-0.209129000
C	3.985992000	-0.228772000	-0.097736000
C	5.857133000	-1.802685000	-0.131533000
C	3.085967000	-1.290814000	0.048218000
C	4.965945000	-2.892298000	0.017026000
C	3.575355000	-2.627704000	0.095932000
C	1.169987000	0.283621000	0.079217000
C	-0.227952000	0.463474000	0.065851000
C	1.665208000	-1.041629000	0.124190000
C	-1.106985000	-0.603773000	0.147006000
C	0.754001000	-2.122708000	0.224139000
C	-0.613900000	-1.900665000	0.247138000
H	-0.656551000	1.447532000	-0.008481000
H	-1.295369000	-2.740348000	0.330131000
C	1.226341000	-3.523338000	0.303207000
C	2.693969000	-3.734091000	0.231494000
C	3.182243000	-5.021517000	0.291714000
C	4.563630000	-5.272446000	0.221802000
C	5.440871000	-4.225148000	0.086498000
H	6.552172000	2.694930000	-0.569485000
H	7.353110000	0.435085000	-0.566713000
H	6.509266000	-4.398095000	0.029325000
H	4.932756000	-6.291501000	0.273522000
H	2.464360000	-5.828859000	0.394401000
O	7.172765000	-2.124271000	-0.194392000
H	7.706550000	-1.327718000	-0.150288000
O	0.428537000	3.073528000	0.325215000
H	0.322902000	4.026976000	0.377640000
C	-2.593432000	-0.379314000	0.146446000
O	-3.381865000	-1.285472000	0.331792000
O	-2.908631000	0.880551000	-0.074938000
H	-3.897877000	1.017206000	-0.017908000
C	4.903153000	4.715248000	-0.346157000
O	6.103206000	4.721264000	-0.532330000
O	4.233796000	5.884921000	-0.244238000
H	4.904862000	6.571129000	-0.351165000
O	0.456753000	-4.466844000	0.418743000
C	-7.820907000	0.615433000	0.310676000
H	-8.302566000	1.396448000	-0.254919000
C	-6.418164000	0.172554000	-0.057597000

H	-6.384077000	-0.162880000	-1.091851000
H	-6.093547000	-0.648339000	0.587878000
O	-5.507612000	1.264029000	0.047606000
Br	-9.008297000	-1.047366000	-0.939835000
H	-8.315494000	0.250763000	1.192092000
C	-5.857473000	2.199663000	1.057886000
O	-7.027862000	2.004817000	1.498029000
O	-5.008547000	3.027900000	1.329240000

### Pdt1- $\omega$ B97XD

SCF Energy (TPSSH/B2) = -4479.36549688

Enthalpy 0K = 0.336500

Enthalpy 298 K = 0.444780

Free Energy 298 K = 0.337459

C	1.782897000	2.823123000	0.230194000
C	2.139464000	1.457795000	0.113439000
C	2.719786000	3.827476000	0.064118000
C	3.517010000	1.172998000	-0.123761000
C	4.055888000	3.557932000	-0.208794000
C	4.479071000	2.216799000	-0.298641000
H	2.398841000	4.859877000	0.150808000
C	5.853687000	1.872331000	-0.568392000
C	6.258250000	0.590264000	-0.614433000
C	5.348103000	-0.499194000	-0.398482000
C	3.959297000	-0.206626000	-0.177982000
C	5.785513000	-1.817872000	-0.403987000
C	3.047744000	-1.254385000	-0.002748000
C	4.881714000	-2.893246000	-0.230243000
C	3.507763000	-2.602576000	-0.037695000
C	1.176110000	0.358192000	0.234131000
C	-0.211908000	0.564557000	0.369350000
C	1.643793000	-0.977938000	0.192967000
C	-1.103274000	-0.489365000	0.486776000
C	0.720401000	-2.044364000	0.331138000
C	-0.634427000	-1.799183000	0.478819000
H	-0.618422000	1.560255000	0.381831000
H	-1.323928000	-2.630146000	0.580294000
C	1.163818000	-3.457659000	0.320279000
C	2.614563000	-3.695574000	0.124998000
C	3.075470000	-4.994345000	0.100351000
C	4.440966000	-5.270992000	-0.084780000
C	5.329420000	-4.237180000	-0.247102000
H	6.555092000	2.675764000	-0.735344000
H	7.304018000	0.402572000	-0.846222000
H	6.386053000	-4.429532000	-0.392122000
H	4.788839000	-6.298578000	-0.099992000
H	2.349027000	-5.790265000	0.228355000
O	7.083246000	-2.165562000	-0.576102000
H	7.637864000	-1.382172000	-0.569383000
O	0.505394000	3.172508000	0.517853000
H	0.435064000	4.129441000	0.564454000
C	-2.575439000	-0.249830000	0.627710000
O	-3.378121000	-1.152246000	-0.743161000
O	-2.890755000	1.039195000	0.608158000
H	-3.864232000	1.124185000	0.740510000
C	4.968397000	4.722334000	-0.380434000
O	6.159405000	4.707172000	-0.615183000
O	4.324548000	5.902907000	-0.245692000
H	5.002477000	6.578330000	-0.376104000
O	0.381688000	-4.386215000	0.464060000

C	-7.569993000	-0.039184000	0.838217000
H	-8.420765000	0.633125000	0.726178000
C	-6.385464000	0.379395000	-0.021692000
H	-6.683374000	1.012176000	-0.853218000
H	-5.787635000	-0.465013000	-0.368939000
O	-5.579402000	1.134099000	0.924722000
Br	-8.867663000	-0.103694000	-2.131444000
H	-7.896285000	-1.058998000	0.656958000
C	-5.942019000	0.804716000	2.193177000
O	-7.045181000	0.062743000	2.187389000
O	-5.332571000	1.160135000	3.163321000

## NGO

SCF Energy (B3LYP-D3/B2) = -1974.13852956  
 Enthalpy 0K = 0.405931  
 Enthalpy 298 K = 0.436232  
 Free Energy 298 K = 0.345586

C	2.302246000	2.737767000	-0.385412000
C	1.475352000	1.625820000	-0.114145000
C	3.677427000	2.587572000	-0.461111000
C	2.089101000	0.341280000	-0.000999000
C	4.300284000	1.353949000	-0.298259000
C	3.524844000	0.193338000	-0.037518000
C	4.080751000	-1.109958000	0.246443000
C	3.203649000	-2.239368000	0.402892000
C	1.785409000	-2.113307000	0.270626000
C	1.236971000	-0.839791000	0.115566000
C	0.977293000	-3.332396000	0.275640000
N	-0.175379000	-0.686595000	0.017526000
C	-0.442484000	-3.114755000	0.051378000
C	-0.977168000	-1.824610000	-0.027375000
C	0.027304000	1.741825000	0.033215000
C	-0.621867000	2.979588000	0.221195000
C	-0.780828000	0.590964000	0.021059000
C	-1.995390000	3.136730000	0.283259000
C	-2.200194000	0.716199000	0.012672000
C	-2.839904000	1.994335000	0.109587000
H	-0.030777000	-3.822203000	0.330067000
C	-4.257157000	2.040310000	0.040835000
C	-3.022446000	-0.442198000	-0.115375000
C	-2.386093000	-1.706934000	-0.140483000
C	5.373265000	-1.580950000	0.462121000
C	3.982291000	-3.352577000	0.689964000
O	1.753885000	3.970945000	-0.607703000
H	2.460342000	4.602085000	-0.793840000
C	-2.422229000	4.542845000	0.534024000
O	-1.663319000	5.495234000	0.564878000
O	-3.751169000	4.724372000	0.766155000
H	-3.848760000	5.678984000	0.918574000
C	5.770762000	1.357713000	-0.545899000
O	6.422223000	0.499876000	-1.107077000
O	6.352887000	2.515882000	-0.125539000
H	7.279764000	2.458457000	-0.411302000
C	-4.431457000	-0.381002000	-0.202054000
N	5.278513000	-2.917546000	0.727592000
H	6.072065000	-3.512689000	0.907547000
H	3.700395000	-4.374742000	0.864129000
H	6.331231000	-1.097749000	0.422698000
C	-1.309775000	-4.232546000	-0.059336000
C	-3.143434000	-2.893199000	-0.244010000
C	-5.045316000	0.916933000	-0.112313000
N	-2.611695000	-4.148388000	-0.220946000
H	-4.743243000	3.001098000	0.123346000

C	-5.183852000	-1.576372000	-0.368063000
C	-4.564203000	-2.804524000	-0.380431000
H	-0.856352000	-5.218462000	-0.007274000
H	4.287704000	3.459795000	-0.672904000
O	-5.262369000	-3.950460000	-0.516177000
H	-4.592828000	-4.663233000	-0.481676000
H	-6.258474000	-1.550905000	-0.504875000
O	1.447923000	-4.466785000	0.438599000
N	-6.424993000	1.030910000	-0.220008000
H	-6.797580000	1.934678000	0.036086000
H	-6.968008000	0.273230000	0.169019000

## Int1a

SCF Energy (B3LYP-D3/B2) = -4702.25249611  
 Enthalpy 0K = 0.464968  
 Enthalpy 298 K = 0.502485  
 Free Energy 298 K = 0.389049

C	-4.451575000	-2.519524000	-0.286798000
C	-3.485643000	-1.509389000	-0.062044000
C	-5.796898000	-2.209638000	-0.340197000
C	-3.945231000	-0.158750000	0.035627000
C	-6.272257000	-0.906183000	-0.194126000
C	-5.355016000	0.156101000	0.030948000
C	-5.744377000	1.518699000	0.315836000
C	-4.737277000	2.538681000	0.431521000
C	-3.346990000	2.247341000	0.259738000
C	-2.955825000	0.916133000	0.109267000
C	-2.404299000	3.364269000	0.229013000
N	-1.576467000	0.598844000	-0.023222000
C	-1.026642000	2.981438000	-0.017739000
C	-0.646559000	1.636664000	-0.097566000
C	-2.062843000	-1.792422000	0.043036000
C	-1.554969000	-3.096721000	0.227135000
C	-1.121482000	-0.741238000	-0.021301000
C	-0.207072000	-3.410463000	0.224611000
C	0.265327000	-1.027120000	-0.079029000
C	0.761606000	-2.372914000	0.003283000
H	-2.252395000	-3.899585000	0.378617000
C	2.146224000	-2.596732000	-0.114690000
C	1.218362000	0.023977000	-0.233211000
C	0.735715000	1.354264000	-0.242022000
C	-6.965533000	2.137660000	0.572715000
C	-5.370343000	3.736514000	0.733475000
O	-4.064309000	-3.819850000	-0.493249000
H	-4.852142000	-4.348872000	-0.669678000
C	0.178717000	-4.822715000	0.441616000
O	1.302244000	-5.298986000	0.399175000
O	-0.885499000	-5.636256000	0.719230000
H	-0.492485000	-6.516091000	0.831508000
C	-7.730831000	-0.742482000	-0.421053000
O	-8.305158000	0.199577000	-0.934258000
O	-8.437681000	-1.851278000	-0.043021000
H	-9.350356000	-1.670660000	-0.321074000
C	2.607199000	-0.202830000	-0.353614000
N	-6.707703000	3.456008000	0.821321000
H	-7.419605000	4.140614000	1.021012000
H	-4.963327000	4.719013000	0.886783000
H	-7.973092000	1.767118000	0.570184000
C	-0.035312000	3.989654000	-0.148349000
C	1.628189000	2.445080000	-0.361462000

C	3.075072000	-1.572603000	-0.305970000
N	1.243950000	3.755022000	-0.330513000
H	2.503178000	-3.614894000	-0.052092000
C	3.496052000	0.893696000	-0.504460000
C	3.023929000	2.186438000	-0.508123000
H	-0.370179000	5.021829000	-0.092242000
H	-6.508287000	-3.007833000	-0.527049000
O	3.861875000	3.239711000	-0.635805000
H	3.291758000	4.031424000	-0.587422000
H	4.563314000	0.731081000	-0.601559000
O	-2.741777000	4.548653000	0.384549000
N	4.390806000	-1.855630000	-0.447064000
H	4.690679000	-2.811920000	-0.345499000
H	5.127855000	-1.151217000	-0.491549000
C	7.015263000	0.737740000	0.731975000
C	7.229215000	1.234111000	-0.630311000
O	6.567629000	-0.037533000	-0.407477000
H	7.891094000	0.325161000	1.234914000
H	6.204580000	1.154456000	1.333128000
H	8.243423000	1.138702000	-1.019350000
H	6.577141000	2.015111000	-1.025332000
Br	10.464937000	0.086975000	0.303243000

### TS1a

SCF Energy (B3LYP-D3/B2) = -4702.24052342

Enthalpy 0K = 0.463228

Enthalpy 298 K = 0.500062

Free Energy 298 K = 0.389266

C	4.015292000	2.817334000	-0.324648000
C	3.208879000	1.676609000	-0.093235000
C	5.392925000	2.716940000	-0.326338000
C	3.865330000	0.416476000	0.062486000
C	6.057062000	1.506359000	-0.120114000
C	5.305830000	0.322126000	0.111783000
C	5.886685000	-0.956517000	0.456180000
C	5.041633000	-2.113734000	0.579203000
C	3.629943000	-2.044248000	0.354063000
C	3.047627000	-0.793573000	0.142461000
C	2.868816000	-3.291452000	0.334557000
N	1.642768000	-0.694527000	-0.047563000
C	1.461282000	-3.130880000	0.022138000
C	0.884844000	-1.863014000	-0.120789000
C	1.758600000	1.742408000	-0.037542000
C	1.052575000	2.954549000	0.104613000
C	0.988063000	0.559585000	-0.102123000
C	-0.326050000	3.061007000	0.068479000
C	-0.421755000	0.629898000	-0.218389000
C	-1.120136000	1.888567000	-0.183004000
H	1.599432000	3.867429000	0.264153000
C	-2.509040000	1.889172000	-0.397980000
C	-1.197262000	-0.558348000	-0.389908000
C	-0.516024000	-1.797954000	-0.332750000
C	7.177533000	-1.374212000	0.771529000
C	5.837212000	-3.191037000	0.943798000
O	3.435649000	4.030596000	-0.589561000
H	4.133024000	4.680670000	-0.739917000
C	-0.821668000	4.441006000	0.311164000
O	-0.106753000	5.425083000	0.425150000
O	-2.170346000	4.569353000	0.438307000

H	-2.314670000	5.514361000	0.609113000
C	7.530162000	1.563367000	-0.293594000
O	8.263466000	0.705318000	-0.749397000
O	8.044117000	2.781036000	0.061860000
H	8.983175000	2.733082000	-0.180260000
C	-2.596753000	-0.553417000	-0.589730000
N	7.113439000	-2.708035000	1.060821000
H	7.913132000	-3.269579000	1.306398000
H	5.577264000	-4.218409000	1.121005000
H	8.116809000	-0.854559000	0.784839000
C	0.641230000	-4.281778000	-0.113165000
C	-1.225515000	-3.015249000	-0.453240000
C	-3.266359000	0.733806000	-0.620875000
N	-0.648188000	-4.250050000	-0.358372000
H	-3.032373000	2.833532000	-0.390228000
C	-3.302290000	-1.777518000	-0.741994000
C	-2.634522000	-2.980729000	-0.673262000
H	1.125429000	-5.248682000	-0.006012000
H	5.979615000	3.609220000	-0.520102000
O	-3.284838000	-4.160098000	-0.798184000
H	-2.592951000	-4.841907000	-0.693061000
H	-4.378030000	-1.791459000	-0.901083000
O	3.374455000	-4.405616000	0.548134000
N	-4.590393000	0.819161000	-0.858585000
H	-5.006766000	1.736861000	-0.817607000
H	-5.252398000	0.008858000	-0.966249000
C	-7.920305000	-0.321731000	-0.613097000
C	-7.060827000	-1.099368000	0.259083000
O	-6.401094000	-1.157330000	-0.995420000
H	-8.656991000	-0.813243000	-1.226620000
H	-7.714564000	0.722828000	-0.781845000
H	-7.453023000	-2.053266000	0.627251000
H	-6.536971000	-0.551337000	1.052332000
Br	-9.964225000	0.594752000	0.842917000

### Int2a

SCF Energy (B3LYP-D3/B2) = -4890.92579550

Enthalpy 0K = 0.477744

Enthalpy 298 K = 0.518424

Free Energy 298 K = 0.397088

C	4.400440000	2.716905000	-0.256718000
C	3.515888000	1.616439000	-0.101664000
C	5.765116000	2.539934000	-0.202808000
C	4.101268000	0.316650000	0.045915000
C	6.360473000	1.287813000	-0.003592000
C	5.529980000	0.143237000	0.164045000
C	6.019217000	-1.172862000	0.512809000
C	5.108604000	-2.285047000	0.559967000
C	3.717556000	-2.135028000	0.257594000
C	3.215492000	-0.847738000	0.051053000
C	2.896537000	-3.338290000	0.160520000
N	1.830212000	-0.668924000	-0.205387000
C	1.520672000	-3.094495000	-0.224368000
C	1.019345000	-1.792355000	-0.355444000
C	2.079557000	1.761724000	-0.116885000
C	1.430184000	3.006191000	0.021082000
C	1.240520000	0.622122000	-0.256658000
C	0.064033000	3.193539000	-0.082410000
C	-0.145358000	0.770798000	-0.441128000

C	-0.789154000	2.071558000	-0.414188000
H	2.015981000	3.882016000	0.239292000
C	-2.149878000	2.152213000	-0.691832000
C	-0.976185000	-0.371110000	-0.687062000
C	-0.363002000	-1.646340000	-0.638808000
C	7.263930000	-1.664943000	0.899193000
C	5.821978000	-3.410276000	0.948693000
O	3.901418000	3.970561000	-0.511326000
H	4.644011000	4.579131000	-0.609050000
C	-0.360438000	4.586876000	0.180516000
O	0.397191000	5.525562000	0.392896000
O	-1.707232000	4.806783000	0.206078000
H	-1.787534000	5.753453000	0.405823000
C	7.833691000	1.268356000	-0.117660000
O	8.554968000	0.360228000	-0.496465000
O	8.397876000	2.480368000	0.198691000
H	9.339604000	2.364536000	-0.004880000
C	-2.356560000	-0.284154000	-0.960396000
N	7.112733000	-2.998651000	1.155556000
H	7.865410000	-3.606448000	1.436052000
H	5.496705000	-4.424920000	1.086917000
H	8.225476000	-1.194727000	0.979437000
C	0.652391000	-4.195628000	-0.446000000
C	-1.124555000	-2.821884000	-0.845765000
C	-2.993423000	1.037964000	-0.974191000
N	-0.616828000	-4.090010000	-0.763985000
H	-2.625455000	3.121874000	-0.674421000
C	-3.102705000	-1.461195000	-1.216318000
C	-2.508786000	-2.703670000	-1.153863000
H	1.081506000	-5.189094000	-0.345417000
H	6.405603000	3.403317000	-0.351365000
O	-3.211247000	-3.844012000	-1.373825000
H	-2.557875000	-4.560345000	-1.250741000
H	-4.155929000	-1.395770000	-1.459545000
O	3.331681000	-4.484872000	0.368923000
N	-4.287697000	1.141618000	-1.227059000
H	-4.567013000	2.122634000	-1.213365000
H	-5.533125000	0.101755000	-1.252140000
C	-6.715216000	0.373715000	1.049386000
C	-6.394500000	-0.873860000	0.230039000
O	-6.329848000	-0.528854000	-1.133495000
H	-7.669930000	0.806554000	0.753916000
H	-5.913704000	1.108112000	0.973670000
H	-7.188194000	-1.616723000	0.363828000
H	-5.453585000	-1.315277000	0.591425000
Br	-6.887084000	-0.059392000	2.988766000
C	-8.545711000	0.254371000	-2.144021000
O	-9.162832000	-0.095002000	-1.209496000
O	-8.050896000	0.649393000	-3.127520000

## TS2a

SCF Energy (B3LYP-D3/B2) = -4890.91907506

Enthalpy 0K = 0.473233

Enthalpy 298 K = 0.513419

Free Energy 298 K = 0.393903

C	4.467577000	2.684597000	-0.264204000
C	3.573673000	1.598127000	-0.085133000
C	5.832193000	2.490366000	-0.218853000
C	4.140096000	0.293104000	0.070054000

C	6.408885000	1.233416000	-0.010939000
C	5.567852000	0.100746000	0.173209000
C	6.044949000	-1.219464000	0.521673000
C	5.120092000	-2.318913000	0.586026000
C	3.727198000	-2.151159000	0.302090000
C	3.239276000	-0.859406000	0.094692000
C	2.887950000	-3.343950000	0.221890000
N	1.853161000	-0.662665000	-0.145161000
C	1.509830000	-3.083319000	-0.144675000
C	1.023810000	-1.776105000	-0.276265000
C	2.134738000	1.762477000	-0.082212000
C	1.506551000	3.017202000	0.053462000
C	1.283269000	0.634534000	-0.197520000
C	0.140809000	3.220512000	-0.030419000
C	-0.108204000	0.801272000	-0.360658000
C	-0.727655000	2.107516000	-0.330825000
H	2.107750000	3.887698000	0.249798000
C	-2.099360000	2.203566000	-0.581954000
C	-0.956966000	-0.329689000	-0.583771000
C	-0.360327000	-1.612625000	-0.538587000
C	7.288758000	-1.727105000	0.890166000
C	5.824165000	-3.452364000	0.967817000
O	3.982622000	3.940405000	-0.529003000
H	4.730436000	4.539750000	-0.642862000
C	-0.262357000	4.625554000	0.217751000
O	0.513112000	5.555016000	0.396332000
O	-1.604277000	4.860211000	0.269781000
H	-1.674394000	5.811050000	0.453346000
C	7.884186000	1.193216000	-0.133296000
O	8.583177000	0.282316000	-0.541734000
O	8.466286000	2.385871000	0.212773000
H	9.406333000	2.266113000	0.002641000
C	-2.343171000	-0.227562000	-0.832160000
N	7.123110000	-3.057728000	1.153164000
H	7.871445000	-3.674980000	1.424848000
H	5.487733000	-4.462196000	1.114456000
H	8.258203000	-1.270764000	0.955101000
C	0.622991000	-4.173560000	-0.346200000
C	-1.141855000	-2.777838000	-0.725475000
C	-2.945379000	1.101831000	-0.839496000
N	-0.649424000	-4.051207000	-0.644431000
H	-2.561321000	3.179350000	-0.563960000
C	-3.114542000	-1.395452000	-1.067143000
C	-2.531172000	-2.642952000	-1.009596000
H	1.039075000	-5.172588000	-0.246645000
H	6.483602000	3.343517000	-0.378921000
O	-3.250231000	-3.773900000	-1.210785000
H	-2.607436000	-4.500531000	-1.095605000
H	-4.176159000	-1.319973000	-1.288011000
O	3.310708000	-4.494388000	0.429916000
N	-4.249450000	1.252812000	-1.077517000
H	-4.552593000	2.220466000	-1.068583000
H	-5.140864000	0.422009000	-1.116262000
C	-7.008410000	0.439411000	0.913587000
C	-6.443686000	-0.782245000	0.188472000
O	-6.104768000	-0.404039000	-1.106483000
H	-7.915211000	0.797695000	0.428399000
H	-6.267810000	1.236021000	0.987973000
H	-7.208465000	-1.573330000	0.180972000
H	-5.578485000	-1.169620000	0.756692000
Br	-7.536435000	0.025288000	2.804402000
C	-7.846015000	-0.042075000	-2.467488000

O -8.707528000 -0.463826000 -1.778167000  
O -7.252464000 0.441930000 -3.361876000

### Int3a

SCF Energy (B3LYP-D3/B2) = -4890.94624281

Enthalpy 0K = 0.480255

Enthalpy 298 K = 0.518977

Free Energy 298 K = 0.406303

C -1.994532000 -3.138719000 -1.121581000  
C -1.992840000 -1.798399000 -0.658263000  
C -3.139644000 -3.907106000 -1.052631000  
C -3.230349000 -1.259057000 -0.178314000  
C -4.345570000 -3.415312000 -0.549411000  
C -4.414057000 -2.081304000 -0.066578000  
C -5.573948000 -1.515556000 0.586797000  
C -5.576587000 -0.128016000 0.962536000  
C -4.457793000 0.725538000 0.702080000  
C -3.291455000 0.158343000 0.177908000  
C -4.592775000 2.148768000 0.990189000  
N -2.156011000 0.975381000 -0.050591000  
C -3.420543000 2.940913000 0.666976000  
C -2.244250000 2.345390000 0.193374000  
C -0.804155000 -0.964352000 -0.689501000  
C 0.503505000 -1.480990000 -0.921529000  
C -0.916453000 0.421986000 -0.466437000  
C 1.604208000 -0.685769000 -1.117296000  
C 0.212801000 1.265779000 -0.635351000  
C 1.478135000 0.732542000 -1.026065000  
H 0.655134000 -2.546257000 -0.941610000  
C 2.575445000 1.605713000 -1.184171000  
C 0.127031000 2.670696000 -0.417626000  
C -1.122118000 3.193116000 -0.010440000  
C -6.785916000 -2.045889000 1.023052000  
C -6.783385000 0.145854000 1.591342000  
O -0.869914000 -3.680117000 -1.685754000  
H -1.064888000 -4.587301000 -1.951586000  
C 2.955450000 -1.340702000 -1.281288000  
O 3.314485000 -2.230971000 -0.521365000  
O 3.661894000 -0.837109000 -2.275290000  
H 4.694260000 -0.849905000 -2.069056000  
C -5.502111000 -4.334238000 -0.692552000  
O -6.661826000 -4.047499000 -0.927959000  
O -5.130112000 -5.648539000 -0.604080000  
H -5.937822000 -6.147674000 -0.806910000  
C 1.234312000 3.542354000 -0.565299000  
N -7.481675000 -1.032441000 1.619818000  
H -8.405048000 -1.136886000 2.008856000  
H -7.159529000 1.064532000 2.002327000  
H -7.214363000 -3.026156000 0.933853000  
C -3.454626000 4.346431000 0.867487000  
C -1.277561000 4.576005000 0.232512000  
C 2.505027000 2.964204000 -0.931547000  
N -2.440474000 5.154618000 0.654934000  
H 3.530879000 1.208202000 -1.490498000  
C 1.055846000 4.937399000 -0.353827000  
C -0.161775000 5.446049000 0.036018000  
H -4.389374000 4.769633000 1.224973000  
H -3.106793000 -4.923904000 -1.430801000

O -0.349162000 6.772035000 0.248653000  
H -1.285621000 6.845595000 0.521462000  
H 1.872711000 5.631219000 -0.516891000  
O -5.621039000 2.660144000 1.467920000  
N 3.639734000 3.736090000 -1.068161000  
H 4.503297000 3.190328000 -1.129524000  
H 3.708417000 4.543943000 -0.466928000  
C 6.214286000 -1.419327000 1.303192000  
C 7.366727000 -0.652875000 0.662491000  
O 6.903180000 0.597803000 0.160067000  
H 5.497289000 -1.785358000 0.570010000  
H 5.718430000 -0.826167000 2.071607000  
H 7.818906000 -1.258202000 -0.127739000  
H 8.123619000 -0.410504000 1.415078000  
Br 6.926312000 -3.031854000 2.238282000  
C 6.145921000 0.557206000 -1.020652000  
O 6.019488000 -0.589880000 -1.552109000  
O 5.696884000 1.652156000 -1.382845000

### TS3a

SCF Energy (B3LYP-D3/B2) = -4890.91949455

Enthalpy 0K = 0.480717

Enthalpy 298 K = 0.519532

Free Energy 298 K = 0.406720

C -2.795159000 2.924178000 0.769614000  
C -2.078892000 1.717564000 0.582524000  
C -4.167426000 2.957448000 0.618648000  
C -2.825734000 0.528811000 0.322526000  
C -4.913331000 1.820063000 0.301369000  
C -4.255051000 0.573935000 0.117705000  
C -4.911208000 -0.638260000 -0.317785000  
C -4.171384000 -1.870201000 -0.365303000  
C -2.791982000 -1.938181000 0.010477000  
C -2.118304000 -0.750445000 0.298844000  
C -2.161647000 -3.251895000 0.094416000  
N -0.740988000 -0.784726000 0.636202000  
C -0.773017000 -3.224015000 0.514095000  
C -0.099112000 -2.015676000 0.725516000  
C -0.630712000 1.647447000 0.671168000  
C 0.191029000 2.793608000 0.609028000  
C 0.013960000 0.400098000 0.774490000  
C 1.559996000 2.775273000 0.786684000  
C 1.413093000 0.342309000 1.011540000  
C 2.218625000 1.529880000 1.059498000  
H -0.253774000 3.749246000 0.392684000  
C 3.612065000 1.391723000 1.247880000  
C 2.065546000 -0.914622000 1.167740000  
C 1.282194000 -2.085076000 1.035990000  
C -6.190600000 -0.925677000 -0.787323000  
C -5.018667000 -2.862570000 -0.837309000  
O -2.138074000 4.067386000 1.147018000  
H -2.779919000 4.786126000 1.200709000  
C 2.210008000 4.103076000 0.591381000  
O 1.651218000 5.071633000 0.102924000  
O 3.490388000 4.192833000 1.022816000  
H 3.805419000 5.062095000 0.728162000  
C -6.384205000 2.014901000 0.314334000  
O -7.242905000 1.225146000 0.663071000  
O -6.740262000 3.283180000 -0.060549000

H	-7.701125000	3.317370000	0.074025000
C	3.456190000	-1.036794000	1.386776000
N	-6.221278000	-2.257455000	-1.092020000
H	-7.034740000	-2.735761000	-1.444469000
H	-4.837292000	-3.908162000	-1.005556000
H	-7.067214000	-0.316397000	-0.900985000
C	-0.072609000	-4.446105000	0.676247000
C	1.871150000	-3.361645000	1.158903000
C	4.247164000	0.165496000	1.362007000
N	1.197255000	-4.538061000	1.003214000
H	4.234679000	2.269420000	1.187683000
C	4.032775000	-2.326182000	1.556440000
C	3.265931000	-3.461708000	1.450740000
H	-0.634222000	-5.362043000	0.514408000
H	-4.686946000	3.896824000	0.778858000
O	3.791830000	-4.701486000	1.599773000
H	3.038508000	-5.304290000	1.434669000
H	5.087372000	-2.438297000	1.779570000
O	-2.755303000	-4.315412000	-0.152009000
N	5.627754000	0.111811000	1.423385000
H	6.039658000	0.885697000	0.887475000
H	5.995619000	-0.750297000	1.040501000
C	2.780245000	0.773393000	-2.295832000
C	3.883753000	-0.268788000	-2.241362000
O	5.015063000	0.180877000	-1.493334000
H	2.514724000	1.261011000	-3.217153000
H	2.350415000	1.153504000	-1.388063000
H	4.184881000	-0.529757000	-3.263848000
H	3.528531000	-1.169791000	-1.741994000
Br	0.885248000	-0.720838000	-2.535291000
C	5.131291000	1.572529000	-1.427453000
O	4.233761000	2.205001000	-2.068139000
O	6.061374000	2.005656000	-0.734352000

### Pdt1a

SCF Energy (B3LYP-D3/B2) = -4890.95314356

Enthalpy 0K = 0.481667

Enthalpy 298 K = 0.520771

Free Energy 298 K = 0.406370

C	4.953702000	1.902048000	-0.159485000
C	3.729105000	1.206222000	-0.023426000
C	6.154701000	1.218837000	-0.160972000
C	3.771384000	-0.219914000	0.028540000
C	6.224336000	-0.170570000	-0.050359000
C	5.028881000	-0.929416000	0.076631000
C	4.990118000	-2.354975000	0.311834000
C	3.725416000	-3.039573000	0.325050000
C	2.491025000	-2.351079000	0.098619000
C	2.509109000	-0.960922000	-0.000873000
C	1.270054000	-3.144815000	-0.044234000
N	1.291708000	-0.252149000	-0.186130000
C	0.081663000	-2.372067000	-0.351606000
C	0.104862000	-0.975641000	-0.375894000
C	2.443775000	1.885667000	0.040664000
C	2.325587000	3.267053000	0.287439000
C	1.245400000	1.156238000	-0.122669000
C	1.126616000	3.960290000	0.269649000
C	0.004711000	1.838638000	-0.223780000
C	-0.084441000	3.264384000	-0.063156000

H	3.208032000	3.839231000	0.514149000
C	-1.348809000	3.876902000	-0.220382000
C	-1.190956000	1.114255000	-0.513759000
C	-1.125306000	-0.299086000	-0.586982000
C	5.961967000	-3.311655000	0.596934000
C	3.964744000	-4.379378000	0.596573000
O	4.962876000	3.263182000	-0.329288000
H	5.877963000	3.554411000	-0.425296000
C	1.271806000	5.397442000	0.613572000
O	2.337222000	5.962314000	0.811786000
O	0.111947000	6.104939000	0.732344000
H	0.401178000	7.001397000	0.968202000
C	7.585629000	-0.741778000	-0.207384000
O	7.900817000	-1.790783000	-0.737721000
O	8.555838000	0.100778000	0.266114000
H	9.392746000	-0.329484000	0.026875000
C	-2.437368000	1.745434000	-0.711862000
N	5.318416000	-4.505189000	0.765010000
H	5.786966000	-5.374533000	0.964370000
H	3.280612000	-5.203881000	0.678853000
H	7.031837000	-3.251286000	0.662931000
C	-1.143406000	-3.041475000	-0.623936000
C	-2.286781000	-1.081816000	-0.839435000
C	-2.505851000	3.174174000	-0.527448000
N	-2.277974000	-2.441324000	-0.884769000
H	-1.427605000	4.943570000	-0.073569000
C	-3.572532000	0.970714000	-1.040062000
C	-3.538950000	-0.411863000	-1.066311000
H	-1.129220000	-4.128047000	-0.622248000
H	7.075137000	1.782330000	-0.276718000
O	-4.665906000	-1.080115000	-1.320290000
H	-4.693165000	-2.011533000	-0.926176000
H	-4.519009000	1.449639000	-1.248500000
O	1.248617000	-4.380408000	0.066228000
N	-3.703777000	3.828718000	-0.676671000
H	-3.709006000	4.792914000	-0.377571000
H	-4.572844000	3.344019000	-0.458639000
C	-6.173487000	-0.358525000	1.528694000
C	-7.305711000	-0.574952000	0.517742000
O	-7.580818000	0.773285000	0.037525000
H	-6.510027000	-0.361897000	2.570062000
H	-5.369883000	-1.080195000	1.384340000
H	-8.219739000	-0.975773000	0.956342000
H	-6.982018000	-1.197940000	-0.315194000
Br	-5.588891000	-3.577476000	0.316473000
C	-6.554101000	1.570777000	0.360902000
O	-5.706607000	0.980638000	1.217348000
O	-6.400329000	2.695031000	-0.073274000

