On the role of stereo-electronic effects in tuning the selectivity and rate of DNA alkylation by duocarmycins

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Supporting Information

List of contents:

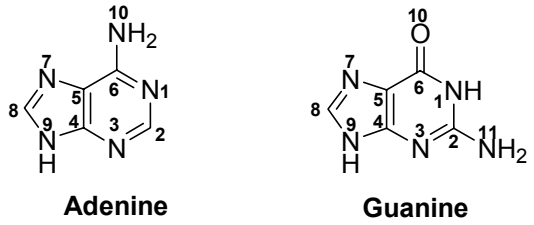

Fig. SI-1: Structure of the studied DNA bases (adenine and guanine).

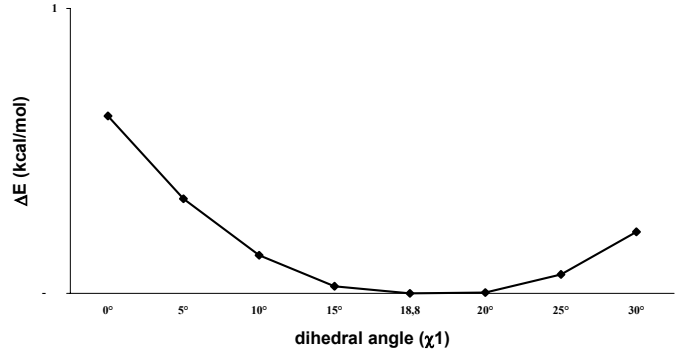

Fig. SI-2: Energy change [PBE0/6-31G(d)] *vs.* variation of the dihedral angle (χ_1) of **3**.

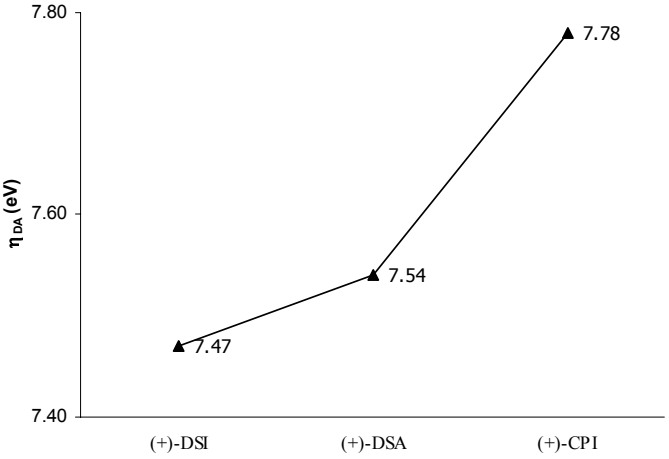

Fig. SI-3: Reactivity indice hardness η_{DA} in eV (298.15 K, 1 atm) in the gas phase [PBE0/6-31G(d))] for the compounds **1**, **2** and **3** with adenine. See text for details.

Table SI-1: Bond lengths and dihedral angles for the reactant structures optimized for the gas phase and for water solution (PBEO/6-31G(d)).

Gas phase (PBE0/6-31G (d))	**(+)DSA**	**(+)DSI**	**(+)CPI**	**(+)-*N*-Boc-CPI**
C1-C2 (Å)	1.485	1.484	1.485	1.485
C1-C10 (Å)	1.528	1.528	1.528	1.528
C2-C10 (Å)	1.515	1.515	1.515	1.518
C2-C3 (Å)	1.510	1.510	1.511	1.511
C3-N4 (Å)	1.468	1.469	1.468	1.470
N4-C5 (Å)	1.403	1.404	1.406	1.399
C5-C10 (Å)	1.484	1.484	1.484	1.485
C5-C6(Å)	1.354	1.354	1.353	1.353
C6-C7 (Å)	1.466	1.467	1.470	1.467
C7-C8 (Å)	1.462	1.462	1.454	1.456
C8-C9 (Å)	1.390	1.390	1.383	1.383
C9-C10 (Å)	1.463	1.464	1.464	1.464
C7-O11 (Å)	1.228	1.227	1.229	1.230
∢(C6-C5-C10-C2)	166.7°	166.5°	166.3°	
∢(C6-C5-C10-C1)	-131.1°	-131.3°	-131.5°	
∢(C6-C5-C10-C9)	14.8°	14.7°	14.4°	
∢(C8-C9-C10-C5)	-13.2°	-13.1°	-12.9°	

Solvent (PCM-PBE0/6-31G (d))	**(+)DSA**	**(+)DSI**	**(+)CPI**
C1-C2 (Å)	1.480	1.480	1.480
C1-C10 (Å)	1.534	1.534	1.534
C2-C10 (Å)	1.519	1.519	1.520
C2-C3 (Å)	1.510	1.510	1.511
C3-N4 (Å)	1.474	1.474	1.473
N4-C5 (Å)	1.398	1.398	1.402
C5-C10 (Å)	1.478	1.477	1.478
C5-C6(Å)	1.359	1.358	1.356
C6-C7 (Å)	1.459	1.459	1.465
C7-C8 (Å)	1.457	1.457	1.448
C8-C9 (Å)	1.394	1.394	1.391
C9-C10 (Å)	1.461	1.461	1.461
C7-O11 (Å)	1.238	1.237	1.240

Table SI-2: Bond lengths and dihedral angles for the transition state structures optimized for the gas phase (PBEO/6-31G(d)).

Gas phase (PBE0/6-31G (d))	**TS-1**	**TS-2**	**TS-3**	**TS-4**
		Pyridine		
Nu-C1 (Å)	1.931	1.910	1.905	1.898
C1-C10 (Å)	2.074	2.086	2.090	2.090
C2-C10 (Å)	1.487	1.485	1.484	1.485
C2-C3 (Å)	1.531	1.522	1.523	1.524
C3-N4 (Å)	1.463	1.464	1.464	1.465
N4-C5 (Å)	1.409	1.423	1.424	1.418
C5-C10 (Å)	1.436	1.426	1.428	1.429
C5-C6(Å)	1.376	1.374	1.372	1.372
C6-C7 (Å)	1.450	1.451	1.454	1.453
C7-C8 (Å)	1.456	1.458	1.450	1.451
C8-C9 (Å)	1.405	1.404	1.396	1.396
C9-C10 (Å)	1.422	1.424	1.423	1.424
C7-O11 (Å)	1.239	1.239	1.242	1.241

Gas-Phase (PBE0/6-31G (d))	**TS-1**	**TS-2**	**TS-3**	**TS-3**
		Adenine		**Guanine**
Nu-C1 (Å)	1.908	1.908	1.892	1.826
C1-C10 (Å)	2.118	2.117	2.128	2.162
C2-C10 (Å)	1.492	1.491	1.490	1.485
C2-C3 (Å)	1.522	1.522	1.522	1.526
C3-N4 (Å)	1.465	1.465	1.464	1.464
N4-C5 (Å)	1.430	1.431	1.432	1.429
C5-C10 (Å)	1.420	1.421	1.422	1.421
C5-C6(Å)	1.375	1.375	1.375	1.376
C6-C7 (Å)	1.449	1.450	1.452	1.452
C7-C8 (Å)	1.457	1.467	1.449	1.450
C8-C9 (Å)	1.406	1.406	1.398	1.397
C9-C10 (Å)	1.423	1.423	1.422	1.420
C7-O11 (Å)	1.240	1.241	1.244	1.243
α (C6-C5-C10-C2)	-178.2°	-178.0°	-177.7°	-175.3°
β (C6-C5-C10-C1)	-131.4°	-131.1°	-131.1°	-129.1°
γ (C6-C5-C10-C9)	0.48°	0.35°	0.04°	-0.9°
δ (C8-C9-C10-C5)	-0.82°	-0.8°	-0.4°	0.4°

Table SI-3: Bond lengths and dihedral angles for the product structures optimized for the gas phase (PBE0/6-31G(d)).

Gas phase (PBE0/6-31G (d))	**P-1**	**P-2**	**P-3**	**P-3**
		Adenine		**Guanine**
Nu-C1 (Å)	1.470	1.470	1.478	
C1-C10 (Å)	2.458	2.455	2.455	
C2-C10 (Å)	1.482	1.481	1.480	
C2-C3 (Å)	1.530	1.530	1.530	
C3-N4 (Å)	1.464	1.462	1.462	
N4-C5 (Å)	1.435	1.435	1.435	
C5-C10 (Å)	1.406	1.406	1.409	
C5-C6(Å)	1.385	1.385	1.384	
C6-C7 (Å)	1.442	1.442	1.445	
C7-C8 (Å)	1.456	1.456	1.449	
C8-C9 (Å)	1.411	1.410	1.402	
C9-C10 (Å)	1.414	1.413	1.412	
C7-O11 (Å)	1.246	1.245	1.248	
α (C6-C5-C10-C2)	-172.5°	-172.1°	-172.2°	
β (C6-C5-C10-C1)	-133.4°	-132.8°	-132.8°	
γ (C6-C5-C10-C9)	-3.2°	-3.4°	-3.2°	
δ (C8-C9-C10-C5)	2.8°	2.8°	2.7°	

Table SI-4: Natural hybrid orbitals for the structure **3** with adenine and guanine.

Transition state	Bond	Center	% Natural hybrid p character
Adenine	C1C2(σ)	C1	65.7 ($sp^{1.92}$)
	C1C2(σ)	C2	75.4 ($sp^{3.07}$)
	C2C10(σ)	C10	69.3 ($sp^{2.26}$)
	C2C10(σ)	C2	75.8 ($sp^{3.14}$)
	C1C10(σ)	C1	97.8 ($sp^{44.43}$ $d^{0.02}$)
	C1C10(σ)	C10	99.5 ($sp^{99.99}$ $d^{0.02}$)
	LP (N3-Adenine)		99.5 ($sp^{99.99}$ $d^{0.22}$)
Guanine	C1C2(σ)	C1	67.1 ($sp^{2.05}$)
	C1C2(σ)	C2	75.8 ($sp^{3.13}$)
	C2C10(σ)	C10	68.7 ($sp^{2.19}$)
	C2C10(σ)	C2	75.2 ($sp^{3.05}$)
	C1Nu(σ)	C1	90.4 ($sp^{9.42}$)
	C1Nu(σ)	Nu	90.1 ($sp^{9.16}$)
	LP (N3-Guanine)		79.7 ($sp^{3.95}$)

Table SI-5: Stabilization energies [E(2)] for the molecule **3** with adenine and guanine.

Transition state	Donor–acceptor	E(2)/kcalmol^{-1}
Adenine–CPI	sp_{C1C2} toσ^*_{C1C10}	10.8
Adenine–CPI	sp_{C1C2} toσ^*_{C2C10}	1.6
Adenine–CPI	sp_{C1C10} toσ^*_{C1C2}	3.0
Adenine–CPI	sp_{C1C10} toσ^*_{C1C10}	24.0
Adenine–CPI	sp_{C1C10} toσ^*_{C2C10}	4.3
Adenine–CPI	sp_{C2C10} toσ^*_{C1C2}	1.8
Adenine–CPI	sp_{C2C10} toσ^*_{C1C10}	3.4
Adenine–CPI	LP_{Nu} toσ^*_{C1C10}	98.1
Guanine–CPI	sp_{C2C10} toσ^*_{C1C2}	1.3
Guanine–CPI	sp_{C2C10} toσ^*_{C1Nu}	7.9
Guanine–CPI	sp_{C1C2} toσ^*_{C2C10}	2.1
Guanine–CPI	sp_{C1Nu} toσ^*_{C2C10}	0.9
Guanine–CPI	sp_{C1Nu} toσ^*_{C1Nu}	2.1
Guanine–CPI	LP_{Nu} toσ^*_{C1Nu}	25.0

Table SI-6: Natural hybrid orbitals and electron population for the structures of the adenine and guanine.