### Int4a

SCF Energy (B3LYP-D3/B2) = -5044.79793238

Enthalpy 0K = 0.540166

Enthalpy 298 K = 0.583623

Free Energy 298 K = 0.460277

C	-2.677963000	-3.176378000	-0.761537000
C	-2.577199000	-1.810715000	-0.392213000
C	-3.890224000	-3.833470000	-0.710215000
C	-3.784869000	-1.130778000	-0.030405000
C	-5.072360000	-3.203411000	-0.311682000

C	-5.042115000	-1.835594000	0.073412000
C	-6.173017000	-1.120644000	0.623471000
C	-6.065996000	0.287722000	0.893666000
C	-4.865995000	1.018393000	0.621114000
C	-3.733874000	0.310826000	0.207219000
C	-4.888314000	2.469453000	0.773421000
N	-2.520542000	1.006577000	-0.031295000
C	-3.648140000	3.130379000	0.409676000
C	-2.507580000	2.397359000	0.057494000
C	-1.318484000	-1.090934000	-0.396874000
C	-0.054913000	-1.736692000	-0.478406000
C	-1.309920000	0.316538000	-0.296803000
C	1.142000000	-1.062907000	-0.562077000
C	-0.102698000	1.038461000	-0.463272000
C	1.153024000	0.368752000	-0.641404000
H	-0.016831000	-2.811059000	-0.453146000
C	2.305356000	1.121346000	-0.920486000
C	-0.095574000	2.463462000	-0.470135000
C	-1.315727000	3.125299000	-0.197785000
C	-7.445400000	-1.506926000	1.038411000
C	-7.268243000	0.714341000	1.440391000
O	-1.575240000	-3.851259000	-1.215838000
H	-1.838828000	-4.747544000	-1.458056000
C	2.408928000	-1.848625000	-0.501688000
O	3.465447000	-1.395231000	-0.081103000
O	2.283739000	-3.113707000	-0.918686000
H	3.184716000	-3.544395000	-0.848884000
C	-6.298574000	-4.024419000	-0.456126000
O	-7.421589000	-3.652660000	-0.746439000
O	-6.047805000	-5.361173000	-0.293369000
H	-6.890107000	-5.795794000	-0.503333000
C	1.070888000	3.224545000	-0.713090000
N	-8.070823000	-0.392901000	1.523056000
H	-9.015158000	-0.385703000	1.873899000
H	-7.576935000	1.691882000	1.762249000
H	-7.955943000	-2.450530000	1.001675000
C	-3.578134000	4.547744000	0.440268000
C	-1.372907000	4.535834000	-0.138159000
C	2.302790000	2.516912000	-1.003872000
N	-2.498908000	5.246245000	0.166438000
H	3.238416000	0.615098000	-1.117913000
C	0.998470000	4.643317000	-0.660515000
C	-0.184975000	5.288082000	-0.383156000
H	-4.486095000	5.080278000	0.709972000
H	-3.930489000	-4.873652000	-1.017119000
O	-0.264448000	6.639910000	-0.313431000
H	-1.198678000	6.818895000	-0.086404000
H	1.883498000	5.252554000	-0.804334000
O	-5.882407000	3.104742000	1.165402000
N	3.446858000	3.170769000	-1.310258000
H	4.245242000	2.596659000	-1.679703000
H	3.392929000	4.132566000	-1.603137000
C	6.094866000	-0.088295000	1.262809000
C	7.067061000	0.772441000	0.470530000
O	6.311113000	1.496046000	-0.483331000
H	5.571794000	-0.777951000	0.609595000
H	5.382512000	0.503763000	1.835716000
H	7.813873000	0.137225000	-0.014063000
H	7.564316000	1.500756000	1.121052000
Br	7.057964000	-1.227843000	2.598599000
C	5.986015000	0.777328000	-1.688150000
O	6.503655000	-0.337528000	-1.847513000

O	5.191899000	1.429063000	-2.407182000
C	5.539858000	-3.673485000	0.291493000
C	5.782429000	-3.239598000	-1.086378000
O	4.728331000	-4.203868000	-0.786762000
H	6.197596000	-4.406440000	0.755821000
H	5.016829000	-3.002904000	0.966146000
H	6.617734000	-3.670157000	-1.635756000
H	5.462248000	-2.252544000	-1.408523000

### TS4a

SCF Energy (B3LYP-D3/B2) = -5044.77454050

Enthalpy 0K = 0.537228

Enthalpy 298 K = 0.579623

Free Energy 298 K = 0.459316

C	-2.800685000	-3.198918000	-0.548549000
C	-2.625215000	-1.817057000	-0.279627000
C	-4.046184000	-3.785949000	-0.446052000
C	-3.794297000	-1.050980000	0.038076000
C	-5.190285000	-3.067335000	-0.093557000
C	-5.086859000	-1.679751000	0.191416000
C	-6.180004000	-0.871009000	0.684914000
C	-6.004270000	0.546482000	0.846500000
C	-4.768235000	1.192925000	0.527131000
C	-3.671368000	0.399791000	0.174694000
C	-4.717526000	2.649852000	0.571995000
N	-2.423340000	1.012562000	-0.098464000
C	-3.441008000	3.217867000	0.179054000
C	-2.337058000	2.403550000	-0.104919000
C	-1.327409000	-1.165393000	-0.334236000
C	-0.097051000	-1.880834000	-0.410948000
C	-1.250215000	0.241199000	-0.308146000
C	1.129256000	-1.271465000	-0.508921000
C	-0.003415000	0.892564000	-0.499526000
C	1.209403000	0.148806000	-0.614893000
H	-0.108974000	-2.955882000	-0.387812000
C	2.414508000	0.828487000	-0.895289000
C	0.081158000	2.311177000	-0.595618000
C	-1.105689000	3.051685000	-0.390663000
C	-7.469328000	-1.162328000	1.124187000
C	-7.184278000	1.072165000	1.354130000
O	-1.742189000	-3.966850000	-0.953551000
H	-2.055417000	-4.863653000	-1.123846000
C	2.381857000	-2.111025000	-0.513941000
O	3.376534000	-1.732369000	0.113445000
O	2.306551000	-3.198978000	-1.227541000
H	3.344187000	-3.627026000	-1.454659000
C	-6.459338000	-3.831442000	-0.178749000
O	-7.557277000	-3.426346000	-0.515176000
O	-6.282005000	-5.159108000	0.105121000
H	-7.144457000	-5.566613000	-0.075758000
C	1.292597000	2.992393000	-0.863729000
N	-8.039929000	0.014895000	1.519211000
H	-8.982651000	0.094981000	1.865207000
H	-7.444317000	2.085493000	1.599093000
H	-8.025797000	-2.079761000	1.158767000
C	-3.296819000	4.628970000	0.111832000
C	-1.088258000	4.463508000	-0.428203000
C	2.487158000	2.203050000	-1.068056000
N	-2.179584000	5.250637000	-0.192401000

H	3.322550000	0.258230000	-1.018810000
C	1.296256000	4.413936000	-0.906365000
C	0.142496000	5.134912000	-0.699515000
H	-4.179133000	5.224576000	0.329837000
H	-4.142058000	-4.842638000	-0.674361000
O	0.132250000	6.490756000	-0.720987000
H	-0.795020000	6.731143000	-0.523421000
H	2.218117000	4.962260000	-1.063134000
O	-5.681464000	3.362624000	0.903093000
N	3.687988000	2.790910000	-1.371002000
H	4.428122000	2.145126000	-1.678619000
H	3.659777000	3.668577000	-1.866581000
C	5.847082000	-0.085885000	1.587525000
C	6.998534000	0.506070000	0.785588000
O	6.458541000	1.071316000	-0.406348000
H	5.350889000	-0.897937000	1.060254000
H	5.115670000	0.671117000	1.867914000
H	7.741886000	-0.261420000	0.558918000
H	7.471224000	1.325681000	1.334894000
Br	6.535017000	-0.854712000	3.291266000
C	6.165690000	0.178555000	-1.447488000
O	6.720589000	-0.959276000	-1.391944000
O	5.376169000	0.628292000	-2.294952000
C	5.527344000	-3.489813000	-1.019340000
C	5.463762000	-2.452937000	-2.039276000
O	4.510604000	-4.027752000	-1.859646000
H	6.437705000	-4.098413000	-0.996798000
H	5.196268000	-3.199114000	-0.021234000
H	5.990249000	-2.599566000	-2.970705000
H	4.659376000	-1.736658000	-2.015592000

## Pdt2a

SCF Energy (B3LYP-D3/B2) = -5044.82551156

Enthalpy 0K = 0.544125

Enthalpy 298 K = 0.586533

Free Energy 298 K = 0.466047

C	-2.670983000	-3.200231000	-0.561031000
C	-2.457204000	-1.815444000	-0.341252000
C	-3.930850000	-3.749822000	-0.420927000
C	-3.601587000	-1.005419000	-0.046960000
C	-5.050479000	-2.986789000	-0.084625000
C	-4.909626000	-1.591911000	0.139912000
C	-5.978583000	-0.733479000	0.602759000
C	-5.764082000	0.684392000	0.702568000
C	-4.512177000	1.283382000	0.352960000
C	-3.438648000	0.446213000	0.029912000
C	-4.420555000	2.738553000	0.339447000
N	-2.176374000	1.011393000	-0.272568000
C	-3.127937000	3.253718000	-0.072704000
C	-2.049209000	2.397162000	-0.329697000
C	-1.139003000	-1.204426000	-0.425728000
C	0.070011000	-1.956272000	-0.467321000
C	-1.027260000	0.197921000	-0.458743000
C	1.318044000	-1.395080000	-0.604390000
C	0.238149000	0.803016000	-0.684891000
C	1.420923000	0.014019000	-0.784134000
H	0.039476000	-3.029162000	-0.393732000
C	2.642639000	0.655733000	-1.112638000
C	0.363754000	2.215340000	-0.823360000

C	-0.799100000	2.998064000	-0.638796000
C	-7.273629000	-0.970524000	1.057200000
C	-6.927595000	1.263250000	1.190033000
O	-1.638951000	-4.004281000	-0.954498000
H	-1.965902000	-4.905476000	-1.065385000
C	2.544103000	-2.313656000	-0.552208000
O	3.594296000	-1.824260000	-0.050447000
O	2.391476000	-3.477525000	-1.007582000
H	3.910953000	-4.342871000	-1.254123000
C	-6.339685000	-3.721613000	-0.121930000
O	-7.428179000	-3.307590000	-0.477393000
O	-6.194649000	-5.034790000	0.235982000
H	-7.067920000	-5.430071000	0.081614000
C	1.596556000	2.852280000	-1.105476000
N	-7.811129000	0.237827000	1.402669000
H	-8.750039000	0.358221000	1.747160000
H	-7.158693000	2.293025000	1.391651000
H	-7.854755000	-1.870086000	1.132497000
C	-2.940256000	4.657080000	-0.185775000
C	-0.737291000	4.406898000	-0.717187000
C	2.759453000	2.018578000	-1.289131000
N	-1.804264000	5.234468000	-0.506878000
H	3.512497000	0.031261000	-1.239992000
C	1.647296000	4.271741000	-1.181910000
C	0.514642000	5.032414000	-1.001304000
H	-3.804155000	5.285907000	0.011928000
H	-4.057316000	-4.811583000	-0.606767000
O	0.545296000	6.387342000	-1.058819000
H	-0.375415000	6.659115000	-0.870434000
H	2.588941000	4.783530000	-1.344020000
O	-5.364139000	3.491619000	0.640983000
N	3.994455000	2.589461000	-1.573341000
H	4.715248000	1.913656000	-1.818875000
H	3.973381000	3.378039000	-2.205231000
C	4.842806000	0.325477000	1.730291000
C	6.287466000	0.159261000	1.282911000
O	6.370459000	0.576956000	-0.098706000
H	4.183790000	-0.402559000	1.248797000
H	4.492797000	1.344835000	1.570468000
H	6.621924000	-0.871278000	1.402004000
H	6.955279000	0.828961000	1.829553000
Br	4.748216000	-0.005270000	3.686371000
C	6.174527000	-0.309055000	-1.098137000
O	6.479754000	-1.555950000	-0.767665000
O	5.797688000	0.081823000	-2.188083000
C	5.705391000	-3.847411000	-0.742622000
C	5.945797000	-2.614674000	-1.620601000
O	4.816799000	-4.728196000	-1.386857000
H	6.650667000	-4.378497000	-0.561205000
H	5.313561000	-3.482637000	0.214147000
H	6.658824000	-2.794445000	-2.431886000
H	4.996805000	-2.278756000	-2.032761000

## Int1a-OH

SCF Energy (B3LYP-D3/B2) = -4702.24781592

Enthalpy 0K = 0.464308

Enthalpy 298 K = 0.501643

Free Energy 298 K = 0.392096

C	4.195241000	1.412372000	-0.654031000
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C	2.920309000	1.043565000	-0.169899000
C	5.214585000	0.481701000	-0.726929000
C	2.692982000	-0.327890000	0.149995000
C	5.035092000	-0.852480000	-0.359528000
C	3.767269000	-1.294158000	0.112313000
C	3.495252000	-2.621817000	0.615860000
C	2.158028000	-2.968774000	1.020966000
C	1.067784000	-2.051495000	0.902269000
C	1.336257000	-0.748335000	0.498879000
C	-0.286787000	-2.532978000	1.190730000
N	0.268609000	0.184111000	0.382042000
C	-1.337538000	-1.595226000	0.847131000
C	-1.049312000	-0.274310000	0.529269000
C	1.834219000	2.003931000	-0.011445000
C	2.046069000	3.395489000	-0.004673000
C	0.510971000	1.550295000	0.173821000
C	1.029525000	4.335984000	0.054074000
C	-0.568587000	2.480294000	0.146309000
C	-0.335334000	3.891943000	0.054411000
H	3.052666000	3.775047000	-0.038444000
C	-1.462377000	4.749275000	-0.017770000
C	-1.915950000	2.009654000	0.193172000
C	-2.140898000	0.622459000	0.366476000
C	4.286056000	-3.742416000	0.865231000
C	2.174189000	-4.274759000	1.487800000
O	4.430919000	2.694219000	-1.086179000
H	5.334480000	2.740803000	-1.421858000
C	1.517298000	5.734304000	0.110950000
O	2.688362000	6.072404000	0.020528000
O	0.564930000	6.694956000	0.307680000
H	1.068967000	7.524704000	0.324919000
C	6.206643000	-1.727297000	-0.617052000
O	6.212790000	-2.888224000	-0.981062000
O	7.393181000	-1.056889000	-0.468656000
H	8.068728000	-1.694326000	-0.751559000
C	-3.027214000	2.877369000	0.097359000
N	3.469852000	-4.706470000	1.387013000
H	3.778727000	-5.634151000	1.629489000
H	1.371420000	-4.887090000	1.855819000
H	5.326052000	-3.940714000	0.689023000
C	-2.696212000	-2.018060000	0.878318000
C	-3.452775000	0.096023000	0.471309000
C	-2.763084000	4.283046000	-0.003745000
N	-3.725493000	-1.205731000	0.736412000
H	-1.298695000	5.815051000	-0.079223000
C	-4.339652000	2.336984000	0.108885000
C	-4.567473000	0.987608000	0.286007000
H	-2.882267000	-3.061951000	1.096841000
H	6.182531000	0.796678000	-1.103690000
O	-5.826932000	0.533590000	0.299261000
H	-5.870379000	-0.455282000	0.248550000
H	-5.207883000	2.965099000	-0.057062000
O	-0.520192000	-3.640733000	1.690784000
N	-3.829857000	5.174814000	-0.119123000
H	-3.582568000	6.137785000	0.064133000
H	-4.667756000	4.904250000	0.377437000
C	-6.201220000	-3.169029000	0.544007000
C	-5.866041000	-2.970192000	-0.869162000
O	-6.671331000	-1.995992000	-0.148136000
H	-6.988271000	-3.869871000	0.825940000
H	-5.438350000	-2.971608000	1.292663000
H	-6.426369000	-3.523170000	-1.622960000

H	-4.855486000	-2.670267000	-1.147436000
Br	-2.379572000	-3.317805000	-1.873960000

### TS1a-OH

SCF Energy (B3LYP-D3/B2) = -4702.23101964

Enthalpy 0K = 0.460859

Enthalpy 298 K = 0.497445

Free Energy 298 K = 0.389609

C	-4.818730000	-0.098379000	0.503574000
C	-3.451729000	-0.006984000	0.156191000
C	-5.431782000	-1.331910000	0.622739000
C	-2.710627000	-1.217575000	0.016546000
C	-4.742310000	-2.529047000	0.429465000
C	-3.361075000	-2.505519000	0.091973000
C	-2.581064000	-3.675269000	-0.242400000
C	-1.171287000	-3.540050000	-0.497329000
C	-0.503183000	-2.279072000	-0.397105000
C	-1.262585000	-1.134951000	-0.178990000
C	0.959506000	-2.257843000	-0.502815000
N	-0.619887000	0.131643000	-0.092981000
C	1.566003000	-0.962504000	-0.238296000
C	0.784136000	0.186260000	-0.092904000
C	-2.775248000	1.269088000	-0.038403000
C	-3.474402000	2.477079000	-0.226019000
C	-1.366047000	1.325163000	-0.070017000
C	-2.863959000	3.717051000	-0.321335000
C	-0.704824000	2.584723000	-0.075019000
C	-1.441852000	3.811882000	-0.167188000
H	-4.546988000	2.458155000	-0.311488000
C	-0.715950000	5.028613000	-0.106295000
C	0.715297000	2.645074000	0.038874000
C	1.452204000	1.433394000	0.039949000
C	-2.891520000	-5.019333000	-0.440296000
C	-0.670591000	-4.792340000	-0.825082000
O	-5.546602000	1.035815000	0.761250000
H	-6.443138000	0.775530000	1.005995000
C	-3.812926000	4.828110000	-0.580192000
O	-5.029628000	4.719943000	-0.587985000
O	-3.250833000	6.041329000	-0.857146000
H	-4.010992000	6.626334000	-1.008655000
C	-5.527248000	-3.754898000	0.725276000
O	-5.135123000	-4.789126000	1.231634000
O	-6.854527000	-3.601166000	0.426309000
H	-7.274153000	-4.417266000	0.743840000
C	1.422567000	3.864960000	0.126676000
N	-1.733370000	-5.654843000	-0.789602000
H	-1.665931000	-6.643354000	-0.972988000
H	0.330845000	-5.097873000	-1.068137000
H	-3.808308000	-5.568070000	-0.335806000
C	2.982079000	-0.850003000	-0.159664000
C	2.871641000	1.427330000	0.119775000
C	0.655975000	5.079281000	0.041278000
N	3.609122000	0.290068000	0.034412000
H	-1.259250000	5.958981000	-0.184147000
C	2.825563000	3.854710000	0.285049000
C	3.580352000	2.682757000	0.288816000
H	3.592078000	-1.750694000	-0.254139000
H	-6.481217000	-1.369300000	0.897520000

O	4.879340000	2.772184000	0.423269000
H	5.527483000	1.900718000	0.559084000
H	3.380978000	4.774456000	0.431576000
O	1.626911000	-3.261809000	-0.772452000
N	1.307354000	6.305223000	0.139658000
H	0.761992000	7.094801000	-0.177505000
H	2.249548000	6.323902000	-0.225316000
C	6.623793000	-0.440082000	0.023598000
C	6.374006000	-0.127901000	1.415900000
O	6.629787000	1.141692000	0.824279000
H	7.635617000	-0.575666000	-0.324382000
H	5.814760000	-0.357208000	-0.679674000
H	7.128460000	-0.443261000	2.143516000
H	5.355927000	-0.286762000	1.775821000
Br	6.228858000	-3.072281000	-0.207050000

### Int2a-OH

SCF Energy (B3LYP-D3/B2) = -4890.93243783

Enthalpy 0K = 0.477503

Enthalpy 298 K = 0.518613

Free Energy 298 K = 0.397315

C	-5.289729000	0.859188000	0.408513000
C	-3.928161000	0.604218000	0.118503000
C	-6.186110000	-0.182652000	0.546347000
C	-3.498133000	-0.755154000	0.061321000
C	-5.801922000	-1.520103000	0.427988000
C	-4.444947000	-1.843020000	0.152144000
C	-3.959804000	-3.180014000	-0.106281000
C	-2.549539000	-3.403818000	-0.279258000
C	-1.596840000	-2.339115000	-0.183824000
C	-2.065674000	-1.031880000	-0.060318000
C	-0.174665000	-2.675857000	-0.193546000
N	-1.143892000	0.045079000	0.003318000
C	0.712486000	-1.547021000	0.013479000
C	0.231935000	-0.235570000	0.066915000
C	-2.960566000	1.669483000	-0.097577000
C	-3.343774000	2.997183000	-0.370132000
C	-1.577990000	1.385526000	-0.064054000
C	-2.445179000	4.044930000	-0.494879000
C	-0.628214000	2.443886000	-0.096940000
C	-1.048769000	3.805636000	-0.282384000
H	-4.385165000	3.231650000	-0.503889000
C	-0.051769000	4.813593000	-0.248308000
C	0.758163000	2.169378000	0.076554000
C	1.180939000	0.817165000	0.168876000
C	-4.582792000	-4.412851000	-0.289929000
C	-2.357766000	-4.752607000	-0.542416000
O	-5.729576000	2.145683000	0.594436000
H	-6.670023000	2.118296000	0.809411000
C	-3.086754000	5.335059000	-0.848920000
O	-4.292712000	5.528805000	-0.893671000
O	-2.239596000	6.355276000	-1.176600000
H	-2.832354000	7.095305000	-1.386123000
C	-6.867881000	-2.504994000	0.736038000
O	-6.754814000	-3.589661000	1.277008000
O	-8.113299000	-2.040181000	0.402189000
H	-8.723089000	-2.719494000	0.732770000
C	1.744947000	3.187085000	0.133377000
N	-3.602051000	-5.327413000	-0.551966000

H	-3.773119000	-6.307961000	-0.707032000
H	-1.451195000	-5.302469000	-0.716959000
H	-5.611522000	-4.713708000	-0.227868000
C	2.110474000	-1.763586000	0.133435000
C	2.554103000	0.477933000	0.314262000
C	1.286242000	4.543122000	-0.044038000
N	2.994468000	-0.808927000	0.305917000
H	-0.350415000	5.841701000	-0.393238000
C	3.094092000	2.861484000	0.346659000
C	3.573605000	1.532546000	0.451638000
H	2.471092000	-2.787459000	0.075633000
H	-7.221270000	0.046875000	0.778461000
O	4.798116000	1.258200000	0.633204000
H	5.555089000	0.026354000	1.491999000
H	3.848068000	3.632892000	0.465742000
O	0.246826000	-3.834466000	-0.342410000
N	2.208532000	5.582798000	0.020220000
H	1.886692000	6.453964000	-0.378310000
H	3.142837000	5.344550000	-0.282799000
C	6.023184000	-1.798739000	-0.228640000
C	5.921382000	-1.872656000	1.290592000
O	6.230195000	-0.613390000	1.840970000
H	7.032617000	-1.572407000	-0.568021000
H	5.306718000	-1.079731000	-0.618616000
H	6.639702000	-2.604144000	1.681928000
H	4.910400000	-2.208892000	1.559451000
Br	5.531635000	-3.557103000	-1.045786000
C	7.500996000	1.596478000	0.535470000
O	7.592427000	1.050299000	-0.496467000
O	7.505545000	2.191560000	1.541781000

### TS2a-OH

SCF Energy (B3LYP-D3/B2) = -4890.91264640

Enthalpy 0K = 0.474966

Enthalpy 298 K = 0.514348

Free Energy 298 K = 0.398941

C	-5.302221000	0.482673000	0.613974000
C	-3.950599000	0.363819000	0.216028000
C	-6.084274000	-0.643613000	0.788851000
C	-3.401506000	-0.946443000	0.084544000
C	-5.586736000	-1.933970000	0.602981000
C	-4.231662000	-2.121423000	0.215919000
C	-3.645828000	-3.400581000	-0.115821000
C	-2.240454000	-3.483948000	-0.411843000
C	-1.388336000	-2.334948000	-0.362821000
C	-1.964681000	-1.083479000	-0.157700000
C	0.054741000	-2.532408000	-0.503764000
N	-1.143229000	0.075674000	-0.129504000
C	0.847613000	-1.330373000	-0.320756000
C	0.251080000	-0.074911000	-0.180560000
C	-3.104101000	1.521239000	-0.038502000
C	-3.625409000	2.814009000	-0.239937000
C	-1.704031000	1.368835000	-0.119263000
C	-2.842668000	3.945855000	-0.399103000
C	-0.864707000	2.514068000	-0.190487000
C	-1.416891000	3.834314000	-0.300256000
H	-4.691545000	2.952492000	-0.286531000
C	-0.518853000	4.931015000	-0.309275000
C	0.552637000	2.367702000	-0.130669000

C	1.101833000	1.060876000	-0.110868000
C	-4.161499000	-4.684778000	-0.277869000
C	-1.944599000	-4.802852000	-0.725928000
O	-5.843598000	1.717202000	0.866122000
H	-6.758047000	1.599454000	1.151439000
C	-3.628421000	5.178072000	-0.661357000
O	-4.846994000	5.250227000	-0.619621000
O	-2.906399000	6.285033000	-1.001724000
H	-3.576942000	6.972843000	-1.144445000
C	-6.530114000	-3.024112000	0.960502000
O	-6.272386000	-4.097691000	1.471573000
O	-7.832214000	-2.678800000	0.717034000
H	-8.353390000	-3.417432000	1.071561000
C	1.436729000	3.471019000	-0.119572000
N	-3.124126000	-5.494592000	-0.645092000
H	-3.213582000	-6.484457000	-0.810353000
H	-1.008748000	-5.260156000	-0.990159000
H	-5.147428000	-5.085865000	-0.137624000
C	2.265662000	-1.415705000	-0.322323000
C	2.508279000	0.849181000	-0.082595000
C	0.851835000	4.783614000	-0.216299000
N	3.067259000	-0.386150000	-0.187122000
H	-0.922703000	5.929005000	-0.396166000
C	2.827415000	3.259245000	-0.012451000
C	3.404503000	1.987855000	0.018256000
H	2.718442000	-2.396911000	-0.443698000
H	-7.115770000	-0.519428000	1.102960000
O	4.700456000	1.868208000	0.080818000
H	5.178275000	1.018615000	0.635459000
H	3.521069000	4.087695000	0.078386000
O	0.567807000	-3.636706000	-0.737361000
N	1.674649000	5.900034000	-0.183447000
H	1.248186000	6.757093000	-0.505263000
H	2.611278000	5.772125000	-0.538383000
C	6.097324000	-1.420457000	-0.387985000
C	5.805724000	-1.177150000	1.086361000
O	5.913891000	0.201957000	1.349271000
H	7.148100000	-1.249762000	-0.614412000
H	5.438150000	-0.824013000	-1.014177000
H	6.527662000	-1.726793000	1.699284000
H	4.792757000	-1.514538000	1.327887000
Br	5.711923000	-3.321579000	-0.883684000
C	7.541826000	0.804728000	1.534920000
O	8.315213000	-0.125273000	1.449610000
O	7.442650000	1.993186000	1.700950000

### Int3a-OH

SCF Energy (B3LYP-D3/B2) = -4890.91454260

Enthalpy 0K = 0.477981

Enthalpy 298 K = 0.517721

Free Energy 298 K = 0.401148

C	5.335133000	0.321736000	-0.220040000
C	3.934497000	0.270172000	-0.032440000
C	6.080286000	-0.841606000	-0.272891000
C	3.309549000	-1.011670000	0.015227000
C	5.498855000	-2.104817000	-0.167015000
C	4.093539000	-2.225288000	0.008131000
C	3.405798000	-3.474926000	0.239541000
C	1.969406000	-3.492898000	0.307659000

C	1.190514000	-2.304563000	0.137475000
C	1.847544000	-1.080360000	0.038409000
C	-0.263990000	-2.436629000	0.046728000
N	1.092585000	0.117639000	-0.094597000
C	-0.967303000	-1.193473000	-0.212948000
C	-0.301504000	0.033845000	-0.234789000
C	3.114688000	1.468349000	0.088553000
C	3.663902000	2.739167000	0.347908000
C	1.711408000	1.382294000	-0.027520000
C	2.924673000	3.909680000	0.378799000
C	0.927112000	2.567321000	-0.080478000
C	1.522940000	3.862460000	0.084180000
H	4.718030000	2.828739000	0.543842000
C	0.689302000	5.001487000	-0.046654000
C	-0.476509000	2.487680000	-0.323613000
C	-1.084611000	1.208963000	-0.394452000
C	3.830173000	-4.780829000	0.475258000
C	1.567059000	-4.796534000	0.562613000
O	5.969220000	1.526065000	-0.387911000
H	6.910322000	1.361838000	-0.525160000
C	3.727407000	5.109003000	0.730420000
O	4.941664000	5.120520000	0.859600000
O	3.021868000	6.256265000	0.947636000
H	3.698470000	6.914474000	1.175885000
C	6.432394000	-3.241103000	-0.379919000
O	6.206257000	-4.297941000	-0.938078000
O	7.693132000	-2.962213000	0.073312000
H	8.228483000	-3.725067000	-0.199564000
C	-1.289729000	3.632614000	-0.477762000
N	2.711463000	-5.541312000	0.667748000
H	2.727882000	-6.533597000	0.842046000
H	0.581449000	-5.210441000	0.672533000
H	4.806339000	-5.227454000	0.492474000
C	-2.371369000	-1.215134000	-0.427809000
C	-2.486300000	1.063507000	-0.598473000
C	-0.661302000	4.918269000	-0.323148000
N	-3.106081000	-0.147663000	-0.634096000
H	1.127501000	5.979989000	0.083435000
C	-2.667030000	3.484928000	-0.747417000
C	-3.297358000	2.246460000	-0.796038000
H	-2.867627000	-2.183600000	-0.424149000
H	7.152553000	-0.768541000	-0.424812000
O	-4.583787000	2.205783000	-1.060941000
H	-5.138282000	1.409094000	-0.680583000
H	-3.305389000	4.343291000	-0.922311000
O	-0.853736000	-3.520172000	0.161224000
N	-1.418049000	6.071235000	-0.482041000
H	-0.989408000	6.912124000	-0.121538000
H	-2.392319000	5.997040000	-0.225006000
C	-5.793898000	-1.738752000	0.592594000
C	-6.209525000	-0.855683000	-0.575889000
O	-6.140499000	0.486748000	-0.151719000
H	-6.562709000	-1.749748000	1.361612000
H	-4.831957000	-1.424077000	0.991376000
H	-7.226056000	-1.115037000	-0.890624000
H	-5.513214000	-0.980379000	-1.409760000
Br	-5.537549000	-3.634455000	0.005074000
C	-7.308577000	1.022324000	0.770048000
O	-8.139469000	0.149169000	1.009677000
O	-7.096192000	2.193524000	1.034466000

### TS3a-OH

SCF Energy (B3LYP-D3/B2) = -4890.89740607  
 Enthalpy 0K = 0.479051  
 Enthalpy 298 K = 0.518136  
 Free Energy 298 K = 0.403471

C	5.230641000	0.116607000	-0.232081000
C	3.829882000	0.138517000	-0.043703000
C	5.917053000	-1.083567000	-0.259666000
C	3.141892000	-1.109009000	0.031548000
C	5.273351000	-2.313325000	-0.127582000
C	3.863626000	-2.360514000	0.049116000
C	3.114052000	-3.568957000	0.305166000
C	1.678690000	-3.511486000	0.380988000
C	0.961163000	-2.288879000	0.189467000
C	1.678682000	-1.103976000	0.059244000
C	-0.501268000	-2.348871000	0.111213000
N	0.983316000	0.127653000	-0.100776000
C	-1.142503000	-1.080775000	-0.194866000
C	-0.412830000	0.108749000	-0.242631000
C	3.069835000	1.378671000	0.051740000
C	3.681569000	2.625922000	0.283404000
C	1.664071000	1.359759000	-0.061699000
C	3.003125000	3.833109000	0.289076000
C	0.940887000	2.582582000	-0.140850000
C	1.599900000	3.849364000	-0.003252000
H	4.739295000	2.666399000	0.476702000
C	0.823071000	5.025557000	-0.154172000
C	-0.464975000	2.567578000	-0.384802000
C	-1.133557000	1.317886000	-0.431181000
C	3.471307000	-4.891266000	0.560629000
C	1.210710000	-4.787861000	0.661258000
O	5.924222000	1.284169000	-0.424840000
H	6.856058000	1.070109000	-0.556407000
C	3.866343000	4.997484000	0.612547000
O	5.078943000	4.948671000	0.748316000
O	3.221955000	6.186657000	0.792647000
H	3.931764000	6.813815000	1.006997000
C	6.149717000	-3.498873000	-0.314502000
O	5.873241000	-4.552788000	-0.854910000
O	7.420599000	-3.275231000	0.141004000
H	7.918118000	-4.069157000	-0.114350000
C	-1.218379000	3.748225000	-0.562529000
N	2.315488000	-5.588742000	0.772176000
H	2.280710000	-6.577551000	0.963096000
H	0.205530000	-5.148171000	0.783412000
H	4.422841000	-5.388087000	0.580130000
C	-2.545118000	-1.041827000	-0.425076000
C	-2.537901000	1.236559000	-0.637878000
C	-0.530391000	5.003261000	-0.427694000
N	-3.222914000	0.060488000	-0.656897000
H	1.308675000	5.983388000	-0.039999000
C	-2.603390000	3.661664000	-0.835389000
C	-3.278674000	2.454701000	-0.860234000
H	-3.091764000	-1.984495000	-0.423187000
H	6.991706000	-1.067271000	-0.411667000
O	-4.577825000	2.458439000	-1.135296000
H	-5.075004000	1.683671000	-0.740675000
H	-3.198244000	4.546790000	-1.028337000
O	-1.141570000	-3.393866000	0.272783000
N	-1.232797000	6.190077000	-0.602997000
H	-0.756928000	7.012411000	-0.258417000
H	-2.202192000	6.167704000	-0.317940000

C	-5.933268000	-1.561784000	0.806593000
C	-6.355053000	-0.626293000	-0.310502000
O	-6.161140000	0.746123000	0.042245000
H	-6.648621000	-2.129308000	1.372967000
H	-4.910967000	-1.554411000	1.146516000
H	-7.409770000	-0.801409000	-0.553678000
H	-5.746275000	-0.799910000	-1.194970000
Br	-5.546865000	-3.515800000	-0.564021000
C	-6.162483000	1.003134000	1.457357000
O	-6.317641000	-0.058292000	2.137464000
O	-6.005158000	2.169837000	1.777546000

### Pdt1a-OH

SCF Energy (B3LYP-D3/B2) = -4890.94333930  
 Enthalpy 0K = 0.482107  
 Enthalpy 298 K = 0.521302  
 Free Energy 298 K = 0.405599

C	-4.557703000	2.429621000	0.707475000
C	-3.597737000	1.478761000	0.285853000
C	-5.894682000	2.091024000	0.786829000
C	-4.042838000	0.145783000	0.032892000
C	-6.362245000	0.811471000	0.481955000
C	-5.446524000	-0.194070000	0.068469000
C	-5.831555000	-1.514682000	-0.376369000
C	-4.816723000	-2.489848000	-0.671628000
C	-3.423092000	-2.196412000	-0.528345000
C	-3.041583000	-0.888335000	-0.231056000
C	-2.464772000	-3.289897000	-0.671884000
N	-1.662551000	-0.561908000	-0.129273000
C	-1.085828000	-2.916469000	-0.420088000
C	-0.712793000	-1.587341000	-0.209005000
C	-2.190002000	1.804888000	0.124724000
C	-1.719383000	3.131492000	0.060309000
C	-1.231235000	0.776581000	-0.003817000
C	-0.382155000	3.478821000	-0.010527000
C	0.152691000	1.086200000	-0.006970000
C	0.617701000	2.447165000	0.024333000
H	-2.426938000	3.942062000	0.055807000
C	2.008941000	2.677417000	0.060857000
C	1.125890000	0.039974000	-0.012589000
C	0.674203000	-1.302361000	-0.090715000
C	-7.055136000	-2.119963000	-0.653864000
C	-5.446519000	-3.651044000	-1.096839000
O	-4.166166000	3.689880000	1.078702000
H	-4.946879000	4.188102000	1.350255000
C	-0.159403000	4.944956000	-0.120207000
O	-1.045432000	5.785450000	-0.080765000
O	1.130920000	5.339558000	-0.296250000
H	1.085838000	6.307306000	-0.361723000
C	-7.805902000	0.593562000	0.751299000
O	-8.348012000	-0.419083000	1.153772000
O	-8.542329000	1.732404000	0.564261000
H	-9.437876000	1.497348000	0.856685000
C	2.511936000	0.288610000	0.051717000
N	-6.791218000	-3.389525000	-1.084625000
H	-7.501993000	-4.057092000	-1.337960000
H	-5.032052000	-4.596327000	-1.395542000
H	-8.066375000	-1.773336000	-0.554963000
C	-0.076899000	-3.915203000	-0.417200000

C	1.587365000	-2.393477000	-0.087505000
C	2.958576000	1.661436000	0.060472000
N	1.201987000	-3.693740000	-0.234043000
H	2.364897000	3.696132000	0.058417000
C	3.416602000	-0.799772000	0.130873000
C	2.987075000	-2.112160000	0.081304000
H	-0.401710000	-4.941143000	-0.573101000
H	-6.603390000	2.841726000	1.121699000
O	3.803908000	-3.176694000	0.170355000
H	4.707049000	-2.902414000	0.419244000
H	4.473095000	-0.595367000	0.242346000
O	-2.793654000	-4.450953000	-0.964505000
N	4.296747000	1.947164000	0.112918000
H	4.518286000	2.931182000	0.026498000
H	4.964603000	1.427667000	-0.484001000
C	7.369740000	-0.272428000	1.041747000
C	7.097911000	-1.407598000	0.061222000
O	6.408770000	-2.375219000	0.904949000
H	8.322125000	0.227668000	0.883315000
H	6.571344000	0.472154000	1.054618000
H	8.012753000	-1.873976000	-0.315964000
H	6.464060000	-1.107269000	-0.769848000
Br	6.868390000	1.353348000	-1.809274000
C	6.711625000	-2.120540000	2.219906000
O	7.396483000	-0.967001000	2.324023000
O	6.401948000	-2.841157000	3.126986000

### Int1a-COOH

SCF Energy (B3LYP-D3/B2) = -4702.28212284

Enthalpy 0K = 0.464806

Enthalpy 298 K = 0.501817

Free Energy 298 K = 0.390885

C	-0.741233000	-3.150914000	-0.658884000
C	-1.222579000	-1.868306000	-0.305035000
C	-1.594599000	-4.239887000	-0.677304000
C	-2.622537000	-1.722175000	-0.055765000
C	-2.952448000	-4.130371000	-0.379813000
C	-3.502954000	-2.866983000	-0.035914000
C	-4.870558000	-2.662551000	0.387777000
C	-5.354691000	-1.327622000	0.615473000
C	-4.519082000	-0.181324000	0.428524000
C	-3.165572000	-0.379922000	0.145277000
C	-5.127353000	1.143067000	0.521242000
N	-2.305612000	0.741343000	0.000414000
C	-4.216628000	2.242193000	0.253278000
C	-2.849551000	2.021402000	0.045801000
C	-0.350515000	-0.704447000	-0.208263000
C	1.060052000	-0.805128000	-0.160089000
C	-0.902689000	0.584802000	-0.130652000
C	1.917987000	0.275192000	-0.149458000
C	-0.053561000	1.726209000	-0.181867000
C	1.371781000	1.594397000	-0.225310000
H	1.523112000	-1.775899000	-0.127086000
C	2.152089000	2.778824000	-0.318900000
C	-0.612380000	3.037869000	-0.210040000
C	-2.018483000	3.162208000	-0.102636000
C	-5.922347000	-3.521868000	0.694957000
C	-6.676153000	-1.413621000	1.031859000
O	0.564182000	-3.319802000	-1.022598000

H	0.724942000	-4.251982000	-1.215087000
C	3.380521000	-0.095492000	-0.056144000
O	3.742696000	-1.265463000	-0.109756000
O	4.217358000	0.916868000	0.108223000
H	5.190397000	0.567292000	0.167095000
C	-3.738255000	-5.377056000	-0.582388000
O	-4.871716000	-5.478591000	-1.012465000
O	-3.008094000	-6.493916000	-0.292352000
H	-3.574984000	-7.240164000	-0.547162000
C	0.175288000	4.206087000	-0.325977000
N	-6.980964000	-2.747452000	1.078720000
H	-7.881303000	-3.115923000	1.341287000
H	-7.376377000	-0.640039000	1.288382000
H	-6.014794000	-4.590313000	0.645444000
C	-4.714238000	3.571395000	0.232462000
C	-2.631951000	4.433656000	-0.106987000
C	1.603809000	4.042688000	-0.371984000
N	-3.973236000	4.640182000	0.042773000
H	3.227119000	2.669491000	-0.328317000
C	-0.455253000	5.479658000	-0.389878000
C	-1.820944000	5.597901000	-0.274962000
H	-5.782394000	3.700862000	0.383774000
H	-1.195303000	-5.209447000	-0.956846000
O	-2.439178000	6.800374000	-0.313673000
H	-3.388962000	6.594867000	-0.199266000
H	0.123689000	6.381994000	-0.547791000
O	-6.324489000	1.333028000	0.790926000
N	2.417179000	5.166305000	-0.510003000
H	3.401110000	4.978104000	-0.368592000
H	2.120720000	5.982220000	0.008665000
C	6.826926000	-1.155665000	0.900391000
C	6.952606000	-1.033775000	-0.550677000
O	6.625374000	0.141976000	0.255912000
H	5.913063000	-1.580233000	1.311622000
H	7.760240000	-1.218280000	1.459046000
H	6.128702000	-1.371424000	-1.176576000
Br	10.347283000	-1.431596000	0.442858000
H	7.968437000	-1.016324000	-0.944361000

### TS1a-COOH

SCF Energy (B3LYP-D3/B2) = -4702.24622197

Enthalpy 0K = 0.461551

Enthalpy 298 K = 0.498054

Free Energy 298 K = 0.388629

C	-0.097820000	-3.037281000	-0.059031000
C	-0.776315000	-1.806096000	0.106603000
C	-0.809229000	-4.220869000	-0.150566000
C	-2.204900000	-1.816078000	0.081222000
C	-2.202853000	-4.259306000	-0.114166000
C	-2.943456000	-3.056087000	0.025593000
C	-4.381412000	-2.994955000	0.174028000
C	-5.041073000	-1.717492000	0.211620000
C	-4.314652000	-0.489756000	0.094776000
C	-2.918154000	-0.539626000	0.075219000
C	-5.068353000	0.755034000	-0.019646000
N	-2.172757000	0.665238000	-0.001742000
C	-4.247246000	1.939375000	-0.199713000
C	-2.849266000	1.871983000	-0.148069000
C	-0.068434000	-0.543060000	0.268089000

C	1.309910000	-0.469610000	0.586334000	C	-2.779239000	-1.670306000	0.043905000
C	-0.759892000	0.670233000	0.128488000	C	-3.156494000	-4.082169000	-0.200501000
C	2.035236000	0.701857000	0.619134000	C	-3.698719000	-2.784309000	-0.007987000
C	-0.042882000	1.899254000	0.127851000	C	-5.105325000	-2.512515000	0.197361000
C	1.373584000	1.931996000	0.326729000	C	-5.566152000	-1.152730000	0.273329000
H	1.851351000	-1.368564000	0.824730000	C	-4.668276000	-0.044452000	0.153630000
C	2.029828000	3.193990000	0.288224000	C	-3.294802000	-0.302372000	0.092778000
C	-0.724400000	3.131805000	-0.090050000	C	-5.230615000	1.299538000	0.084066000
C	-2.132200000	3.094499000	-0.232473000	N	-2.381363000	0.777904000	0.029065000
C	-5.373544000	-3.956976000	0.3444002000	C	-4.246434000	2.352310000	-0.088015000
C	-6.400405000	-1.939428000	0.383988000	C	-2.872879000	2.076218000	-0.068679000
O	1.261309000	-3.060956000	-0.166412000	C	-0.465210000	-0.738394000	0.181382000
H	1.562545000	-3.970324000	-0.286561000	C	0.927138000	-0.880222000	0.424800000
C	3.499480000	0.532365000	0.991363000	C	-0.979695000	0.567954000	0.120764000
O	3.859277000	-0.488295000	1.573736000	C	1.811726000	0.171352000	0.524378000
O	4.292271000	1.507919000	0.625546000	C	-0.093170000	1.678163000	0.153425000
H	5.363342000	1.328616000	0.913729000	C	1.311755000	1.495079000	0.340440000
C	-2.795524000	-5.601849000	-0.358814000	H	1.362091000	-1.858401000	0.536308000
O	-3.805183000	-5.865110000	-0.984285000	C	2.143763000	2.648328000	0.348222000
O	-2.021365000	-6.603039000	0.153298000	C	-0.585213000	3.005450000	-0.016067000
H	-2.442110000	-7.425972000	-0.144902000	C	-1.983460000	3.181520000	-0.135868000
C	-0.056214000	4.376301000	-0.153669000	C	-6.222772000	-3.320051000	0.393727000
N	-6.563522000	-3.296264000	0.470241000	C	-6.936728000	-1.173471000	0.491175000
H	-7.452411000	-3.755907000	0.587241000	O	0.443927000	-3.421715000	-0.382287000
H	-7.215389000	-1.242298000	0.450254000	H	0.591936000	-4.367570000	-0.504388000
H	-5.338917000	-5.029975000	0.355011000	C	3.286986000	-0.198731000	0.803860000
C	-4.872073000	3.198193000	-0.401306000	O	3.577136000	-1.409830000	0.751419000
C	-2.867261000	4.282766000	-0.433620000	O	4.075304000	0.765824000	1.073872000
C	1.367689000	4.379039000	0.054839000	H	5.692018000	0.574041000	1.233177000
N	-4.228337000	4.336449000	-0.533416000	C	-3.950316000	-5.312734000	-0.449343000
H	3.099738000	3.196694000	0.450951000	O	-5.017107000	-5.410973000	-1.027516000
C	-0.798565000	5.561657000	-0.414315000	O	-3.308611000	-6.436315000	-0.005578000
C	-2.167850000	5.523743000	-0.542404000	H	-3.864711000	-7.173871000	-0.304876000
H	-5.957608000	3.207626000	-0.448520000	C	0.262223000	4.138409000	-0.060775000
H	-0.261338000	-5.148709000	-0.278639000	N	-7.296952000	-2.492953000	0.569591000
O	-2.895614000	6.642170000	-0.771845000	H	-8.239635000	-2.817779000	0.713027000
H	-3.822046000	6.329516000	-0.809152000	H	-7.635345000	-0.363643000	0.594553000
H	-0.299217000	6.515713000	-0.536375000	H	-6.347201000	-4.386400000	0.391709000
O	-6.308944000	0.815160000	0.017920000	C	-4.679654000	3.695547000	-0.246482000
N	2.065975000	5.587099000	-0.022920000	C	-2.536042000	4.471724000	-0.294279000
H	3.027950000	5.514528000	0.282451000	C	1.671723000	3.922613000	0.132701000
H	1.604469000	6.375525000	0.412002000	N	-3.876353000	4.728855000	-0.365682000
C	7.045058000	-0.141927000	1.401867000	H	3.187360000	2.477329000	0.574116000
C	7.373148000	0.167126000	0.026605000	C	-0.298884000	5.426780000	-0.281676000
O	6.644364000	1.224737000	1.179984000	C	-1.660510000	5.596262000	-0.386211000
H	6.219228000	-0.828153000	1.587209000	H	-5.752478000	3.866856000	-0.270360000
H	7.870562000	-0.245664000	2.108555000	H	-1.376785000	-5.245264000	-0.464314000
H	6.642559000	0.001576000	-0.749849000	O	-2.218621000	6.817787000	-0.575773000
Br	8.588386000	-2.063736000	-0.996950000	H	-3.181007000	6.643632000	-0.601068000
H	8.315555000	0.623269000	-0.225950000	H	0.339663000	6.296377000	-0.385809000
				O	-6.449070000	1.541606000	0.151995000
				N	2.555979000	5.005083000	0.059859000
				H	3.508607000	4.747028000	0.291259000
				H	2.261899000	5.830800000	0.566446000
				C	7.184808000	-0.700116000	1.080042000
				C	6.646950000	-1.398980000	-0.166256000
				O	6.689248000	0.613925000	1.150046000
				H	6.918538000	-1.301554000	1.964605000
				H	8.280211000	-0.648465000	1.036273000
				H	5.578470000	-1.602169000	-0.077081000
				Br	7.530912000	-3.185391000	-0.398483000
				H	6.872487000	-0.836056000	-1.070587000

## Int2a-COOH

SCF Energy (B3LYP-D3/B2) = -4890.94870192

Enthalpy 0K = 0.478393

Enthalpy 298 K = 0.519116

Free Energy 298 K = 0.400209

C	-0.889398000	-3.190570000	-0.210160000
C	-1.362861000	-1.872763000	0.010539000
C	-1.773886000	-4.249913000	-0.293112000

C	5.527046000	2.254757000	-0.838569000
O	5.553813000	1.398491000	-1.633045000
O	5.502537000	3.183491000	-0.123782000

### TS2a-COOH

SCF Energy (B3LYP-D3/B2) = -4890.93805169

Enthalpy 0K = 0.475303

Enthalpy 298 K = 0.514488

Free Energy 298 K = 0.400739

C	-1.528899000	-3.287404000	-0.165784000
C	-1.781674000	-1.904758000	0.020546000
C	-2.571647000	-4.190929000	-0.238421000
C	-3.148399000	-1.477518000	0.051326000
C	-3.909810000	-3.801742000	-0.157422000
C	-4.234606000	-2.430645000	0.018500000
C	-5.577917000	-1.935090000	0.226883000
C	-5.815451000	-0.518545000	0.288520000
C	-4.753385000	0.430168000	0.146768000
C	-3.439406000	-0.044508000	0.079386000
C	-5.094941000	1.845742000	0.062720000
N	-2.366352000	0.875333000	-0.009928000
C	-3.958220000	2.725464000	-0.139208000
C	-2.646081000	2.234594000	-0.129999000
C	-0.714394000	-0.925515000	0.160003000
C	0.644587000	-1.279923000	0.393593000
C	-1.015589000	0.446650000	0.074671000
C	1.667475000	-0.366169000	0.480927000
C	0.032234000	1.406240000	0.068517000
C	1.391061000	1.012420000	0.248495000
H	0.915704000	-2.314564000	0.511100000
C	2.405873000	1.999180000	0.180966000
C	-0.240127000	2.790262000	-0.130213000
C	-1.594182000	3.183655000	-0.233624000
C	-6.807926000	-2.551979000	0.442200000
C	-7.169673000	-0.317997000	0.516882000
O	-0.248153000	-3.741253000	-0.314727000
H	-0.266924000	-4.695388000	-0.458561000
C	3.068025000	-0.883709000	0.776940000
O	3.420257000	-1.969287000	0.299451000
O	3.760772000	-0.104898000	1.540565000
H	4.997841000	-0.041649000	1.411210000
C	-4.891420000	-4.889362000	-0.398293000
O	-5.963798000	-4.816887000	-0.969979000
O	-4.435649000	-6.101333000	0.044655000
H	-5.105299000	-6.739756000	-0.249835000
C	0.779522000	3.769096000	-0.214023000
N	-7.734626000	-1.562329000	0.615025000
H	-8.715652000	-1.730952000	0.769857000
H	-7.729530000	0.593837000	0.615151000
H	-7.100597000	-3.584823000	0.455417000
C	-4.175230000	4.117520000	-0.319299000
C	-1.937066000	4.541980000	-0.411692000
C	2.145167000	3.334141000	-0.053171000
N	-3.220171000	5.007791000	-0.469796000
H	3.426987000	1.695932000	0.358042000
C	0.424701000	5.126063000	-0.451727000
C	-0.894155000	5.509523000	-0.539154000
H	-5.207495000	4.456701000	-0.333081000
H	-2.339770000	-5.240206000	-0.390386000
O	-1.252012000	6.801146000	-0.745454000

H	-2.230009000	6.785042000	-0.753356000
H	1.188551000	5.883743000	-0.583284000
O	-6.258082000	2.279649000	0.140722000
N	3.191950000	4.238519000	-0.172573000
H	4.096698000	3.851903000	0.082740000
H	3.032456000	5.152744000	0.227212000
C	6.935088000	-0.937407000	1.000161000
C	6.546315000	-1.546696000	-0.341651000
O	6.128428000	0.189692000	1.273416000
H	6.808205000	-1.678292000	1.800155000
H	7.982182000	-0.620227000	0.977310000
H	5.524811000	-1.927854000	-0.330715000
Br	7.724545000	-3.108207000	-0.746774000
H	6.708649000	-0.835848000	-1.150380000
C	6.520166000	1.727384000	0.357099000
O	7.540089000	1.526922000	-0.237924000
O	5.632950000	2.486322000	0.645631000

### Int3a-COOH

SCF Energy (B3LYP-D3/B2) = -4890.94134900

Enthalpy 0K = 0.480131

Enthalpy 298 K = 0.519349

Free Energy 298 K = 0.405434

C	-1.831138000	-3.356421000	-0.244732000
C	-2.024790000	-1.967829000	-0.031644000
C	-2.909460000	-4.214122000	-0.334809000
C	-3.373701000	-1.486813000	0.020060000
C	-4.230958000	-3.773326000	-0.239849000
C	-4.497559000	-2.394552000	-0.026290000
C	-5.817375000	-1.851106000	0.209076000
C	-5.996755000	-0.428446000	0.312756000
C	-4.898734000	0.480077000	0.183803000
C	-3.606307000	-0.044639000	0.086632000
C	-5.183880000	1.910309000	0.143560000
N	-2.497846000	0.834837000	0.006372000
C	-4.015873000	2.750050000	-0.051494000
C	-2.724479000	2.208086000	-0.075439000
C	-0.919592000	-1.035621000	0.112697000
C	0.428685000	-1.449113000	0.317608000
C	-1.164978000	0.351994000	0.060840000
C	1.481067000	-0.572663000	0.406371000
C	-0.083619000	1.270732000	0.056517000
C	1.263593000	0.823265000	0.201013000
H	0.653120000	-2.496565000	0.419781000
C	2.314911000	1.757230000	0.120745000
C	-0.298713000	2.669543000	-0.105403000
C	-1.637746000	3.117906000	-0.173120000
C	-7.069028000	-2.423955000	0.422140000
C	-7.339165000	-0.180260000	0.563107000
O	-0.569055000	-3.863168000	-0.403395000
H	-0.633750000	-4.808803000	-0.585081000
C	2.863162000	-1.117564000	0.641514000
O	3.288774000	-2.111251000	0.074393000
O	3.543871000	-0.391793000	1.526938000
H	4.523850000	-0.363279000	1.292745000
C	-5.256959000	-4.812033000	-0.506139000
O	-6.332803000	-4.677657000	-1.060127000
O	-4.844403000	-6.056715000	-0.113026000
H	-5.542678000	-6.656698000	-0.421395000

C	0.759140000	3.608747000	-0.185009000
N	-7.952670000	-1.403233000	0.633409000
H	-8.938016000	-1.536600000	0.795340000
H	-7.861010000	0.749891000	0.693444000
H	-7.402915000	-3.444204000	0.410378000
C	-4.180887000	4.153613000	-0.190833000
C	-1.929746000	4.493084000	-0.309123000
C	2.112955000	3.115335000	-0.071361000
N	-3.193775000	5.009827000	-0.332780000
H	3.335621000	1.433281000	0.256647000
C	0.452344000	4.984595000	-0.373380000
C	-0.851321000	5.422339000	-0.426460000
H	-5.198996000	4.533116000	-0.178859000
H	-2.721151000	-5.268165000	-0.512030000
O	-1.160008000	6.732670000	-0.587266000
H	-2.137683000	6.756980000	-0.578869000
H	1.240760000	5.719426000	-0.490204000
O	-6.327150000	2.387314000	0.250446000
N	3.201131000	3.943728000	-0.182760000
H	4.101748000	3.512837000	0.057840000
H	3.093604000	4.906068000	0.097063000
C	6.616651000	-1.010652000	-0.096782000
C	8.012694000	-1.112489000	0.498600000
O	5.916937000	0.018265000	0.592777000
H	6.686346000	-0.781718000	-1.163531000
H	6.045599000	-1.933133000	0.043285000
H	8.577319000	-0.207039000	0.287317000
Br	9.028293000	-2.619563000	-0.324231000
H	7.982790000	-1.320768000	1.568019000
C	6.158565000	1.428646000	0.125808000
O	7.084911000	1.555498000	-0.669855000
O	5.346586000	2.195619000	0.669194000

### TS3a-COOH

SCF Energy (B3LYP-D3/B2) = -4890.91922501

Enthalpy 0K = 0.480038

Enthalpy 298 K = 0.518988

Free Energy 298 K = 0.404880

C	-1.800731000	-3.354753000	-0.078579000
C	-2.007845000	-1.961838000	0.079570000
C	-2.872751000	-4.218400000	-0.197240000
C	-3.357057000	-1.482120000	0.045380000
C	-4.196394000	-3.777230000	-0.185147000
C	-4.476036000	-2.393397000	-0.031063000
C	-5.807141000	-1.846430000	0.114888000
C	-5.992917000	-0.421595000	0.163975000
C	-4.890175000	0.484796000	0.064664000
C	-3.594373000	-0.039133000	0.052575000
C	-5.173600000	1.912919000	-0.037857000
N	-2.483634000	0.840354000	0.001036000
C	-3.997469000	2.748489000	-0.202107000
C	-2.706578000	2.209326000	-0.139986000
C	-0.911987000	-1.020877000	0.252710000
C	0.422454000	-1.424272000	0.542312000
C	-1.155988000	0.362906000	0.142870000
C	1.467208000	-0.540907000	0.661832000
C	-0.076463000	1.284448000	0.166832000
C	1.259505000	0.845853000	0.402354000
H	0.641799000	-2.467798000	0.686903000

C	2.312512000	1.781772000	0.349434000
C	-0.283160000	2.675728000	-0.058208000
C	-1.617004000	3.117891000	-0.213123000
C	-7.068187000	-2.415260000	0.276327000
C	-7.347238000	-0.168982000	0.332610000
O	-0.531719000	-3.861675000	-0.152683000
H	-0.582072000	-4.812387000	-0.311272000
C	2.830807000	-1.081392000	0.981885000
O	3.293655000	-2.084866000	0.469665000
O	3.464677000	-0.330677000	1.891422000
H	4.445679000	-0.422523000	1.795961000
C	-5.207872000	-4.827393000	-0.469448000
O	-6.246123000	-4.713854000	-1.094112000
O	-4.822773000	-6.052419000	0.001165000
H	-5.500626000	-6.667805000	-0.322409000
C	0.776728000	3.613657000	-0.119105000
N	-7.962618000	-1.390451000	0.406965000
H	-8.955319000	-1.521046000	0.519002000
H	-7.876495000	0.763303000	0.405055000
H	-7.400670000	-3.436065000	0.278272000
C	-4.155772000	4.145859000	-0.400373000
C	-1.901815000	4.486011000	-0.415065000
C	2.121581000	3.126854000	0.084481000
N	-3.163018000	4.998552000	-0.522811000
H	3.321003000	1.462232000	0.560066000
C	0.480870000	4.980387000	-0.377253000
C	-0.818830000	5.412849000	-0.512615000
H	-5.173239000	4.523339000	-0.454623000
H	-2.674938000	-5.277364000	-0.328784000
O	-1.118566000	6.714585000	-0.738686000
H	-2.095359000	6.738866000	-0.781953000
H	1.274441000	5.711107000	-0.483890000
O	-6.320497000	2.390505000	-0.005137000
N	3.214963000	3.955246000	-0.016142000
H	4.102883000	3.532747000	0.262229000
H	3.100868000	4.921085000	0.249621000
C	6.745133000	-1.060379000	0.472119000
C	7.763844000	-0.502522000	-0.505097000
O	6.031843000	-0.002287000	1.156067000
H	6.019835000	-1.694850000	-0.043565000
H	7.242144000	-1.646817000	1.243211000
H	7.599302000	-0.531013000	-1.566959000
Br	8.951595000	-2.657451000	-0.779548000
H	8.682363000	-0.068108000	-0.146810000
C	6.091335000	1.244302000	0.504417000
O	6.895139000	1.268392000	-0.476212000
O	5.373758000	2.134164000	0.966883000

### Pdt1a-COOH

SCF Energy (B3LYP-D3/B2) = -4890.97189662

Enthalpy 0K = 0.482927

Enthalpy 298 K = 0.521637

Free Energy 298 K = 0.409209

C	2.020825000	1.105779000	0.084123000
C	0.634154000	0.903165000	-0.118782000
C	2.535075000	2.404858000	0.078242000
C	-0.223952000	2.045167000	-0.211327000
C	1.719583000	3.517046000	-0.074797000
C	0.317070000	3.378317000	-0.234558000
C	-0.588276000	4.481968000	-0.474199000

C	-2.003275000	4.240274000	-0.546738000
C	-2.550328000	2.930501000	-0.359444000
C	-1.670202000	1.850576000	-0.231194000
C	-3.999283000	2.790197000	-0.273732000
N	-2.190109000	0.538033000	-0.062506000
C	-4.457149000	1.441065000	0.015366000
C	-3.562605000	0.364971000	0.072275000
C	0.046301000	-0.430889000	-0.204390000
C	0.818933000	-1.594273000	-0.443576000
C	-1.342368000	-0.599215000	-0.088806000
C	0.299276000	-2.876487000	-0.418926000
C	-1.901030000	-1.906991000	-0.001522000
C	-1.081357000	-3.069484000	-0.113421000
H	1.869317000	-1.474315000	-0.645791000
C	-1.693559000	-4.347761000	0.017304000
C	-3.297701000	-2.086397000	0.215890000
C	-4.113763000	-0.930423000	0.255691000
C	-0.406718000	5.841984000	-0.703396000
C	-2.635370000	5.450077000	-0.804251000
O	2.858419000	0.072392000	0.293740000
H	3.746695000	0.407823000	0.655986000
C	1.209900000	-4.022983000	-0.715444000
O	1.040728000	-5.178903000	-0.360358000
O	2.267153000	-3.654256000	-1.461955000
H	2.887022000	-4.411984000	-1.523588000
C	2.428943000	4.822683000	0.067773000
O	2.061713000	5.789510000	0.709289000
O	3.629036000	4.814582000	-0.566643000
H	4.073130000	5.636503000	-0.300935000
C	-3.893334000	-3.359342000	0.370476000
N	-1.645904000	6.390682000	-0.901624000
H	-1.806723000	7.370457000	-1.071116000
H	-3.679049000	5.679142000	-0.918110000
H	0.472797000	6.458331000	-0.706895000
C	-5.841128000	1.201656000	0.216137000
C	-5.507423000	-1.040524000	0.444450000
C	-3.039810000	-4.511477000	0.256307000
N	-6.369415000	0.018614000	0.442554000
H	-1.055817000	-5.217621000	-0.071147000
C	-5.290691000	-3.457282000	0.622542000
C	-6.082170000	-2.332657000	0.650373000
H	-6.499912000	2.065035000	0.178701000
H	3.601798000	2.523707000	0.235468000
O	-7.417065000	-2.401205000	0.867035000
H	-7.718777000	-1.470888000	0.823064000
H	-5.756789000	-4.416640000	0.814822000
O	-4.796000000	3.733727000	-0.414517000
N	-3.588641000	-5.787340000	0.428874000
H	-2.954553000	-6.531678000	0.168215000
H	-4.494490000	-5.918258000	-0.003073000
C	5.169361000	-2.272589000	0.774253000
C	5.641881000	-1.637626000	-0.540894000
O	4.723875000	-3.591754000	0.360480000
H	5.970849000	-2.384886000	1.507391000
H	4.330961000	-1.750943000	1.227249000
H	6.607290000	-1.144091000	-0.465050000
Br	5.602983000	0.994644000	1.425695000
H	4.908739000	-0.942779000	-0.952152000
C	5.085855000	-3.819478000	-0.912459000
O	5.750927000	-2.779489000	-1.437971000
O	4.815914000	-4.836580000	-1.516542000

## Int1a-pyrrolic-H

SCF Energy (B3LYP-D3/B2) = -4702.28119017

Enthalpy 0K = 0.464525

Enthalpy 298 K = 0.501605

Free Energy 298 K = 0.392229

C	0.295950000	3.157791000	-0.674586000
C	-0.335916000	1.942841000	-0.354168000
C	1.684439000	3.243347000	-0.697086000
C	0.477230000	0.771808000	-0.229484000
C	2.489344000	2.153854000	-0.422778000
C	1.914170000	0.868815000	-0.251484000
C	2.693253000	-0.339047000	-0.171249000
C	2.026505000	-1.613255000	-0.086630000
C	0.601128000	-1.707994000	-0.073796000
C	-0.160314000	-0.531628000	-0.120588000
C	-0.007903000	-3.036733000	-0.056898000
N	-1.589087000	-0.604788000	-0.108175000
C	-1.463285000	-3.040996000	-0.099655000
C	-2.201665000	-1.850859000	-0.095032000
C	-1.777892000	1.827098000	-0.144963000
C	-2.603012000	2.952288000	0.049408000
C	-2.388123000	0.563059000	-0.065937000
C	-3.976686000	2.894401000	0.228811000
C	-3.808235000	0.462906000	0.052688000
C	-4.634098000	1.625483000	0.182059000
H	-2.152225000	3.930134000	0.066838000
C	-6.042927000	1.440250000	0.263479000
C	-4.442432000	-0.814581000	0.023362000
C	-3.616138000	-1.962312000	-0.062735000
C	4.061538000	-0.606322000	-0.212375000
C	3.010515000	-2.599720000	-0.065403000
O	-0.445569000	4.276235000	-0.970948000
H	0.164868000	4.998441000	-1.164875000
C	-4.604631000	4.222018000	0.458635000
O	-4.025965000	5.290871000	0.361452000
O	-5.918598000	4.204912000	0.832751000
H	-6.145725000	5.142362000	0.946392000
C	3.967566000	2.458831000	-0.379817000
O	4.516884000	3.060681000	-1.285295000
O	4.520721000	2.073032000	0.759361000
H	5.531492000	1.985329000	0.676686000
C	-5.845467000	-0.980539000	0.079000000
N	4.211825000	-1.958730000	-0.142370000
H	5.130551000	-2.413874000	-0.118984000
H	2.923670000	-3.669030000	-0.004587000
H	4.941030000	0.015595000	-0.250740000
C	-2.149992000	-4.280503000	-0.128767000
C	-4.182251000	-3.253937000	-0.092613000
C	-6.646729000	0.203253000	0.217039000
N	-3.459764000	-4.410402000	-0.138305000
H	-6.667939000	2.313643000	0.378272000
C	-6.410848000	-2.284130000	-0.001498000
C	-5.604564000	-3.395038000	-0.077312000
H	-1.539724000	-5.179390000	-0.144159000
H	2.164600000	4.192867000	-0.923634000
O	-6.112127000	-4.647208000	-0.141174000
H	-5.322775000	-5.226526000	-0.179971000
H	-7.484606000	-2.428208000	-0.029270000
O	0.638760000	-4.094102000	-0.018386000

N	-8.040358000	0.085011000	0.259296000
H	-8.506569000	0.933616000	0.552609000
H	-8.378848000	-0.710548000	0.785023000
C	7.960737000	-2.417586000	-0.458874000
C	7.703440000	-2.549009000	0.976945000
O	6.801000000	-3.144221000	0.013412000
H	7.757384000	-1.447430000	-0.909670000
H	8.711224000	-3.045386000	-0.939751000
H	7.324951000	-1.667082000	1.491829000
H	8.262037000	-3.274498000	1.568698000
Br	7.420892000	1.041932000	0.504302000