Structure	Bond	Center	Electron population	% Natural hybrid p character
Adenine	N1C2(σ)	N1	1.98696	63.8 ($sp^{1.77}$)
	N1C2(σ)	C2	1.98696	65.6 ($sp^{1.91}$)
	C2N3(σ)	C2	1.98166	65.4 ($sp^{1.89}$)
	C2N3(σ)	N3	1.98166	65.0 ($sp^{1.87}$)
	C2N3(π)	C2	1.78118	99.9 ($sp^{1.00}$)
	C2N3(π)	N3	1.78118	99.7 ($sp^{1.00}$)
	N1C6(σ)	N1	1.97955	65.4 ($sp^{1.90}$)
	N1C6(σ)	C6	1.97955	67.9 ($sp^{2.12}$)
	N1C6(π)	N1	1.70579	99.8 ($sp^{1.00}$)
	N1C6(π)	C6	1.70579	99.9 ($sp^{1.00}$)
	LP	N3	1.90275	68.1 ($sp^{2.15}d^{0.01}$)
Guanine	N1C2(σ)	N1	1.98810	62.6 ($sp^{1.68}$)
	N1C2(σ)	C2	1.98810	67.4 ($sp^{2.07}$)
	C2N3(σ)	C2	1.97774	63.8 ($sp^{1.76}$)
	C2N3(σ)	N3	1.97774	64.6 ($sp^{1.83}$)
	C2N3(π)	C2	1.83253	99.9 ($sp^{1.00}$)
	C2N3(π)	N3	1.83253	99.7 ($sp^{1.00}$)
	N1C6(σ)	N1	1.98379	64.4 ($sp^{1.81}$)
	N1C6(σ)	C6	1.98379	73.3 ($sp^{2.76}$)
	LP	N3	1.88500	68.8 ($sp^{2.21}d^{0.01}$)

Z-matrix

Vacuum PBE0/6-31G(d)

Structure: ch3oh

```
 c
 o   1 oc2
 h   2 ho3        1 hoc3
 h   1 hc4        2 hco4         3 dih4
 h   1 hc5        2 hco5         3 dih5
 h   1 hc6        2 hco6         3 dih6

oc2         1.407928
ho3         0.964799
hoc3        107.660
hc4         1.101004
hco4        112.821
dih4        -61.586
hc5         1.093190
hco5        106.844
dih5        180.000
hc6         1.101004
hco6        112.821
dih6         61.586
```

Number of immaginary frequency: 0

Thermochemical Data

```
 Electronic Energy=                             -115.579175189
(Hartree/Particle)
 Zero-point correction=                          0.051972 (Hartree/Particle)
 Thermal correction to Energy=                   0.055255
 Thermal correction to Enthalpy=                 0.056199
 Thermal correction to Gibbs Free Energy=        0.029268
 Sum of electronic and zero-point Energies=          -115.527203
 Sum of electronic and thermal Energies=             -115.523920
 Sum of electronic and thermal Enthalpies=           -115.522976
 Sum of electronic and thermal Free Energies=        -115.549907
```

Structure: CH3NH2

```
c
n   1 nc2
h   2 hn3        1 hnc3
h   2 hn4        3 hnh4         1 dih4
h   1 hc5        2 hcn5         3 dih5
h   1 hc6        2 hcn6         3 dih6
h   1 hc7        2 hcn7         3 dih7

nc2         1.454834
hn3         1.015848
hnc3        109.800
hn4         1.015848
hnh4        106.001
dih4       -118.540
hc5         1.095248
hcn5        109.199
dih5       -179.758
hc6         1.104202
hcn6        115.869
dih6        -58.084
```

```
hc7         1.095248
hcn7        109.199
dih7         63.590

Number of immaginary frequency: 0

Zero-point correction=                           0.065036 (Hartree/Particle)
Thermal correction to Energy=                    0.068406
Thermal correction to Enthalpy=                  0.069350
Thermal correction to Gibbs Free Energy=         0.042161
Sum of electronic and zero-point Energies=           -95.667297
Sum of electronic and thermal Energies=              -95.663927
Sum of electronic and thermal Enthalpies=            -95.662983
Sum of electronic and thermal Free Energies=         -95.690172
```

Structure: Pyridine

```
c
c   1 cc2
n   2 nc3        1 ncc3
c   3 cn4        2 cnc4         1 dih4
c   4 cc5        3 ccn5         2 dih5
c   5 cc6        4 ccc6         3 dih6
h   4 hc7        3 hcn7         2 dih7
h   5 hc8        4 hcc8         3 dih8
h   6 hc9        5 hcc9         4 dih9
h   1 hc10       2 hcc10        3 dih10
h   2 hc11       3 hcn11        4 dih11

cc2         1.392473
nc3         1.333980
ncc3        123.868
cn4         1.333980
cnc4        117.026
dih4          0.000
cc5         1.392514
ccn5        123.866
dih5          0.000
cc6         1.390838
ccc6        118.363
dih6          0.000
hc7         1.089292
hcn7        115.869
dih7        180.000
hc8         1.086012
hcc8        120.329
dih8        180.000
hc9         1.086855
hcc9        120.743
dih9        180.000
hc10        1.086012
hcc10       120.329
dih10       180.000
hc11        1.089293
hcn11       115.869
dih11       180.000

Number of immaginary frequency: 0

Zero-point correction=                           0.089766 (Hartree/Particle)
Thermal correction to Energy=                    0.094027
Thermal correction to Enthalpy=                  0.094971
Thermal correction to Gibbs Free Energy=         0.062373
Sum of electronic and zero-point Energies=          -247.899041
Sum of electronic and thermal Energies=             -247.894780
```

Sum of electronic and thermal Enthalpies= -247.893836
Sum of electronic and thermal Free Energies= -247.926434

Structure: Adenine

N						
C	1	B1				
C	2	B2	1	A1		
N	3	B3	2	A2	1	D1
C	1	B4	2	A3	3	D2
N	3	B5	2	A4	1	D3
C	6	B6	3	A5	2	D4
N	7	B7	6	A6	3	D5
C	8	B8	7	A7	6	D6
N	9	B9	8	A8	7	D7
H	4	B10	3	A9	2	D8
H	5	B11	1	A10	2	D9
H	7	B12	6	A11	3	D10
H	10	B13	9	A12	8	D11
H	10	B14	9	A13	8	D12

B1	1.37817762
B2	1.39519040
B3	1.37124359
B4	1.30640042
B5	1.33439582
B6	1.33097428
B7	1.33828201
B8	1.33920270
B9	1.34936427
B10	1.00843686
B11	1.08260067
B12	1.08853293
B13	1.00743928
B14	1.00699913
A1	111.63798993
A2	104.26100765
A3	103.72630692
A4	127.11498899
A5	110.89500972
A6	129.15298546
A7	118.29900337
A8	118.92664785
A9	125.73504121
A10	125.04246482
A11	115.77100477
A12	118.07003278
A13	119.30798175
D1	-0.14102456
D2	0.10729452
D3	179.65398708
D4	-0.18104602
D5	0.06500805
D6	0.25903285
D7	178.49020875
D8	-179.93794322
D9	180.00000000
D10	-179.78700978
D11	10.40088859
D12	169.87397993

Number of immaginary frequency:0

Zero-point correction= 0.113803 (Hartree/Particle)

```
 Thermal correction to Energy=                  0.121023
 Thermal correction to Enthalpy=                0.121967
 Thermal correction to Gibbs Free Energy=       0.082107
 Sum of electronic and zero-point Energies=          -466.688843
 Sum of electronic and thermal Energies=             -466.681623
 Sum of electronic and thermal Enthalpies=           -466.680679
 Sum of electronic and thermal Free Energies=        -466.720538
```

Structure: Guanine

```
 C
 C                  1             B1
 C                  2             B2    1             A1
 N                  3             B3    2             A2    1             D1
 C                  4             B4    3             A3    2             D2
 N                  5             B5    4             A4    3             D3
 N                  3             B6    2             A5    1             D4
 C                  7             B7    3             A6    2             D5
 N                  8             B8    7             A7    3             D6
 N                  5             B9    4             A8    3             D7
 O                  1            B10    6             A9    5             D8
 H                  7            B11    3            A10    2             D9
 H                  8            B12    7            A11    3            D10
 H                 10            B13    5            A12    4            D11
 H                 10            B14    5            A13    4            D12
 H                  6            B15    5            A14    4            D13

   B1            1.43754320
   B2            1.39154503
   B3            1.35341724
   B4            1.30762418
   B5            1.36503148
   B6            1.36357845
   B7            1.37616890
   B8            1.30356794
   B9            1.37131512
   B10           1.21384080
   B11           1.00853652
   B12           1.08220409
   B13           1.01000519
   B14           1.01047933
   B15           1.01246461
   A1          118.55197804
   A2          129.46398228
   A3          112.17606455
   A4          123.69595323
   A5          104.74098040
   A6          106.81198004
   A7          112.96203613
   A8          119.47703511
   A9          119.26379024
   A10         125.46598734
   A11         121.54994010
   A12         117.36199801
   A13         112.58702458
   A14         119.88499061
   D1            1.31192562
   D2           -1.49494963
   D3            0.84498055
   D4         -179.44602043
   D5            0.08498186
   D6           -0.05500294
   D7         -176.57104949
   D8         -179.68326505
```

D9	179.88094371
D10	179.96797444
D11	-147.27100628
D12	-12.26098716
D13	-175.34901400

Number of immaginary frequency:0

Zero-point correction=	0.118818 (Hartree/Particle)
Thermal correction to Energy=	0.126930
Thermal correction to Enthalpy=	0.127875
Thermal correction to Gibbs Free Energy=	0.085911
Sum of electronic and zero-point Energies=	-541.843682
Sum of electronic and thermal Energies=	-541.835569
Sum of electronic and thermal Enthalpies=	-541.834625
Sum of electronic and thermal Free Energies=	-541.876589

Structure: NBocCPI (4)

C							
C	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	
C	4	B4	3	A3	2	D2	
C	1	B5	2	A4	3	D3	
C	4	B6	3	A5	2	D4	
C	7	B7	4	A6	3	D5	
N	8	B8	7	A7	4	D6	
C	5	B9	4	A8	3	D7	
C	10	B10	5	A9	4	D8	
N	6	B11	1	A10	2	D9	
C	10	B12	5	A11	4	D10	
H	8	B13	7	A12	4	D11	
O	2	B14	1	A13	6	D12	
C	12	B15	6	A14	1	D13	
O	16	B16	12	A15	6	D14	
C	17	B17	16	A16	12	D15	
C	18	B18	17	A17	16	D16	
O	16	B19	12	A18	6	D17	
C	18	B20	17	A19	16	D18	
C	18	B21	17	A20	16	D19	
H	7	B22	4	A21	3	D20	
H	9	B23	8	A22	7	D21	
H	1	B24	6	A23	12	D22	
H	10	B25	5	A24	4	D23	
H	13	B26	10	A25	5	D24	
H	13	B27	10	A26	5	D25	
H	11	B28	10	A27	5	D26	
H	11	B29	10	A28	5	D27	
H	22	B30	18	A29	17	D28	
H	22	B31	18	A30	17	D29	
H	22	B32	18	A31	17	D30	
H	21	B33	18	A32	17	D31	
H	21	B34	18	A33	17	D32	
H	21	B35	18	A34	17	D33	
H	19	B36	18	A35	17	D34	
H	19	B37	18	A36	17	D35	
H	19	B38	18	A37	17	D36	

B1	1.46747776
B2	1.45582377
B3	1.38318936
B4	1.46423872
B5	1.35342461

B6	1.41539757
B7	1.38413601
B8	1.35968473
B9	1.51841618
B10	1.51160330
B11	1.39903263
B12	1.48493635
B13	1.08085651
B14	1.23029315
B15	1.38031181
B16	1.34233409
B17	1.46193491
B18	1.52383918
B19	1.21205641
B20	1.52270432
B21	1.52382925
B22	1.08223977
B23	1.00887666
B24	1.08171232
B25	1.08531409
B26	1.08777987
B27	1.08567860
B28	1.09708793
B29	1.09295146
B30	1.09522014
B31	1.09531995
B32	1.09128257
B33	1.09443635
B34	1.09479906
B35	1.09470720
B36	1.09527774
B37	1.09122397
B38	1.09534018
A1	114.35514876
A2	126.54613681
A3	117.50192434
A4	120.50364785
A5	107.25490518
A6	106.61142203
A7	108.61401342
A8	129.94607381
A9	106.84840703
A10	128.77239696
A11	61.15298585
A12	130.05006328
A13	123.76322569
A14	124.57425120
A15	109.17697723
A16	120.40001897
A17	110.11855008
A18	124.35175457
A19	102.53489025
A20	110.00823735
A21	127.91975576
A22	127.90722399
A23	121.69516854
A24	120.80734956
A25	118.96718066
A26	118.18523777
A27	111.63187710
A28	112.85056795
A29	109.39818608
A30	110.29724558
A31	111.15667261

A32	109.95858336
A33	110.69082625
A34	110.68693139
A35	109.38576159
A36	111.22313781
A37	110.27819422
D1	4.39602127
D2	4.32468501
D3	-3.62008223
D4	179.96395744
D5	0.51235072
D6	-0.48865321
D7	-157.08275883
D8	145.70157033
D9	170.70320553
D10	-104.98888369
D11	178.89884546
D12	179.85239130
D13	11.36134401
D14	-173.10054276
D15	-179.86771034
D16	62.09750634
D17	7.07220554
D18	179.92211592
D19	-62.26399168
D20	179.97980285
D21	179.68341480
D22	-4.66203641
D23	5.55617678
D24	-107.85879402
D25	103.67385987
D26	-107.29241067
D27	130.56858730
D28	-173.39239877
D29	-54.64948015
D30	66.42610311
D31	179.76301165
D32	-60.42573619
D33	59.91689023
D34	172.82320792
D35	-66.98664987
D36	54.11296764