### TS1a-pyrollic-H

SCF Energy (B3LYP-D3/B2) = -4702.23842761

Enthalpy 0K = 0.462316

Enthalpy 298 K = 0.499329

Free Energy 298 K = 0.387476

C	-1.075786000	3.726867000	-0.425350000
C	-1.267253000	2.361817000	-0.132401000
C	0.203077000	4.263222000	-0.472732000
C	-0.113252000	1.540733000	0.057374000
C	1.336468000	3.491801000	-0.250834000
C	1.215848000	2.109649000	0.061059000
C	2.319966000	1.268797000	0.427944000
C	2.107331000	-0.142360000	0.632681000
C	0.819575000	-0.728640000	0.463952000
C	-0.279208000	0.103421000	0.220477000
C	0.700432000	-2.187947000	0.527861000
N	-1.586021000	-0.461201000	0.080379000
C	-0.633323000	-2.701355000	0.244838000
C	-1.726410000	-1.843374000	0.076718000
C	-2.594739000	1.754704000	-0.030487000
C	-3.774009000	2.518334000	0.070887000
C	-2.734609000	0.354477000	-0.001914000
C	-5.053517000	1.984371000	0.086865000
C	-4.035169000	-0.232290000	-0.056438000
C	-5.221414000	0.569752000	-0.045140000
H	-3.698455000	3.589360000	0.144314000
C	-6.475777000	-0.090837000	-0.152688000
C	-4.178758000	-1.648765000	-0.144552000
C	-3.004221000	-2.437960000	-0.082206000
C	3.670548000	1.496824000	0.703715000
C	3.333081000	-0.696459000	1.002577000
O	-2.146172000	4.542721000	-0.702502000
H	-1.813474000	5.427029000	-0.898869000
C	-6.122808000	3.004180000	0.246860000
O	-5.937937000	4.209724000	0.248508000
O	-7.385928000	2.519785000	0.430427000
H	-7.936227000	3.314435000	0.525577000
C	2.631234000	4.185446000	-0.503225000
O	3.595122000	3.740297000	-1.088191000
O	2.610736000	5.479719000	-0.063340000
H	3.461241000	5.853740000	-0.348010000
C	-5.431528000	-2.290661000	-0.272560000
N	4.242132000	0.313682000	1.045186000
H	5.282224000	0.227877000	1.329641000
H	3.590222000	-1.714088000	1.235605000
H	4.266599000	2.390888000	0.671064000
C	-0.836820000	-4.102166000	0.170592000

C	-3.078564000	-3.845095000	-0.140563000
C	-6.603049000	-1.459204000	-0.266769000
N	-2.003550000	-4.677098000	-0.033577000
H	-7.373871000	0.508823000	-0.133383000
C	-5.494048000	-3.707363000	-0.393149000
C	-4.352032000	-4.470019000	-0.320682000
H	0.038652000	-4.734392000	0.291065000
H	0.322432000	5.315951000	-0.712406000
O	-4.384457000	-5.817761000	-0.411397000
H	-3.448807000	-6.093013000	-0.318437000
H	-6.436189000	-4.215672000	-0.562059000
O	1.644452000	-2.945533000	0.781725000
N	-7.860397000	-2.046493000	-0.414817000
H	-8.629540000	-1.426745000	-0.198071000
H	-7.971905000	-2.941917000	0.041591000
C	7.759821000	-0.903020000	0.855911000
C	7.587951000	0.513499000	0.603656000
O	6.753460000	0.274895000	1.727172000
H	7.071044000	-1.612848000	0.425767000
H	8.462501000	-1.237467000	1.600427000
H	7.076478000	0.789501000	-0.326803000
H	8.448704000	1.164350000	0.792006000
Br	9.547279000	-1.802888000	-0.921488000

### Int2a-pyrollic-H

SCF Energy (B3LYP-D3/B2) = -4702.27135759

Enthalpy 0K = 0.464268

Enthalpy 298 K = 0.501315

Free Energy 298 K = 0.390009

C	-0.858418000	3.786174000	-0.423760000
C	-1.047523000	2.429516000	-0.096982000
C	0.416207000	4.336337000	-0.433971000
C	0.102475000	1.629480000	0.185878000
C	1.546842000	3.589061000	-0.130236000
C	1.428428000	2.218144000	0.247082000
C	2.511102000	1.422212000	0.721482000
C	2.310354000	0.012069000	0.969048000
C	1.053027000	-0.600794000	0.738303000
C	-0.049871000	0.202994000	0.394789000
C	0.948377000	-2.060331000	0.836337000
N	-1.340411000	-0.390397000	0.202612000
C	-0.362081000	-2.603839000	0.499612000
C	-1.460377000	-1.771051000	0.241573000
C	-2.371056000	1.803925000	-0.047075000
C	-3.564626000	2.550040000	-0.042134000
C	-2.492331000	0.402279000	0.025996000
C	-4.837535000	1.996634000	-0.078707000
C	-3.781284000	-0.206902000	-0.078942000
C	-4.977549000	0.575677000	-0.163883000
H	-3.506697000	3.624219000	-0.007113000
C	-6.214766000	-0.111028000	-0.313392000
C	-3.899162000	-1.627847000	-0.120559000
C	-2.717557000	-2.393742000	0.036183000
C	3.848056000	1.667758000	1.084321000
C	3.536812000	-0.477786000	1.443139000
O	-1.925431000	4.584249000	-0.780112000
H	-1.585576000	5.464359000	-0.981559000
C	-5.926873000	3.002416000	-0.020775000
O	-5.763409000	4.211745000	-0.045577000

O	-7.195922000	2.506146000	0.095012000
H	-7.756383000	3.298500000	0.127699000
C	2.842644000	4.275874000	-0.374881000
O	3.831620000	3.815605000	-0.904967000
O	2.801761000	5.597316000	-0.006793000
H	3.660120000	5.953172000	-0.289864000
C	-5.133798000	-2.295581000	-0.292619000
N	4.442288000	0.532468000	1.522087000
H	6.068296000	0.288696000	1.939696000
H	3.777466000	-1.485167000	1.742278000
H	4.405625000	2.590186000	1.048194000
C	-0.542378000	-4.007995000	0.464322000
C	-2.768182000	-3.803111000	0.025505000
C	-6.314539000	-1.483876000	-0.381541000
N	-1.687411000	-4.613084000	0.219835000
H	-7.121727000	0.473195000	-0.365879000
C	-5.168778000	-3.716879000	-0.362129000
C	-4.019825000	-4.455029000	-0.199140000
H	0.335556000	-4.619609000	0.654499000
H	0.535057000	5.378963000	-0.716268000
O	-4.022489000	-5.807735000	-0.240164000
H	-3.086104000	-6.053341000	-0.085484000
H	-6.092884000	-4.246347000	-0.563295000
O	1.886456000	-2.801050000	1.158507000
N	-7.556195000	-2.099929000	-0.573803000
H	-8.340346000	-1.480876000	-0.414548000
H	-7.675892000	-2.968952000	-0.069597000
C	6.957233000	-1.515761000	0.232215000
C	7.478848000	-0.154608000	0.690990000
O	7.050324000	0.072485000	2.005608000
H	5.871684000	-1.518663000	0.136186000
H	7.283093000	-2.310849000	0.902495000
H	7.131961000	0.615651000	-0.016464000
H	8.576456000	-0.156915000	0.666793000
Br	7.667935000	-1.999037000	-1.577465000

## BGO

SCF Energy (B3LYP-D3/B2) = -1599.43715355

Enthalpy 0K = 0.336871

Enthalpy 298 K = 0.364223

Free Energy 298 K = 0.276871

C	2.839507000	1.579825000	0.015485000
C	1.589773000	0.938126000	0.005647000
C	4.049451000	0.860674000	0.012671000
C	1.644313000	-0.519137000	0.000430000
C	4.137557000	-0.520675000	0.002428000
C	2.899578000	-1.235105000	-0.001986000
H	4.971145000	1.439291000	0.018618000
C	2.875856000	-2.664976000	-0.006795000
C	1.707627000	-3.375079000	-0.007971000
C	0.458269000	-2.692757000	-0.004397000
C	0.437715000	-1.278628000	-0.000664000
C	-0.797395000	-3.399878000	-0.003812000
B	-0.920473000	-0.562809000	0.003584000
C	-2.112183000	-2.770847000	0.000004000
C	-2.174946000	-1.341564000	0.003190000
C	0.296459000	1.686826000	0.002504000
C	0.202970000	3.093550000	-0.004754000
C	-0.923741000	0.962497000	0.004448000

C	-1.039940000	3.739368000	-0.006542000
C	-2.170079000	1.620364000	0.003429000
C	-2.234852000	3.011638000	-0.001285000
H	1.074967000	3.724831000	-0.009627000
H	-3.198740000	3.505888000	-0.001841000
C	-3.463900000	0.841391000	0.006533000
C	-3.446159000	-0.676817000	0.005484000
C	-4.651247000	-1.350510000	0.005882000
B	-4.653337000	-2.877087000	0.003495000
C	-3.261294000	-3.563108000	0.000026000
H	3.819010000	-3.192268000	-0.009371000
H	1.782881000	-4.462340000	-0.011289000
H	-3.152593000	-4.645319000	-0.002506000
H	-5.547790000	-0.730741000	0.007511000
O	-0.799829000	-4.728645000	-0.007067000
H	0.103112000	-5.077098000	-0.009585000
O	2.924421000	2.941128000	0.028307000
H	3.853647000	3.203279000	0.034724000
C	-1.026507000	5.226856000	-0.014505000
O	-0.025377000	5.919008000	-0.020494000
O	-2.271332000	5.767972000	-0.014656000
H	-2.141291000	6.729946000	-0.020129000
B	5.591673000	-1.120686000	-0.003007000
O	5.808414000	-2.477014000	-0.032928000
O	6.620901000	-0.209514000	0.021703000
H	7.508104000	-0.583684000	0.015082000
O	-4.528757000	1.450335000	0.009341000
O	-5.770221000	-3.691437000	0.003784000
H	-6.583282000	-3.172787000	0.005993000
H	6.734744000	-2.742978000	-0.034561000

## Int1b

SCF Energy (B3LYP-D3/B2) = -4327.54352943

Enthalpy 0K = 0.395682

Enthalpy 298 K = 0.430270

Free Energy 298 K = 0.320297

C	-5.172284000	0.640172000	0.609541000
C	-3.822818000	0.432418000	0.251977000
C	-6.076493000	-0.417889000	0.747598000
C	-3.435513000	-0.962436000	0.083466000
C	-5.746263000	-1.756683000	0.562668000
C	-4.389916000	-2.036307000	0.231505000
H	-7.101297000	-0.167672000	1.015706000
C	-3.939907000	-3.389221000	0.047875000
C	-2.646646000	-3.692373000	-0.248887000
C	-1.673341000	-2.654122000	-0.389929000
C	-2.077096000	-1.295522000	-0.226714000
C	-0.312525000	-2.929372000	-0.684971000
B	-1.040763000	-0.188254000	-0.378778000
C	0.725031000	-1.902804000	-0.843670000
C	0.360157000	-0.518394000	-0.692125000
C	-2.859248000	1.553748000	0.069889000
C	-3.213905000	2.916529000	0.153514000
C	-1.499420000	1.256855000	-0.219831000
C	-2.261893000	3.927925000	-0.021349000
C	-0.546034000	2.284101000	-0.388976000
C	-0.921019000	3.619857000	-0.286335000
H	-4.223838000	3.232425000	0.350981000
H	-0.176602000	4.395894000	-0.417819000

C	0.899497000	1.969186000	-0.691366000
C	1.351953000	0.529057000	-0.842296000
C	2.671637000	0.281853000	-1.117863000
B	3.143171000	-1.180928000	-1.293618000
C	2.023586000	-2.280323000	-1.131261000
H	-4.662714000	-4.185423000	0.152893000
H	-2.392083000	-4.745091000	-0.372576000
H	2.257689000	-3.337939000	-1.234773000
H	3.332124000	1.141513000	-1.210475000
O	0.109965000	-4.191432000	-0.839797000
H	-0.619935000	-4.810077000	-0.703315000
O	-5.645420000	1.904337000	0.837943000
H	-6.577121000	1.846592000	1.083299000
C	-2.737625000	5.329007000	0.084900000
O	-3.886418000	5.673356000	0.303564000
O	-1.746722000	6.243987000	-0.089763000
H	-2.175177000	7.109628000	0.003331000
B	-6.916306000	-2.782847000	0.748906000
O	-8.124893000	-2.265799000	1.167255000
O	-6.754681000	-4.127243000	0.499055000
H	-7.540713000	-4.663082000	0.652149000
O	1.697865000	2.892549000	-0.818196000
O	4.392799000	-1.606557000	-1.570201000
H	5.063566000	-0.863730000	-1.620448000
H	-8.833921000	-2.910734000	1.257996000
C	6.204142000	0.753323000	-0.081700000
C	7.274921000	-0.069140000	-0.622567000
O	6.130864000	0.351053000	-1.477001000
H	5.453601000	0.300790000	0.565219000
H	6.361139000	1.819440000	0.070210000
H	7.312186000	-1.124437000	-0.377291000
H	8.227153000	0.380637000	-0.875651000
Br	9.482992000	-0.605408000	1.601616000

## TS1b

SCF Energy (B3LYP-D3/B2) = -4327.53011464

Enthalpy 0K = 0.393272

Enthalpy 298 K = 0.427224

Free Energy 298 K = 0.319496

C	-5.276859000	0.578549000	0.316929000
C	-3.886790000	0.397299000	0.138083000
C	-6.157464000	-0.498249000	0.439696000
C	-3.449075000	-0.989920000	0.053765000
C	-5.766677000	-1.834495000	0.389737000
C	-4.381842000	-2.084670000	0.182903000
H	-7.211663000	-0.269258000	0.584591000
C	-3.881592000	-3.431248000	0.087667000
C	-2.566981000	-3.706544000	-0.123217000
C	-1.613445000	-2.647116000	-0.260240000
C	-2.064454000	-1.292563000	-0.168372000
C	-0.239732000	-2.894237000	-0.486369000
B	-1.058360000	-0.163836000	-0.312967000
C	0.775759000	-1.843805000	-0.633165000
C	0.368097000	-0.461760000	-0.541969000
C	-2.936047000	1.537808000	0.035489000
C	-3.313703000	2.890960000	0.166323000
C	-1.557573000	1.270760000	-0.196216000
C	-2.374297000	3.923043000	0.057664000
C	-0.618645000	2.320537000	-0.309001000
C	-1.022064000	3.645523000	-0.185940000
H	-4.332175000	3.182758000	0.356414000

H	-0.288055000	4.437355000	-0.275181000
C	0.843596000	2.041155000	-0.561880000
C	1.338462000	0.612752000	-0.671600000
C	2.672673000	0.394661000	-0.885897000
B	3.198005000	-1.064552000	-1.003625000
C	2.093971000	-2.189871000	-0.854494000
H	-4.585994000	-4.244384000	0.188368000
H	-2.276024000	-4.755542000	-0.183610000
H	2.359531000	-3.243552000	-0.917355000
H	3.323104000	1.262661000	-0.971580000
O	0.227645000	-4.152361000	-0.583260000
H	-0.494563000	-4.783942000	-0.471482000
O	-5.813456000	1.838312000	0.375018000
H	-6.767883000	1.759684000	0.494799000
C	-2.873275000	5.310000000	0.212316000
O	-4.029851000	5.630704000	0.428948000
O	-1.894811000	6.248240000	0.088478000
H	-2.341619000	7.100899000	0.209908000
B	-6.911521000	-2.887752000	0.569796000
O	-8.197399000	-2.391677000	0.654244000
O	-6.658342000	-4.239574000	0.652930000
H	-7.442507000	-4.788785000	0.761585000
O	1.620304000	2.985397000	-0.675332000
O	4.462676000	-1.448659000	-1.212529000
H	5.135912000	-0.645165000	-1.266927000
H	-8.879767000	-3.057380000	0.788706000
C	6.543866000	0.601606000	0.102357000
C	7.596263000	-0.143956000	-0.563566000
O	6.049663000	0.477546000	-1.223081000
H	5.976524000	0.068566000	0.873880000
H	6.775850000	1.625011000	0.413121000
H	7.513422000	-1.215429000	-0.653139000
H	8.341072000	0.377039000	-1.141835000
Br	9.525993000	-0.595731000	1.212982000

## Int2b

SCF Energy (B3LYP-D3/B2) = -4516.22035360

Enthalpy 0K = 0.408631

Enthalpy 298 K = 0.446702

Free Energy 298 K = 0.328715

C	-5.501561000	0.680662000	0.256546000
C	-4.113790000	0.470940000	0.065995000
C	-6.407738000	-0.373507000	0.341233000
C	-3.709848000	-0.919991000	-0.078893000
C	-6.045671000	-1.718384000	0.237965000
C	-4.670575000	-1.993251000	0.012314000
H	-7.455856000	-0.125235000	0.498749000
C	-4.203135000	-3.348866000	-0.145997000
C	-2.899150000	-3.648785000	-0.377381000
C	-1.911376000	-2.612989000	-0.475552000
C	-2.330760000	-1.246816000	-0.323994000
C	-0.553878000	-2.889687000	-0.718418000
B	-1.307451000	-0.144389000	-0.429931000
C	0.485938000	-1.864212000	-0.831683000
C	0.117218000	-0.468048000	-0.684594000
C	-3.135657000	1.587343000	0.007737000
C	-3.475241000	2.942473000	0.206846000
C	-1.764112000	1.294116000	-0.249016000
C	-2.510933000	3.954893000	0.136973000
C	-0.799202000	2.327409000	-0.323511000

C	-1.167782000	3.653522000	-0.135226000
H	-4.484064000	3.249795000	0.422691000
H	-0.413949000	4.429310000	-0.195963000
C	0.652173000	2.025171000	-0.603294000
C	1.108604000	0.593325000	-0.778920000
C	2.433351000	0.347799000	-1.016028000
B	2.958112000	-1.131945000	-1.194710000
C	1.795656000	-2.226300000	-1.072633000
H	-4.927865000	-4.147625000	-0.077218000
H	-2.638068000	-4.701790000	-0.489136000
H	2.030549000	-3.285234000	-1.175955000
H	3.099383000	1.207935000	-1.072082000
O	-0.114650000	-4.164816000	-0.867438000
H	-0.855499000	-4.774218000	-0.763888000
O	-6.005056000	1.953893000	0.363074000
H	-6.960977000	1.890480000	0.479130000
C	-2.969990000	5.342973000	0.363032000
O	-4.114224000	5.688918000	0.610020000
O	-1.968188000	6.263828000	0.271472000
H	-2.397228000	7.117579000	0.439283000
B	-7.210906000	-2.749264000	0.387042000
O	-8.493013000	-2.233670000	0.451870000
O	-6.989775000	-4.108784000	0.469340000
H	-7.790946000	-4.637460000	0.552569000
O	1.452072000	2.956223000	-0.683350000
O	4.197291000	-1.499943000	-1.404005000
H	5.188300000	-0.295176000	-1.339411000
H	-9.182909000	-2.892798000	0.580216000
C	5.839509000	0.460135000	0.335564000
C	6.393900000	-0.875450000	0.825302000
O	5.822811000	0.456396000	-1.071140000
H	4.836101000	0.616902000	0.759717000
H	6.483124000	1.278086000	0.677835000
H	5.752384000	-1.698389000	0.512165000
H	7.418169000	-1.027305000	0.488235000
Br	6.464735000	-0.945425000	2.822534000
C	8.110717000	0.434345000	-2.152542000
O	7.695619000	0.265884000	-3.233313000
O	8.671467000	0.602080000	-1.135104000

## TS2b

SCF Energy (B3LYP-D3/B2) = -4516.21049558

Enthalpy 0K = 0.405558

Enthalpy 298 K = 0.442396

Free Energy 298 K = 0.328622

C	-5.503957000	0.710672000	0.251508000
C	-4.118026000	0.481312000	0.082937000
C	-6.421875000	-0.333463000	0.360825000
C	-3.728985000	-0.918499000	-0.016805000
C	-6.075516000	-1.683395000	0.303952000
C	-4.700754000	-1.979785000	0.099307000
H	-7.468595000	-0.069358000	0.500341000
C	-4.247624000	-3.343680000	-0.009855000
C	-2.944857000	-3.663720000	-0.223848000
C	-1.950755000	-2.638921000	-0.351417000
C	-2.353921000	-1.267008000	-0.243249000
C	-0.592129000	-2.933961000	-0.583293000
B	-1.313545000	-0.174746000	-0.376322000
C	0.460227000	-1.918753000	-0.718784000
C	0.104070000	-0.519463000	-0.611735000

C	-3.127383000	1.587105000	0.002656000
C	-3.454571000	2.949887000	0.166787000
C	-1.759068000	1.274176000	-0.237734000
C	-2.478924000	3.949425000	0.076706000
C	-0.783193000	2.292831000	-0.333219000
C	-1.138433000	3.627986000	-0.180988000
H	-4.460854000	3.273485000	0.370177000
H	-0.376314000	4.394227000	-0.257381000
C	0.667307000	1.967311000	-0.595938000
C	1.110513000	0.525134000	-0.730621000
C	2.433825000	0.262354000	-0.954457000
B	2.919497000	-1.219903000	-1.082988000
C	1.764488000	-2.305997000	-0.941100000
H	-4.980786000	-4.132085000	0.082741000
H	-2.691690000	-4.721975000	-0.294288000
H	1.991987000	-3.368222000	-1.015002000
H	3.115804000	1.106171000	-1.036127000
O	-0.167138000	-4.210156000	-0.697845000
H	-0.913760000	-4.814189000	-0.598504000
O	-5.995420000	1.989723000	0.311049000
H	-6.953453000	1.942925000	0.417760000
C	-2.925340000	5.348883000	0.266515000
O	-4.067593000	5.708542000	0.499653000
O	-1.914009000	6.254539000	0.156529000
H	-2.330615000	7.118855000	0.300334000
B	-7.255248000	-2.697271000	0.473769000
O	-8.527932000	-2.161756000	0.527343000
O	-7.048179000	-4.056012000	0.581406000
H	-7.853155000	-4.576625000	0.677880000
O	1.476877000	2.885856000	-0.694240000
O	4.164796000	-1.632440000	-1.275823000
H	4.928526000	-0.769989000	-1.300978000
H	-9.230496000	-2.805894000	0.662855000
C	5.981792000	0.429223000	0.186990000
C	6.588910000	-0.833266000	0.795721000
O	5.734704000	0.197832000	-1.171318000
H	5.049922000	0.685796000	0.714987000
H	6.684228000	1.262683000	0.310735000
H	5.919872000	-1.687006000	0.692446000
H	7.562791000	-1.044007000	0.357619000
Br	6.909224000	-0.626247000	2.762589000
C	7.300988000	0.199329000	-2.303445000
O	6.870372000	-0.159304000	-3.354730000
O	8.197194000	0.556823000	-1.593650000

## Int3b

SCF Energy (B3LYP-D3/B2) = -4516.21301617

Enthalpy 0K = 0.410286

Enthalpy 298 K = 0.447056

Free Energy 298 K = 0.333957

C	5.850892000	0.240748000	-0.203179000
C	4.441283000	0.189885000	-0.103285000
C	6.641341000	-0.907377000	-0.140242000
C	3.875304000	-1.148040000	0.000617000
C	6.132149000	-2.197085000	0.007046000
C	4.717051000	-2.319651000	0.064007000
H	7.719975000	-0.778353000	-0.209027000
C	4.091596000	-3.613134000	0.170299000
C	2.741912000	-3.768488000	0.202289000

C	1.874504000	-2.630549000	0.129997000
C	2.451106000	-1.323224000	0.030281000
C	0.468881000	-2.752145000	0.148103000
B	1.540126000	-0.111445000	-0.055716000
C	-0.460402000	-1.614341000	0.078707000
C	0.073636000	-0.276167000	-0.027733000
C	3.593758000	1.411451000	-0.116415000
C	4.108112000	2.725062000	-0.103283000
C	2.177643000	1.269987000	-0.119117000
C	3.259404000	3.837847000	-0.122817000
C	1.330490000	2.399825000	-0.149667000
C	1.866121000	3.682827000	-0.158403000
H	5.165878000	2.923112000	-0.072646000
H	1.200613000	4.537426000	-0.183807000
C	-0.174080000	2.254133000	-0.175647000
C	-0.807437000	0.881978000	-0.072392000
C	-2.172371000	0.791147000	-0.015819000
B	-2.826136000	-0.616210000	0.046200000
C	-1.819637000	-1.837848000	0.127005000
H	4.729269000	-4.483805000	0.224473000
H	2.353682000	-4.784230000	0.282753000
H	-2.185475000	-2.859518000	0.212526000
H	-2.762880000	1.703528000	0.001530000
O	-0.120312000	-3.959950000	0.231429000
H	0.551604000	-4.652129000	0.280100000
O	6.492312000	1.440378000	-0.371799000
H	7.441326000	1.274307000	-0.429069000
C	3.898036000	5.174895000	-0.102917000
O	5.098020000	5.390926000	-0.063192000
O	3.000744000	6.197879000	-0.133535000
H	3.535349000	7.007267000	-0.113552000
B	7.193267000	-3.344825000	0.087859000
O	8.508657000	-2.986170000	-0.133237000
O	6.845949000	-4.646212000	0.380123000
H	7.585497000	-5.263527000	0.398675000
O	-0.865334000	3.261201000	-0.288274000
O	-4.132787000	-0.916913000	-0.011117000
H	-4.753607000	-0.115755000	-0.071848000
H	9.143272000	-3.704892000	-0.046064000
C	-7.109032000	0.503750000	-0.679921000
C	-7.538319000	-0.691636000	0.163123000
O	-5.863914000	0.967219000	-0.202618000
H	-6.987867000	0.208167000	-1.729500000
H	-7.864987000	1.291677000	-0.607098000
H	-6.794658000	-1.488028000	0.144931000
H	-7.755190000	-0.372741000	1.180466000
Br	-9.226206000	-1.503446000	-0.541138000
C	-5.899436000	1.787964000	1.139859000
O	-4.748519000	1.988401000	1.502241000
O	-7.041801000	2.026945000	1.522764000

### TS3b

SCF Energy (B3LYP-D3/B2) = -4516.19572003

Enthalpy 0K = 0.410323

Enthalpy 298 K = 0.446761

Free Energy 298 K = 0.332909

C	5.838823000	0.789639000	-0.382337000
C	4.468356000	0.504619000	-0.190115000
C	6.811476000	-0.212597000	-0.391558000

C	4.140887000	-0.909883000	-0.071202000
C	6.535548000	-1.568994000	-0.232823000
C	5.166908000	-1.926073000	-0.083215000
H	7.846430000	0.094909000	-0.529733000
C	4.773482000	-3.304969000	0.044381000
C	3.472550000	-3.682543000	0.162312000
C	2.428080000	-2.703327000	0.163651000
C	2.772013000	-1.320076000	0.048853000
C	1.062771000	-3.056213000	0.269733000
B	1.666469000	-0.275101000	0.043509000
C	-0.044012000	-2.088589000	0.280532000
C	0.254739000	-0.682723000	0.164141000
C	3.430556000	1.568797000	-0.126854000
C	3.719803000	2.949462000	-0.125899000
C	2.061205000	1.194024000	-0.038888000
C	2.698744000	3.905367000	-0.071494000
C	1.038385000	2.166293000	0.005256000
C	1.351618000	3.521108000	-0.017812000
H	4.729612000	3.321057000	-0.161660000
H	0.553746000	4.253354000	0.014700000
C	-0.418799000	1.770891000	0.077549000
C	-0.806720000	0.310652000	0.195597000
C	-2.131661000	-0.006681000	0.335217000
B	-2.535326000	-1.498942000	-0.421666000
C	-1.342743000	-2.536643000	0.411081000
H	5.548671000	-4.057719000	0.043839000
H	3.264015000	-4.748786000	0.254060000
H	-1.528303000	-3.605342000	0.500625000
H	-2.855595000	0.800769000	0.399598000
O	0.690892000	-4.343530000	0.368719000
H	1.468983000	-4.916176000	0.356404000
O	6.260004000	2.079313000	-0.572273000
H	7.217146000	2.075143000	-0.696426000
C	3.107124000	5.330640000	-0.072111000
O	4.254929000	5.741387000	-0.107451000
O	2.052743000	6.189159000	-0.027707000
H	2.443953000	7.077052000	-0.030485000
B	7.775892000	-2.525016000	-0.243925000
O	8.995119000	-1.948510000	-0.538460000
O	7.666779000	-3.868887000	0.039414000
H	8.496954000	-4.356320000	-0.000603000
O	-1.274872000	2.648136000	0.033275000
O	-3.778877000	-2.018952000	0.462952000
H	-4.495137000	-1.336270000	0.456655000
H	9.745539000	-2.551002000	-0.510580000
C	-6.921091000	-0.153258000	-0.467833000
C	-8.146902000	0.216717000	0.348549000
O	-5.736801000	-0.186908000	0.335180000
H	-7.037788000	-1.148154000	-0.896194000
H	-6.798360000	0.566984000	-1.284877000
H	-8.479652000	-0.433827000	1.141309000
H	-8.627550000	1.171976000	0.245917000
Br	-9.796767000	-0.693135000	-1.180959000
C	-5.785351000	0.640695000	1.501857000
O	-4.744823000	0.703320000	2.139540000
O	-6.929562000	1.161644000	1.679981000

### Pdt1b

SCF Energy (B3LYP-D3/B2) = -4516.27344737

Enthalpy 0K = 0.412877

Enthalpy 298 K = 0.448761

Free Energy 298 K = 0.340054

C	4.195943000	2.072246000	0.061493000
C	3.209879000	1.075157000	0.029416000
C	3.876034000	3.442419000	0.054388000
C	1.832271000	1.557557000	0.052162000
C	2.584582000	3.935631000	0.028857000
C	1.526122000	2.968485000	0.047028000
H	4.705282000	4.148618000	0.063958000
C	0.160142000	3.372037000	0.086440000
C	-0.874865000	2.473234000	0.129763000
C	-0.593608000	1.082154000	0.133743000
C	0.744604000	0.632201000	0.094594000
C	-1.662984000	0.091804000	0.186680000
B	1.028175000	-0.874957000	0.111148000
C	-1.424816000	-1.368085000	0.214884000
C	-0.077212000	-1.849140000	0.163071000
C	3.539376000	-0.382007000	-0.009310000
C	4.849973000	-0.886551000	-0.123828000
C	2.485110000	-1.332051000	0.053941000
C	5.099551000	-2.265839000	-0.147595000
C	2.745793000	-2.718800000	0.037914000
C	4.050969000	-3.190795000	-0.057688000
H	5.705425000	-0.236970000	-0.200210000
H	4.233745000	-4.258505000	-0.067941000
C	1.621676000	-3.729371000	0.119431000
C	0.183580000	-3.265098000	0.178327000
C	-0.815857000	-4.213217000	0.235439000
B	-2.284453000	-3.769077000	0.271232000
C	-2.512193000	-2.230784000	0.286267000
H	-0.067441000	4.428661000	0.081944000
H	-1.892620000	2.849302000	0.159664000
H	-3.496642000	-1.783186000	0.376023000
H	-0.504173000	-5.256109000	0.238411000
O	-2.911916000	0.440105000	0.205534000
H	-3.241649000	1.425556000	0.133347000
O	5.528964000	1.747009000	0.100267000
H	6.040796000	2.564359000	0.133308000
C	6.511576000	-2.695515000	-0.272311000
O	7.477853000	-1.956648000	-0.363099000
O	6.663408000	-4.049969000	-0.279606000
H	7.618769000	-4.195572000	-0.365674000
B	2.439241000	5.494001000	-0.025230000
O	3.571223000	6.231648000	0.265395000
O	1.254513000	6.093918000	-0.377648000
H	1.261944000	7.057195000	-0.363830000
O	1.905255000	-4.925372000	0.134473000
O	-3.307929000	-4.688048000	0.284582000
H	-4.190321000	-4.287137000	0.228989000
H	3.461788000	7.183009000	0.163444000
C	-6.102553000	-0.135167000	0.608220000
C	-5.993168000	-0.047714000	-0.915966000
O	-5.870649000	-1.541143000	0.865495000
H	-5.347336000	0.458728000	1.116717000
H	-7.099291000	0.121834000	0.981127000
H	-5.000931000	0.267433000	-1.238910000
H	-6.746792000	0.588599000	-1.378007000
Br	-4.512104000	2.966369000	-0.026798000
C	-5.991324000	-2.237883000	-0.284998000
O	-5.900824000	-3.439979000	-0.359512000
O	-6.215317000	-1.421275000	-1.332428000

## Int4b

SCF Energy (B3LYP-D3/B2) = -4670.09556981

Enthalpy 0K = 0.471602

Enthalpy 298 K = 0.512080

Free Energy 298 K = 0.391801

C	5.536477000	-0.796850000	0.512080000
C	4.245918000	-0.344032000	0.191576000
C	5.815753000	-2.154480000	0.742238000
C	3.229530000	-1.385671000	0.097897000
C	4.872818000	-3.167161000	0.673769000
C	3.538161000	-2.777081000	0.330847000
H	6.842988000	-2.415328000	0.992219000
C	2.494772000	-3.746248000	0.195608000
C	1.214064000	-3.400506000	-0.144101000
C	0.889332000	-2.034241000	-0.349303000
C	1.882759000	-1.041764000	-0.232842000
C	-0.447571000	-1.641522000	-0.745710000
B	1.502452000	0.418587000	-0.495412000
C	-0.885410000	-0.243297000	-0.857782000
C	0.110480000	0.788193000	-0.807547000
C	3.927365000	1.099436000	-0.034858000
C	4.877482000	2.136005000	0.058154000
C	2.594727000	1.475148000	-0.357373000
C	4.519384000	3.474017000	-0.158275000
C	2.241287000	2.824979000	-0.567393000
C	3.200742000	3.828093000	-0.472126000
H	5.909256000	1.943639000	0.298134000
H	2.914395000	4.859697000	-0.637711000
C	0.816407000	3.221501000	-0.890403000
C	-0.273921000	2.171863000	-0.935193000
C	-1.581791000	2.578650000	-1.071406000
B	-2.711933000	1.534606000	-1.054395000
C	-2.241879000	0.047730000	-0.917948000
H	2.735969000	-4.785718000	0.367037000
H	0.446818000	-4.159177000	-0.250243000
H	-2.968889000	-0.757130000	-0.839854000
H	-1.759278000	3.649036000	-1.155910000
O	-1.254167000	-2.630519000	-1.019244000
H	-2.083476000	-2.401440000	-1.556768000
O	6.585559000	0.080195000	0.616927000
H	7.380594000	-0.418184000	0.842237000
C	5.592977000	4.488419000	-0.036783000
O	6.760625000	4.261662000	0.232386000
O	5.158220000	5.759709000	-0.259911000
H	5.943467000	6.319153000	-0.151210000
B	5.390904000	-4.610826000	0.990658000
O	6.756487000	-4.758469000	1.137999000
O	4.532667000	-5.676959000	1.134856000
H	4.962012000	-6.518276000	1.325039000
O	0.565130000	4.405754000	-1.098694000
O	-4.029758000	1.874493000	-1.151431000
H	-4.624445000	1.090288000	-1.065013000
H	7.041669000	-5.648268000	1.370216000
C	-5.388432000	-0.403880000	0.916477000
C	-5.950393000	0.902035000	1.462810000
O	-5.403205000	-0.357905000	-0.500118000
H	-4.347037000	-0.531527000	1.236760000
H	-5.989261000	-1.242495000	1.281952000
H	-5.379828000	1.762753000	1.115439000