Number of immaginary frequency = 0

Zero-point correction=	0.323255 (Hartree/Particle)
Thermal correction to Energy=	0.341789
Thermal correction to Enthalpy=	0.342733
Thermal correction to Gibbs Free Energy=	0.276888
Sum of electronic and zero-point Energies=	-954.325001
Sum of electronic and thermal Energies=	-954.306468
Sum of electronic and thermal Enthalpies=	-954.305524
Sum of electronic and thermal Free Energies=	-954.371368

Structure: CPI (3)

N								
C		1	B1					
C		2	B2	1	A1			
C		3	B3	2	A2	1		D1
C		1	B4	2	A3	3		D2
C		3	B5	2	A4	1		D3
C		6	B6	3	A5	2		D4
C		7	B7	6	A6	3		D5

C	2	B8	1	A7	5	D6
C	6	B9	3	A8	2	D7
C	10	B10	6	A9	3	D8
N	7	B11	6	A10	3	D9
C	10	B12	6	A11	3	D10
O	9	B13	2	A12	1	D11
C	12	B14	7	A13	6	D12
O	15	B15	12	A14	7	D13
C	15	B16	12	A15	7	D14
C	17	B17	15	A16	12	D15
C	18	B18	17	A17	15	D16
C	19	B19	18	A18	17	D17
N	20	B20	19	A19	18	D18
C	20	B21	19	A20	18	D19
C	22	B22	20	A21	19	D20
C	23	B23	22	A22	20	D21
C	24	B24	23	A23	22	D22
H	25	B25	24	A24	23	D23
H	18	B26	17	A25	15	D24
H	8	B27	7	A26	6	D25
H	11	B28	10	A27	6	D26
H	11	B29	10	A28	6	D27
H	10	B30	6	A29	3	D28
H	13	B31	10	A30	6	D29
H	13	B32	10	A31	6	D30
H	4	B33	3	A32	2	D31
H	21	B34	20	A33	19	D32
H	1	B35	5	A34	4	D33
H	24	B36	23	A35	22	D34
H	23	B37	22	A36	20	D35
H	22	B38	20	A37	19	D36
H	5	B39	1	A38	2	D37

B1	1.36281853
B2	1.38324486
B3	1.41514809
B4	1.35957550
B5	1.46399016
B6	1.48455125
B7	1.35290865
B8	1.45443136
B9	1.51546530
B10	1.51081245
B11	1.40584114
B12	1.48475414
B13	1.22970719
B14	1.37772708
B15	1.22706280
B16	1.47827136
B17	1.38352250
B18	1.42429995
B19	1.42069661
B20	1.36096963
B21	1.39943013
B22	1.38248167
B23	1.41110465
B24	1.38104528
B25	1.08686334
B26	1.07875135
B27	1.08107630
B28	1.09369622
B29	1.09767959
B30	1.08518318
B31	1.08778608

B32	1.08556842
B33	1.08220681
B34	1.01010028
B35	1.00888839
B36	1.08630082
B37	1.08650298
B38	1.08627355
B39	1.08088175
A1	108.16176098
A2	107.26232752
A3	109.34110017
A4	117.55733750
A5	115.69123996
A6	123.72786344
A7	125.40846634
A8	129.72936670
A9	106.73251078
A10	107.57351726
A11	61.21903887
A12	122.00613169
A13	123.69753699
A14	121.71441670
A15	120.07617609
A16	138.16380944
A17	107.13704296
A18	106.92374324
A19	107.22042263
A20	122.09484996
A21	117.26273911
A22	121.58980487
A23	121.12053582
A24	120.76438465
A25	127.51104694
A26	121.91700246
A27	112.16590769
A28	111.02945957
A29	120.95287545
A30	119.02214800
A31	118.10185718
A32	127.92969394
A33	128.92030414
A34	127.86195515
A35	119.11214927
A36	119.25355585
A37	121.34976194
A38	121.33834838
D1	-0.33814358
D2	0.04300083
D3	-176.03368168
D4	-12.91166574
D5	14.37836658
D6	179.67634346
D7	-156.92933773
D8	145.38937615
D9	-162.30196846
D10	-105.19146578
D11	1.34878090
D12	-164.75709351
D13	7.43116313
D14	-172.95874639
D15	11.78546519
D16	176.38930402
D17	-0.03911012
D18	0.06583967

D19	-179.98271839
D20	0.07518328
D21	-0.08969347
D22	0.04118457
D23	179.98490795
D24	-1.76503449
D25	178.14819702
D26	130.55808161
D27	-107.31630848
D28	5.51439558
D29	-107.85832557
D30	103.69328898
D31	-179.99564911
D32	-175.78487923
D33	179.69454421
D34	-179.95760716
D35	179.88902970
D36	-179.99493641
D37	-179.17019002

Number of immaginary frequency = 0

Zero-point correction=	0.316889 (Hartree/Particle)
Thermal correction to Energy=	0.335328
Thermal correction to Enthalpy=	0.336273
Thermal correction to Gibbs Free Energy=	0.269479
Sum of electronic and zero-point Energies=	-1084.320810
Sum of electronic and thermal Energies=	-1084.302371
Sum of electronic and thermal Enthalpies=	-1084.301427
Sum of electronic and thermal Free Energies=	-1084.368220

Structure: DSI (2)

C							
C	1	B1					
C	2	B2	1	A1			
N	3	B3	2	A2	1	D1	
C	4	B4	3	A3	2	D2	
C	1	B5	2	A4	3	D3	
C	2	B6	1	A5	6	D4	
C	7	B7	2	A6	1	D5	
C	8	B8	7	A7	2	D6	
C	3	B9	2	A8	1	D7	
C	7	B10	2	A9	1	D8	
C	11	B11	7	A10	2	D9	
N	8	B12	7	A11	2	D10	
C	4	B13	3	A12	2	D11	
O	14	B14	4	A13	3	D12	
O	9	B15	8	A14	7	D13	
C	12	B16	11	A15	7	D14	
O	17	B17	12	A16	11	D15	
C	14	B18	4	A17	3	D16	
N	19	B19	14	A18	4	D17	
C	20	B20	19	A19	14	D18	
C	21	B21	20	A20	19	D19	
C	19	B22	14	A21	4	D20	
C	21	B23	20	A22	19	D21	
C	24	B24	21	A23	20	D22	
C	25	B25	24	A24	21	D23	
C	26	B26	25	A25	24	D24	
O	17	B27	12	A26	11	D25	
C	28	B28	17	A27	12	D26	
H	24	B29	21	A28	20	D27	
H	25	B30	24	A29	21	D28	
H	26	B31	25	A30	24	D29	

H	27	B32	26	A31	25	D30	
H	23	B33	19	A32	14	D31	
H	10	B34	3	A33	2	D32	
H	5	B35	4	A34	3	D33	
H	5	B36	4	A35	3	D34	
H	6	B37	1	A36	2	D35	
H	1	B38	6	A37	5	D36	
H	1	B39	6	A38	5	D37	
H	11	B40	7	A39	2	D38	
H	29	B41	28	A40	17	D39	
H	29	B42	28	A41	17	D40	
H	29	B43	28	A42	17	D41	
H	20	B44	19	A43	14	D42	
H	13	B45	8	A44	7	D43	

B1	1.52781265
B2	1.48403046
B3	1.40369532
B4	1.46861020
B5	1.48458353
B6	1.46405039
B7	1.39048538
B8	1.46197239
B9	1.35400649
B10	1.40721307
B11	1.39162868
B12	1.35256463
B13	1.37989268
B14	1.22646889
B15	1.22728687
B16	1.45963214
B17	1.21431879
B18	1.47706811
B19	1.37642525
B20	1.36100390
B21	1.42066989
B22	1.38361638
B23	1.39956132
B24	1.38242312
B25	1.41117500
B26	1.38082192
B27	1.34158986
B28	1.42523498
B29	1.08623258
B30	1.08646428
B31	1.08624708
B32	1.08684016
B33	1.07872477
B34	1.08115054
B35	1.09365962
B36	1.09754051
B37	1.08524567
B38	1.08777160
B39	1.08563336
B40	1.08148306
B41	1.09008900
B42	1.09325605
B43	1.09329552
B44	1.01002355
B45	1.01103304
A1	113.97702818
A2	107.58602111
A3	111.25893957
A4	60.38121825

A5	120.48165647
A6	117.71899797
A7	125.96099983
A8	123.80554221
A9	134.80969200
A10	106.45697535
A11	108.39713847
A12	123.70004850
A13	121.60298478
A14	121.71617447
A15	132.54595340
A16	123.60001034
A17	120.01701587
A18	113.41602040
A19	110.24302511
A20	107.22898150
A21	138.04191321
A22	130.70198213
A23	117.25497448
A24	121.61303248
A25	121.11397739
A26	112.14404240
A27	114.58302807
A28	121.36198611
A29	119.23899509
A30	119.10601987
A31	120.77370934
A32	127.54723272
A33	121.82301666
A34	109.92399665
A35	110.23401227
A36	120.86345527
A37	119.13086662
A38	118.05545313
A39	128.61796397
A40	105.64298951
A41	110.64398193
A42	110.64802540
A43	120.78751526
A44	125.57896863
D1	51.90098025
D2	18.64503551
D3	-95.26758264
D4	120.50965036
D5	130.51743417
D6	4.30597491
D7	-131.29653545
D8	-43.93938489
D9	175.37267051
D10	-176.23542287
D11	-164.67900579
D12	7.82405612
D13	-178.93012989
D14	179.15997812
D15	-179.75797087
D16	-172.60995055
D17	-171.56598862
D18	-177.22503704
D19	-0.02600118
D20	12.32514849
D21	-179.98244036
D22	-179.92415341
D23	-0.08093837
D24	-0.00000000

D25	0.34608627
D26	179.88100744
D27	-0.02403363
D28	179.87601692
D29	-179.98025709
D30	-179.99238515
D31	-1.88508103
D32	177.91173366
D33	-139.59098263
D34	100.29607234
D35	-110.80288211
D36	-11.66124752
D37	-160.12222162
D38	-5.04197082
D39	-179.79703962
D40	-60.12909274
D41	60.55095003
D42	-1.11166932
D43	-179.40972343

Number of immaginary frequency:0

Energy= -1312.2788961(a.u.)

Structure: DSA (1)

C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1
C	4	B4	3	A3	2	D2
C	1	B5	2	A4	3	D3
N	3	B6	2	A5	1	D4
C	7	B7	3	A6	2	D5
C	8	B8	7	A7	3	D6
C	8	B9	7	A8	3	D7
O	10	B10	8	A9	7	D8
O	4	B11	3	A10	2	D9
C	12	B12	4	A11	3	D10
O	5	B13	4	A12	3	D11
C	14	B14	5	A13	4	D12
O	6	B15	1	A14	2	D13
C	16	B16	6	A15	1	D14
N	10	B17	8	A16	7	D15
C	18	B18	10	A17	8	D16
C	19	B19	18	A18	10	D17
C	20	B20	19	A19	18	D18
C	18	B21	10	A20	8	D19
C	19	B22	18	A21	10	D20
C	23	B23	19	A22	18	D21
C	24	B24	23	A23	19	D22
C	25	B25	24	A24	23	D23
C	26	B26	25	A25	24	D24
C	27	B27	26	A26	25	D25
N	25	B28	24	A27	23	D26
C	21	B29	20	A28	19	D27
C	28	B30	27	A29	26	D28
O	31	B31	28	A30	27	D29
C	32	B32	31	A31	28	D30
O	24	B33	23	A32	19	D31
O	31	B34	28	A33	27	D32
H	1	B35	6	A34	16	D33
H	9	B36	8	A35	7	D34
H	23	B37	19	A36	18	D35

H	22	B38	18	A37	10	D36
H	22	B39	18	A38	10	D37
H	21	B40	20	A39	19	D38
H	30	B41	21	A40	20	D39
H	30	B42	21	A41	20	D40
H	13	B43	12	A42	4	D41
H	13	B44	12	A43	4	D42
H	13	B45	12	A44	4	D43
H	15	B46	14	A45	5	D44
H	15	B47	14	A46	5	D45
H	15	B48	14	A47	5	D46
H	27	B49	26	A48	25	D47
H	17	B50	16	A49	6	D48
H	17	B51	16	A50	6	D49
H	17	B52	16	A51	6	D50
H	33	B53	32	A52	31	D51
H	33	B54	32	A53	31	D52
H	33	B55	32	A54	31	D53
H	7	B56	3	A55	2	D54
H	29	B57	25	A56	24	D55

B1	1.41131726
B2	1.41204768
B3	1.40362417
B4	1.38524308
B5	1.38142193
B6	1.35782916
B7	1.37376835
B8	1.38838451
B9	1.47492791
B10	1.22613823
B11	1.36238924
B12	1.42440979
B13	1.36601930
B14	1.42075840
B15	1.35839820
B16	1.40659968
B17	1.38224985
B18	1.40264846
B19	1.48441257
B20	1.51511982
B21	1.46797305
B22	1.35439751
B23	1.46636772
B24	1.46230111
B25	1.39037426
B26	1.40726601
B27	1.39169706
B28	1.35240101
B29	1.48479003
B30	1.45924091
B31	1.34193905
B32	1.42509273
B33	1.22749772
B34	1.21440870
B35	1.08401809
B36	1.07891966
B37	1.08108378
B38	1.09363188
B39	1.09769758
B40	1.08525684
B41	1.08776245
B42	1.08563552
B43	1.09275889

B44	1.09716182
B45	1.09198768
B46	1.09693046
B47	1.09531105
B48	1.09231259
B49	1.08147914
B50	1.09135150
B51	1.09864756
B52	1.09820957
B53	1.09011430
B54	1.09328706
B55	1.09328335
B56	1.00941365
B57	1.01099778
A1	119.70301918
A2	122.31797755
A3	117.37902490
A4	118.29006057
A5	108.25801893
A6	109.74797486
A7	108.29199715
A8	113.63397080
A9	118.61999320
A10	118.36598515
A11	115.58298603
A12	119.60700003
A13	113.79900633
A14	124.93199709
A15	117.19499048
A16	119.94198934
A17	123.67895382
A18	107.58696345
A19	106.51399645
A20	124.98308882
A21	128.56112760
A22	120.78398726
A23	114.43499835
A24	125.98600243
A25	107.28898550
A26	106.46400659
A27	125.60217885
A28	61.23041268
A29	132.55867938
A30	112.16101517
A31	114.55799865
A32	123.84102394
A33	123.62696276
A34	121.45091845
A35	127.33899348
A36	121.77803319
A37	109.92031417
A38	110.28129784
A39	120.93103093
A40	119.09720516
A41	118.07978901
A42	111.19394018
A43	110.64102725
A44	105.89895404
A45	110.80198942
A46	110.99997153
A47	106.29100359
A48	128.62595114
A49	106.10301589
A50	111.61501006

A51	111.42700785
A52	105.64602744
A53	110.65101213
A54	110.65203451
A55	127.79577038
A56	125.54503568
D1	-0.80795551
D2	0.08197015
D3	0.65531281
D4	179.68696507
D5	0.17607376
D6	-0.27706296
D7	-177.67212984
D8	8.42560832
D9	-177.50201827
D10	-120.05999135
D11	178.94800767
D12	101.46798100
D13	179.68668830
D14	1.24177682
D15	-170.96833903
D16	-172.79199177
D17	-164.34803005
D18	-10.21799317
D19	3.76247128
D20	18.96490112
D21	169.92841799
D22	-3.42997774
D23	4.40699496
D24	-179.65996594
D25	0.48897872
D26	-174.81442258
D27	108.23485452
D28	179.09227942
D29	0.37461027
D30	179.93999123
D31	-179.94793428
D32	-179.69549919
D33	-0.29943277
D34	-177.87369120
D35	-5.97455514
D36	43.24431117
D37	-76.83421205
D38	-141.12721186
D39	-107.73200182
D40	103.77149451
D41	-63.45804554
D42	58.61198642
D43	176.97302607
D44	-59.83101030
D45	62.46600416
D46	-178.68603664
D47	-179.93795992
D48	179.27300154
D49	-61.73598384
D50	60.41504172
D51	-179.96907003
D52	-60.30205939
D53	60.36693233
D54	-177.84151236
D55	-0.03792072

Number of immaginary frequency:0

Energy= -1655.45841659(a.u.)

Structure: N-Boc-CPI (4) in water

C							
C	1	B1					
C	2	B2	1	A1			
N	3	B3	2	A2	1	D1	
C	4	B4	3	A3	2	D2	
C	1	B5	2	A4	3	D3	
C	3	B6	2	A5	1	D4	
C	7	B7	3	A6	2	D5	
C	8	B8	7	A7	3	D6	
C	9	B9	8	A8	7	D7	
C	10	B10	9	A9	8	D8	
C	11	B11	10	A10	9	D9	
N	12	B12	11	A11	10	D10	
O	8	B13	7	A12	3	D11	
C	4	B14	3	A13	2	D12	
O	15	B15	4	A14	3	D13	
O	15	B16	4	A15	3	D14	
C	17	B17	15	A16	4	D15	
C	18	B18	17	A17	15	D16	
C	18	B19	17	A18	15	D17	
C	18	B20	17	A19	15	D18	
H	12	B21	11	A20	10	D19	
H	11	B22	10	A21	9	D20	
H	13	B23	12	A22	11	D21	
H	7	B24	3	A23	2	D22	
H	6	B25	1	A24	2	D23	
H	1	B26	6	A25	5	D24	
H	1	B27	6	A26	5	D25	
H	5	B28	4	A27	3	D26	
H	5	B29	4	A28	3	D27	
H	19	B30	18	A29	17	D28	
H	19	B31	18	A30	17	D29	
H	19	B32	18	A31	17	D30	
H	21	B33	18	A32	17	D31	
H	21	B34	18	A33	17	D32	
H	21	B35	18	A34	17	D33	
H	20	B36	18	A35	17	D34	
H	20	B37	18	A36	17	D35	
H	20	B38	18	A37	17	D36	

B1	1.53363197
B2	1.47902479
B3	1.39277775
B4	1.47375930
B5	1.48072848
B6	1.35806730
B7	1.46222923
B8	1.44928452
B9	1.39027699
B10	1.41290945
B11	1.38683554
B12	1.35721214
B13	1.24140261
B14	1.38022067
B15	1.21714561
B16	1.33337605
B17	1.46664979
B18	1.52295682
B19	1.52288274
B20	1.52205665

B21	1.08470331
B22	1.08502617
B23	1.02232585
B24	1.08326277
B25	1.08817964
B26	1.08886531
B27	1.08665836
B28	1.09665220
B29	1.09306035
B30	1.09516833
B31	1.09535248
B32	1.09155113
B33	1.09451147
B34	1.09485589
B35	1.09479475
B36	1.09520390
B37	1.09160246
B38	1.09533154
A1	113.94955042
A2	107.68833439
A3	111.96171161
A4	60.64107947
A5	123.29813513
A6	120.93413644
A7	114.91300751
A8	125.48179414
A9	107.40195343
A10	106.45933029
A11	108.97560563
A12	122.47891876
A13	124.85742858
A14	123.90474307
A15	109.39023029
A16	121.30729033
A17	109.91631667
A18	109.98906115
A19	102.47234661
A20	130.09350195
A21	127.70914544
A22	125.99239502
A23	121.64073874
A24	120.79400755
A25	119.08551063
A26	118.07186463
A27	109.81370039
A28	110.05927744
A29	109.20710774
A30	110.29907074
A31	111.32983275
A32	109.75428120
A33	110.66428146
A34	110.67079756
A35	109.21091985
A36	111.36565003
A37	110.31006217
D1	51.54239209
D2	18.30758117
D3	-95.05142560
D4	-131.62950894
D5	-5.73685196
D6	-3.48997922
D7	4.26141089
D8	179.86189209
D9	0.56184959

D10	-0.55332990
D11	179.68417006
D12	-170.64475133
D13	7.15862253
D14	-173.03224405
D15	-179.36961714
D16	-62.33440146
D17	62.16607348
D18	179.92212444
D19	178.89209456
D20	-179.85361973
D21	179.39442888
D22	179.34827976
D23	-110.43338098
D24	-11.22533289
D25	-160.21669495
D26	101.31529883
D27	-139.18766791
D28	-173.02965056
D29	-54.33251682
D30	66.90919960
D31	179.84930935
D32	-60.38947996
D33	60.06348211
D34	172.56907198
D35	-67.41052539
D36	53.86085236

Number of immaginary frequency=0

Energy=-954.6736301 (a.u.)

Structure: CPI (3) in water

C								
C	1	B1						
C	2	B2	1	A1				
N	3	B3	2	A2	1	D1		
C	4	B4	3	A3	2	D2		
C	1	B5	2	A4	3	D3		
C	2	B6	1	A5	6	D4		
C	7	B7	2	A6	1	D5		
C	8	B8	7	A7	2	D6		
C	3	B9	2	A8	1	D7		
C	7	B10	2	A9	1	D8		
C	11	B11	7	A10	2	D9		
N	12	B12	11	A11	7	D10		
C	4	B13	3	A12	2	D11		
O	14	B14	4	A13	3	D12		
O	9	B15	8	A14	7	D13		
C	14	B16	4	A15	3	D14		
N	17	B17	14	A16	4	D15		
C	18	B18	17	A17	14	D16		
C	19	B19	18	A18	17	D17		
C	17	B20	14	A19	4	D18		
C	19	B21	18	A20	17	D19		
C	22	B22	19	A21	18	D20		
C	23	B23	22	A22	19	D21		
C	24	B24	23	A23	22	D22		
H	25	B25	24	A24	23	D23		
H	21	B26	17	A25	14	D24		
H	10	B27	3	A26	2	D25		
H	5	B28	4	A27	3	D26		
H	5	B29	4	A28	3	D27		

H	6	B30	1	A29	2	D28	
H	1	B31	6	A30	5	D29	
H	1	B32	6	A31	5	D30	
H	11	B33	7	A32	2	D31	
H	18	B34	17	A33	14	D32	
H	13	B35	12	A34	11	D33	
H	24	B36	23	A35	22	D34	
H	23	B37	22	A36	19	D35	
H	22	B38	19	A37	18	D36	
H	12	B39	11	A38	7	D37	

B1	1.53407859
B2	1.47776418
B3	1.40170033
B4	1.47338676
B5	1.47994671
B6	1.46159253
B7	1.39071959
B8	1.44770784
B9	1.35641582
B10	1.41251777
B11	1.38691087
B12	1.35694375
B13	1.37732730
B14	1.23081725
B15	1.24059020
B16	1.47381943
B17	1.37795652
B18	1.36107108
B19	1.42166063
B20	1.38481541
B21	1.40148167
B22	1.38364743
B23	1.41381448
B24	1.38221006
B25	1.08956385
B26	1.08145833
B27	1.08328213
B28	1.09365903
B29	1.09704503
B30	1.08810715
B31	1.08882316
B32	1.08660704
B33	1.08499812
B34	1.02114506
B35	1.02232553
B36	1.08895571
B37	1.08924427
B38	1.08909671
B39	1.08470804
A1	113.71298045
A2	108.04702090
A3	110.81898480
A4	60.53224197
A5	120.46531223
A6	118.18897516
A7	125.43002588
A8	123.23190848
A9	134.24957896
A10	106.44999588
A11	109.00899178
A12	123.63998688
A13	121.40598275
A14	122.75730282

A15	119.66495439
A16	115.12095652
A17	109.88299274
A18	107.49201078
A19	135.99968902
A20	130.39699109
A21	117.16696393
A22	121.65600703
A23	121.15801582
A24	120.92764826
A25	127.63332356
A26	121.89803073
A27	110.00601521
A28	110.07900109
A29	120.96355951
A30	119.18545106
A31	117.97854878
A32	127.74400888
A33	123.47580995
A34	125.97670209
A35	119.07596276
A36	119.23295756
A37	121.20996547
A38	130.06101329
D1	51.18498944
D2	19.36395750
D3	-95.09091644
D4	120.67065282
D5	131.46495788
D6	4.17295995
D7	-132.78726748
D8	-43.18159517
D9	175.56436362
D10	-0.51997930
D11	-160.83001265
D12	7.74698715
D13	-179.23500867
D14	-172.83000917
D15	-166.72002182
D16	-176.65101145
D17	0.51703972
D18	18.45484550
D19	-179.47963714
D20	-179.72371784
D21	-0.07605453
D22	-0.06992240
D23	-179.90350875
D24	-2.47655254
D25	179.21526179
D26	-140.57252451
D27	99.06251840
D28	-110.48614034
D29	-11.48494944
D30	-160.51201720
D31	-4.83394518
D32	1.92983182
D33	179.23913756
D34	180.00000000
D35	179.86398354
D36	0.14521885
D37	178.94897906

Number of immaginary frequency=0

Zero-point correction=	0.316637 (Hartree/Particle)
Thermal correction to Energy=	0.334767
Thermal correction to Enthalpy=	0.335711
Thermal correction to Gibbs Free Energy=	0.270337
Sum of electronic and zero-point Energies=	-1084.319469
Sum of electronic and thermal Energies=	-1084.301339
Sum of electronic and thermal Enthalpies=	-1084.300394
Sum of electronic and thermal Free Energies=	-1084.365768