H	-7.004747000	0.992278000	1.210413000
Br	-5.844591000	0.930994000	3.454508000
C	-6.796505000	-0.567899000	-1.176363000
O	-6.678544000	-0.398840000	-2.386084000
O	-7.683712000	-0.858310000	-0.378886000
C	-4.602882000	-2.818982000	-2.344822000
C	-4.225341000	-1.699848000	-3.197676000
O	-3.197595000	-2.588437000	-2.657925000
H	-4.888657000	-2.595170000	-1.321154000
H	-5.003368000	-3.732761000	-2.779127000
H	-4.267216000	-0.702158000	-2.778832000
H	-4.338923000	-1.780470000	-4.275982000

### TS4b

SCF Energy (B3LYP-D3/B2) = -4670.08823894

Enthalpy 0K = 0.469046

Enthalpy 298 K = 0.508529

Free Energy 298 K = 0.391615

C	5.751669000	-0.614022000	0.502595000
C	4.432296000	-0.224852000	0.228660000
C	6.099022000	-1.953519000	0.761409000
C	3.457247000	-1.308369000	0.205296000
C	5.197685000	-3.002226000	0.766634000
C	3.831489000	-2.677544000	0.467344000
H	7.146456000	-2.163385000	0.973328000
C	2.826246000	-3.686997000	0.402411000
C	1.517679000	-3.397889000	0.097331000
C	1.136596000	-2.058730000	-0.136775000
C	2.086103000	-1.030857000	-0.084883000
C	-0.257642000	-1.740857000	-0.516125000
B	1.627977000	0.405471000	-0.369006000
C	-0.753148000	-0.347782000	-0.602667000
C	0.205275000	0.715491000	-0.628372000
C	4.039981000	1.198823000	-0.018610000
C	4.946577000	2.276775000	0.015663000
C	2.680592000	1.510622000	-0.295461000
C	4.522159000	3.593449000	-0.213161000
C	2.260284000	2.839104000	-0.516774000
C	3.178059000	3.884256000	-0.480326000
H	5.994217000	2.133469000	0.218844000
H	2.840230000	4.898795000	-0.653942000
C	0.805332000	3.169722000	-0.786434000
C	-0.237351000	2.075931000	-0.772715000
C	-1.568911000	2.420773000	-0.884848000
B	-2.649365000	1.329623000	-0.831144000
C	-2.120238000	-0.111088000	-0.617426000
H	3.112657000	-4.711213000	0.596848000
H	0.772493000	-4.183757000	0.036626000
H	-2.784889000	-0.955422000	-0.442984000
H	-1.793676000	3.480522000	-0.993096000
O	-1.006327000	-2.725576000	-0.799330000
H	-1.990522000	-2.674374000	-1.633132000
O	6.769150000	0.306278000	0.534139000
H	7.592066000	-0.155374000	0.736128000
C	5.554020000	4.655389000	-0.154849000
O	6.740277000	4.486143000	0.072746000
O	5.056137000	5.902214000	-0.386662000
H	5.820702000	6.495865000	-0.320534000
B	5.784932000	-4.412018000	1.109664000
O	7.162174000	-4.514528000	1.163111000

O	4.974362000	-5.494211000	1.369232000
H	5.445163000	-6.312573000	1.561609000
O	0.499134000	4.340832000	-0.998459000
O	-3.986111000	1.621364000	-0.992959000
H	-4.546415000	0.819967000	-0.958057000
H	7.489116000	-5.381949000	1.423432000
C	-5.902175000	-0.477467000	0.836562000
C	-6.523113000	0.900419000	1.026174000
O	-5.518885000	-0.649080000	-0.525062000
H	-4.990371000	-0.569220000	1.436000000
H	-6.619174000	-1.248622000	1.131813000
H	-5.832261000	1.697088000	0.752874000
H	-7.458729000	0.971658000	0.476485000
Br	-6.972884000	1.184997000	2.945933000
C	-6.627854000	-0.964222000	-1.481512000
O	-6.174431000	-1.123960000	-2.630376000
O	-7.751968000	-1.017552000	-0.989251000
C	-4.110968000	-3.041897000	-1.853308000
C	-3.964863000	-1.931007000	-2.762870000
O	-2.760364000	-2.945650000	-2.423738000
H	-4.172150000	-2.817515000	-0.791905000
H	-4.636791000	-3.936929000	-2.174495000
H	-3.742257000	-0.945809000	-2.388376000
H	-4.210113000	-2.050279000	-3.807567000

### Pdt2b

SCF Energy (B3LYP-D3/B2) = -4670.16876228

Enthalpy 0K = 0.476547

Enthalpy 298 K = 0.516065

Free Energy 298 K = 0.399889

C	-4.144232000	1.528468000	-0.000186000
C	-2.935395000	0.888961000	-0.308197000
C	-4.233829000	2.925246000	0.158228000
C	-1.797659000	1.773226000	-0.517501000
C	-3.164686000	3.788868000	0.012545000
C	-1.906557000	3.202161000	-0.356846000
H	-5.208734000	3.336065000	0.417426000
C	-0.753759000	4.004441000	-0.593576000
C	0.450829000	3.459581000	-0.974947000
C	0.567589000	2.064292000	-1.135568000
C	-0.531547000	1.233962000	-0.906736000
C	1.892535000	1.492407000	-1.561960000
B	-0.351534000	-0.277565000	-1.088314000
C	2.085031000	0.007939000	-1.690419000
C	0.965976000	-0.856190000	-1.456306000
C	-2.809078000	-0.597696000	-0.424790000
C	-3.858133000	-1.491781000	-0.132767000
C	-1.568302000	-1.166770000	-0.819111000
C	-3.686351000	-2.878130000	-0.247204000
C	-1.404746000	-2.562180000	-0.929794000
C	-2.460968000	-3.422974000	-0.652385000
H	-4.824750000	-1.146873000	0.193436000
H	-2.315365000	-4.492789000	-0.738936000
C	-0.072331000	-3.166750000	-1.319513000
C	1.127395000	-2.280092000	-1.555674000
C	2.343743000	-2.875265000	-1.842587000
B	3.567744000	-1.996396000	-2.100030000
C	3.339811000	-0.480394000	-2.020253000
H	-0.837439000	5.075652000	-0.469535000
H	1.318282000	4.084438000	-1.159221000
H	4.124780000	0.255874000	-2.193711000
H	2.357912000	-3.963284000	-1.879507000

O	2.812009000	2.292295000	-1.792285000
H	4.621920000	2.305417000	-1.757177000
O	-5.304294000	0.811622000	0.162530000
H	-6.016444000	1.430069000	0.365984000
C	-4.849146000	-3.733492000	0.084793000
O	-5.944123000	-3.341253000	0.452841000
O	-4.596540000	-5.065523000	-0.057784000
H	-5.424634000	-5.505452000	0.191145000
B	-3.459689000	5.301439000	0.280314000
O	-4.789333000	5.673579000	0.358259000
O	-2.447603000	6.217536000	0.460983000
H	-2.745858000	7.121362000	0.611112000
O	0.006004000	-4.387988000	-1.435958000
O	4.811399000	-2.569845000	-2.378664000
H	5.469522000	-1.878894000	-2.515723000
H	-4.930448000	6.598442000	0.586277000
C	2.057644000	0.002467000	1.883198000
C	2.022603000	-1.514420000	1.819018000
O	3.367451000	0.445158000	1.465020000
H	1.364226000	0.438799000	1.165978000
H	1.849737000	0.363544000	2.892231000
H	2.226933000	-1.878526000	0.812834000
H	2.701860000	-1.954051000	2.548375000
Br	0.207964000	-2.135118000	2.284425000
C	4.346534000	0.391970000	2.395487000
O	5.551464000	0.666730000	1.879156000
O	4.188390000	0.132888000	3.567086000
C	5.368468000	2.269185000	0.011846000
C	5.701090000	0.840715000	0.444700000
O	5.523804000	2.386347000	-1.389129000
H	4.346169000	2.508797000	0.327157000
H	6.052189000	2.968094000	0.513324000
H	5.072177000	0.127969000	-0.090856000
H	6.752446000	0.618193000	0.247254000

### Int1b-COOH

SCF Energy (B3LYP-D3/B2) = -4327.54633235

Enthalpy 0K = 0.395724

Enthalpy 298 K = 0.429911

Free Energy 298 K = 0.322328

C	0.923395000	2.982399000	-0.072910000
C	1.428122000	1.669977000	-0.034764000
C	1.767111000	4.108592000	-0.054030000
C	2.882565000	1.572270000	-0.002253000
C	3.150687000	4.052709000	-0.006121000
C	3.729968000	2.743973000	0.014703000
H	1.288136000	5.085610000	-0.078115000
C	5.145580000	2.564802000	0.047940000
C	5.726061000	1.323570000	0.058264000
C	4.913098000	0.158058000	0.035783000
C	3.508399000	0.292532000	0.008129000
C	5.481441000	-1.174245000	0.038404000
B	2.651046000	-0.984858000	-0.014520000
C	4.724542000	-2.410549000	0.019062000
C	3.298453000	-2.317529000	-0.005503000
C	0.547852000	0.463455000	-0.033041000
C	-0.861611000	0.520193000	-0.023011000
C	1.137888000	-0.826521000	-0.033007000
C	-1.640241000	-0.642408000	-0.023890000
C	0.348969000	-1.994608000	-0.036430000
C	-1.043983000	-1.906858000	-0.034552000
H	-1.401432000	1.451440000	-0.012804000
H	-1.648754000	-2.805589000	-0.037702000
C	0.989190000	-3.361001000	-0.039213000

C	2.504001000	-3.504615000	-0.020357000
C	3.050231000	-4.777574000	-0.015448000
B	4.564083000	-4.947194000	0.007634000
C	5.391880000	-3.643360000	0.026180000
H	5.772982000	3.444614000	0.064239000
H	6.815391000	1.282224000	0.084078000
H	6.479626000	-3.645988000	0.045276000
H	2.335360000	-5.600845000	-0.027524000
O	6.805598000	-1.306721000	0.060225000
H	7.233622000	-0.438934000	0.069917000
O	-0.418887000	3.208764000	-0.130859000
H	-0.586046000	4.159362000	-0.149318000
C	-3.133844000	-0.465888000	-0.011770000
O	-3.654499000	0.643967000	0.003559000
O	-3.799141000	-1.609370000	-0.018947000
H	-4.807068000	-1.423970000	-0.010582000
B	3.898428000	5.429867000	0.017523000
O	3.107895000	6.556515000	-0.040481000
O	5.271469000	5.507574000	0.095556000
H	5.623355000	6.404559000	0.103778000
O	0.278671000	-4.361086000	-0.055037000
O	5.246830000	-6.157365000	0.014344000
H	4.627845000	-6.896434000	0.001754000
H	3.581265000	7.394424000	-0.017621000
C	-6.731451000	0.021303000	0.747012000
C	-6.740811000	0.036660000	-0.713734000
O	-6.333112000	-1.171188000	0.001387000
H	-5.906713000	0.502972000	1.268549000
H	-7.700557000	-0.069253000	1.235299000
H	-5.922879000	0.529525000	-1.235549000
H	-7.716257000	-0.043553000	-1.191227000
Br	-10.247406000	0.279429000	0.039535000

### TS1b-COOH

SCF Energy (B3LYP-D3/B2) = -4327.53580163

Enthalpy 0K = 0.392456

Enthalpy 298 K = 0.426091

Free Energy 298 K = 0.321469

C	0.112993000	2.743948000	-0.108802000
C	0.862712000	1.556207000	-0.040172000
C	0.722366000	4.013842000	-0.075587000
C	2.307532000	1.743298000	0.002512000
C	2.088575000	4.226583000	0.005319000
C	2.910907000	3.056330000	0.031663000
H	0.063218000	4.878848000	-0.114519000
C	4.334634000	3.153868000	0.074773000
C	5.143585000	2.048318000	0.076827000
C	4.571408000	0.747421000	0.035585000
C	3.168851000	0.609380000	0.003857000
C	5.388085000	-0.451581000	0.020579000
B	2.574243000	-0.810495000	-0.038439000
C	4.888134000	-1.808872000	-0.015800000
C	3.471016000	-1.992265000	-0.040716000
C	0.232956000	0.202273000	-0.025667000
C	-1.159883000	-0.012879000	0.028526000
C	1.061152000	-0.948477000	-0.047806000
C	-1.702000000	-1.302587000	0.032953000
C	0.511490000	-2.246723000	-0.047385000
C	-0.873624000	-2.426863000	-0.014518000
H	-1.871860000	0.793771000	0.071577000
H	-1.300900000	-3.422425000	-0.017118000
C	1.404964000	-3.461024000	-0.075662000

C	2.921023000	-3.307924000	-0.065978000
C	3.705904000	-4.450967000	-0.075360000
B	5.223962000	-4.326788000	-0.056098000
C	5.783092000	-2.890995000	-0.022424000
H	4.780253000	4.138158000	0.104747000
H	6.220262000	2.218366000	0.110939000
H	6.850478000	-2.681465000	-0.002235000
H	3.162999000	-5.396713000	-0.093615000
O	6.712750000	-0.321543000	0.041709000
H	6.961271000	0.613392000	0.060802000
O	-1.241538000	2.699664000	-0.212011000
H	-1.602063000	3.594846000	-0.240036000
C	-3.209866000	-1.417481000	0.093195000
O	-3.906149000	-0.405485000	0.165733000
O	-3.651452000	-2.647254000	0.063828000
H	-4.759387000	-2.659379000	0.082329000
B	2.554626000	5.722538000	0.055657000
O	1.570621000	6.675306000	-0.083843000
O	3.876640000	6.062699000	0.240544000
H	4.048079000	7.010817000	0.255232000
O	0.906029000	-4.581872000	-0.102213000
O	6.124998000	-5.387595000	-0.063838000
H	5.654463000	-6.228680000	-0.084968000
H	1.868010000	7.589053000	-0.026169000
C	-6.699482000	-1.774688000	0.967650000
C	-6.934972000	-1.289831000	-0.376037000
O	-6.093634000	-2.750376000	0.113463000
H	-6.001005000	-1.188991000	1.569680000
H	-7.554099000	-2.145969000	1.538787000
H	-6.193889000	-0.647432000	-0.825146000
H	-7.769329000	-1.655726000	-0.949648000
Br	-8.536460000	0.903001000	-0.131497000

## Int2b-COOH

SCF Energy (B3LYP-D3/B2) = -4516.23097978

Enthalpy 0K = 0.408265

Enthalpy 298 K = 0.446314

Free Energy 298 K = 0.328550

C	-1.053006000	2.937827000	0.082709000
C	-1.599720000	1.642122000	0.080429000
C	-1.857380000	4.088149000	0.202522000
C	-3.056637000	1.594883000	0.125268000
C	-3.239323000	4.075055000	0.300303000
C	-3.863161000	2.787900000	0.242514000
H	-1.345107000	5.048449000	0.221175000
C	-5.282457000	2.650235000	0.283725000
C	-5.902279000	1.430082000	0.197893000
C	-5.128003000	0.246707000	0.063025000
C	-3.724334000	0.340955000	0.035091000
C	-5.743210000	-1.068727000	-0.053650000
B	-2.908497000	-0.958987000	-0.109076000
C	-5.039416000	-2.318267000	-0.187016000
C	-3.610523000	-2.267824000	-0.208546000
C	-0.761635000	0.408740000	0.017817000
C	0.647821000	0.412748000	0.100394000
C	-1.397606000	-0.853268000	-0.106114000
C	1.393118000	-0.769810000	0.027918000
C	-0.645494000	-2.044649000	-0.185071000
C	0.750449000	-2.001082000	-0.128208000
H	1.226284000	1.312592000	0.227143000
H	1.344686000	-2.905155000	-0.191773000

C	-1.335144000	-3.377326000	-0.323711000
C	-2.858241000	-3.468564000	-0.324129000
C	-3.454056000	-4.719771000	-0.429238000
B	-4.971451000	-4.845708000	-0.420219000
C	-5.751037000	-3.529872000	-0.286190000
H	-5.882209000	3.544091000	0.382790000
H	-6.992291000	1.421962000	0.238046000
H	-6.838175000	-3.492422000	-0.262620000
H	-2.764592000	-5.561405000	-0.510706000
O	-7.073431000	-1.145795000	-0.037607000
H	-7.460789000	-0.263516000	0.047959000
O	0.290422000	3.121644000	-0.033823000
H	0.491469000	4.065461000	-0.012688000
C	2.924482000	-0.681067000	0.125008000
O	3.405048000	0.457194000	0.322928000
O	3.531470000	-1.786794000	-0.011576000
H	5.101032000	-1.807012000	0.197091000
B	-3.937694000	5.466374000	0.457034000
O	-3.124185000	6.577529000	0.385715000
O	-5.295855000	5.577841000	0.667095000
H	-5.614540000	6.483543000	0.747879000
O	-0.669175000	-4.402634000	-0.432740000
O	-5.683848000	-6.042089000	-0.519515000
H	-5.074821000	-6.785088000	-0.596700000
H	-3.571488000	7.420749000	0.510486000
C	6.586873000	-0.918492000	-0.731650000
C	6.520859000	0.482482000	-0.130781000
O	6.113706000	-1.841330000	0.216571000
H	5.994357000	-0.943371000	-1.658347000
H	7.624510000	-1.169719000	-0.986343000
H	5.486607000	0.770525000	0.068566000
H	7.147282000	0.561152000	0.756592000
Br	7.262083000	1.840198000	-1.415808000
C	7.375188000	-2.040573000	2.383491000
O	8.298681000	-1.434047000	1.987054000
O	6.540455000	-2.662481000	2.917549000

## TS2b-COOH

SCF Energy (B3LYP-D3/B2) = -4516.21719299

Enthalpy 0K = 0.405666

Enthalpy 298 K = 0.442279

Free Energy 298 K = 0.329193

C	-1.038280000	2.948080000	0.090234000
C	-1.589105000	1.654243000	0.078838000
C	-1.841575000	4.101395000	0.179333000
C	-3.046617000	1.609693000	0.096196000
C	-3.225469000	4.092094000	0.241137000
C	-3.851383000	2.806921000	0.183295000
H	-1.327575000	5.060523000	0.203006000
C	-5.272782000	2.675650000	0.197168000
C	-5.895428000	1.457827000	0.117203000
C	-5.123247000	0.268760000	0.016594000
C	-3.716899000	0.356217000	0.012091000
C	-5.739468000	-1.042315000	-0.087078000
B	-2.903307000	-0.947265000	-0.096717000
C	-5.031513000	-2.297661000	-0.189486000
C	-3.602923000	-2.253177000	-0.189219000
C	-0.752821000	0.418143000	0.037618000
C	0.655746000	0.420941000	0.122018000
C	-1.388570000	-0.844681000	-0.072667000
C	1.395781000	-0.765375000	0.075919000
C	-0.639815000	-2.038099000	-0.127333000
C	0.755366000	-2.000319000	-0.057944000
H	1.230872000	1.325032000	0.228533000

H	1.337872000	-2.913003000	-0.097792000
C	-1.329386000	-3.372767000	-0.256466000
C	-2.851187000	-3.460993000	-0.275738000
C	-3.445199000	-4.710972000	-0.370589000
B	-4.963514000	-4.830040000	-0.382335000
C	-5.743527000	-3.506035000	-0.280650000
H	-5.869993000	3.573507000	0.271031000
H	-6.985907000	1.453714000	0.133964000
H	-6.830830000	-3.468190000	-0.274934000
H	-2.758155000	-5.556047000	-0.429227000
O	-7.068691000	-1.121912000	-0.089925000
H	-7.460699000	-0.240075000	-0.021117000
O	0.308777000	3.127757000	0.013289000
H	0.512637000	4.070992000	0.036211000
C	2.908894000	-0.655822000	0.172998000
O	3.424773000	0.459389000	0.299727000
O	3.520058000	-1.796286000	0.101013000
H	4.672115000	-1.730796000	0.204324000
B	-3.923419000	5.489071000	0.363935000
O	-3.101718000	6.593707000	0.307023000
O	-5.286136000	5.606375000	0.530459000
H	-5.605537000	6.513197000	0.594590000
O	-0.660663000	-4.397461000	-0.344732000
O	-5.683194000	-6.018737000	-0.473420000
H	-5.082866000	-6.770911000	-0.529036000
H	-3.545632000	7.441951000	0.407731000
C	6.541639000	-0.791254000	-0.627050000
C	6.621931000	0.544820000	0.102013000
O	5.929716000	-1.730667000	0.218547000
H	5.949397000	-0.679533000	-1.546059000
H	7.549299000	-1.128782000	-0.896333000
H	5.628117000	0.916094000	0.343176000
H	7.262110000	0.465414000	0.978225000
Br	7.475829000	1.940389000	-1.062906000
C	6.911805000	-2.375989000	1.566030000
O	8.033101000	-1.948805000	1.430374000
O	6.162243000	-3.053546000	2.213167000

### Int3b-COOH

SCF Energy (B3LYP-D3/B2) = -4516.21805326

Enthalpy 0K = 0.409261

Enthalpy 298 K = 0.446074

Free Energy 298 K = 0.332052

C	-0.934224000	2.898998000	-0.242469000
C	-1.529060000	1.629662000	-0.129368000
C	-1.696389000	4.082927000	-0.257186000
C	-2.986259000	1.638892000	-0.071588000
C	-3.078485000	4.128259000	-0.177586000
C	-3.747895000	2.867244000	-0.090798000
H	-1.150028000	5.020938000	-0.335546000
C	-5.172446000	2.790419000	-0.029115000
C	-5.837667000	1.595246000	0.038420000
C	-5.109121000	0.374454000	0.049439000
C	-3.700372000	0.408594000	-0.001669000
C	-5.771249000	-0.914394000	0.109148000
B	-2.934790000	-0.927261000	0.014844000
C	-5.106567000	-2.199440000	0.129832000
C	-3.678087000	-2.208258000	0.085952000
C	-0.736231000	0.365052000	-0.080502000
C	0.673775000	0.323188000	-0.072563000
C	-1.416076000	-0.878354000	-0.024994000
C	1.370456000	-0.889232000	-0.031359000
C	-0.710306000	-2.097965000	0.014893000
C	0.686752000	-2.107656000	0.005545000

H	1.280781000	1.211986000	-0.094783000
H	1.232128000	-3.043513000	0.032061000
C	-1.447027000	-3.412804000	0.075072000
C	-2.969862000	-3.446777000	0.111278000
C	-3.606273000	-4.676471000	0.172584000
B	-5.127633000	-4.739088000	-0.216928000
C	-5.860275000	-3.382263000	0.192804000
H	-5.736333000	3.712404000	-0.037831000
H	-6.926655000	1.632531000	0.082813000
H	-6.945066000	-3.305446000	0.223574000
H	-2.950624000	-5.547789000	0.187238000
O	-7.101493000	-0.948128000	0.149373000
H	-7.464412000	-0.051504000	0.127233000
O	0.417271000	3.024745000	-0.343769000
H	0.653941000	3.958497000	-0.406529000
C	2.880717000	-0.815993000	-0.021658000
O	3.453473000	0.271191000	-0.028013000
O	3.456949000	-1.992921000	0.002400000
H	4.504561000	-1.911731000	-0.002125000
B	-3.726496000	5.553890000	-0.195042000
O	-2.863684000	6.618236000	-0.347147000
O	-5.085188000	5.736171000	-0.058781000
H	-5.372389000	6.655602000	-0.084218000
O	-0.813811000	-4.462836000	0.099711000
O	-5.891285000	-5.900075000	0.278059000
H	-5.322145000	-6.678162000	0.287000000
H	-3.275982000	7.488115000	-0.341362000
C	6.507461000	-0.660333000	0.751382000
C	6.660257000	0.463318000	-0.263909000
O	5.951090000	-1.783318000	0.101203000
H	7.483783000	-0.914015000	1.176408000
H	5.822428000	-0.351114000	1.548956000
H	7.371229000	0.181332000	-1.037058000
H	5.693255000	0.760727000	-0.662330000
Br	7.417970000	2.105579000	0.605805000
C	6.915087000	-2.638058000	-0.832660000
O	8.067210000	-2.215190000	-0.807724000
O	6.261141000	-3.521481000	-1.358301000

### TS3b-COOH

SCF Energy (B3LYP-D3/B2) = -4516.19913487

Enthalpy 0K = 0.410197

Enthalpy 298 K = 0.446375

Free Energy 298 K = 0.334247

C	-1.126731000	2.944118000	0.142625000
C	-1.702706000	1.662019000	0.108099000
C	-1.910120000	4.113558000	0.184562000
C	-3.159433000	1.644398000	0.054231000
C	-3.295116000	4.130551000	0.175852000
C	-3.942955000	2.858209000	0.094549000
H	-1.379545000	5.062711000	0.229115000
C	-5.366559000	2.756285000	0.039420000
C	-6.009433000	1.551689000	-0.062870000
C	-5.257954000	0.345547000	-0.117653000
C	-3.849921000	0.403439000	-0.054477000
C	-5.893725000	-0.950250000	-0.241612000
B	-3.058785000	-0.915496000	-0.115246000
C	-5.202578000	-2.222175000	-0.301261000
C	-3.775105000	-2.207067000	-0.233100000
C	-0.889394000	0.409703000	0.112119000
C	0.512935000	0.386646000	0.259351000
C	-1.542629000	-0.841853000	-0.019759000
C	1.228726000	-0.815382000	0.252020000
C	-0.816674000	-2.049737000	-0.033592000

C	0.573632000	-2.040493000	0.097597000
H	1.096360000	1.282512000	0.386826000
H	1.131390000	-2.969128000	0.088500000
C	-1.524135000	-3.373383000	-0.185141000
C	-3.043328000	-3.432633000	-0.276093000
C	-3.654244000	-4.670531000	-0.390794000
B	-5.173100000	-4.757542000	-0.473941000
C	-5.932078000	-3.414589000	-0.418076000
H	-5.947345000	3.666960000	0.078106000
H	-7.099136000	1.569206000	-0.099769000
H	-7.017495000	-3.357581000	-0.464719000
H	-2.983317000	-5.529924000	-0.411289000
O	-7.221703000	-1.009012000	-0.308230000
H	-7.603811000	-0.121129000	-0.264509000
O	0.225703000	3.095670000	0.135403000
H	0.449332000	4.034375000	0.163425000
C	2.723303000	-0.720042000	0.415006000
O	3.286940000	0.354891000	0.567463000
O	3.325356000	-1.898245000	0.365118000
H	4.317279000	-1.777748000	0.510435000
B	-3.970663000	5.543572000	0.254039000
O	-3.123233000	6.628506000	0.233459000
O	-5.336870000	5.687690000	0.348321000
H	-5.642720000	6.600473000	0.390979000
O	-0.868452000	-4.408878000	-0.232952000
O	-5.914849000	-5.927183000	-0.591274000
H	-5.333601000	-6.696018000	-0.614381000
H	-3.550616000	7.488241000	0.303916000
C	6.399040000	-0.354391000	-0.118794000
C	7.778324000	0.043963000	0.367569000
O	5.905782000	-1.486659000	0.616310000
H	5.700268000	0.480412000	-0.015039000
H	6.437660000	-0.663266000	-1.162753000
H	7.950777000	0.973868000	0.877219000
H	8.580012000	-0.676532000	0.344602000
Br	8.576994000	1.094691000	-1.668086000
C	6.310448000	-1.483307000	2.001010000
O	7.254153000	-0.662790000	2.219477000
O	5.707536000	-2.258994000	2.723575000

### Pdt1b-COOH

SCF Energy (B3LYP-D3/B2) = -4516.26634365

Enthalpy 0K = 0.413169

Enthalpy 298 K = 0.449252

Free Energy 298 K = 0.339925

C	1.261808000	1.303819000	-0.067711000
C	-0.035905000	0.755333000	-0.111360000
C	1.471651000	2.709553000	-0.181672000
C	-1.127952000	1.716382000	-0.157230000
C	0.453024000	3.636691000	-0.259350000
C	-0.886566000	3.140084000	-0.229937000
H	2.506940000	3.039939000	-0.184792000
C	-1.999635000	4.027126000	-0.292417000
C	-3.295791000	3.581737000	-0.245890000
C	-3.558687000	2.188930000	-0.132041000
C	-2.478785000	1.278672000	-0.101351000
C	-4.905339000	1.669579000	-0.038089000
B	-2.795487000	-0.219810000	0.011868000
C	-5.267038000	0.268324000	0.059085000
C	-4.204333000	-0.687345000	0.078799000
C	-0.291993000	-0.717499000	-0.086868000
C	0.727874000	-1.690446000	-0.187727000

C	-1.624966000	-1.193316000	0.008265000
C	0.426283000	-3.059364000	-0.151408000
C	-1.918816000	-2.572470000	0.053704000
C	-0.892220000	-3.508783000	-0.014132000
H	1.757110000	-1.395600000	-0.302428000
H	-1.105884000	-4.570590000	0.021726000
C	-3.342987000	-3.063612000	0.162714000
C	-4.499817000	-2.078644000	0.163596000
C	-5.795644000	-2.570780000	0.237097000
B	-6.972209000	-1.604330000	0.226910000
C	-6.615933000	-0.110217000	0.128844000
H	-1.802832000	5.088901000	-0.363127000
H	-4.086852000	4.330223000	-0.305646000
H	-7.374095000	0.669922000	0.109440000
H	-5.886587000	-3.656243000	0.295888000
O	-5.924007000	2.528368000	-0.036216000
H	-5.594621000	3.437333000	-0.079151000
O	2.348378000	0.533705000	0.069315000
H	3.180147000	1.091151000	0.252467000
C	1.493169000	-4.097758000	-0.262564000
O	1.291427000	-5.296360000	-0.189541000
O	2.721652000	-3.579143000	-0.464110000
H	3.365460000	-4.311776000	-0.510323000
B	0.896948000	5.139078000	-0.333773000
O	2.127215000	5.386159000	-0.882259000
O	0.085907000	6.140326000	0.161814000
H	0.458655000	7.024288000	0.066220000
O	-3.558816000	-4.269715000	0.243387000
O	-8.317193000	-1.966424000	0.295970000
H	-8.401029000	-2.924862000	0.354230000
H	2.466163000	6.281393000	-0.777767000
C	5.080652000	-1.198852000	0.854965000
C	5.362409000	-0.890549000	-0.624396000
O	5.383338000	-2.613246000	0.964672000
H	5.714400000	-0.636854000	1.537297000
H	4.032804000	-1.049532000	1.120186000
H	6.287401000	-0.332281000	-0.775632000
H	4.542325000	-0.367505000	-1.111671000
Br	4.935362000	2.144323000	0.669627000
C	5.481505000	-3.150343000	-0.264257000
O	5.494765000	-2.206288000	-1.221172000
O	5.529930000	-4.340061000	-0.484472000

### Int1b-B(OH)<sub>2</sub>

SCF Energy (B3LYP-D3/B2) = -4327.57228387

Enthalpy 0K = 0.397146

Enthalpy 298 K = 0.431347

Free Energy 298 K = 0.323276

C	-0.058425000	2.336287000	0.002471000
C	-1.087260000	1.383770000	0.001799000
C	1.304764000	1.972851000	0.015367000
C	-0.641741000	-0.004299000	0.010294000
C	1.762423000	0.670122000	0.026783000
C	0.761229000	-0.349835000	0.022713000
H	2.040990000	2.775270000	0.016630000
C	1.129936000	-1.730950000	0.029751000
C	0.198238000	-2.733159000	0.024694000
C	-1.191107000	-2.418726000	0.012168000
C	-1.593906000	-1.062300000	0.005653000
C	-2.206570000	-3.440232000	0.005683000

B	-3.093095000	-0.747839000	-0.006870000
C	-3.642616000	-3.200797000	-0.005076000
C	-4.091504000	-1.841497000	-0.011246000
C	-2.536797000	1.749713000	-0.007603000
C	-3.012712000	3.076406000	-0.010482000
C	-3.513507000	0.719105000	-0.012700000
C	-4.386213000	3.357217000	-0.019285000
C	-4.893548000	1.009724000	-0.021813000
C	-5.336886000	2.329224000	-0.025478000
H	-2.343575000	3.920317000	-0.005893000
H	-6.399350000	2.539741000	-0.032563000
C	-5.924632000	-0.095608000	-0.027392000
C	-5.492068000	-1.548762000	-0.021627000
C	-6.467398000	-2.530955000	-0.026319000
B	-6.052627000	-3.998762000	-0.020322000
C	-4.535247000	-4.277425000	-0.009127000
H	2.184732000	-1.970802000	0.039432000
H	0.567899000	-3.759012000	0.031033000
H	-4.130574000	-5.287215000	-0.004128000
H	-7.499657000	-2.178904000	-0.034166000
O	-1.840181000	-4.723788000	0.009562000
H	-0.875436000	-4.797869000	0.014960000
O	-0.340938000	3.673738000	-0.008930000
H	0.490860000	4.164223000	-0.008649000
C	-4.783374000	4.787297000	-0.021505000
O	-4.019259000	5.736009000	-0.015483000
O	-6.132773000	4.968228000	-0.031192000
H	-6.260905000	5.930158000	-0.031733000
B	3.338172000	0.477566000	0.043897000
O	3.902851000	-0.767437000	0.070538000
O	4.081423000	1.627079000	0.033548000
H	5.038086000	1.431444000	0.047890000
O	-7.116770000	0.201857000	-0.036407000
O	-6.924817000	-5.082754000	-0.024070000
H	-7.839529000	-4.778546000	-0.031258000
H	4.880279000	-0.708808000	0.081400000
C	7.805524000	0.045314000	-0.430301000
C	7.605788000	0.094888000	1.005530000
O	6.446372000	0.223431000	0.128832000
H	8.205703000	0.912860000	-0.942364000
H	7.981125000	-0.910448000	-0.910438000
H	7.868385000	0.998829000	1.549784000
H	7.643800000	-0.826803000	1.581130000
Br	10.914381000	-0.364125000	-0.158099000