Structure: DSI (2) in water

C								
C	1	B1						
C	2	B2	1	A1				
N	3	B3	2	A2	1	D1		
C	4	B4	3	A3	2	D2		
C	2	B5	1	A4	5	D3		
C	6	B6	2	A5	1	D4		
C	7	B7	6	A6	2	D5		
C	3	B8	2	A7	1	D6		
C	6	B9	2	A8	1	D7		
C	10	B10	6	A9	2	D8		
N	7	B11	6	A10	2	D9		
C	10	B12	6	A11	2	D10		
C	12	B13	7	A12	6	D11		
O	14	B14	12	A13	7	D12		
O	9	B15	3	A14	2	D13		
C	5	B16	4	A15	3	D14		
O	17	B17	5	A16	4	D15		
C	14	B18	12	A17	7	D16		
C	19	B19	14	A18	12	D17		
C	20	B20	19	A19	14	D18		
C	21	B21	20	A20	19	D19		
N	22	B22	21	A21	20	D20		
C	22	B23	21	A22	20	D21		
C	24	B24	22	A23	21	D22		
C	25	B25	24	A24	22	D23		
C	26	B26	25	A25	24	D24		
O	17	B27	5	A26	4	D25		
C	28	B28	17	A27	5	D26		
H	24	B29	22	A28	21	D27		
H	25	B30	24	A29	22	D28		
H	26	B31	25	A30	24	D29		
H	27	B32	26	A31	25	D30		
H	20	B33	19	A32	14	D31		
H	8	B34	7	A33	6	D32		
H	11	B35	10	A34	6	D33		
H	11	B36	10	A35	6	D34		
H	10	B37	6	A36	2	D35		
H	13	B38	10	A37	6	D36		
H	13	B39	10	A38	6	D37		
H	1	B40	5	A39	4	D38		
H	29	B41	28	A40	17	D39		
H	29	B42	28	A41	17	D40		
H	29	B43	28	A42	17	D41		
H	23	B44	22	A43	21	D42		
H	4	B45	3	A44	2	D43		

B1	1.40549287
B2	1.39420875
B3	1.35530075
B4	1.36344767
B5	1.46142413
B6	1.47758964

B7	1.35897898
B8	1.45720592
B9	1.51948227
B10	1.51037325
B11	1.39831984
B12	1.47969749
B13	1.38045789
B14	1.22978473
B15	1.23731819
B16	1.46018277
B17	1.21802188
B18	1.47265036
B19	1.38509251
B20	1.42317296
B21	1.42169721
B22	1.36095074
B23	1.40158847
B24	1.38351235
B25	1.41399602
B26	1.38198637
B27	1.33706471
B28	1.42922972
B29	1.08909801
B30	1.08925703
B31	1.08896550
B32	1.08956646
B33	1.08134402
B34	1.08322006
B35	1.09360518
B36	1.09687725
B37	1.08827255
B38	1.08883486
B39	1.08668824
B40	1.08488078
B41	1.08991801
B42	1.09323706
B43	1.09322242
B44	1.02119326
B45	1.02446811
A1	107.30475658
A2	108.48881016
A3	108.95397718
A4	134.33660556
A5	115.77194523
A6	123.42536120
A7	125.23393570
A8	129.96740600
A9	106.45058598
A10	108.05063327
A11	61.51103259
A12	123.58165440
A13	121.20691214
A14	122.05720985
A15	119.68210116
A16	123.89784521
A17	119.70926479
A18	135.94704265
A19	107.01637735
A20	106.89574876
A21	107.51288838
A22	122.09361688
A23	117.16348152
A24	121.66908816
A25	121.15554716

A26	112.03134888
A27	115.22049679
A28	121.21368641
A29	119.22881854
A30	119.08593859
A31	120.93499418
A32	127.69168308
A33	121.80331941
A34	112.26043545
A35	110.79763625
A36	120.59259204
A37	119.30035782
A38	117.96081352
A39	125.51679686
A40	105.57044298
A41	110.50730382
A42	110.51576382
A43	126.56851107
A44	125.61129251
D1	-0.35541283
D2	0.05916291
D3	175.72542594
D4	172.82423900
D5	13.71605475
D6	-179.73137905
D7	28.18855837
D8	145.29516059
D9	-162.61186039
D10	-104.82435082
D11	-161.41812266
D12	8.09176262
D13	-179.15543546
D14	-179.48242668
D15	-0.11881302
D16	-172.47034366
D17	17.72556313
D18	175.36018856
D19	0.16426255
D20	-0.47641069
D21	179.58772913
D22	0.28476474
D23	-0.09074322
D24	-0.04165591
D25	-179.95474175
D26	179.80586500
D27	-179.86591823
D28	179.87305058
D29	-180.00000000
D30	-179.90852858
D31	-2.23945558
D32	178.84363376
D33	131.37818290
D34	-106.15884710
D35	6.22064734
D36	-107.35141075
D37	103.49398626
D38	179.80245176
D39	179.98225178
D40	-60.57632639
D41	60.52994154
D42	-178.76506044
D43	-179.27331826

Number of immaginary frequency:0

Energy= -1312.3152893(a.u.)