### TS1b-B(OH)<sub>2</sub>

SCF Energy (B3LYP-D3/B2) = -4327.56528471

Enthalpy 0K = 0.396002

Enthalpy 298 K = 0.429419

Free Energy 298 K = 0.324458

C	-0.047054000	2.364001000	-0.088143000
C	-1.064777000	1.401660000	-0.059273000
C	1.321752000	2.014383000	-0.128706000
C	-0.603452000	0.019240000	-0.075655000
C	1.794152000	0.719163000	-0.144492000
C	0.803111000	-0.310816000	-0.117376000
H	2.051474000	2.822872000	-0.148890000
C	1.191221000	-1.685305000	-0.131528000
C	0.271706000	-2.699679000	-0.106949000
C	-1.119444000	-2.399166000	-0.066279000

C	-1.540176000	-1.049617000	-0.051065000
C	-2.124616000	-3.433137000	-0.040022000
B	-3.045094000	-0.752972000	-0.007140000
C	-3.564002000	-3.211654000	0.001716000
C	-4.029372000	-1.859323000	0.018571000
C	-2.518367000	1.750447000	-0.015160000
C	-3.009822000	3.071197000	0.004455000
C	-3.482493000	0.709042000	0.009694000
C	-4.386220000	3.334861000	0.045997000
C	-4.865069000	0.981957000	0.051254000
C	-5.324454000	2.296199000	0.069540000
H	-2.350638000	3.922926000	-0.011489000
H	-6.388791000	2.494354000	0.101556000
C	-5.881773000	-0.136441000	0.077162000
C	-5.431598000	-1.585164000	0.059873000
C	-6.394522000	-2.580145000	0.084958000
B	-5.962327000	-4.041972000	0.068427000
C	-4.440665000	-4.300623000	0.024024000
H	2.250681000	-1.905670000	-0.163083000
H	0.653427000	-3.721060000	-0.120024000
H	-4.023186000	-5.305068000	0.009475000
H	-7.430551000	-2.241053000	0.115933000
O	-1.742928000	-4.707530000	-0.054072000
H	-0.777122000	-4.771095000	-0.081799000
O	-0.342538000	3.697285000	-0.078026000
H	0.484034000	4.196366000	-0.101661000
C	-4.800616000	4.760828000	0.063884000
O	-4.047493000	5.717638000	0.045395000
O	-6.151165000	4.924666000	0.104489000
H	-6.292188000	5.884803000	0.112558000
B	3.377272000	0.538492000	-0.191641000
O	3.947686000	-0.699959000	-0.214115000
O	4.106051000	1.693814000	-0.208759000
H	5.068740000	1.474765000	-0.237983000
O	-7.076821000	0.144777000	0.112455000
O	-6.816762000	-5.138606000	0.089969000
H	-7.736304000	-4.850531000	0.117356000
H	4.936844000	-0.600791000	-0.242253000
C	8.062113000	0.017915000	-0.490508000
C	7.376571000	0.161980000	0.777406000
O	6.377112000	0.301796000	-0.231306000
H	8.432047000	0.886899000	-1.009665000
H	8.129901000	-0.947370000	-0.964964000
H	7.583668000	1.062029000	1.362865000
H	7.290311000	-0.726784000	1.408832000
Br	10.659728000	-0.399291000	0.152472000

### Int2b-B(OH)<sub>2</sub>

SCF Energy (B3LYP-D3/B2) = -4516.25589864

Enthalpy 0K = 0.410870

Enthalpy 298 K = 0.447947

Free Energy 298 K = 0.337138

C	-0.573451000	-3.314112000	-0.233725000
C	-1.141633000	-2.036581000	-0.290543000
C	0.819215000	-3.536949000	-0.399670000
C	-0.197291000	-0.962946000	-0.556832000
C	1.734428000	-2.547087000	-0.679581000
C	1.195432000	-1.228323000	-0.812601000
H	1.187200000	-4.556658000	-0.282179000

C	2.041834000	-0.152133000	-1.206498000
C	1.619790000	1.151733000	-1.184384000
C	0.295041000	1.443073000	-0.759748000
C	-0.613517000	0.391419000	-0.521124000
C	-0.145171000	2.795439000	-0.521333000
B	-2.070392000	0.742252000	-0.213969000
C	-1.532134000	3.199069000	-0.303929000
C	-2.505900000	2.158949000	-0.159084000
C	-2.595563000	-1.760458000	-0.079105000
C	-3.574589000	-2.763424000	0.061713000
C	-3.048673000	-0.414322000	-0.026903000
C	-4.924814000	-2.438120000	0.261713000
C	-4.405444000	-0.093820000	0.181059000
C	-5.351222000	-1.104829000	0.329435000
H	-3.321263000	-3.810472000	0.018105000
H	-6.392061000	-0.850301000	0.487586000
C	-4.866567000	1.347949000	0.244043000
C	-3.874607000	2.484713000	0.075463000
C	-4.332274000	3.791699000	0.154006000
B	-3.344596000	4.943305000	0.001819000
C	-1.870469000	4.552038000	-0.225508000
H	3.055788000	-0.412434000	-1.481786000
H	2.303207000	1.930548000	-1.508822000
H	-1.078311000	5.289824000	-0.337495000
H	-5.401844000	3.913126000	0.331531000
O	0.763262000	3.757811000	-0.464394000
H	1.665762000	3.387192000	-0.418496000
O	-1.350213000	-4.410758000	0.023799000
H	-0.777571000	-5.188312000	0.038184000
C	-5.878934000	-3.566134000	0.395612000
O	-5.594857000	-4.749877000	0.340954000
O	-7.165272000	-3.161848000	0.594106000
H	-7.678910000	-3.982102000	0.663983000
B	3.319584000	-2.861375000	-0.687756000
O	4.231093000	-1.924475000	-0.617423000
O	3.583592000	-4.245089000	-0.688438000
H	4.543369000	-4.335474000	-0.618941000
O	-6.057963000	1.581734000	0.433234000
O	-3.674151000	6.296986000	0.059437000
H	-4.620493000	6.401984000	0.209206000
H	5.504365000	-1.034248000	-0.786762000
C	4.829258000	1.069011000	0.565789000
C	5.625550000	0.908125000	-0.728574000
O	6.239810000	-0.348507000	-0.743162000
H	5.458633000	0.960848000	1.446921000
H	3.986207000	0.382728000	0.613778000
H	6.401329000	1.682576000	-0.780620000
H	4.949066000	1.070897000	-1.586182000
Br	4.060232000	2.931772000	0.706570000
C	5.900886000	-2.536328000	1.358985000
O	6.382878000	-3.418963000	0.756342000
O	5.492986000	-1.703081000	2.071733000

## TS2b-B(OH)<sub>2</sub>

SCF Energy (B3LYP-D3/B2) = -4516.24775618

Enthalpy 0K = 0.407659

Enthalpy 298 K = 0.443716

Free Energy 298 K = 0.333555

C	-0.559638000	-2.876000000	-0.133068000
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C	-1.361893000	-1.729357000	-0.138534000
C	0.840326000	-2.825452000	-0.342271000
C	-0.643205000	-0.483418000	-0.369545000
C	1.553864000	-1.670468000	-0.573821000
C	0.785373000	-0.462791000	-0.589114000
H	1.390907000	-3.765587000	-0.318263000
C	1.435343000	0.786208000	-0.823118000
C	0.745884000	1.970695000	-0.828969000
C	-0.659503000	1.976625000	-0.599382000
C	-1.336475000	0.754739000	-0.381399000
C	-1.426561000	3.197788000	-0.580318000
B	-2.853614000	0.788854000	-0.156811000
C	-2.868154000	3.292548000	-0.383990000
C	-3.589551000	2.076576000	-0.170868000
C	-2.840999000	-1.759056000	0.075335000
C	-3.582780000	-2.939193000	0.284055000
C	-3.569474000	-0.540376000	0.068716000
C	-4.971254000	-2.901586000	0.477606000
C	-4.965519000	-0.510005000	0.264316000
C	-5.674265000	-1.690432000	0.470624000
H	-3.111957000	-3.908165000	0.301776000
H	-6.746440000	-1.656182000	0.619908000
C	-5.727979000	0.796242000	0.254220000
C	-5.002208000	2.109156000	0.029264000
C	-5.737298000	3.284917000	0.026453000
B	-5.026086000	4.613730000	-0.196565000
C	-3.500159000	4.539945000	-0.405876000
H	2.505976000	0.745509000	-1.001038000
H	1.314956000	2.880866000	-1.023697000
H	-2.892498000	5.426928000	-0.572139000
H	-6.810253000	3.176335000	0.190001000
O	-0.796655000	4.356493000	-0.751172000
H	0.155406000	4.208082000	-0.851987000
O	-1.103964000	-4.111546000	0.080230000
H	-0.392580000	-4.764204000	0.048454000
C	-5.659719000	-4.199447000	0.688739000
O	-5.124436000	-5.293561000	0.706729000
O	-7.003667000	-4.070473000	0.870132000
H	-7.330166000	-4.975642000	0.995457000
B	3.151813000	-1.780919000	-0.794813000
O	3.906262000	-0.723644000	-1.048318000
O	3.594547000	-3.095436000	-0.683384000
H	4.554516000	-3.152831000	-0.802624000
O	-6.943800000	0.777529000	0.430185000
O	-5.640381000	5.863814000	-0.224002000
H	-6.589187000	5.773083000	-0.080391000
H	5.186058000	-0.809295000	-1.183940000
C	6.133854000	0.636924000	0.725303000
C	6.712537000	0.477516000	-0.679899000
O	6.318675000	-0.761327000	-1.207918000
H	6.555337000	-0.097220000	1.410766000
H	5.046857000	0.575936000	0.711372000
H	7.807041000	0.524529000	-0.631889000
H	6.363607000	1.306260000	-1.315157000
Br	6.591947000	2.423228000	1.491706000
C	7.245989000	-2.397866000	-0.362781000
O	6.533695000	-3.269960000	-0.743590000
O	8.166534000	-1.908926000	0.199178000

## Int3b-B(OH)<sub>2</sub>

SCF Energy (B3LYP-D3/B2) = -4516.25296775

Enthalpy 0K = 0.411740  
 Enthalpy 298 K = 0.446202  
 Free Energy 298 K = 0.339985

C	-0.954043000	-2.732267000	-0.000162000
C	-1.771318000	-1.595268000	-0.000131000
C	0.457874000	-2.649353000	-0.000252000
C	-1.054801000	-0.326465000	-0.000200000
C	1.170501000	-1.470011000	-0.000315000
C	0.390745000	-0.271027000	-0.000291000
H	1.025030000	-3.579686000	-0.000270000
C	1.033273000	1.004125000	-0.000362000
C	0.323544000	2.175794000	-0.000354000
C	-1.099772000	2.145270000	-0.000270000
C	-1.769954000	0.900538000	-0.000188000
C	-1.890377000	3.351442000	-0.000274000
B	-3.305069000	0.897065000	-0.000090000
C	-3.346506000	3.410195000	-0.000197000
C	-4.061205000	2.171802000	-0.000097000
C	-3.265224000	-1.660370000	-0.000040000
C	-4.000187000	-2.863028000	0.000021000
C	-4.013874000	-0.454499000	-0.000015000
C	-5.402403000	-2.858792000	0.000100000
C	-5.423734000	-0.457934000	0.000075000
C	-6.125930000	-1.660241000	0.000131000
H	-3.514552000	-3.824661000	0.000004000
H	-7.208971000	-1.651773000	0.000203000
C	-6.208272000	0.834453000	0.000140000
C	-5.489395000	2.170572000	-0.000011000
C	-6.244916000	3.332228000	-0.000035000
B	-5.541695000	4.684204000	-0.000150000
C	-3.998867000	4.647016000	-0.000226000
H	2.116123000	1.013878000	-0.000430000
H	0.893203000	3.105846000	-0.000416000
H	-3.396243000	5.552737000	-0.000306000
H	-7.327132000	3.197062000	0.000042000
O	-1.271888000	4.528725000	-0.000366000
H	-0.311353000	4.404768000	-0.000419000
O	-1.495705000	-3.985645000	-0.000110000
H	-0.775578000	-4.629620000	-0.000146000
C	-6.082133000	-4.179012000	0.000154000
O	-5.526597000	-5.262715000	0.000279000
O	-7.440218000	-4.081815000	0.000413000
H	-7.761044000	-4.997692000	0.000551000
B	2.769316000	-1.607843000	-0.000406000
O	3.539768000	-0.480535000	-0.000549000
O	3.238438000	-2.872683000	-0.000338000
H	4.244877000	-2.956105000	-0.000550000
O	-7.435670000	0.787015000	0.000016000
O	-6.172803000	5.924321000	-0.000185000
H	-7.130505000	5.814721000	-0.000128000
H	4.507799000	-0.679127000	-0.000450000
C	8.502764000	0.074661000	0.000255000
C	6.981403000	0.239131000	0.000721000
O	6.185709000	-0.944502000	0.000202000
H	8.901585000	-0.396460000	-0.889925000
H	8.902028000	-0.397428000	0.889721000
H	6.701050000	0.827675000	-0.882335000
H	6.701475000	0.826641000	0.884600000
Br	9.269266000	1.949350000	0.001085000
C	6.729529000	-2.303448000	-0.000632000
O	5.808279000	-3.142698000	-0.000947000

O 7.955039000 -2.416746000 -0.000883000

### TS3b-B(OH)<sub>2</sub>

SCF Energy (B3LYP-D3/B2) = -4516.24019791  
 Enthalpy 0K = 0.412029  
 Enthalpy 298 K = 0.447775  
 Free Energy 298 K = 0.336202

C	0.979099000	-2.693247000	-0.000027000
C	1.814268000	-1.569133000	-0.000013000
C	-0.430586000	-2.587165000	-0.000014000
C	1.118429000	-0.288601000	0.000010000
C	-1.123841000	-1.395754000	0.000014000
C	-0.325766000	-0.208644000	0.000025000
H	-1.010228000	-3.509445000	-0.000028000
C	-0.945550000	1.077900000	0.000047000
C	-0.216089000	2.237052000	0.000053000
C	1.206210000	2.182270000	0.000037000
C	1.855031000	0.926530000	0.000017000
C	2.017005000	3.375514000	0.000037000
B	3.390041000	0.896656000	0.000002000
C	3.473815000	3.408253000	0.000033000
C	4.167320000	2.157734000	0.000013000
C	3.307013000	-1.659687000	-0.000021000
C	4.021066000	-2.874823000	-0.000032000
C	4.075778000	-0.466723000	-0.000016000
C	5.423017000	-2.894771000	-0.000040000
C	5.485295000	-0.494587000	-0.000024000
C	6.166741000	-1.708813000	-0.000037000
H	3.519660000	-3.828216000	-0.000034000
H	7.249784000	-1.718861000	-0.000043000
C	6.291941000	0.783882000	-0.000018000
C	5.595958000	2.132140000	0.000006000
C	6.371360000	3.279943000	0.000021000
B	5.691383000	4.644072000	0.000045000
C	4.147236000	4.633472000	0.000049000
H	-2.027328000	1.110897000	0.000063000
H	-0.770042000	3.176304000	0.000076000
H	3.560798000	5.549702000	0.000064000
H	7.451025000	3.126302000	0.000014000
O	1.419561000	4.562921000	0.000041000
H	0.456735000	4.458307000	0.000039000
O	1.500854000	-3.954952000	-0.000056000
H	0.772011000	-4.588960000	-0.000063000
C	6.079685000	-4.226869000	-0.000051000
O	5.504505000	-5.300204000	-0.000052000
O	7.438809000	-4.153023000	-0.000062000
H	7.744804000	-5.073988000	-0.000069000
B	-2.720329000	-1.508197000	0.000027000
O	-3.475462000	-0.369420000	0.000183000
O	-3.210375000	-2.768601000	-0.000117000
H	-4.204225000	-2.850729000	-0.000012000
O	7.518174000	0.715470000	-0.000032000
O	6.341793000	5.872938000	0.000063000
H	7.297878000	5.749760000	0.000058000
H	-4.440897000	-0.534359000	0.000097000
C	-8.615323000	-0.374247000	0.000199000
C	-7.208466000	0.201767000	-0.000410000
O	-6.195107000	-0.828931000	-0.000257000
H	-9.132689000	-0.573915000	0.922448000

H	-9.133296000	-0.574399000	-0.921601000
H	-7.057596000	0.819948000	0.885898000
H	-7.058087000	0.819238000	-0.887299000
Br	-9.651280000	1.864625000	-0.000107000
C	-6.682297000	-2.136454000	0.000189000
O	-5.837213000	-3.038329000	0.000312000
O	-7.945425000	-2.223349000	0.000414000

### Pdt1b-B(OH)<sub>2</sub>

SCF Energy (B3LYP-D3/B2) = -4516.26019600

Enthalpy 0K = 0.414316

Enthalpy 298 K = 0.450488

Free Energy 298 K = 0.337785

C	-1.039041000	-2.697812000	-0.000063000
C	-1.866118000	-1.566803000	-0.000078000
C	0.369542000	-2.601688000	-0.000315000
C	-1.161909000	-0.290392000	-0.000335000
C	1.070422000	-1.413110000	-0.000599000
C	0.282144000	-0.219503000	-0.000583000
H	0.939106000	-3.529838000	-0.000276000
C	0.907895000	1.064970000	-0.000771000
C	0.185298000	2.227604000	-0.000752000
C	-1.237545000	2.182745000	-0.000544000
C	-1.893079000	0.929953000	-0.000336000
C	-2.039958000	3.380896000	-0.000538000
B	-3.426830000	0.908608000	-0.000110000
C	-3.496050000	3.420686000	-0.000338000
C	-4.196852000	2.173299000	-0.000121000
C	-3.359258000	-1.648595000	0.000160000
C	-4.080214000	-2.859689000	0.000411000
C	-4.120661000	-0.450679000	0.000135000
C	-5.482102000	-2.872059000	0.000621000
C	-5.530501000	-0.471217000	0.000344000
C	-6.218598000	-1.681494000	0.000590000
H	-3.584993000	-3.816142000	0.000449000
H	-7.301720000	-1.684984000	0.000748000
C	-6.330356000	0.811342000	0.000298000
C	-5.626956000	2.155177000	0.000081000
C	-6.396065000	3.306229000	0.000080000
B	-5.708072000	4.667095000	-0.000146000
C	-4.163994000	4.648855000	-0.000361000
H	1.988946000	1.098185000	-0.000964000
H	0.744910000	3.163291000	-0.000899000
H	-3.573208000	5.562258000	-0.000530000
H	-7.476572000	3.158593000	0.000244000
O	-1.435994000	4.567115000	-0.000728000
H	-0.473942000	4.458809000	-0.000853000
O	-1.570893000	-3.956218000	0.000194000
H	-0.847903000	-4.596506000	0.000191000
C	-6.145840000	-4.200251000	0.000873000
O	-5.576506000	-5.276931000	0.001041000
O	-7.504498000	-4.119137000	0.001223000
H	-7.815565000	-5.038390000	0.001474000
B	2.658837000	-1.534703000	-0.000917000
O	3.430395000	-0.406386000	-0.001988000
O	3.145845000	-2.804000000	-0.000270000
H	4.122357000	-2.894647000	-0.000514000
O	-7.557073000	0.748859000	0.000543000
O	-6.352598000	5.898715000	-0.000175000

H	-7.309299000	5.780201000	-0.000030000
H	4.390548000	-0.561571000	-0.001869000
C	8.593693000	-0.903640000	-0.001668000
C	7.396672000	0.058551000	0.000546000
O	6.238090000	-0.858609000	-0.001048000
H	9.214957000	-0.810521000	-0.889087000
H	9.218134000	-0.810752000	0.883491000
H	7.342971000	0.685570000	-0.885744000
H	7.343417000	0.681837000	0.889535000
Br	9.874354000	1.975688000	0.001828000
C	6.651938000	-2.140627000	-0.001250000
O	5.886189000	-3.085438000	-0.001514000
O	7.974636000	-2.239966000	-0.000820000

### Cl<sup>-</sup>

SCF Energy (B3LYP-D3/B2) = -460.303727292

Enthalpy 0K = 0.000000

Enthalpy 298 K = 0.001416

Free Energy 298 K = -0.015023

Cl	0.000000000	0.000000000	0.000000000
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### I<sup>-</sup>

SCF Energy (B3LYP-D3/B2) = -11.4721100531

Enthalpy 0K = 0.000000

Enthalpy 298 K = 0.001416

Free Energy 298 K = -0.016848

I	0.000000000	0.000000000	0.000000000
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### CN<sup>-</sup>

SCF Energy (B3LYP-D3/B2) = -92.8883409232

Enthalpy 0K = 0.004870

Enthalpy 298 K = 0.007231

Free Energy 298 K = -0.014182

C	0.000000000	0.000000000	-0.637379000
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N	0.000000000	0.000000000	0.546325000
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### N<sub>3</sub><sup>-</sup>

SCF Energy (B3LYP-D3/B2) = -164.285543536

Enthalpy 0K = 0.011058

Enthalpy 298 K = 0.013677

Free Energy 298 K = -0.009492

N	0.000000000	0.000000000	1.191064000
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N	0.000000000	0.000000000	0.000000000
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N	0.000000000	0.000000000	-1.191064000
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### Int3-Cl

SCF Energy (B3LYP-D3/B2) = -2366.11381931

Enthalpy 0K = 0.401324

Enthalpy 298 K = 0.435272

Free Energy 298 K = 0.329556

C	-1.033016000	2.825401000	0.073330000
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C	-1.440972000	1.462461000	0.025214000
C	-1.952387000	3.860195000	-0.007877000
C	-2.853535000	1.220816000	-0.051652000
C	-3.325551000	3.636641000	-0.125286000
C	-3.801066000	2.300586000	-0.140959000
H	-1.584500000	4.879979000	0.023484000
C	-5.202466000	1.995090000	-0.252871000
C	-5.651697000	0.717445000	-0.229534000
C	-4.760459000	-0.394395000	-0.091147000
C	-3.341349000	-0.141932000	-0.031601000
C	-5.239425000	-1.704931000	-0.019680000
C	-2.444245000	-1.225731000	0.056959000
C	-4.356892000	-2.810050000	0.066948000
C	-2.950918000	-2.561000000	0.095591000
C	-0.506808000	0.336164000	0.059389000
C	0.897934000	0.493938000	0.044256000
C	-1.021318000	-0.994417000	0.090527000
C	1.771041000	-0.586372000	0.080291000
C	-0.116130000	-2.091674000	0.143068000
C	1.261352000	-1.884135000	0.139140000
H	1.352560000	1.468391000	0.000236000
H	1.928250000	-2.737521000	0.175234000
C	-0.602609000	-3.488594000	0.202536000
C	-2.076134000	-3.681071000	0.174204000
C	-2.581216000	-4.970999000	0.224339000
C	-3.967622000	-5.204846000	0.201979000
C	-4.842971000	-4.141204000	0.125800000
H	-5.894982000	2.816169000	-0.359206000
H	-6.720875000	0.553907000	-0.349264000
H	-5.914584000	-4.303346000	0.107995000
H	-4.347102000	-6.221518000	0.244728000
H	-1.868728000	-5.787608000	0.282367000
O	-6.570906000	-2.006137000	-0.033983000
H	-7.088328000	-1.199037000	0.070455000
O	0.285433000	3.138165000	0.210751000
H	0.390762000	4.097804000	0.220318000
C	3.255286000	-0.298014000	0.058432000
O	3.661032000	0.860465000	0.006085000
O	3.987959000	-1.380367000	0.108782000
H	5.026900000	-1.163194000	0.076433000
C	-4.213972000	4.823767000	-0.216476000
O	-5.430703000	4.846887000	-0.311032000
O	-3.519406000	5.998628000	-0.184755000
H	-4.196556000	6.690392000	-0.250291000
O	0.161467000	-4.451016000	0.274321000
C	6.854684000	1.455207000	-0.150432000
H	5.845283000	1.635463000	-0.515814000
C	6.865882000	0.276398000	0.815686000
H	6.182038000	0.473798000	1.650166000
H	7.879994000	0.121785000	1.198628000
O	6.420286000	-0.878699000	0.139527000
Cl	7.396982000	2.999133000	0.695290000
H	7.561107000	1.274859000	-0.958987000
C	7.446843000	-1.588295000	-0.866370000
O	8.543119000	-1.040314000	-0.850104000
O	6.871533000	-2.513147000	-1.409494000

### TS3-C1

SCF Energy (B3LYP-D3/B2) = -2366.08928143

Enthalpy 0K = 0.402369

Enthalpy 298 K = 0.435592

Free Energy 298 K = 0.332184

C	-0.632698000	2.715513000	-0.029490000
C	-1.173376000	1.400084000	-0.072801000
C	-1.449957000	3.834271000	-0.103557000
C	-2.602466000	1.293324000	-0.108508000
C	-2.839614000	3.741264000	-0.202058000
C	-3.443297000	2.457624000	-0.193778000
H	-0.985676000	4.813996000	-0.082098000
C	-4.869474000	2.284861000	-0.273672000
C	-5.437754000	1.056533000	-0.211718000
C	-4.653487000	-0.132206000	-0.060672000
C	-3.216381000	-0.015891000	-0.042664000
C	-5.252033000	-1.388561000	0.066177000
C	-2.424161000	-1.177870000	0.058502000
C	-4.476166000	-2.569931000	0.171170000
C	-3.052600000	-2.456341000	0.156200000
C	-0.350817000	0.190003000	-0.059332000
C	1.056909000	0.213069000	-0.165296000
C	-0.985784000	-1.083330000	0.038960000
C	1.824971000	-0.944747000	-0.118515000
C	-0.186852000	-2.259568000	0.099516000
C	1.202636000	-2.184048000	0.034678000
H	1.594358000	1.137754000	-0.287745000
H	1.784446000	-3.096465000	0.089440000
C	-0.800425000	-3.600540000	0.229892000
C	-2.285280000	-3.651841000	0.251726000
C	-2.909088000	-4.884960000	0.362027000
C	-4.311502000	-4.985192000	0.384141000
C	-5.084009000	-3.845759000	0.290774000
H	-5.482883000	3.165962000	-0.385763000
H	-6.519850000	0.992757000	-0.307552000
H	-6.166233000	-3.905354000	0.305983000
H	-4.784408000	-5.958668000	0.474177000
H	-2.276486000	-5.764115000	0.430924000
O	-6.605635000	-1.561082000	0.094163000
H	-7.040932000	-0.705359000	0.186196000
O	0.709475000	2.889541000	0.097974000
H	0.920432000	3.830705000	0.144319000
C	3.316517000	-0.788472000	-0.233700000
O	3.828988000	0.290268000	-0.487957000
O	3.974649000	-1.919728000	-0.019970000
H	4.967598000	-1.735959000	-0.094533000
C	-3.612465000	5.007645000	-0.295901000
O	-4.822227000	5.143509000	-0.383242000
O	-2.809632000	6.110211000	-0.277471000
H	-3.416699000	6.864209000	-0.343434000
O	-0.126676000	-4.627844000	0.314794000
C	6.871914000	1.154653000	0.175569000
H	6.020245000	1.537600000	-0.362425000
C	6.732727000	-0.181105000	0.878842000
H	5.879919000	-0.148977000	1.555878000
H	7.638572000	-0.396508000	1.456177000
O	6.487414000	-1.252444000	-0.044509000
Cl	6.418513000	2.455071000	2.014336000
H	7.814504000	1.664794000	0.103959000
C	6.970388000	-0.990476000	-1.383954000
O	7.474396000	0.168334000	-1.488512000
O	6.811762000	-1.900841000	-2.178092000

### Pdt1-C1

SCF Energy (B3LYP-D3/B2) = -2366.15524999  
 Enthalpy 0K = 0.404704  
 Enthalpy 298 K = 0.437508  
 Free Energy 298 K = 0.338436

C	0.831011000	2.015809000	-0.348388000
C	-0.210137000	1.039577000	-0.366489000
C	0.517410000	3.377902000	-0.240988000
C	-1.557829000	1.495236000	-0.221518000
C	-0.796631000	3.829815000	-0.163962000
C	-1.868569000	2.894641000	-0.153811000
H	1.347960000	4.073456000	-0.205833000
C	-3.247144000	3.297052000	-0.101596000
C	-4.252931000	2.388804000	-0.031291000
C	-3.989783000	0.980506000	0.019648000
C	-2.627596000	0.526963000	-0.107626000
C	-5.016084000	0.048594000	0.199701000
C	-2.348982000	-0.857548000	-0.082568000
C	-4.757807000	-1.344191000	0.236966000
C	-3.408854000	-1.793658000	0.091332000
C	0.057860000	-0.394834000	-0.456744000
C	1.334534000	-0.913858000	-0.741708000
C	-0.997420000	-1.328772000	-0.247356000
C	1.615692000	-2.276186000	-0.670357000
C	-0.706530000	-2.722697000	-0.214880000
C	0.599682000	-3.184695000	-0.375861000
H	2.141433000	-0.249234000	-0.994213000
C	0.793307000	-4.247988000	-0.294055000
C	-1.776212000	-3.722977000	-0.001035000
C	-3.157966000	-3.195940000	0.139418000
C	-4.200166000	-4.092614000	0.321253000
C	-5.524184000	-3.640742000	0.464207000
C	-5.798935000	-2.288461000	0.424824000
H	-3.468963000	4.353992000	-0.112250000
H	-5.276874000	2.757683000	-0.033753000
H	-6.813915000	-1.924496000	0.538141000
H	-6.328793000	-4.356087000	0.608448000
H	-3.955564000	-5.149590000	0.351765000
O	-6.322688000	0.419698000	0.358072000
H	-6.365457000	1.371038000	0.512782000
O	2.106891000	1.644204000	-0.427653000
H	2.780157000	2.381372000	-0.150910000
C	3.046542000	-2.649166000	-0.855709000
O	3.844249000	-1.941223000	-1.448112000
O	3.387302000	-3.798263000	-0.248152000
H	4.367248000	-3.801960000	-0.178055000
C	-1.015794000	5.300914000	-0.068220000
O	-2.054180000	5.882336000	0.209976000
O	0.111960000	6.010532000	-0.327274000
H	-0.131768000	6.939651000	-0.191609000
O	-1.543300000	-4.933431000	0.051659000
C	5.476877000	0.433491000	-0.004978000
H	4.902785000	0.498180000	-0.930753000
C	4.587806000	0.149175000	1.206958000
H	3.548069000	0.423924000	1.048576000
H	4.959430000	0.610862000	2.124959000
O	4.680651000	-1.295151000	1.339822000
Cl	4.121714000	3.459443000	0.515146000
H	6.102684000	1.314601000	0.113045000
C	5.698197000	-1.751896000	0.583298000
O	6.311051000	-0.757624000	-0.074992000
O	6.014662000	-2.922002000	0.521794000

### Int3-CN

SCF Energy (B3LYP-D3/B2) = -1998.76118095  
 Enthalpy 0K = 0.409369  
 Enthalpy 298 K = 0.443747  
 Free Energy 298 K = 0.338118

C	-0.809567000	2.746389000	0.093329000
C	-1.264133000	1.400790000	-0.004366000
C	-1.698880000	3.811062000	0.090274000
C	-2.684351000	1.203028000	-0.019267000
C	-3.081787000	3.632058000	0.015352000
C	-3.600509000	2.312620000	-0.028188000
H	-1.298314000	4.816908000	0.151204000
C	-5.014145000	2.051029000	-0.087308000
C	-5.500747000	0.786665000	-0.077741000
C	-4.638173000	-0.354305000	-0.007032000
C	-3.211306000	-0.144968000	-0.012816000
C	-5.151642000	-1.651796000	0.063342000
C	-2.343852000	-1.256329000	0.005403000
C	-4.299379000	-2.783863000	0.083513000
C	-2.886793000	-2.576741000	0.042516000
C	-0.365191000	0.247884000	-0.069378000
C	1.038485000	0.370597000	-0.191470000
C	-0.915321000	-1.067096000	-0.036204000
C	1.879433000	-0.735890000	-0.227912000
C	-0.041039000	-2.190855000	-0.060975000
C	1.337749000	-2.018443000	-0.143278000
H	1.503740000	1.337558000	-0.260215000
H	1.989661000	-2.884722000	-0.153000000
C	-0.564567000	-3.574025000	-0.004113000
C	-2.042442000	-3.723085000	0.050286000
C	-2.582999000	-4.998538000	0.103350000
C	-3.975026000	-5.191294000	0.153052000
C	-4.821024000	-4.101360000	0.143797000
H	-5.685437000	2.894652000	-0.140790000
H	-6.578410000	0.656787000	-0.154963000
H	-5.896443000	-4.232173000	0.180987000
H	-4.382147000	-6.197127000	0.198157000
H	-1.893739000	-5.836857000	0.105921000
O	-6.490874000	-1.913213000	0.111992000
H	-6.975857000	-1.094534000	0.269342000
O	0.520718000	3.002991000	0.203867000
H	0.674721000	3.954355000	0.263988000
C	3.375038000	-0.562720000	-0.339169000
O	4.128048000	-1.529058000	-0.254899000
O	3.726275000	0.685966000	-0.525545000
H	4.769514000	0.824750000	-0.544834000
C	-3.936527000	4.847744000	0.000239000
O	-5.154350000	4.908764000	-0.056039000
O	-3.206363000	5.998815000	0.057496000
H	-3.862744000	6.713128000	0.040847000
O	0.173934000	-4.559520000	-0.003318000
C	7.235124000	-0.813501000	0.516104000
H	6.250097000	-1.212355000	0.778234000
C	7.093951000	0.014207000	-0.782873000
H	6.707431000	-0.626491000	-1.584037000
H	8.074612000	0.409626000	-1.067311000
O	6.188045000	1.075201000	-0.600423000
H	7.580743000	-0.132017000	1.299490000
C	6.686217000	2.313872000	0.265467000

O	7.863612000	2.199851000	0.592423000
O	5.756252000	3.090673000	0.398729000
C	8.182358000	-1.918270000	0.380374000
N	8.940923000	-2.789209000	0.248122000