Structure: DSA (1) in water

```
 C
 C                    1             B1
 C                    2             B2     1              A1
 C                    3             B3     2              A2     1              D1
 C                    4             B4     3              A3     2              D2
 C                    1             B5     2              A4     3              D3
 N                    3             B6     2              A5     1              D4
 C                    7             B7     3              A6     2              D5
 C                    8             B8     7              A7     3              D6
 C                    8             B9     7              A8     3              D7
 O                   10            B10     8              A9     7              D8
 O                    4            B11     3             A10     2              D9
 C                   12            B12     4             A11     3             D10
 O                    5            B13     4             A12     3             D11
 C                   14            B14     5             A13     4             D12
 O                    6            B15     1             A14     2             D13
 C                   16            B16     6             A15     1             D14
 N                   10            B17     8             A16     7             D15
 C                   18            B18    10             A17     8             D16
 C                   19            B19    18             A18    10             D17
 C                   20            B20    19             A19    18             D18
 C                   18            B21    10             A20     8             D19
 C                   19            B22    18             A21    10             D20
 C                   23            B23    19             A22    18             D21
 C                   24            B24    23             A23    19             D22
 C                   25            B25    24             A24    23             D23
 C                   26            B26    25             A25    24             D24
 C                   27            B27    26             A26    25             D25
 N                   25            B28    24             A27    23             D26
 C                   21            B29    20             A28    19             D27
 C                   28            B30    27             A29    26             D28
 O                   31            B31    28             A30    27             D29
 C                   32            B32    31             A31    28             D30
 O                   24            B33    23             A32    19             D31
 O                   31            B34    28             A33    27             D32
 H                    1            B35     6             A34    16             D33
 H                    9            B36     8             A35     7             D34
 H                   23            B37    19             A36    18             D35
 H                   22            B38    18             A37    10             D36
 H                   22            B39    18             A38    10             D37
 H                   21            B40    20             A39    19             D38
 H                   30            B41    21             A40    20             D39
 H                   30            B42    21             A41    20             D40
 H                   13            B43    12             A42     4             D41
 H                   13            B44    12             A43     4             D42
 H                   13            B45    12             A44     4             D43
 H                   15            B46    14             A45     5             D44
 H                   15            B47    14             A46     5             D45
 H                   15            B48    14             A47     5             D46
 H                   27            B49    26             A48    25             D47
 H                   17            B50    16             A49     6             D48
 H                   17            B51    16             A50     6             D49
 H                   17            B52    16             A51     6             D50
 H                   33            B53    32             A52    31             D51
 H                   33            B54    32             A53    31             D52
 H                   33            B55    32             A54    31             D53
 H                    7            B56     3             A55     2             D54
 H                   29            B57    25             A56    24             D55
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B1	1.41221610
B2	1.41384967
B3	1.40544680
B4	1.38611081
B5	1.38157279
B6	1.35919747
B7	1.37680798
B8	1.38825816
B9	1.47145929
B10	1.23024707
B11	1.36364515
B12	1.42775588
B13	1.36789450
B14	1.42496591
B15	1.35762050
B16	1.41279167
B17	1.38089729
B18	1.39785324
B19	1.47786881
B20	1.51903713
B21	1.47375716
B22	1.35934085
B23	1.45919126
B24	1.45697346
B25	1.39408871
B26	1.40561769
B27	1.39339358
B28	1.35498356
B29	1.47983772
B30	1.46008902
B31	1.33695210
B32	1.42914681
B33	1.23759423
B34	1.21805079
B35	1.08599033
B36	1.08122428
B37	1.08292084
B38	1.09356423
B39	1.09689881
B40	1.08818512
B41	1.08880758
B42	1.08664749
B43	1.09262435
B44	1.09667881
B45	1.09205420
B46	1.09645985
B47	1.09534468
B48	1.09238197
B49	1.08477973
B50	1.09133955
B51	1.09761482
B52	1.09759917
B53	1.08991526
B54	1.09322112
B55	1.09319815
B56	1.01997790
B57	1.02394905
A1	120.19821032
A2	121.85564016
A3	117.37337028
A4	118.12029539
A5	108.35176561
A6	109.39763970
A7	108.58762975

A8	114.99233818
A9	119.08203127
A10	118.84661149
A11	115.41219917
A12	119.67827636
A13	113.44912304
A14	125.09961713
A15	117.07161234
A16	119.76641130
A17	123.64536027
A18	108.02617947
A19	106.52011929
A20	125.35141119
A21	128.48107262
A22	121.05378841
A23	114.86586969
A24	125.25437421
A25	107.30586136
A26	106.34975070
A27	126.25132797
A28	61.53252184
A29	131.47168857
A30	112.04571193
A31	115.24338626
A32	123.05991418
A33	123.87092974
A34	121.94328140
A35	127.70876321
A36	121.78824572
A37	109.97735288
A38	110.03267967
A39	120.61665803
A40	119.25562736
A41	117.97932319
A42	111.07038852
A43	110.52724805
A44	105.98401178
A45	110.69386203
A46	110.85927377
A47	106.39314659
A48	128.14378016
A49	106.05034075
A50	111.36584112
A51	111.33548112
A52	105.57011842
A53	110.51620669
A54	110.50735011
A55	126.87407821
A56	125.56790412
D1	-1.04139145
D2	0.32686814
D3	0.79957954
D4	179.50916832
D5	0.49896564
D6	-0.56417184
D7	-177.24738583
D8	11.45640271
D9	-177.24088145
D10	-118.80204392
D11	179.20384255
D12	98.14082800
D13	179.73801381
D14	-1.37974687
D15	-167.89044471

D16	-172.45599597
D17	-162.11154496
D18	-10.02152837
D19	6.58069169
D20	21.77560406
D21	169.62292913
D22	-3.13328088
D23	3.99749996
D24	-179.51287852
D25	0.48225889
D26	-175.07524442
D27	108.04780694
D28	178.99311503
D29	0.33679372
D30	-179.87700226
D31	-179.88126116
D32	-179.55650957
D33	-0.05223572
D34	-177.49140071
D35	-5.60957138
D36	40.85933612
D37	-79.55571084
D38	-140.91471961
D39	-107.32847774
D40	103.50157609
D41	-64.52155000
D42	57.63970887
D43	176.04091224
D44	-59.93624580
D45	62.22036480
D46	-178.81034588
D47	-179.89672791
D48	-179.45360006
D49	-60.43539197
D50	61.62155770
D51	-179.99617910
D52	-60.54234456
D53	60.55616823
D54	-179.62262121
D55	0.07306545

Number of immaginary frequency:0

Energy= -1655.4950636(a.u.)

Structure: N-Boc-CPI (4) with 1 explicit molecule of water

C							
C	1	B1					
C	2	B2	1	A1			
N	3	B3	2	A2	1	D1	
C	4	B4	3	A3	2	D2	
C	1	B5	2	A4	3	D3	
C	2	B6	1	A5	6	D4	
C	7	B7	2	A6	1	D5	
C	8	B8	7	A7	2	D6	
C	3	B9	2	A8	1	D7	
N	8	B10	7	A9	2	D8	
C	11	B11	8	A10	7	D9	
C	12	B12	11	A11	8	D10	
O	9	B13	8	A12	7	D11	
C	4	B14	3	A13	2	D12	
O	15	B15	4	A14	3	D13	
C	16	B16	15	A15	4	D14	

C	17	B17	16	A16	15	D15
O	15	B18	4	A17	3	D16
C	17	B19	16	A18	15	D17
C	17	B20	16	A19	15	D18
O	14	B21	9	A20	8	D19
H	12	B22	11	A21	8	D20
H	11	B23	8	A22	7	D21
H	22	B24	14	A23	9	D22
H	13	B25	12	A24	11	D23
H	22	B26	14	A25	9	D24
H	6	B27	1	A26	2	D25
H	1	B28	6	A27	5	D26
H	1	B29	6	A28	5	D27
H	5	B30	4	A29	3	D28
H	5	B31	4	A30	3	D29
H	10	B32	3	A31	2	D30
H	18	B33	17	A32	16	D31
H	18	B34	17	A33	16	D32
H	18	B35	17	A34	16	D33
H	20	B36	17	A35	16	D34
H	20	B37	17	A36	16	D35
H	20	B38	17	A37	16	D36
H	21	B39	17	A38	16	D37
H	21	B40	17	A39	16	D38
H	21	B41	17	A40	16	D39

B1	1.52930151
B2	1.48043700
B3	1.39666612
B4	1.47045354
B5	1.48367805
B6	1.46237154
B7	1.39133291
B8	1.45104594
B9	1.35357115
B10	1.36760011
B11	1.35306898
B12	1.38723055
B13	1.24244599
B14	1.38132885
B15	1.34138076
B16	1.46265382
B17	1.52370956
B18	1.21193462
B19	1.52266061
B20	1.52363779
B21	2.71968252
B22	1.08132040
B23	1.03217446
B24	0.98884028
B25	1.08221522
B26	0.96548703
B27	1.08528829
B28	1.08781218
B29	1.08552678
B30	1.09291460
B31	1.09692619
B32	1.08148163
B33	1.09118892
B34	1.09523450
B35	1.09533767
B36	1.09474861
B37	1.09468931
B38	1.09438449

B39	1.09523117
B40	1.09121219
B41	1.09531487
A1	113.98605191
A2	107.54993962
A3	111.90997538
A4	60.54152595
A5	120.29370563
A6	118.32297913
A7	124.92400844
A8	123.32797486
A9	108.06699356
A10	108.93496840
A11	109.34904241
A12	123.79797063
A13	124.56992733
A14	109.16796002
A15	120.42702771
A16	110.11797358
A17	124.25308836
A18	102.52100976
A19	109.99599434
A20	115.34003462
A21	120.93780951
A22	123.11401939
A23	12.03999500
A24	125.77590046
A25	103.01503551
A26	120.73130550
A27	119.02946491
A28	118.21161303
A29	110.09095776
A30	110.01002599
A31	121.81250214
A32	111.24598235
A33	109.34296785
A34	110.30599601
A35	110.72101854
A36	110.67999095
A37	109.94397554
A38	109.39496995
A39	111.20097412
A40	110.31700496
D1	51.77096710
D2	18.44508616
D3	-95.12644624
D4	120.94650432
D5	130.04341425
D6	4.23999952
D7	-131.00782156
D8	-175.84504148
D9	0.12203272
D10	0.21395334
D11	-178.50499066
D12	-172.21714171
D13	-173.41594207
D14	-179.73397649
D15	61.88100391
D16	6.72309689
D17	179.71698765
D18	-62.50498164
D19	-1.67902682
D20	-179.29928109
D21	-179.60002650

D22	156.80912188
D23	-179.97942793
D24	-108.38199495
D25	-110.50871933
D26	-11.46062736
D27	-160.24297457
D28	-139.71107834
D29	101.10196979
D30	178.45305156
D31	-66.94000284
D32	172.87204339
D33	54.18402151
D34	-60.50001925
D35	59.86601703
D36	179.66899476
D37	-173.37904664
D38	66.48498317
D39	-54.64203870

Number of immaginary frequency:0

Zero-point correction=	0.349082	(Hartree/Particle)
Thermal correction to Energy=	0.370053	
Thermal correction to Enthalpy=	0.370998	
Thermal correction to Gibbs Free Energy=	0.299778	
Sum of electronic and zero-point Energies=	-1030.653288	
Sum of electronic and thermal Energies=	-1030.632316	
Sum of electronic and thermal Enthalpies=	-1030.631372	
Sum of electronic and thermal Free Energies=	-1030.702592	

Structure: N-Boc-CPI (4) with 2 explicit molecules of water

C						
C	1	B1				
C	2	B2	1	A1		
N	3	B3	2	A2	1	D1
C	4	B4	3	A3	2	D2
C	3	B5	2	A4	1	D3
C	6	B6	3	A5	2	D4
C	7	B7	6	A6	3	D5
C	2	B8	1	A7	5	D6
N	8	B9	7	A8	6	D7
C	10	B10	8	A9	7	D8
C	11	B11	10	A10	8	D9
C	12	B12	11	A11	10	D10
C	10	B13	8	A12	7	D11
O	14	B14	10	A13	8	D12
O	6	B15	3	A14	2	D13
O	14	B16	10	A15	8	D14
C	17	B17	14	A16	10	D15
C	18	B18	17	A17	14	D16
C	18	B19	17	A18	14	D17
C	18	B20	17	A19	14	D18
O	16	B21	6	A20	3	D19
O	16	B22	6	A21	3	D20
H	5	B23	4	A22	3	D21
H	4	B24	3	A23	2	D22
H	22	B25	16	A24	6	D23
H	1	B26	5	A25	4	D24
H	22	B27	16	A26	6	D25
H	12	B28	11	A27	10	D26
H	13	B29	12	A28	11	D27
H	13	B30	12	A29	11	D28
H	11	B31	10	A30	8	D29

H	11	B32	10	A31	8	D30
H	7	B33	6	A32	3	D31
H	21	B34	18	A33	17	D32
H	21	B35	18	A34	17	D33
H	21	B36	18	A35	17	D34
H	19	B37	18	A36	17	D35
H	19	B38	18	A37	17	D36
H	19	B39	18	A38	17	D37
H	20	B40	18	A39	17	D38
H	20	B41	18	A40	17	D39
H	20	B42	18	A41	17	D40
H	23	B43	16	A42	6	D41
H	23	B44	16	A43	6	D42

B1	1.40871778
B2	1.39263064
B3	1.36817565
B4	1.35221690
B5	1.44520765
B6	1.45701779
B7	1.35533504
B8	1.46120810
B9	1.39361337
B10	1.46930383
B11	1.51213772
B12	1.48232713
B13	1.38394938
B14	1.21058079
B15	1.25166500
B16	1.34014068
B17	1.46417705
B18	1.52251188
B19	1.52342376
B20	1.52360502
B21	2.73490335
B22	2.84010159
B23	1.08131963
B24	1.03232726
B25	0.98592041
B26	1.08208049
B27	0.96560010
B28	1.08520588
B29	1.08775371
B30	1.08551341
B31	1.09278613
B32	1.09684015
B33	1.08401107
B34	1.09116771
B35	1.09521321
B36	1.09541388
B37	1.09482721
B38	1.09464873
B39	1.09436728
B40	1.09519496
B41	1.09132267
B42	1.09525215
B43	0.96470136
B44	0.97635548
A1	107.30398573
A2	108.08101517
A3	108.86498623
A4	124.70896023
A5	115.97303565
A6	120.30900623

A7	134.28771835
A8	128.78330183
A9	111.87099085
A10	103.78903282
A11	114.78001002
A12	124.51168137
A13	124.02102153
A14	122.85899383
A15	109.12599328
A16	120.30701375
A17	102.50897599
A18	109.92096414
A19	110.07200719
A20	115.89499257
A21	109.97201117
A22	120.91099732
A23	123.32400191
A24	13.01195403
A25	125.76524292
A26	103.78799595
A27	118.97602576
A28	119.05901902
A29	118.23504259
A30	110.12149854
A31	110.06765621
A32	117.13465481
A33	111.23698637
A34	109.31693331
A35	110.34097588
A36	110.76802020
A37	110.67599512
A38	109.91697974
A39	109.35500344
A40	111.25201189
A41	110.34903839
A42	101.36393760
A43	7.87101156
D1	-0.37496843
D2	0.06498431
D3	179.85799178
D4	4.72903118
D5	-4.50206304
D6	175.03677939
D7	171.07470248
D8	-156.92395255
D9	-19.52302529
D10	-53.84497197
D11	14.28222726
D12	8.01050995
D13	-178.34796666
D14	-172.34345406
D15	179.63404867
D16	-179.89003620
D17	-62.05507580
D18	62.27394092
D19	-2.41801232
D20	-171.54797820
D21	-179.23794256
D22	-179.15000247
D23	159.93516770
D24	179.98123079
D25	-108.09192676
D26	152.14795521
D27	-11.43898883

D28	-160.38007783
D29	-140.58237599
D30	100.11623147
D31	170.69272424
D32	-67.09301414
D33	172.78201502
D34	54.10104544
D35	-60.60103888
D36	59.82197491
D37	179.58596430
D38	-173.75202021
D39	66.10305537
D40	-55.02796487
D41	-79.11507595
D42	175.72003865

Number of immaginary frequency:0

Zero-point correction=	0.373925 (Hartree/Particle)
Thermal correction to Energy=	0.398199
Thermal correction to Enthalpy=	0.399143
Thermal correction to Gibbs Free Energy=	0.319845
Sum of electronic and zero-point Energies=	-1106.969126
Sum of electronic and thermal Energies=	-1106.944852
Sum of electronic and thermal Enthalpies=	-1106.943908
Sum of electronic and thermal Free Energies=	-1107.023205

Structure: Transition State of N-Boc-CPI (4) with Pyridine

C							
H	1	B1					
H	1	B2	2	A1			
C	1	B3	3	A2	2	D1	
H	4	B4	1	A3	3	D2	
C	4	B5	1	A4	3	D3	
H	6	B6	4	A5	1	D4	
H	6	B7	4	A6	1	D5	
C	4	B8	1	A7	6	D6	
C	9	B9	4	A8	1	D7	
N	10	B10	9	A9	4	D8	
C	9	B11	4	A10	1	D9	
C	12	B12	9	A11	4	D10	
C	13	B13	12	A12	9	D11	
C	10	B14	9	A13	4	D12	
C	12	B15	9	A14	4	D13	
C	16	B16	12	A15	9	D14	
N	17	B17	16	A16	12	D15	
H	16	B18	12	A17	9	D16	
H	17	B19	16	A18	12	D17	
H	18	B20	17	A19	16	D18	
O	14	B21	13	A20	12	D19	
H	15	B22	10	A21	9	D20	
N	1	B23	4	A22	9	D21	
C	24	B24	1	A23	4	D22	
C	25	B25	24	A24	1	D23	
C	26	B26	25	A25	24	D24	
C	27	B27	26	A26	25	D25	
C	24	B28	1	A27	4	D26	
H	29	B29	24	A28	1	D27	
H	28	B30	27	A29	26	D28	
H	27	B31	26	A30	25	D29	
H	26	B32	25	A31	24	D30	
H	25	B33	24	A32	1	D31	
C	11	B34	10	A33	9	D32	

O	35	B35	11	A34	10	D33
O	35	B36	11	A35	10	D34
C	37	B37	35	A36	11	D35
C	38	B38	37	A37	35	D36
C	38	B39	37	A38	35	D37
C	38	B40	37	A39	35	D38
H	39	B41	38	A40	37	D39
H	39	B42	38	A41	37	D40
H	39	B43	38	A42	37	D41
H	40	B44	38	A43	37	D42
H	40	B45	38	A44	37	D43
H	40	B46	38	A45	37	D44
H	41	B47	38	A46	37	D45
H	41	B48	38	A47	37	D46
H	41	B49	38	A48	37	D47

B1	1.08629726
B2	1.08553637
B3	1.48783562
B4	1.09445253
B5	1.52373596
B6	1.09221779
B7	1.09781641
B8	1.48539740
B9	1.42880422
B10	1.41811619
B11	1.42385043
B12	1.39550301
B13	1.45114359
B14	1.37226142
B15	1.42696435
B16	1.38085420
B17	1.36198457
B18	1.08279667
B19	1.08131643
B20	1.00858369
B21	1.24197104
B22	1.08136236
B23	1.89786789
B24	1.34178239
B25	1.38535429
B26	1.39418178
B27	1.39313435
B28	1.34170169
B29	1.08773922
B30	1.08544745
B31	1.08560216
B32	1.08540678
B33	1.08775893
B34	1.36873384
B35	1.21359463
B36	1.35356472
B37	1.45625257
B38	1.52368436
B39	1.52455766
B40	1.52470386
B41	1.09456315
B42	1.09525960
B43	1.09477450
B44	1.09540709
B45	1.09536508
B46	1.09101257
B47	1.09541707
B48	1.09104678

B49	1.09584235
A1	115.08400127
A2	116.48009021
A3	114.90832320
A4	113.75885649
A5	113.71336023
A6	110.31539077
A7	89.34083203
A8	109.55002526
A9	107.16379396
A10	132.14165374
A11	116.69620990
A12	126.82656724
A13	124.39473033
A14	136.56603776
A15	106.77907127
A16	108.82065317
A17	127.83659869
A18	129.92576259
A19	128.36906232
A20	121.27274192
A21	121.56505139
A22	111.32432247
A23	117.72593754
A24	122.38979664
A25	118.89451059
A26	118.61538170
A27	116.11429123
A28	115.82614903
A29	121.31892818
A30	120.68852316
A31	119.77715326
A32	115.85367870
A33	125.79589676
A34	125.15976134
A35	109.27509246
A36	120.10936842
A37	102.63645730
A38	110.26843268
A39	110.36412398
A40	110.09216489
A41	110.69751498
A42	110.61216003
A43	109.55136619
A44	110.21689775
A45	111.01638950
A46	109.56554066
A47	111.00637690
A48	110.23676763
D1	-141.11007692
D2	-53.49938966
D3	172.35984937
D4	48.29825873
D5	170.03117498
D6	-104.58892760
D7	96.64858632
D8	4.26269145
D9	-81.34529615
D10	176.19684074
D11	0.47070910
D12	-176.68387815
D13	-3.87879289
D14	-179.82929173
D15	-0.05552128

D16	-0.75105158
D17	179.50688466
D18	178.98155390
D19	-179.99736672
D20	-179.23996802
D21	177.23557934
D22	81.75091023
D23	-149.55137916
D24	0.69814726
D25	-0.45229148
D26	-68.01786930
D27	-30.73276832
D28	-179.31223698
D29	179.43944346
D30	-178.93717569
D31	30.73598752
D32	-177.97820330
D33	6.75910368
D34	-173.84762017
D35	179.22980311
D36	-179.59593198
D37	-61.92159168
D38	62.58408206
D39	179.38508483
D40	-60.76539960
D41	59.48241797
D42	-173.37269306
D43	-54.51507578
D44	66.32333944
D45	172.95852326
D46	-66.65031178
D47	54.17071730

Number of immaginary frequency = 1 (eigenvalue=-560.6820)

Zero-point correction=	0.412647 (Hartree/Particle)
Thermal correction to Energy=	0.436801
Thermal correction to Enthalpy=	0.437746
Thermal correction to Gibbs Free Energy=	0.357010
Sum of electronic and zero-point Energies=	-1202.172838
Sum of electronic and thermal Energies=	-1202.148683
Sum of electronic and thermal Enthalpies=	-1202.147739
Sum of electronic and thermal Free Energies=	-1202.228475

Structure: Transition State of N-Boc-CPI (4) with Pyridine (1 water explicit molecule)

C								
N	1	B1						
C	2	B2	1	A1				
C	3	B3	2	A2	1	D1		
C	4	B4	3	A3	2	D2		
C	1	B5	2	A4	3	D3		
C	2	B6	1	A5	6	D4		
C	7	B7	2	A6	1	D5		
C	8	B8	7	A7	2	D6		
N	9	B9	8	A8	7	D7		
C	10	B10	9	A9	8	D8		
C	11	B11	10	A10	9	D9		
C	11	B12	10	A11	9	D10		
C	13	B13	11	A12	10	D11		
C	14	B14	13	A13	11	D12		
C	15	B15	14	A14	13	D13		
N	15	B16	14	A15	13	D14		

C	17	B17	15	A16	14	D15
C	18	B18	17	A17	15	D16
C	10	B19	9	A18	8	D17
O	20	B20	10	A19	9	D18
C	21	B21	20	A20	10	D19
C	22	B22	21	A21	20	D20
O	14	B23	13	A22	11	D21
O	20	B24	10	A23	9	D22
C	22	B25	21	A24	20	D23
C	22	B26	21	A25	20	D24
O	24	B27	14	A26	13	D25
H	7	B28	2	A27	1	D26
H	7	B29	2	A28	1	D27
H	8	B30	7	A29	2	D28
H	9	B31	8	A30	7	D29
H	9	B32	8	A31	7	D30
H	19	B33	18	A32	17	D31
H	18	B34	17	A33	15	D32
H	17	B35	15	A34	14	D33
H	13	B36	11	A35	10	D34
H	1	B37	2	A36	3	D35
H	6	B38	1	A37	2	D36
H	5	B39	4	A38	3	D37
H	4	B40	3	A39	2	D38
H	3	B41	2	A40	1	D39
H	26	B42	22	A41	21	D40
H	26	B43	22	A42	21	D41
H	26	B44	22	A43	21	D42
H	27	B45	22	A44	21	D43
H	27	B46	22	A45	21	D44
H	27	B47	22	A46	21	D45
H	23	B48	22	A47	21	D46
H	23	B49	22	A48	21	D47
H	23	B50	22	A49	21	D48
H	28	B51	24	A50	14	D49
H	28	B52	24	A51	14	D50

B1	1.33906226
B2	1.33921250
B3	1.38619781
B4	1.39350461
B5	1.38659354
B6	1.90870948
B7	1.48528601
B8	1.52380999
B9	1.46521771
B10	1.41679403
B11	1.42323862
B12	1.37306884
B13	1.44537830
B14	1.44706605
B15	1.40366117
B16	1.36983082
B17	1.35607502
B18	1.38235366
B19	1.36909027
B20	1.35307317
B21	1.45663065
B22	1.52469699
B23	1.25749806
B24	1.21346844
B25	1.52346383
B26	1.52449820
B27	2.66800990

B28	1.08614663
B29	1.08546873
B30	1.09373382
B31	1.09237977
B32	1.09780510
B33	1.08276560
B34	1.08179217
B35	1.03165335
B36	1.08123372
B37	1.08774917
B38	1.08532895
B39	1.08571042
B40	1.08529432
B41	1.08780681
B42	1.09453910
B43	1.09518622
B44	1.09473794
B45	1.09541766
B46	1.09540522
B47	1.09105844
B48	1.09543996
B49	1.09108245
B50	1.09591243
B51	0.99852892
B52	0.96553626
A1	119.18942425
A2	122.22385868
A3	118.78825752
A4	122.22470653
A5	116.95465792
A6	111.51482781
A7	113.82882051
A8	103.45373497
A9	110.12170677
A10	107.50233657
A11	128.77201486
A12	120.32738810
A13	114.83579097
A14	125.04286811
A15	127.10774857
A16	109.18894396
A17	109.62696633
A18	123.27058915
A19	109.27710155
A20	120.09638576
A21	110.28405012
A22	121.72555518
A23	125.05080301
A24	102.63848911
A25	110.30048136
A26	115.86008300
A27	96.51401922
A28	96.23060397
A29	115.29272408
A30	113.71118795
A31	110.30498662
A32	125.76912594
A33	120.76831042
A34	122.73765696
A35	121.73260011
A36	115.91054691
A37	119.85792338
A38	120.61024718
A39	119.85249571

A40	115.95141185
A41	110.07795604
A42	110.64659927
A43	110.63027726
A44	109.51995848
A45	110.21410894
A46	111.10247064
A47	109.61083328
A48	111.01225888
A49	110.23435137
A50	9.54856010
A51	100.84482225
D1	-0.73694583
D2	0.67392545
D3	0.47227110
D4	153.90020479
D5	-70.56289892
D6	-78.54557931
D7	-70.75564341
D8	-22.59642346
D9	11.79508245
D10	-167.34750767
D11	178.94476133
D12	-1.26143538
D13	1.13551581
D14	-178.57530168
D15	179.92662005
D16	-0.12818788
D17	167.11268126
D18	-4.79540002
D19	179.29793911
D20	62.84841970
D21	179.47080457
D22	175.79532291
D23	-179.35320041
D24	-61.64890982
D25	177.85353533
D26	167.81269277
D27	51.34096432
D28	56.33963077
D29	49.34726932
D30	171.10730260
D31	-178.94832220
D32	-179.73009705
D33	0.44877081
D34	-0.52889477
D35	-179.98153198
D36	179.41086759
D37	179.53543714
D38	-179.02194005
D39	179.58335874
D40	179.83812634
D41	-60.33736467
D42	59.93078711
D43	-172.98790395
D44	-54.17226372
D45	66.67445058
D46	173.24302828
D47	-66.36952458
D48	54.48972272
D49	150.14959429
D50	-105.76257941

Number of immaginary frequency = 1 (eigenvalue=-543.5000)

Zero-point correction=	0.438739 (Hartree/Particle)
Thermal correction to Energy=	0.465197
Thermal correction to Enthalpy=	0.466141
Thermal correction to Gibbs Free Energy=	0.380555
Sum of electronic and zero-point Energies=	-1278.504185
Sum of electronic and thermal Energies=	-1278.477727
Sum of electronic and thermal Enthalpies=	-1278.476783
Sum of electronic and thermal Free Energies=	-1278.562369

Structure: Transition State of N-Boc-CPI (5) with Pyridine (2 water explicit molecules)

C							
N	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1
C	4	B4	3	A3	2	D2
C	1	B5	2	A4	3	D3
C	2	B6	1	A5	6	D4
C	7	B7	2	A6	1	D5
C	8	B8	7	A7	2	D6
N	9	B9	8	A8	7	D7
C	10	B10	9	A9	8	D8
C	11	B11	10	A10	9	D9
C	11	B12	10	A11	9	D10
C	13	B13	11	A12	10	D11
C	14	B14	13	A13	11	D12
C	15	B15	14	A14	13	D13
N	15	B16	14	A15	13	D14
C	17	B17	15	A16	14	D15
C	18	B18	17	A17	15	D16
C	10	B19	9	A18	8	D17
O	20	B20	10	A19	9	D18
C	21	B21	20	A20	10	D19
C	22	B22	21	A21	20	D20
O	14	B23	13	A22	11	D21
O	20	B24	10	A23	9	D22
C	22	B25	21	A24	20	D23
C	22	B26	21	A25	20	D24
O	24	B27	14	A26	13	D25
H	7	B28	2	A27	1	D26
H	7	B29	2	A28	1	D27
H	8	B30	7	A29	2	D28
H	9	B31	8	A30	7	D29
H	9	B32	8	A31	7	D30
H	19	B33	18	A32	17	D31
H	18	B34	17	A33	15	D32
H	17	B35	15	A34	14	D33
H	13	B36	11	A35	10	D34
H	1	B37	2	A36	3	D35
H	6	B38	1	A37	2	D36
H	5	B39	4	A38	3	D37
H	4	B40	3	A39	2	D38
H	3	B41	2	A40	1	D39
H	26	B42	22	A41	21	D40
H	26	B43	22	A42	21	D41
H	26	B44	22	A43	21	D42
H	27	B45	22	A44	21	D43
H	27	B46	22	A45	21	D44
H	27	B47	22	A46	21	D45
H	23	B48	22	A47	21	D46
H	23	B49	22	A48	21	D47
H	23	B50	22	A49	21	D48
H	28	B51	24	A50	14	D49

H	28	B52	24	A51	14	D50
H	24	B53	14	A52	13	D51
O	24	B54	14	A53	13	D52
H	55	B55	24	A54	14	D53

B1	1.33672501
B2	1.33696670
B3	1.38702612
B4	1.39284191
B5	1.38719690
B6	1.91909863
B7	1.48228696
B8	1.52399863
B9	1.46418183
B10	1.41495996
B11	1.42098740
B12	1.37540361
B13	1.43839438
B14	1.44005805
B15	1.40504681
B16	1.37071031
B17	1.35548244
B18	1.38238118
B19	1.37066382
B20	1.35251182
B21	1.45790784
B22	1.52455789
B23	1.26931457
B24	1.21227407
B25	1.52346591
B26	1.52423316
B27	2.68271641
B28	1.08603262
B29	1.08554696
B30	1.09304069
B31	1.09210776
B32	1.09786860
B33	1.08263187
B34	1.08179418
B35	1.03139116
B36	1.08314456
B37	1.08772966
B38	1.08522603
B39	1.08581563
B40	1.08519780
B41	1.08785978
B42	1.09452400
B43	1.09539294
B44	1.09471016
B45	1.09537779
B46	1.09532610
B47	1.09117110
B48	1.09538363
B49	1.09098967
B50	1.09601353
B51	0.99456530
B52	0.96557882
B53	1.82154528
B54	2.79298502
B55	0.96447908
A1	119.53902871
A2	122.05719032
A3	118.69783546
A4	122.08014371

A5	117.90954861
A6	111.52335431
A7	114.00452672
A8	103.30732722
A9	110.00703695
A10	107.60547860
A11	128.60541028
A12	119.84106898
A13	115.57503216
A14	124.79495369
A15	127.34482503
A16	109.10660326
A17	109.73718483
A18	123.73955364
A19	109.29538664
A20	119.96850249
A21	110.31910115
A22	121.97858627
A23	124.85544496
A24	102.58218496
A25	110.21889918
A26	116.47977146
A27	95.83665321
A28	95.92710606
A29	115.54321284
A30	113.78942468
A31	110.23245115
A32	125.74676255
A33	120.72316725
A34	122.96529164
A35	122.17536489
A36	116.00154459
A37	119.94079043
A38	120.52989659
A39	119.91846247
A40	116.04696814
A41	110.09185066
A42	110.70158815
A43	110.62506642
A44	109.51771844
A45	110.24326622
A46	111.08186800
A47	109.52267420
A48	110.99272642
A49	110.29918522
A50	10.30845095
A51	101.51856668
A52	113.98028316
A53	111.03899320
A54	98.10026972
D1	-0.81579468
D2	0.65327568
D3	0.58821401
D4	158.30106122
D5	-73.74870681
D6	-78.25214407
D7	-69.57992713
D8	-23.80986595
D9	13.15027868
D10	-165.44528953
D11	178.95966949
D12	-1.53256192
D13	0.92433907
D14	-178.43453558

D15	179.58206098
D16	-0.08024963
D17	163.50523717
D18	-2.49550120
D19	178.28517877
D20	63.10755897
D21	179.06937105
D22	178.23349637
D23	-179.08037607
D24	-61.33226086
D25	177.91919622
D26	164.71381848
D27	48.23729091
D28	57.45003068
D29	50.51586174
D30	172.36681139
D31	-178.90753875
D32	-179.67033614
D33	0.39136835
D34	0.60833831
D35	-179.82901330
D36	179.48187662
D37	179.60230873
D38	-179.16390836
D39	179.44584031
D40	179.76539416
D41	-60.39447581
D42	59.87187244
D43	-173.50603665
D44	-54.66977645
D45	66.20024468
D46	172.98826219
D47	-66.69542593
D48	54.24326272
D49	153.16946723
D50	-106.53811367
D51	4.31470546
D52	2.33521328
D53	-76.40323019

Number of immaginary frequency = 1 (eigenvalue=-518.2779)

Zero-point correction=	0.463654 (Hartree/Particle)
Thermal correction to Energy=	0.493464
Thermal correction to Enthalpy=	0.494409
Thermal correction to Gibbs Free Energy=	0.399701
Sum of electronic and zero-point Energies=	-1354.823081
Sum of electronic and thermal Energies=	-1354.793270
Sum of electronic and thermal Enthalpies=	-1354.792326
Sum of electronic and thermal Free Energies=	-1354.887034

Structure: Transition State of CPI (3) with Pyridine

C								
C	1	B1						
N	2	B2	1	A1				
C	3	B3	2	A2	1	D1		
C	2	B4	1	A3	3	D2		
O	5	B5	2	A4	1	D3		
N	5	B6	2	A5	1	D4		
C	7	B7	5	A6	2	D5		
C	8	B8	7	A7	5	D6		
C	9	B9	8	A8	7	D7		
C	7	B10	5	A9	2	D8		

C	8	B11	7	A10	5	D9
C	12	B12	8	A11	7	D10
C	13	B13	12	A12	8	D11
C	14	B14	13	A13	12	D12
N	14	B15	13	A14	12	D13
C	16	B16	14	A15	13	D14
C	17	B17	16	A16	14	D15
O	13	B18	12	A17	8	D16
C	10	B19	9	A18	8	D17
N	20	B20	10	A19	9	D18
C	21	B21	20	A20	10	D19
C	22	B22	21	A21	20	D20
C	23	B23	22	A22	21	D21
C	24	B24	23	A23	22	D22
C	21	B25	20	A24	10	D23
H	20	B26	10	A25	9	D24
H	20	B27	10	A26	9	D25
H	10	B28	9	A27	8	D26
H	12	B29	8	A28	7	D27
H	11	B30	7	A29	5	D28
H	11	B31	7	A30	5	D29
H	22	B32	21	A31	20	D30
H	23	B33	22	A32	21	D31
H	24	B34	23	A33	22	D32
H	25	B35	24	A34	23	D33
H	26	B36	21	A35	20	D34
H	16	B37	14	A36	13	D35
H	18	B38	17	A37	16	D36
H	17	B39	16	A38	14	D37
H	3	B40	2	A39	1	D38
H	1	B41	2	A40	3	D39
C	4	B42	3	A41	2	D40
C	43	B43	4	A42	3	D41
C	44	B44	43	A43	4	D42
C	45	B45	44	A44	43	D43
C	46	B46	45	A45	44	D44
H	43	B47	4	A46	3	D45
H	44	B48	43	A47	4	D46
H	45	B49	44	A48	43	D47
H	46	B50	45	A49	44	D48

B1	1.38246815
B2	1.37478696
B3	1.36232977
B4	1.48591481
B5	1.22911038
B6	1.36617245
B7	1.42388849
B8	1.42812770
B9	1.48441019
B10	1.46354646
B11	1.37253923
B12	1.45382335
B13	1.45037731
B14	1.39605691
B15	1.36385729
B16	1.36202162
B17	1.38060214
B18	1.24171578
B19	1.48679433
B20	1.90552600
B21	1.34031701
B22	1.38637853
B23	1.39297774

B24	1.39381481
B25	1.34081412
B26	1.08556774
B27	1.08616582
B28	1.09401742
B29	1.08081098
B30	1.09822795
B31	1.09245890
B32	1.08773541
B33	1.08540303
B34	1.08566479
B35	1.08528732
B36	1.08783637
B37	1.00863426
B38	1.08273459
B39	1.08129989
B40	1.01073167
B41	1.07956550
B42	1.39886565
B43	1.38336135
B44	1.41011198
B45	1.38212008
B46	1.40526061
B47	1.08639387
B48	1.08653678
B49	1.08646126
B50	1.08712878
A1	108.52033408
A2	110.29973142
A3	138.05872998
A4	117.56527844
A5	119.55581376
A6	125.11231130
A7	107.43463572
A8	109.43980591
A9	125.33064883
A10	128.18531469
A11	120.02057629
A12	113.73292146
A13	126.86080056
A14	125.08638744
A15	109.59142642
A16	108.85599928
A17	124.88028039
A18	89.43018561
A19	111.52843697
A20	116.77524874
A21	122.29193326
A22	118.84115270
A23	118.72568671
A24	117.76434389
A25	116.48714273
A26	116.28711254
A27	118.51808147
A28	121.71574938
A29	110.64410832
A30	110.56039675
A31	115.89973519
A32	119.82539835
A33	120.64796269
A34	121.43172148
A35	116.00982107
A36	122.03631044
A37	125.38839322

A38	121.24106030
A39	120.16210754
A40	127.20608140
A41	130.73098937
A42	117.35568223
A43	121.50106532
A44	121.10991157
A45	118.88534429
A46	121.30282984
A47	119.28130253
A48	119.13816884
A49	120.68565144
D1	0.34395349
D2	175.86798643
D3	-164.82909405
D4	15.90735637
D5	-174.93487509
D6	-166.54497418
D7	4.63222454
D8	6.63993551
D9	15.25023180
D10	177.68698945
D11	-0.72398223
D12	0.62509780
D13	-178.58865124
D14	179.41835453
D15	-0.03795919
D16	-179.92365202
D17	95.74486853
D18	178.09743566
D19	-70.02414615
D20	151.59306298
D21	-0.16159149
D22	0.17322998
D23	81.57015182
D24	68.41394449
D25	-72.42868750
D26	-145.61039477
D27	-2.05456183
D28	-86.73825371
D29	33.98348566
D30	-28.86099347
D31	179.40878711
D32	-179.69152035
D33	179.42047302
D34	28.60705759
D35	0.33726492
D36	-179.19149718
D37	-179.63480092
D38	173.73135164
D39	-177.27765964
D40	179.85630718
D41	179.87254151
D42	-0.08746619
D43	0.03094421
D44	0.01752162
D45	-0.34352266
D46	179.76642065
D47	179.87072324
D48	179.73449326

Number of immaginary frequency : 1 (eigenvalue=-548.8549)

Zero-point correction= 0.406306 (Hartree/Particle)