### TS3-CN

SCF Energy (B3LYP-D3/B2) = -1998.67766075

Enthalpy 0K = 0.409164

Enthalpy 298 K = 0.443554

Free Energy 298 K = 0.336740

C	0.827153000	2.804034000	-0.020755000
C	1.305691000	1.464617000	0.010851000
C	1.693517000	3.883825000	0.067451000
C	2.728603000	1.293315000	0.069107000
C	3.076373000	3.728182000	0.174072000
C	3.620459000	2.418348000	0.166852000
H	1.274293000	4.883860000	0.050667000
C	5.036556000	2.182743000	0.261794000
C	5.549861000	0.930247000	0.210663000
C	4.714693000	-0.222690000	0.058126000
C	3.284577000	-0.042382000	0.018100000
C	5.258503000	-1.505831000	-0.047101000
C	2.442989000	-1.168966000	-0.084651000
C	4.432236000	-2.652609000	-0.150119000
C	3.015282000	-2.475499000	-0.158463000
C	0.429952000	0.291977000	-0.026691000
C	-0.978771000	0.377833000	0.023252000
C	1.010305000	-1.009652000	-0.095254000
C	-1.795514000	-0.746273000	-0.026990000
C	0.161866000	-2.150525000	-0.160322000
C	-1.223644000	-2.014770000	-0.131771000
H	-1.478097000	1.327697000	0.105707000
H	-1.842040000	-2.903024000	-0.182138000
C	0.717376000	-3.519985000	-0.258110000
C	2.197860000	-3.637265000	-0.252648000
C	2.767755000	-4.898228000	-0.338038000
C	4.164355000	-5.060826000	-0.336394000
C	4.984855000	-3.955367000	-0.244825000
H	5.687405000	3.036046000	0.377243000
H	6.627034000	0.819188000	0.317508000
H	6.063454000	-4.062731000	-0.242267000
H	4.594901000	-6.055263000	-0.406990000
H	2.097823000	-5.749277000	-0.406816000
O	6.602479000	-1.739266000	-0.052954000
H	7.078747000	-0.905230000	-0.140995000
O	-0.505989000	3.046994000	-0.149302000
H	-0.665130000	3.999313000	-0.162101000
C	-3.281900000	-0.527169000	0.032579000
O	-3.764088000	0.586991000	0.169888000
O	-3.973400000	-1.652367000	-0.086609000
H	-4.955663000	-1.448474000	-0.024873000
C	3.904751000	4.958681000	0.277488000
O	5.118800000	5.039673000	0.369579000
O	3.151388000	6.095484000	0.261782000
H	3.790337000	6.822176000	0.333551000
O	-0.000789000	-4.516554000	-0.340686000
C	-8.055815000	0.891788000	0.121476000
H	-7.861113000	1.725317000	0.774609000
C	-6.924597000	0.240597000	-0.664948000
H	-6.048882000	0.888403000	-0.698285000

H	-7.245168000	-0.001036000	-1.678033000
O	-6.532107000	-1.000766000	-0.027372000
H	-9.084525000	0.699892000	-0.135619000
C	-7.153314000	-1.208826000	1.221015000
O	-8.036194000	-0.307228000	1.473335000
O	-6.799386000	-2.170897000	1.873885000
C	-8.171331000	2.436138000	-1.452294000
N	-8.366166000	3.319122000	-2.199177000

### Pdt1-CN

SCF Energy (B3LYP-D3/B2) = -1998.74165036

Enthalpy 0K = 0.408916

Enthalpy 298 K = 0.442849

Free Energy 298 K = 0.341063

C	0.765744000	2.143620000	-0.277814000
C	-0.244808000	1.110707000	-0.310601000
C	0.326910000	3.490392000	-0.212962000
C	-1.618371000	1.481493000	-0.184056000
C	-1.009879000	3.860579000	-0.159188000
C	-2.024755000	2.858677000	-0.134097000
H	1.098862000	4.249195000	-0.204722000
C	-3.422995000	3.169895000	-0.086503000
C	-4.372400000	2.200407000	-0.009233000
C	-4.017730000	0.813390000	0.046234000
C	-2.628267000	0.447651000	-0.078669000
C	-4.982218000	-0.182553000	0.226094000
C	-2.266154000	-0.918459000	-0.065212000
C	-4.639990000	-1.556287000	0.250644000
C	-3.266264000	-1.920906000	0.094933000
C	0.107683000	-0.300358000	-0.412880000
C	1.417637000	-0.731581000	-0.699724000
C	-0.888835000	-1.303296000	-0.233124000
C	1.776584000	-2.078170000	-0.674523000
C	-0.514478000	-2.677647000	-0.233014000
C	0.815734000	-3.055287000	-0.409954000
H	2.174336000	0.003912000	-0.916017000
H	1.072436000	-4.107051000	-0.361460000
C	-1.520447000	-3.745392000	-0.038531000
C	-2.930462000	-3.305796000	0.119823000
C	-3.914956000	-4.267588000	0.293372000
C	-5.262807000	-3.898962000	0.451130000
C	-5.619817000	-2.565351000	0.431821000
H	-3.713451000	4.209953000	-0.110010000
H	-5.418225000	2.501029000	-0.021565000
H	-6.654494000	-2.265355000	0.555112000
H	-6.021659000	-4.663927000	0.589956000
H	-3.606281000	-5.308036000	0.305345000
O	-6.309943000	0.111148000	0.392782000
H	-6.397898000	1.052307000	0.586862000
O	2.036460000	1.888943000	-0.304096000
H	2.999730000	2.804492000	0.058530000
C	3.218685000	-2.377902000	-0.876608000
O	3.998356000	-1.604713000	-1.411345000
O	3.602204000	-3.559449000	-0.357962000
H	4.580445000	-3.545451000	-0.311217000
C	-1.322299000	5.315390000	-0.104859000
O	-2.405713000	5.843972000	0.098358000
O	-0.225935000	6.098959000	-0.308893000
H	-0.553320000	7.007951000	-0.221616000

O	-1.214374000	-4.941045000	-0.013171000
C	5.575252000	0.686114000	-0.011513000
H	5.019329000	0.739565000	-0.949270000
C	4.659861000	0.366861000	1.177546000
H	3.610296000	0.578099000	0.974423000
H	4.972527000	0.866134000	2.099055000
O	4.833559000	-1.060556000	1.345046000
H	6.175379000	1.583063000	0.131384000
C	5.868298000	-1.485169000	0.590951000
O	6.447789000	-0.468417000	-0.069342000
O	6.230133000	-2.639462000	0.534853000
C	4.854407000	3.940964000	0.810073000
N	3.886928000	3.406638000	0.409720000

### Int3-N<sub>3</sub>

SCF Energy (B3LYP-D3/B2) = -2070.11772083

Enthalpy 0K = 0.414561

Enthalpy 298 K = 0.449632

Free Energy 298 K = 0.343679

C	0.573764000	2.596291000	-0.038738000
C	1.155242000	1.303208000	0.092100000
C	1.364284000	3.737074000	-0.048777000
C	2.582570000	1.225098000	0.075028000
C	2.759633000	3.677393000	0.030098000
C	3.397240000	2.409729000	0.071685000
H	0.876541000	4.701936000	-0.126507000
C	4.828709000	2.264942000	0.112267000
C	5.418227000	1.044206000	0.082932000
C	4.654037000	-0.165927000	0.005887000
C	3.216142000	-0.075715000	0.040397000
C	5.268612000	-1.416441000	-0.103612000
C	2.441129000	-1.253808000	0.009218000
C	4.509569000	-2.613520000	-0.144807000
C	3.085666000	-2.523391000	-0.077003000
C	0.361252000	0.082065000	0.197499000
C	-1.028427000	0.092494000	0.427999000
C	1.004298000	-1.183921000	0.096915000
C	-1.790779000	-1.068801000	0.435134000
C	0.216110000	-2.369470000	0.107619000
C	-1.172133000	-2.304061000	0.237840000
H	-1.558736000	1.013816000	0.594329000
H	-1.751654000	-3.219735000	0.206950000
C	0.845779000	-3.702479000	-0.022376000
C	2.331556000	-3.731308000	-0.107376000
C	2.970998000	-4.956997000	-0.209294000
C	4.373389000	-5.035830000	-0.285066000
C	5.131861000	-3.883407000	-0.253210000
H	5.429465000	3.160327000	0.165624000
H	6.504141000	1.003994000	0.143688000
H	6.213495000	-3.928356000	-0.309734000
H	4.857762000	-6.004399000	-0.367728000
H	2.351352000	-5.847839000	-0.228431000
O	6.623882000	-1.567515000	-0.177960000
H	7.038485000	-0.707475000	-0.314745000
O	-0.768959000	2.693899000	-0.176596000
H	-1.082866000	3.605709000	-0.235112000
C	-3.275370000	-0.880055000	0.614436000
O	-3.703170000	0.176600000	1.069718000
O	-3.999000000	-1.892384000	0.196795000
H	-5.003404000	-1.593501000	0.099746000

C	3.506533000	4.961740000	0.043417000
O	4.714723000	5.126378000	0.105312000
O	2.682005000	6.046918000	-0.021319000
H	3.276434000	6.813505000	-0.003789000
O	0.187758000	-4.743112000	-0.053054000
C	-6.333229000	1.416754000	0.114055000
H	-5.797576000	1.151479000	1.026753000
C	-6.096984000	0.310725000	-0.926249000
H	-5.066985000	0.381377000	-1.300520000
H	-6.793221000	0.433894000	-1.763147000
O	-6.251714000	-0.961246000	-0.338657000
H	-7.401704000	1.496049000	0.308546000
C	-7.723335000	-1.444665000	-0.025973000
O	-8.560405000	-0.622909000	-0.392180000
O	-7.672243000	-2.536289000	0.514290000
N	-5.892468000	2.753828000	-0.379861000
N	-4.701224000	3.036267000	-0.314364000
N	-3.630965000	3.453472000	-0.308489000

### TS3-N<sub>3</sub>

SCF Energy (B3LYP-D3/B2) = -2070.07242035

Enthalpy 0K = 0.414318

Enthalpy 298 K = 0.449339

Free Energy 298 K = 0.339463

C	1.131958000	2.813437000	-0.284113000
C	1.584056000	1.471317000	-0.144387000
C	2.017602000	3.880723000	-0.279823000
C	3.001961000	1.283081000	-0.025984000
C	3.396031000	3.711105000	-0.144680000
C	3.913551000	2.396886000	-0.016700000
H	1.617035000	4.882909000	-0.386494000
C	5.322516000	2.148679000	0.133414000
C	5.812046000	0.889701000	0.231239000
C	4.957822000	-0.258214000	0.188736000
C	3.533068000	-0.059401000	0.083551000
C	5.478454000	-1.553523000	0.254006000
C	2.672502000	-1.176221000	0.082821000
C	4.632487000	-2.690281000	0.261348000
C	3.220614000	-2.491819000	0.182391000
C	0.688341000	0.312968000	-0.119970000
C	-0.718719000	0.420585000	-0.189591000
C	1.245047000	-0.996658000	-0.010178000
C	-1.553865000	-0.690415000	-0.163949000
C	0.377824000	-2.125134000	0.010859000
C	-1.003437000	-1.968815000	-0.067409000
H	-1.203301000	1.378297000	-0.264709000
H	-1.636241000	-2.848097000	-0.050806000
C	0.907468000	-3.503959000	0.118920000
C	2.383831000	-3.643307000	0.196674000
C	2.930105000	-4.914548000	0.283520000
C	4.322100000	-5.098700000	0.355507000
C	5.161368000	-4.003753000	0.343044000
H	5.987479000	2.998059000	0.170387000
H	6.884628000	0.773445000	0.373124000
H	6.236869000	-4.127455000	0.396671000
H	4.734296000	-6.101307000	0.419798000
H	2.245334000	-5.756469000	0.291703000
O	6.816724000	-1.808935000	0.321014000
H	7.313269000	-0.997925000	0.160497000

O	-0.196365000	3.075426000	-0.430785000
H	-0.332549000	4.028312000	-0.505690000
C	-3.037259000	-0.449924000	-0.241808000
O	-3.502016000	0.677137000	-0.333184000
O	-3.740845000	-1.570180000	-0.192542000
H	-4.722551000	-1.359502000	-0.286585000
C	4.246250000	4.930611000	-0.149508000
O	5.461256000	4.998906000	-0.059452000
O	3.513817000	6.074991000	-0.273511000
H	4.166552000	6.792868000	-0.265483000
O	0.172322000	-4.491099000	0.142882000
C	-7.894228000	0.905718000	-0.280872000
H	-8.875532000	0.468877000	-0.171999000
C	-6.687571000	0.257502000	0.371457000
H	-6.926578000	-0.074281000	1.384304000
H	-5.849012000	0.956766000	0.397865000
O	-6.281839000	-0.922506000	-0.350547000
H	-7.807849000	1.827775000	-0.827395000
C	-6.748181000	-0.954612000	-1.698960000
O	-7.622527000	-0.052016000	-1.926467000
O	-6.269713000	-1.814990000	-2.415362000
N	-8.250233000	2.132778000	1.339057000
N	-8.597835000	1.460072000	2.278079000
N	-8.923475000	0.802247000	3.187308000

### Pdt1-N<sub>3</sub>

SCF Energy (B3LYP-D3/B2) = -2070.09601471

Enthalpy 0K = 0.416236

Enthalpy 298 K = 0.451862

Free Energy 298 K = 0.340065

C	0.880675000	2.749053000	-0.150121000
C	1.422357000	1.435899000	-0.083044000
C	1.696324000	3.871202000	-0.150003000
C	2.852182000	1.335394000	0.000233000
C	3.086701000	3.787237000	-0.075907000
C	3.691511000	2.505917000	0.007218000
H	1.228755000	4.848020000	-0.209243000
C	5.115415000	2.345245000	0.114466000
C	5.684723000	1.117253000	0.187265000
C	4.903620000	-0.081036000	0.157134000
C	3.468648000	0.029114000	0.081947000
C	5.504500000	-1.343283000	0.208933000
C	2.679645000	-1.141924000	0.090714000
C	4.733124000	-2.531218000	0.231440000
C	3.309525000	-2.422372000	0.176195000
C	0.604232000	0.220289000	-0.087671000
C	-0.803202000	0.236374000	-0.187847000
C	1.245599000	-1.052620000	0.011465000
C	-1.563567000	-0.929888000	-0.174665000
C	0.453399000	-2.236610000	0.026221000
C	-0.934119000	-2.169465000	-0.061771000
H	-1.344852000	1.161387000	-0.278853000
H	-1.504359000	-3.090487000	-0.046245000
C	1.068622000	-3.579151000	0.132674000
C	2.547169000	-3.624386000	0.197938000
C	3.175793000	-4.861271000	0.275232000
C	4.575423000	-4.955210000	0.327560000
C	5.345070000	-3.808688000	0.303238000
H	5.727499000	3.233759000	0.142978000
H	6.765780000	1.067272000	0.301273000

H	6.426848000	-3.864487000	0.339703000
H	5.052064000	-5.929792000	0.384779000
H	2.545784000	-5.744645000	0.290058000
O	6.858705000	-1.513211000	0.249491000
H	7.297891000	-0.673259000	0.071941000
O	-0.468734000	2.930745000	-0.216457000
H	-0.666748000	3.875388000	-0.239272000
C	-3.048695000	-0.786851000	-0.286292000
O	-3.601778000	0.292788000	-0.428271000
O	-3.693803000	-1.954494000	-0.206881000
H	-4.658309000	-1.775032000	-0.322909000
C	3.857162000	5.057760000	-0.089599000
O	5.068619000	5.201705000	-0.056031000
O	3.049640000	6.156592000	-0.150319000
H	3.657002000	6.913195000	-0.156015000
O	0.391872000	-4.610149000	0.160713000
C	-7.384087000	0.957200000	-0.549079000
H	-8.472070000	0.865470000	-0.532196000
C	-6.694408000	-0.039768000	0.383835000
H	-7.362113000	-0.473468000	1.129832000
H	-5.792055000	0.372664000	0.834914000
O	-6.286471000	-1.099814000	-0.537352000
H	-7.102215000	1.987582000	-0.352752000
C	-6.318028000	-0.627818000	-1.821797000
O	-6.910356000	0.572279000	-1.872664000
O	-5.876659000	-1.237840000	-2.759064000
N	-8.102334000	2.093844000	2.049136000
N	-8.625781000	1.080477000	2.389709000
N	-9.126037000	0.051566000	2.704185000

### Int3-I

SCF Energy (B3LYP-D3/B2) = -1917.27250796

Enthalpy 0K = 0.400194

Enthalpy 298 K = 0.434549

Free Energy 298 K = 0.326683

C	-1.425950000	2.695226000	0.030021000
C	-2.050882000	1.416674000	-0.000990000
C	-2.165481000	3.865160000	-0.054901000
C	-3.484470000	1.407319000	-0.064595000
C	-3.557659000	3.866885000	-0.159968000
C	-4.244449000	2.626008000	-0.158393000
H	-1.636344000	4.811694000	-0.036485000
C	-5.677804000	2.551566000	-0.257166000
C	-6.328620000	1.364311000	-0.216798000
C	-5.628866000	0.123645000	-0.072565000
C	-4.187194000	0.142313000	-0.026082000
C	-6.313928000	-1.090790000	0.016923000
C	-3.477612000	-1.072186000	0.068032000
C	-5.622180000	-2.323928000	0.109585000
C	-4.194231000	-2.306772000	0.125319000
C	-1.312212000	0.153601000	0.037821000
C	0.099049000	0.080607000	0.008474000
C	-2.035798000	-1.075193000	0.088239000
C	0.785081000	-1.127094000	0.050308000
C	-1.320642000	-2.304554000	0.146310000
C	0.072127000	-2.324103000	0.129290000
H	0.705240000	0.967776000	-0.051676000
H	0.591316000	-3.274414000	0.170626000
C	-2.027299000	-3.603138000	0.225069000
C	-3.512600000	-3.553470000	0.210086000

C	-4.220334000	-4.743445000	0.278433000
C	-5.626448000	-4.748714000	0.268753000
C	-6.317761000	-3.557586000	0.186874000
H	-6.228528000	3.473290000	-0.367607000
H	-7.411162000	1.375794000	-0.327193000
H	-7.401595000	-3.543399000	0.178570000
H	-6.165861000	-5.689579000	0.325695000
H	-3.649749000	-5.664554000	0.340432000
O	-7.676618000	-1.171422000	0.015603000
H	-8.055038000	-0.289898000	0.114440000
O	-0.073130000	2.789830000	0.154494000
H	0.188440000	3.719194000	0.151997000
C	2.295188000	-1.083073000	0.011385000
O	2.883389000	-0.006848000	-0.061678000
O	2.845557000	-2.268971000	0.070737000
H	3.902009000	-2.217472000	0.029030000
C	-4.242012000	5.182059000	-0.256546000
O	-5.439543000	5.401756000	-0.342907000
O	-3.365412000	6.228292000	-0.240978000
H	-3.921248000	7.020668000	-0.308533000
O	-1.428993000	-4.676179000	0.301384000
C	6.067017000	0.043833000	-0.456567000
H	5.088737000	0.358582000	-0.810294000
C	5.952807000	-1.007314000	0.635544000
H	5.323816000	-0.638780000	1.453870000
H	6.944762000	-1.270223000	1.015952000
O	5.332644000	-2.141412000	0.070428000
I	7.013326000	1.929426000	0.325207000
H	6.732138000	-0.288922000	-1.249437000
C	6.241198000	-3.092219000	-0.871099000
O	7.400684000	-2.701710000	-0.908150000
O	5.528743000	-3.971225000	-1.315198000

### TS3-I

SCF Energy (B3LYP-D3/B2) = -1917.25704890

Enthalpy 0K = 0.401229

Enthalpy 298 K = 0.434880

Free Energy 298 K = 0.328048

C	-1.880785000	2.754888000	0.542922000
C	-2.399341000	1.454340000	0.287982000
C	-2.694545000	3.877580000	0.516187000
C	-3.810545000	1.365483000	0.042404000
C	-4.062520000	3.806378000	0.249394000
C	-4.646975000	2.536375000	0.010884000
H	-2.244597000	4.844807000	0.711750000
C	-6.049778000	2.388380000	-0.271477000
C	-6.606524000	1.169540000	-0.468600000
C	-5.832836000	-0.033274000	-0.405300000
C	-4.412608000	0.066751000	-0.174086000
C	-6.426245000	-1.287839000	-0.568800000
C	-3.626477000	-1.103400000	-0.153232000
C	-5.655512000	-2.476824000	-0.556767000
C	-4.245418000	-2.375013000	-0.355645000
C	-1.576855000	0.242974000	0.272707000
C	-0.174402000	0.256951000	0.444801000
C	-2.202958000	-1.021822000	0.060262000
C	0.590364000	-0.903635000	0.430788000
C	-1.408159000	-2.202559000	0.054183000
C	-0.029889000	-2.139043000	0.241732000
H	0.362071000	1.177779000	0.593516000

H	0.547439000	-3.055820000	0.235027000
C	-2.012269000	-3.538316000	-0.154708000
C	-3.483561000	-3.577467000	-0.353959000
C	-4.099085000	-4.805704000	-0.539667000
C	-5.489253000	-4.895044000	-0.730253000
C	-6.256764000	-3.748606000	-0.737517000
H	-6.654386000	3.280823000	-0.326186000
H	-7.667255000	1.129938000	-0.708106000
H	-7.329780000	-3.799165000	-0.882372000
H	-5.956516000	-5.865227000	-0.870664000
H	-3.469762000	-5.689830000	-0.530357000
O	-7.767940000	-1.451177000	-0.755143000
H	-8.224499000	-0.617646000	-0.591207000
O	-0.559090000	2.919654000	0.826891000
H	-0.373252000	3.855963000	0.971522000
C	2.077862000	-0.763706000	0.621070000
O	2.602731000	0.329994000	0.777667000
O	2.709145000	-1.924214000	0.587521000
H	3.698716000	-1.783077000	0.764930000
C	-4.832029000	5.078082000	0.239412000
O	-6.026340000	5.231454000	0.041164000
O	-4.045317000	6.164505000	0.489718000
H	-4.648873000	6.923581000	0.458475000
O	-1.340948000	-4.570224000	-0.164852000
C	7.163769000	-0.017276000	0.650445000
H	7.858895000	-0.841549000	0.704139000
C	5.731409000	-0.312323000	0.252189000
H	5.657029000	-0.550577000	-0.809268000
H	5.090119000	0.548047000	0.466238000
O	5.246088000	-1.470632000	0.940074000
I	8.198720000	0.964787000	-1.500689000
H	7.411533000	0.869289000	1.206823000
C	5.582289000	-1.472857000	2.365216000
O	6.501327000	-0.652449000	2.635155000
O	4.933943000	-2.264304000	3.030159000

### Pdt1-I

SCF Energy (B3LYP-D3/B2) = -1917.28716486

Enthalpy 0K = 0.405010

Enthalpy 298 K = 0.438856

Free Energy 298 K = 0.330704

C	-1.293037000	2.589916000	0.367923000
C	-2.021059000	1.374537000	0.247693000
C	-1.940323000	3.814837000	0.446473000
C	-3.445994000	1.486849000	0.133562000
C	-3.329809000	3.931713000	0.394233000
C	-4.110939000	2.759622000	0.224650000
H	-1.338189000	4.710642000	0.551163000
C	-5.546535000	2.805406000	0.146726000
C	-6.278983000	1.685478000	-0.065479000
C	-5.666352000	0.401382000	-0.226007000
C	-4.235291000	0.294856000	-0.092347000
C	-6.426396000	-0.738526000	-0.504876000
C	-3.617459000	-0.968648000	-0.200878000
C	-5.827314000	-2.017937000	-0.618691000
C	-4.412919000	-2.127444000	-0.454127000
C	-1.388958000	0.054211000	0.216583000
C	-0.011900000	-0.146784000	0.449093000

C	-2.192249000	-1.097999000	-0.035474000
C	0.575023000	-1.406929000	0.387653000
C	-1.575601000	-2.379034000	-0.106401000
C	-0.205677000	-2.524971000	0.092093000
H	0.639199000	0.677108000	0.685378000
H	0.231603000	-3.514056000	0.026425000
C	-2.363853000	-3.601171000	-0.388286000
C	-3.826227000	-3.420433000	-0.560456000
C	-4.610932000	-4.534066000	-0.822180000
C	-6.001053000	-4.413629000	-0.990709000
C	-6.601204000	-3.174738000	-0.891312000
H	-6.031989000	3.762420000	0.263011000
H	-7.362408000	1.784305000	-0.084949000
H	-7.671962000	-3.064442000	-1.018410000
H	-6.600774000	-5.294749000	-1.198541000
H	-4.112434000	-5.495483000	-0.892234000
O	-7.778293000	-0.697892000	-0.680142000
H	-8.071881000	0.218297000	-0.748759000
O	0.067460000	2.565945000	0.398081000
H	0.411043000	3.466885000	0.451573000
C	2.046433000	-1.493079000	0.647798000
O	2.709627000	-0.534082000	1.008411000
O	2.545063000	-2.714220000	0.433792000
H	3.511938000	-2.683044000	0.635406000
C	-3.913745000	5.295226000	0.507343000
O	-5.092453000	5.609146000	0.482518000
O	-2.959999000	6.258032000	0.655040000
H	-3.450448000	7.093017000	0.716638000
O	-1.840972000	-4.713192000	-0.474796000
C	6.486797000	-0.323617000	1.352347000
H	7.562624000	-0.507115000	1.350992000
C	5.750735000	-1.096011000	0.253590000
H	6.408938000	-1.459182000	-0.531490000
H	4.922059000	-0.530137000	-0.170678000
O	5.196238000	-2.235838000	0.986252000
I	7.768620000	1.238305000	-1.567925000
H	6.307978000	0.747940000	1.311859000
C	5.216457000	-1.969213000	2.330080000
O	5.916964000	-0.857931000	2.583439000
O	4.676117000	-2.667640000	3.146018000

#### Int4-Cl

SCF Energy (B3LYP-D3/B2) = -2519.98482765

Enthalpy 0K = 0.461907

Enthalpy 298 K = 0.499852

Free Energy 298 K = 0.385361

C	-0.877564000	2.453624000	0.224508000
C	-1.475080000	1.168558000	0.072008000
C	-1.652664000	3.608083000	0.144702000
C	-2.901708000	1.110051000	-0.001593000
C	-3.039573000	3.565131000	-0.016574000
C	-3.696943000	2.305982000	-0.058774000
H	-1.147960000	4.562883000	0.227599000
C	-5.126687000	2.182311000	-0.160303000
C	-5.737714000	0.971489000	-0.146597000
C	-4.994896000	-0.249688000	-0.040024000
C	-3.555760000	-0.180826000	-0.009473000
C	-5.631441000	-1.492013000	0.028998000
C	-2.800621000	-1.372168000	0.030369000

C	-4.893511000	-2.701556000	0.071678000
C	-3.466439000	-2.632984000	0.054145000
C	-0.693620000	-0.065391000	-0.002801000
C	0.709915000	-0.069811000	-0.144873000
C	-1.360405000	-1.322232000	0.007918000
C	1.450025000	-1.243727000	-0.212148000
C	-0.591987000	-2.521376000	-0.030434000
C	0.797385000	-2.475104000	-0.127533000
H	1.242948000	0.859953000	-0.202914000
H	1.365405000	-3.398330000	-0.152708000
C	-1.246383000	-3.848068000	0.023736000
C	-2.733398000	-3.854455000	0.069741000
C	-3.395091000	-5.071826000	0.115844000
C	-4.800114000	-5.129142000	0.149350000
C	-5.538576000	-3.963469000	0.126694000
H	-5.710057000	3.086542000	-0.248102000
H	-6.820370000	0.946643000	-0.254674000
H	-6.622109000	-3.991598000	0.147942000
H	-5.302374000	-6.091321000	0.190120000
H	-2.790622000	-5.973198000	0.124341000
O	-6.991780000	-1.620564000	0.051780000
H	-7.393089000	-0.756795000	0.204529000
O	0.436697000	2.544364000	0.476845000
H	0.858236000	3.431144000	0.293662000
C	2.946851000	-1.185514000	-0.359431000
O	3.638628000	-2.196015000	-0.321015000
O	3.393889000	0.046043000	-0.528615000
H	4.426386000	0.090681000	-0.603999000
C	-3.764982000	4.859873000	-0.109450000
O	-4.966059000	5.039344000	-0.240604000
O	-2.929289000	5.934236000	-0.035810000
H	-3.509705000	6.707923000	-0.111414000
O	-0.605227000	-4.900169000	0.027748000
C	6.799103000	-1.603131000	0.508882000
H	5.814211000	-1.951441000	0.818297000
C	6.721627000	-0.912890000	-0.847015000
H	6.260748000	-1.582844000	-1.579977000
H	7.724212000	-0.624802000	-1.175005000
O	5.900352000	0.238359000	-0.742828000
Cl	7.875380000	-3.086283000	0.416094000
H	7.247072000	-0.930764000	1.239033000
C	6.520521000	1.490365000	-0.089985000
O	7.701055000	1.349282000	0.216658000
O	5.669568000	2.375007000	-0.018558000
C	3.274149000	3.597001000	-0.272050000
C	3.097623000	4.089933000	1.085415000
O	2.120395000	4.450265000	0.065853000
H	4.007712000	4.067377000	-0.916106000
H	3.046047000	2.558473000	-0.489852000
H	3.698649000	4.922507000	1.444421000
H	2.725117000	3.410376000	1.849987000

#### TS4-Cl

SCF Energy (B3LYP-D3/B2) = -2519.96518236

Enthalpy 0K = 0.459194

Enthalpy 298 K = 0.496115

Free Energy 298 K = 0.385633

C	-0.671691000	2.386140000	0.057972000
C	-1.388078000	1.144190000	-0.026011000

C	-1.383050000	3.590747000	-0.062711000
C	-2.813639000	1.184515000	-0.088137000
C	-2.769596000	3.639383000	-0.196179000
C	-3.522793000	2.430616000	-0.185422000
H	-0.805109000	4.505831000	-0.033161000
C	-4.956322000	2.405212000	-0.273224000
C	-5.655400000	1.242550000	-0.217206000
C	-5.000153000	-0.024058000	-0.071071000
C	-3.559454000	-0.056785000	-0.043637000
C	-5.722339000	-1.215871000	0.042056000
C	-2.893782000	-1.300063000	0.043472000
C	-5.074544000	-2.473122000	0.130675000
C	-3.645929000	-2.508054000	0.116136000
C	-0.706559000	-0.147738000	-0.033547000
C	0.691506000	-0.255537000	-0.145856000
C	-1.454895000	-1.355100000	0.029520000
C	1.355819000	-1.477355000	-0.129608000
C	-0.768820000	-2.604750000	0.060139000
C	0.623774000	-2.659530000	-0.002787000
H	1.267980000	0.643807000	-0.238089000
H	1.122356000	-3.621685000	0.035384000
C	-1.516689000	-3.878423000	0.157061000
C	-3.000626000	-3.776973000	0.186222000
C	-3.747954000	-4.941628000	0.276268000
C	-5.153594000	-4.896995000	0.302702000
C	-5.807234000	-3.683232000	0.231292000
H	-5.474870000	3.345267000	-0.389270000
H	-6.737425000	1.291761000	-0.323681000
H	-6.890170000	-3.633517000	0.248897000
H	-5.723583000	-5.818636000	0.378183000
H	-3.209796000	-5.882836000	0.325935000
O	-7.089951000	-1.243324000	0.067992000
H	-7.421836000	-0.346731000	0.197138000
O	0.626411000	2.400338000	0.262417000
H	1.299887000	3.287188000	0.037879000
C	2.850674000	-1.490719000	-0.209809000
O	3.533865000	-2.490591000	-0.049495000
O	3.335134000	-0.274799000	-0.473639000
H	4.327212000	-0.187108000	-0.397219000
C	-3.404196000	4.978927000	-0.325869000
O	-4.591553000	5.239433000	-0.452768000
O	-2.497758000	5.996969000	-0.294896000
H	-3.029130000	6.802828000	-0.391372000
O	-0.950633000	-4.972752000	0.209330000
C	6.888939000	-1.686872000	-0.010409000
H	5.924168000	-2.195457000	0.033843000
C	6.825764000	-0.444869000	-0.891764000
H	6.514390000	-0.711193000	-1.906768000
H	7.800319000	0.047744000	-0.918866000
O	5.836930000	0.454256000	-0.386299000
Cl	8.095198000	-2.874163000	-0.702368000
H	7.238360000	-1.414044000	0.984212000
C	6.244258000	1.284043000	0.756784000
O	7.379660000	1.106469000	1.182087000
O	5.321590000	2.054459000	1.120714000
C	3.725659000	2.910668000	0.050260000
C	3.144857000	3.819864000	1.022582000
O	2.309422000	4.058756000	-0.111818000
H	4.411881000	3.294610000	-0.688463000
H	3.276169000	1.942594000	-0.101288000
H	3.743174000	4.683783000	1.322932000
H	2.639226000	3.357756000	1.875667000

## Pdt2-Cl

SCF Energy (B3LYP-D3/B2) = -2520.01774480

Enthalpy 0K = 0.466370

Enthalpy 298 K = 0.503300

Free Energy 298 K = 0.393057

C	-0.608960000	2.389140000	-0.423981000
C	-1.351910000	1.138737000	-0.341400000
C	-1.366051000	3.594747000	-0.322002000
C	-2.766523000	1.175911000	-0.150936000
C	-2.740408000	3.634487000	-0.162763000
C	-3.487030000	2.417807000	-0.076866000
H	-0.789765000	4.510386000	-0.370509000
C	-4.911777000	2.390629000	0.040476000
C	-5.605814000	1.224774000	0.147382000
C	-4.932688000	-0.038755000	0.163743000
C	-3.501279000	-0.066858000	-0.017111000
C	-5.629378000	-1.236374000	0.354383000
C	-2.831227000	-1.312811000	-0.044842000
C	-4.978040000	-2.492417000	0.330840000
C	-3.563634000	-2.524315000	0.121541000
C	-0.678832000	-0.149541000	-0.421955000
C	0.704989000	-0.252106000	-0.668555000
C	-1.407757000	-1.362237000	-0.246977000
C	1.369327000	-1.478802000	-0.672062000
C	-0.720009000	-2.611325000	-0.275566000
C	0.659084000	-2.663610000	-0.462374000
H	1.245969000	0.664028000	-0.838017000
H	1.161451000	-3.624201000	-0.450001000
C	-1.446647000	-3.889085000	-0.100382000
C	-2.914692000	-3.792996000	0.102322000
C	-3.642025000	-4.961372000	0.279800000
C	-5.032000000	-4.919660000	0.487750000
C	-5.689072000	-3.705456000	0.515936000
H	-5.440555000	3.332712000	0.044543000
H	-6.692464000	1.270916000	0.180345000
H	-6.759870000	-3.656849000	0.680052000
H	-5.587294000	-5.842757000	0.629441000
H	-3.099608000	-5.901142000	0.256461000
O	-6.982534000	-1.260525000	0.575765000
H	-7.270630000	-0.370086000	0.811567000
O	0.658094000	2.462024000	-0.577829000
H	1.714413000	3.748960000	-0.580202000
C	2.843040000	-1.511257000	-0.821631000
O	3.557872000	-2.472973000	-0.581913000
O	3.342610000	-0.323067000	-1.235990000
H	4.302855000	-0.305802000	-1.089211000
C	-3.386484000	4.971623000	-0.061137000
O	-4.531710000	5.229084000	0.281038000
O	-2.546888000	5.994268000	-0.393941000
H	-3.074963000	6.796037000	-0.254279000
O	-0.870648000	-4.981039000	-0.120060000
C	6.669007000	-1.645554000	0.311175000
H	5.756297000	-2.104091000	-0.074660000
C	6.938294000	-0.283582000	-0.318368000
H	7.031618000	-0.367456000	-1.403092000
H	7.843408000	0.161494000	0.099616000
O	5.818003000	0.608383000	-0.108919000
Cl	8.058359000	-2.747004000	-0.096052000
H	6.626165000	-1.560725000	1.395723000

C	5.752875000	1.170147000	1.144460000
O	6.508984000	0.873855000	2.041601000
O	4.792867000	2.068226000	1.270003000
C	3.989611000	2.543935000	0.142806000
C	3.209645000	3.763251000	0.636936000
O	2.496043000	4.341878000	-0.423110000
H	4.647989000	2.818226000	-0.686004000
H	3.309933000	1.754904000	-0.178073000
H	3.919348000	4.501989000	1.032889000
H	2.560260000	3.449188000	1.469296000

### Int4-CN

SCF Energy (B3LYP-D3/B2) = -2152.62989672

Enthalpy 0K = 0.469829

Enthalpy 298 K = 0.508256

Free Energy 298 K = 0.392748

C	-0.817216000	2.437838000	-0.658676000
C	-1.378086000	1.154032000	-0.401008000
C	-1.576773000	3.590808000	-0.476325000
C	-2.780216000	1.092512000	-0.122053000
C	-2.926764000	3.547300000	-0.121691000
C	-3.566844000	2.286612000	0.021435000
H	-1.091341000	4.545046000	-0.639630000
C	-4.970604000	2.161566000	0.310833000
C	-5.571127000	0.949151000	0.403942000
C	-4.839520000	-0.271856000	0.238188000
C	-3.417537000	-0.199235000	0.015894000
C	-5.469649000	-1.518075000	0.297965000
C	-2.663770000	-1.388539000	-0.073371000
C	-4.732544000	-2.725726000	0.212176000
C	-3.315336000	-2.651363000	0.046628000
C	-0.583770000	-0.074845000	-0.392648000
C	0.825549000	-0.069697000	-0.455990000
C	-1.233700000	-1.332123000	-0.242956000
C	1.580000000	-1.235158000	-0.395582000
C	-0.455226000	-2.525254000	-0.234774000
C	0.934927000	-2.469991000	-0.305881000
H	1.351140000	0.861629000	-0.550391000
H	1.510984000	-3.388149000	-0.279271000
C	-1.097973000	-3.855642000	-0.137799000
C	-2.578917000	-3.869841000	-0.002179000
C	-3.229873000	-5.090313000	0.090992000
C	-4.627713000	-5.153987000	0.233843000
C	-5.368091000	-3.990954000	0.295019000
H	-5.542758000	3.066105000	0.452435000
H	-6.630808000	0.923773000	0.650442000
H	-6.445464000	-4.023573000	0.411015000
H	-5.122293000	-6.118672000	0.300117000
H	-2.622665000	-5.988995000	0.051093000
O	-6.820245000	-1.651967000	0.454285000
H	-7.245691000	-0.796680000	0.320200000
O	0.445077000	2.542411000	-1.114493000
H	0.908602000	3.380527000	-0.829793000
C	3.082667000	-1.164658000	-0.405998000
O	3.776207000	-2.169709000	-0.300968000
O	3.533418000	0.070763000	-0.526169000
H	4.564197000	0.130404000	-0.468815000
C	-3.636648000	4.841410000	0.060099000
O	-4.813405000	5.019263000	0.334730000
O	-2.816033000	5.915987000	-0.110613000

H	-3.383415000	6.689686000	0.033279000
O	-0.450827000	-4.903505000	-0.166179000
C	6.921266000	-1.700038000	0.591832000
H	5.901010000	-2.061525000	0.756138000
C	6.914937000	-0.762579000	-0.635987000
H	6.551547000	-1.306259000	-1.514826000
H	7.928455000	-0.394158000	-0.820442000
O	6.042778000	0.327601000	-0.423968000
H	7.247974000	-1.108313000	1.452461000
C	6.528034000	1.437263000	0.531571000
O	7.672185000	1.260747000	0.942435000
O	5.635504000	2.269625000	0.674419000
C	3.270539000	3.499121000	-0.029400000
C	2.390876000	3.598494000	1.129394000
O	2.037910000	4.303234000	-0.092041000
H	4.189034000	4.072262000	-0.056207000
H	3.263260000	2.584836000	-0.614186000
H	2.654078000	4.248820000	1.960823000
H	1.741740000	2.758779000	1.374253000
C	7.817526000	-2.841611000	0.418616000
N	8.537331000	-3.739837000	0.257590000

### TS4-CN

SCF Energy (B3LYP-D3/B2) = -2152.60977877

Enthalpy 0K = 0.467476

Enthalpy 298 K = 0.504718

Free Energy 298 K = 0.394397

C	-0.583496000	2.359526000	-0.700121000
C	-1.268594000	1.123481000	-0.454225000
C	-1.273455000	3.568087000	-0.516910000
C	-2.672109000	1.167849000	-0.187874000
C	-2.630785000	3.624930000	-0.207766000
C	-3.372827000	2.416948000	-0.073752000
H	-0.704190000	4.479461000	-0.648804000
C	-4.785791000	2.398293000	0.184811000
C	-5.476449000	1.234873000	0.295526000
C	-4.828927000	-0.038487000	0.180262000
C	-3.402666000	-0.072225000	-0.025540000
C	-5.543890000	-1.236266000	0.275047000
C	-2.735466000	-1.316752000	-0.064106000
C	-4.893367000	-2.494741000	0.246756000
C	-3.472545000	-2.525743000	-0.096374000
C	-0.576224000	-0.163518000	-0.433988000
C	0.823794000	-0.261600000	-0.538567000
C	-1.306216000	-1.367895000	-0.232206000
C	1.501050000	-1.472056000	-0.431743000
C	-0.609846000	-2.610900000	-0.178992000
C	0.781218000	-2.655956000	-0.261426000
H	1.390259000	0.636128000	-0.697114000
H	1.289452000	-3.610861000	-0.187184000
C	-1.342566000	-3.887585000	-0.020854000
C	-2.821304000	-3.793369000	0.103504000
C	-3.556452000	-4.961465000	0.238129000
C	-4.956538000	-4.922207000	0.366774000
C	-5.615190000	-3.709090000	0.371599000
H	-5.294706000	3.344531000	0.292721000
H	-6.539174000	1.291737000	0.523147000
H	-6.693471000	-3.662773000	0.474924000
H	-5.517793000	-5.846938000	0.465722000
H	-3.013188000	-5.901042000	0.240819000

O	-6.904012000	-1.267789000	0.416022000
H	-7.261377000	-0.389599000	0.237814000
O	0.671106000	2.382873000	-1.110742000
H	1.344555000	3.210951000	-0.753254000
C	2.996006000	-1.470460000	-0.442516000
O	3.678743000	-2.447361000	-0.170269000
O	3.488526000	-0.272243000	-0.765611000
H	4.456540000	-0.162786000	-0.546518000
C	-3.248437000	4.969577000	-0.051006000
O	-4.422038000	5.237866000	0.159750000
O	-2.342284000	5.981307000	-0.165398000
H	-2.861236000	6.792273000	-0.046576000
O	-0.767358000	-4.977977000	0.004137000
C	6.967991000	-1.686873000	0.213364000
H	5.991545000	-2.164162000	0.062856000
C	7.020154000	-0.352870000	-0.560493000
H	6.930995000	-0.530489000	-1.636828000
H	7.959559000	0.164126000	-0.349525000
O	5.920025000	0.477497000	-0.202320000
H	7.081830000	-1.457772000	1.277217000
C	6.021215000	1.152800000	1.096514000
O	7.045823000	0.951046000	1.737940000
O	4.996040000	1.835531000	1.343510000
C	3.711374000	2.877202000	0.073634000
C	2.667720000	3.337229000	0.974121000
O	2.255032000	3.965119000	-0.236520000
H	4.519048000	3.547572000	-0.174427000
H	3.518480000	2.021140000	-0.554107000
H	2.960130000	4.034453000	1.763598000
H	1.987333000	2.565676000	1.350212000
C	8.031690000	-2.597047000	-0.206805000
N	8.886307000	-3.298674000	-0.563403000

## Pdt2-CN

SCF Energy (B3LYP-D3/B2) = -2152.66007065

Enthalpy 0K = 0.474015

Enthalpy 298 K = 0.511504

Free Energy 298 K = 0.400510

C	-0.477862000	2.378140000	-0.466023000
C	-1.234614000	1.138318000	-0.357994000
C	-1.215177000	3.594107000	-0.345040000
C	-2.643880000	1.194777000	-0.133867000
C	-2.585223000	3.652367000	-0.158574000
C	-3.345286000	2.446404000	-0.045597000
H	-0.629660000	4.502186000	-0.419208000
C	-4.753927000	2.441265000	0.199385000
C	-5.460716000	1.285439000	0.327852000
C	-4.819543000	0.009466000	0.225757000
C	-3.392477000	-0.037784000	0.016467000
C	-5.542457000	-1.183272000	0.333062000
C	-2.740292000	-1.292868000	-0.026205000
C	-4.906968000	-2.447478000	0.309185000
C	-3.487839000	-2.495140000	0.139364000
C	-0.578739000	-0.158868000	-0.437623000
C	0.800491000	-0.280828000	-0.699556000
C	-1.319189000	-1.360867000	-0.238249000
C	1.451937000	-1.514641000	-0.686285000
C	-0.645233000	-2.617710000	-0.252482000

C	0.731858000	-2.687993000	-0.447029000
H	1.348505000	0.626495000	-0.892491000
H	1.224008000	-3.653564000	-0.419890000
C	-1.384623000	-3.884874000	-0.053691000
C	-2.854289000	-3.771646000	0.125701000
C	-3.600205000	-4.932240000	0.274853000
C	-4.996060000	-4.875517000	0.434126000
C	-5.639582000	-3.653827000	0.448017000
H	-5.259531000	3.392262000	0.284168000
H	-6.520585000	1.352805000	0.564895000
H	-6.715662000	-3.594202000	0.567928000
H	-5.567222000	-5.793148000	0.544526000
H	-3.068740000	-5.878416000	0.259946000
O	-6.905405000	-1.195112000	0.479815000
H	-7.246042000	-0.318629000	0.263049000
O	0.784980000	2.433679000	-0.659608000
H	1.862499000	3.701257000	-0.638031000
C	2.922964000	-1.563221000	-0.845295000
O	3.632799000	-2.522641000	-0.578462000
O	3.430826000	-0.393733000	-1.300642000
H	4.390658000	-0.379759000	-1.151472000
C	-3.217779000	4.998555000	-0.097374000
O	-4.406300000	5.273755000	-0.176215000
O	-2.310006000	6.005355000	0.054292000
H	-2.842886000	6.816052000	0.044760000
O	-0.818278000	-4.981903000	-0.046236000
C	6.707437000	-1.801728000	0.325027000
H	5.762970000	-2.204849000	-0.063542000
C	7.006706000	-0.429087000	-0.303622000
H	7.119984000	-0.511231000	-1.386745000
H	7.911079000	0.003566000	0.129605000
O	5.903415000	0.481541000	-0.117684000
H	6.606325000	-1.677068000	1.406904000
C	5.814188000	1.029868000	1.141263000
O	6.542523000	0.706859000	2.052489000
O	4.868206000	1.942251000	1.253925000
C	4.100175000	2.447374000	0.114020000
C	3.336586000	3.678822000	0.603367000
O	2.654049000	4.276934000	-0.466069000
H	4.782885000	2.714184000	-0.697287000
H	3.409956000	1.676839000	-0.228217000
H	4.053490000	4.400793000	1.016708000
H	2.666210000	3.372219000	1.421611000
C	7.795635000	-2.737285000	0.044712000
N	8.677312000	-3.453114000	-0.196856000

## Int4-N<sub>3</sub>

SCF Energy (B3LYP-D3/B2) = -2223.98711484

Enthalpy 0K = 0.474426

Enthalpy 298 K = 0.513872

Free Energy 298 K = 0.395302

C	1.012825000	2.497410000	-0.234962000
C	1.558693000	1.189968000	-0.078905000
C	1.833840000	3.619979000	-0.160231000
C	2.982014000	1.074393000	-0.007957000
C	3.218325000	3.521981000	-0.002102000
C	3.824778000	2.237587000	0.042445000
H	1.367629000	4.593963000	-0.245219000
C	5.248727000	2.057000000	0.140092000
C	5.810519000	0.822533000	0.129792000

C	5.018889000	-0.368274000	0.031525000
C	3.583600000	-0.241780000	0.004809000
C	5.604811000	-1.635553000	-0.032620000
C	2.781168000	-1.402085000	-0.025871000
C	4.818800000	-2.814706000	-0.065848000
C	3.395725000	-2.688747000	-0.044011000
C	0.728825000	-0.011402000	0.004082000
C	-0.673159000	0.041547000	0.148624000
C	1.344211000	-1.294185000	0.000395000
C	-1.459918000	-1.100870000	0.227506000
C	0.528084000	-2.461048000	0.049307000
C	-0.858082000	-2.358427000	0.150743000
H	-1.168159000	0.992435000	0.199178000
H	-1.462622000	-3.257954000	0.184837000
C	1.128636000	-3.813348000	0.001310000
C	2.614094000	-3.879767000	-0.049643000
C	3.226131000	-5.123014000	-0.090511000
C	4.627613000	-5.236957000	-0.128476000
C	5.412440000	-4.101849000	-0.115424000
H	5.868248000	2.937408000	0.222098000
H	6.891658000	0.754627000	0.234516000
H	6.493881000	-4.173666000	-0.140153000
H	5.090603000	-6.218796000	-0.165088000
H	2.585906000	-5.999397000	-0.091375000
O	6.958799000	-1.818747000	-0.059019000
H	7.393956000	-0.972681000	-0.218047000
O	-0.297209000	2.640859000	-0.486947000
H	-0.684687000	3.540412000	-0.291461000
C	-2.952244000	-0.977690000	0.378173000
O	-3.687334000	-1.958509000	0.351941000
O	-3.345996000	0.273435000	0.532509000
H	-4.379297000	0.365645000	0.609549000
C	3.995299000	4.786850000	0.084718000
O	5.203163000	4.918471000	0.210241000
O	3.202902000	5.893642000	0.012356000
H	3.814179000	6.643610000	0.083615000
O	0.445828000	-4.838722000	0.005742000
C	-6.676015000	-1.181531000	-0.738872000
H	-5.650568000	-1.375494000	-1.069184000
C	-6.647111000	-0.612634000	0.683740000
H	-6.200359000	-1.347969000	1.362901000
H	-7.665000000	-0.371872000	1.004346000
O	-5.836454000	0.547688000	0.738407000
H	-7.152953000	-0.453837000	-1.394302000
C	-6.424136000	1.848706000	0.154365000
O	-7.593110000	1.739090000	-0.204895000
O	-5.566782000	2.729570000	0.180277000
C	-3.082552000	3.802821000	0.339665000
C	-2.921803000	4.281254000	-1.025015000
O	-1.903520000	4.604791000	-0.033959000
H	-3.778194000	4.306965000	0.999915000
H	-2.891697000	2.756774000	0.557676000
H	-3.497130000	5.136517000	-1.372570000
H	-2.598415000	3.583218000	-1.795338000
N	-7.493803000	-2.418730000	-0.830227000
N	-7.024323000	-3.435530000	-0.316328000
N	-6.715793000	-4.454514000	0.107386000

#### TS4-N<sub>3</sub>

SCF Energy (B3LYP-D3/B2) = -2223.96709267  
 Enthalpy 0K = 0.471648

Enthalpy 298 K = 0.510144  
 Free Energy 298 K = 0.395169

C	0.838112000	2.425027000	-0.041451000
C	1.503797000	1.153947000	0.022702000
C	1.593086000	3.597044000	0.126215000
C	2.928206000	1.136472000	0.116470000
C	2.977305000	3.587653000	0.288485000
C	3.682970000	2.350796000	0.261069000
H	1.051732000	4.534561000	0.110006000
C	5.112181000	2.266920000	0.377907000
C	5.766679000	1.079416000	0.307096000
C	5.066076000	-0.156492000	0.115791000
C	3.626146000	-0.131788000	0.056768000
C	5.743845000	-1.372800000	-0.010896000
C	2.914921000	-1.345598000	-0.074830000
C	5.049931000	-2.601204000	-0.143695000
C	3.621089000	-2.580224000	-0.160503000
C	0.772818000	-0.110107000	-0.018737000
C	-0.630686000	-0.165472000	0.056826000
C	1.475068000	-1.344279000	-0.093579000
C	-1.341167000	-1.359810000	-0.000758000
C	0.741984000	-2.565051000	-0.168625000
C	-0.652723000	-2.566863000	-0.136538000
H	-1.173922000	0.753837000	0.153718000
H	-1.186941000	-3.507906000	-0.206018000
C	1.441881000	-3.864552000	-0.280267000
C	2.928849000	-3.820848000	-0.275033000
C	3.632247000	-5.011572000	-0.377170000
C	5.038788000	-5.021647000	-0.372449000
C	5.737226000	-3.836488000	-0.257818000
H	5.664166000	3.182731000	0.528441000
H	6.847220000	1.083488000	0.437271000
H	6.821398000	-3.828950000	-0.251069000
H	5.574138000	-5.962973000	-0.457892000
H	3.059201000	-5.929471000	-0.461018000
O	7.109553000	-1.453368000	-0.008352000
H	7.478796000	-0.567660000	-0.107755000
O	-0.453956000	2.496763000	-0.270990000
H	-1.096414000	3.402748000	-0.029928000
C	-2.836601000	-1.316276000	0.048897000
O	-3.554673000	-2.288132000	-0.132477000
O	-3.279148000	-0.084814000	0.312191000
H	-4.266853000	0.041295000	0.230138000
C	3.660513000	4.897494000	0.466020000
O	4.854437000	5.108052000	0.620864000
O	2.794683000	5.950558000	0.446865000
H	3.354806000	6.732247000	0.574529000
O	0.835038000	-4.934149000	-0.371692000
C	-6.883803000	-1.363239000	-0.256736000
H	-5.910838000	-1.859748000	-0.348350000
C	-6.773078000	-0.155387000	0.680864000
H	-6.478411000	-0.479391000	1.686357000
H	-7.731335000	0.367526000	0.729368000
O	-5.750838000	0.734767000	0.235030000
H	-7.211740000	-1.009880000	-1.233607000
C	-6.115675000	1.632976000	-0.868859000
O	-7.255254000	1.524415000	-1.306227000
O	-5.159186000	2.379635000	-1.193493000
C	-3.539159000	3.130553000	-0.082233000
C	-2.903962000	4.036514000	-1.023166000
O	-2.075079000	4.210447000	0.127592000

H	-4.217288000	3.527480000	0.657084000
H	-3.135069000	2.139989000	0.050988000
H	-3.459114000	4.933214000	-1.310049000
H	-2.406970000	3.573109000	-1.880627000
N	-7.926242000	-2.312012000	0.212481000
N	-7.622241000	-3.040659000	1.158673000
N	-7.474709000	-3.777376000	2.023607000

### Pdt2-N<sub>3</sub>

SCF Energy (B3LYP-D3/B2) = -2224.01954266

Enthalpy 0K = 0.478787

Enthalpy 298 K = 0.517309

Free Energy 298 K = 0.402459

C	0.779459000	2.408441000	0.415622000
C	1.476229000	1.132002000	0.329433000
C	1.585261000	3.585314000	0.363898000
C	2.895642000	1.117700000	0.175656000
C	2.963990000	3.574594000	0.241749000
C	3.665117000	2.331775000	0.146341000
H	1.043692000	4.521529000	0.419327000
C	5.090192000	2.251243000	0.061774000
C	5.741037000	1.061564000	-0.054219000
C	5.020324000	-0.174172000	-0.112630000
C	3.585015000	-0.149997000	0.034232000
C	5.674728000	-1.394097000	-0.311781000
C	2.867132000	-1.369336000	0.021588000
C	4.975235000	-2.624120000	-0.328302000
C	3.556167000	-2.605044000	-0.151683000
C	0.752766000	-0.130479000	0.370413000
C	-0.639065000	-0.183546000	0.584226000
C	1.438533000	-1.367287000	0.190243000
C	-1.349874000	-1.383541000	0.551737000
C	0.702890000	-2.589124000	0.180627000
C	-0.681042000	-2.591292000	0.336556000
H	-1.148447000	0.749857000	0.757178000
H	-1.219342000	-3.531417000	0.295727000
C	1.383825000	-3.890633000	-0.003345000
C	2.858727000	-3.847737000	-0.171658000
C	3.544642000	-5.039914000	-0.355675000
C	4.939615000	-5.048242000	-0.531767000
C	5.643282000	-3.860138000	-0.521327000
H	5.654912000	3.171785000	0.090562000
H	6.829135000	1.065865000	-0.061134000
H	6.718681000	-3.850058000	-0.660319000
H	5.462207000	-5.989369000	-0.679076000
H	2.966253000	-5.958252000	-0.362669000
O	7.030741000	-1.466558000	-0.502713000
H	7.358383000	-0.583574000	-0.713626000
O	-0.488187000	2.527298000	0.530949000
H	-1.493125000	3.852108000	0.601368000
C	-2.826621000	-1.359984000	0.667138000
O	-3.573048000	-2.290355000	0.399869000
O	-3.288323000	-0.157268000	1.082571000
H	-4.243125000	-0.096868000	0.913854000
C	3.663716000	4.887391000	0.189367000
O	4.827307000	5.107483000	-0.114835000
O	2.854954000	5.934340000	0.522841000
H	3.417438000	6.717727000	0.417422000
O	0.765991000	-4.959550000	-0.017855000

C	-6.619860000	-1.313840000	-0.614686000
H	-5.688427000	-1.781744000	-0.276358000
C	-6.848424000	0.022722000	0.099919000
H	-6.943279000	-0.124479000	1.179526000
H	-7.745375000	0.512339000	-0.285249000
O	-5.710706000	0.902549000	-0.049540000
H	-6.565769000	-1.136661000	-1.688338000
C	-5.631030000	1.543220000	-1.262873000
O	-6.401927000	1.335352000	-2.172226000
O	-4.639563000	2.412879000	-1.336355000
C	-3.805561000	2.775680000	-0.189841000
C	-2.991486000	4.002531000	-0.604541000
O	-2.251217000	4.483751000	0.485154000
H	-4.442437000	3.009196000	0.667731000
H	-3.149210000	1.942624000	0.060983000
H	-3.681554000	4.788546000	-0.939467000
H	-2.360015000	3.729042000	-1.464772000
N	-7.790060000	-2.195985000	-0.393899000
N	-7.777463000	-2.868056000	0.642643000
N	-7.895642000	-3.547031000	1.555159000

### Int4-I

SCF Energy (B3LYP-D3/B2) = -2071.14329429

Enthalpy 0K = 0.460794

Enthalpy 298 K = 0.499134

Free Energy 298 K = 0.382300

C	-2.171512000	2.473994000	0.227266000
C	-2.538112000	1.105649000	0.069572000
C	-3.137449000	3.475955000	0.174391000
C	-3.933771000	0.799597000	0.017508000
C	-4.498214000	3.192921000	0.035032000
C	-4.926355000	1.838756000	-0.012405000
H	-2.805741000	4.503475000	0.260674000
C	-6.314198000	1.468406000	-0.092783000
C	-6.704289000	0.169449000	-0.085162000
C	-5.758127000	-0.904250000	-0.006029000
C	-4.352726000	-0.585534000	0.003693000
C	-6.167029000	-2.239292000	0.056222000
C	-3.400870000	-1.627122000	0.017493000
C	-5.228860000	-3.301797000	0.072748000
C	-3.836127000	-2.985009000	0.035540000
C	-1.554808000	0.027657000	-0.030848000
C	-0.174328000	0.269325000	-0.191819000
C	-1.992000000	-1.326350000	-0.025245000
C	0.757908000	-0.756936000	-0.282149000
C	-1.027024000	-2.372656000	-0.088320000
C	0.331351000	-2.084075000	-0.203431000
H	0.187505000	1.278285000	-0.246175000
H	1.050944000	-2.893984000	-0.246816000
C	-1.439165000	-3.793742000	-0.040993000
C	-2.901274000	-4.059932000	0.025615000
C	-3.339742000	-5.374509000	0.065868000
C	-4.712511000	-5.676490000	0.118416000
C	-5.643109000	-4.657387000	0.120935000
H	-7.047788000	2.257738000	-0.159427000
H	-7.767829000	-0.042803000	-0.176100000
H	-6.704658000	-4.874339000	0.157139000
H	-5.038605000	-6.711902000	0.154125000
H	-2.587322000	-6.156597000	0.054630000
O	-7.483359000	-2.603769000	0.097022000

H	-8.027172000	-1.824770000	0.264008000
O	-0.888641000	2.791050000	0.457941000
H	-0.633879000	3.740774000	0.284654000
C	2.219052000	-0.437202000	-0.446620000
O	3.077434000	-1.311234000	-0.427769000
O	2.442290000	0.855398000	-0.607086000
H	3.448187000	1.079609000	-0.692897000
C	-5.439963000	4.341913000	-0.030420000
O	-6.655970000	4.309992000	-0.140984000
O	-4.803386000	5.544926000	0.043927000
H	-5.511037000	6.206119000	-0.013107000
O	-0.624294000	-4.717603000	-0.058540000
C	6.063859000	-0.180059000	0.361875000
H	5.169612000	-0.722642000	0.660616000
C	5.885939000	0.497553000	-0.986734000
H	5.545340000	-0.225209000	-1.734613000
H	6.820774000	0.964654000	-1.306992000
O	4.877347000	1.486675000	-0.855692000
I	7.663271000	-1.741566000	0.266755000
H	6.410307000	0.529953000	1.108874000
C	5.280883000	2.819653000	-0.177194000
O	6.469798000	2.873644000	0.121403000
O	4.290621000	3.541078000	-0.087137000
C	1.710691000	4.334378000	-0.296113000
C	1.464399000	4.772008000	1.069677000
O	0.430102000	4.969488000	0.062253000
H	2.345146000	4.933147000	-0.938933000
H	1.664348000	3.274843000	-0.527052000
H	1.915078000	5.691816000	1.435936000
H	1.222787000	4.028449000	1.827226000

#### TS4-I

SCF Energy (B3LYP-D3/B2) = -2071.12346554

Enthalpy 0K = 0.458052

Enthalpy 298 K = 0.495349

Free Energy 298 K = 0.382529

C	-1.942900000	2.447728000	0.049953000
C	-2.451227000	1.106350000	-0.023368000
C	-2.833105000	3.521543000	-0.112854000
C	-3.863066000	0.918464000	-0.119724000
C	-4.205932000	3.346923000	-0.278076000
C	-4.758060000	2.034147000	-0.258829000
H	-2.408330000	4.517199000	-0.090303000
C	-6.166674000	1.779834000	-0.378874000
C	-6.673888000	0.521925000	-0.315703000
C	-5.830104000	-0.621897000	-0.129629000
C	-4.403642000	-0.424774000	-0.068151000
C	-6.356977000	-1.911464000	-0.010202000
C	-3.551896000	-1.545100000	0.058136000
C	-5.520669000	-3.048344000	0.117202000
C	-4.104696000	-2.856049000	0.136150000
C	-1.573831000	-0.060952000	0.011859000
C	-0.173894000	0.053239000	-0.062772000
C	-2.122670000	-1.370949000	0.079238000
O	0.674968000	-1.047294000	-0.009290000
C	-1.248230000	-2.495139000	0.149239000
C	0.136622000	-2.329056000	0.120163000
H	0.254618000	1.031759000	-0.155374000
H	0.780057000	-3.199322000	0.186676000
C	-1.787074000	-3.869991000	0.252021000

C	-3.268529000	-4.005153000	0.245019000
C	-3.823923000	-5.272275000	0.339818000
C	-5.219080000	-5.451130000	0.333229000
C	-6.054716000	-4.357815000	0.223961000
H	-6.824470000	2.623578000	-0.525333000
H	-7.746903000	0.396796000	-0.447993000
H	-7.131943000	-4.480471000	0.215938000
H	-5.637576000	-6.450369000	0.413076000
H	-3.144885000	-6.115188000	0.419569000
O	-7.703131000	-2.155412000	-0.015160000
H	-8.176097000	-1.321127000	0.089674000
O	-0.669337000	2.672752000	0.282925000
H	-0.138068000	3.651837000	0.048106000
C	2.154072000	-0.823607000	-0.055366000
O	2.984155000	-1.700233000	0.131806000
O	2.445263000	0.451899000	-0.322979000
H	3.408784000	0.695646000	-0.232560000
C	-5.041337000	4.566187000	-0.449913000
O	-6.252094000	4.632769000	-0.602886000
O	-4.307847000	5.715294000	-0.427383000
H	-4.957800000	6.424780000	-0.550947000
O	-1.056180000	-4.859492000	0.337514000
C	6.126064000	-0.367408000	0.266254000
H	5.261498000	-1.030897000	0.290915000
C	5.926920000	0.816503000	-0.667039000
H	5.686813000	0.482104000	-1.680775000
H	6.815934000	1.450257000	-0.683022000
O	4.799531000	1.573502000	-0.215767000
I	7.814222000	-1.630305000	-0.444492000
H	6.417449000	-0.029036000	1.257602000
C	5.047258000	2.486231000	0.911412000
O	6.184117000	2.491671000	1.368010000
O	4.010512000	3.119510000	1.229001000
C	2.318780000	3.672897000	0.112101000
C	1.574259000	4.493870000	1.051171000
O	0.734743000	4.570244000	-0.102356000
H	2.946554000	4.150258000	-0.624159000
H	2.036383000	2.641557000	-0.025563000
H	2.016262000	5.450131000	1.342309000
H	1.133166000	3.971997000	1.905618000

#### Pdt2-I

SCF Energy (B3LYP-D3/B2) = -2071.17613365

Enthalpy 0K = 0.465241

Enthalpy 298 K = 0.502529

Free Energy 298 K = 0.390064

C	-1.867849000	2.444699000	-0.420413000
C	-2.405552000	1.093358000	-0.337279000
C	-2.804931000	3.516731000	-0.322282000
C	-3.809060000	0.908255000	-0.151070000
C	-4.168923000	3.340474000	-0.166340000
C	-4.715653000	2.021799000	-0.080757000
H	-2.379251000	4.511367000	-0.371011000
C	-6.118850000	1.771523000	0.032622000
C	-6.621695000	0.511283000	0.138676000
C	-5.758809000	-0.631058000	0.158128000
C	-4.340136000	-0.434337000	-0.018140000
C	-6.259685000	-1.923123000	0.347275000
C	-3.482834000	-1.559790000	-0.042500000

C	-5.419290000	-3.061471000	0.326926000
C	-4.016672000	-2.871127000	0.122552000
C	-1.538403000	-0.073428000	-0.413611000
C	-0.154772000	0.042425000	-0.654713000
C	-2.068564000	-1.385397000	-0.239821000
C	0.693933000	-1.064789000	-0.654748000
C	-1.193156000	-2.511080000	-0.264795000
C	0.177735000	-2.346409000	-0.446805000
H	0.236182000	1.032201000	-0.822580000
H	0.824550000	-3.216284000	-0.431880000
C	-1.710969000	-3.886957000	-0.090876000
C	-3.176637000	-4.022282000	0.106658000
C	-3.712298000	-5.290244000	0.282581000
C	-5.092346000	-5.467080000	0.485583000
C	-5.931882000	-4.370999000	0.510463000
H	-6.788882000	2.618987000	0.034208000
H	-7.702254000	0.386591000	0.168650000
H	-6.997629000	-4.490996000	0.670745000
H	-5.496443000	-6.465834000	0.626023000
H	-3.029078000	-6.133278000	0.261910000
O	-7.592966000	-2.159284000	0.564062000
H	-8.018685000	-1.324683000	0.795701000
O	-0.627447000	2.715166000	-0.571533000
H	0.208813000	4.152623000	-0.590653000
C	2.154750000	-0.864657000	-0.798761000
O	3.011230000	-1.702776000	-0.557997000
O	2.462325000	0.388175000	-1.208993000
H	3.406818000	0.557901000	-1.057953000
C	-5.017080000	4.559744000	-0.067885000
O	-6.189592000	4.634443000	0.270577000
O	-4.347224000	5.701262000	-0.398974000
H	-4.994970000	6.410344000	-0.261773000
O	-0.970741000	-4.875017000	-0.107571000
C	5.900880000	-0.383546000	0.376127000
H	5.079406000	-0.990605000	-0.006316000
C	5.995387000	0.979066000	-0.290738000
H	6.094582000	0.889641000	-1.374296000
H	6.825726000	1.560964000	0.113337000
O	4.758507000	1.712819000	-0.096844000
I	7.744929000	-1.524108000	-0.051009000
H	5.858807000	-0.288768000	1.458213000
C	4.617036000	2.285444000	1.145282000
O	5.415663000	2.127896000	2.040745000
O	3.532242000	3.029501000	1.262015000
C	2.651619000	3.342368000	0.135562000
C	1.688643000	4.429834000	0.614819000
O	0.884860000	4.866910000	-0.448189000
H	3.248888000	3.701660000	-0.706963000
H	2.106769000	2.446192000	-0.160645000
H	2.273358000	5.279951000	0.991150000
H	1.103587000	4.031629000	1.458916000