```
 Thermal correction to Energy=                  0.430376
 Thermal correction to Enthalpy=                0.431320
 Thermal correction to Gibbs Free Energy=       0.349621
 Sum of electronic and zero-point Energies=         -1332.170826
 Sum of electronic and thermal Energies=            -1332.146756
 Sum of electronic and thermal Enthalpies=          -1332.145812
 Sum of electronic and thermal Free Energies=       -1332.227511
```

Structure: Transition State of CPI (3) with Adenine

```
 N
 C                  1             B1
 C                  2             B2    1             A1
 N                  3             B3    2             A2    1             D1
 C                  1             B4    2             A3    3             D2
 C                  2             B5    1             A4    5             D3
 N                  6             B6    2             A5    1             D4
 C                  7             B7    6             A6    2             D5
 N                  8             B8    7             A7    6             D6
 N                  6             B9    2             A8    1             D7
 C                  9            B10    8             A9    7             D8
 C                 11            B11    9            A10    8             D9
 C                 12            B12   11            A11    9            D10
 C                 13            B13   12            A12   11            D11
 N                 14            B14   13            A13   12            D12
 C                 15            B15   14            A14   13            D13
 C                 13            B16   12            A15   11            D14
 C                 17            B17   13            A16   12            D15
 C                 18            B18   17            A17   13            D16
 C                 14            B19   13            A18   12            D17
 C                 17            B20   13            A19   12            D18
 C                 21            B21   17            A20   13            D19
 N                 22            B22   21            A21   17            D20
 C                 15            B23   14            A22   13            D21
 O                 24            B24   15            A23   14            D22
 O                 19            B25   18            A24   17            D23
 C                 24            B26   15            A25   14            D24
 N                 27            B27   24            A26   15            D25
 C                 28            B28   27            A27   24            D26
 C                 29            B29   28            A28   27            D27
 C                 27            B30   24            A29   15            D28
 C                 29            B31   28            A30   27            D29
 C                 32            B32   29            A31   28            D30
 C                 33            B33   32            A32   29            D31
 C                 34            B34   33            A33   32            D32
 H                 11            B35    9            A34    8            D33
 H                 11            B36    9            A35    8            D34
 H                 12            B37   11            A36    9            D35
 H                 20            B38   14            A37   13            D36
 H                 16            B39   15            A38   14            D37
 H                 16            B40   15            A39   14            D38
 H                  8            B41    7            A40    6            D39
 H                 23            B42   22            A41   21            D40
 H                 21            B43   17            A42   13            D41
 H                 22            B44   21            A43   17            D42
 H                 28            B45   27            A44   24            D43
 H                 31            B46   27            A45   24            D44
 H                 32            B47   29            A46   28            D45
 H                 33            B48   32            A47   29            D46
 H                 34            B49   33            A48   32            D47
 H                 35            B50   34            A49   33            D48
 H                 10            B51    6            A50    2            D49
 H                 10            B52    6            A51    2            D50
 H                  5            B53    1            A52    2            D51
```

H	4	B54	3	A53	2	D52
B1	1.37295904					
B2	1.39473357					
B3	1.36385500					
B4	1.30609696					
B5	1.40933684					
B6	1.34627711					
B7	1.32237428					
B8	1.33698717					
B9	1.33647140					
B10	1.89223209					
B11	1.48446901					
B12	1.49088298					
B13	1.42158606					
B14	1.43236618					
B15	1.46441408					
B16	1.42160073					
B17	1.39791359					
B18	1.44903550					
B19	1.37466451					
B20	1.42777474					
B21	1.38075474					
B22	1.36155977					
B23	1.36045521					
B24	1.22897374					
B25	1.24379886					
B26	1.49469878					
B27	1.37414378					
B28	1.36305407					
B29	1.42094719					
B30	1.38592028					
B31	1.39893305					
B32	1.38337167					
B33	1.41019035					
B34	1.38275400					
B35	1.08608759					
B36	1.08649487					
B37	1.09343857					
B38	1.08104538					
B39	1.09749571					
B40	1.08909872					
B41	1.08828813					
B42	1.00849630					
B43	1.08290604					
B44	1.08145914					
B45	1.01197834					
B46	1.08037670					
B47	1.08620272					
B48	1.08632011					
B49	1.08628446					
B50	1.08705711					
B51	1.00767200					
B52	1.00778901					
B53	1.08266192					
B54	1.01588693					
A1	111.35403021					
A2	104.79197579					
A3	103.87531998					
A4	131.65047642					
A5	119.03200900					
A6	118.49994182					
A7	127.89405645					
A8	122.14303093					

A9	118.63599345
A10	115.42999278
A11	91.35000074
A12	109.65899479
A13	107.25000838
A14	108.21597494
A15	132.25387087
A16	116.59501417
A17	127.19401248
A18	124.88937857
A19	136.70744212
A20	106.78802349
A21	108.90199510
A22	124.40999885
A23	123.38398429
A24	121.43466230
A25	119.96097148
A26	112.68696604
A27	110.51900426
A28	107.16100737
A29	138.96255220
A30	130.72407603
A31	117.32201016
A32	121.52800797
A33	121.16097541
A34	94.83401060
A35	97.43032922
A36	115.39191266
A37	121.77398919
A38	110.11697416
A39	111.41896537
A40	116.66554850
A41	128.53500791
A42	127.83004799
A43	129.84695072
A44	119.66951076
A45	127.08485981
A46	121.30702616
A47	119.27802528
A48	119.14004337
A49	120.73698636
A50	120.24500968
A51	119.43398278
A52	125.83817561
A53	128.78998318
D1	-0.35698360
D2	-0.11245208
D3	179.42126597
D4	-179.30761367
D5	-0.40603315
D6	0.01504905
D7	0.43938052
D8	174.38812031
D9	-97.32905141
D10	175.68499638
D11	94.38897495
D12	2.99101107
D13	16.41697770
D14	-82.88700369
D15	176.63760223
D16	0.36197426
D17	-177.67567950
D18	-3.66972607
D19	-179.64307417

D20	-0.02001294
D21	-154.58700847
D22	-4.28701107
D23	179.62159025
D24	172.38000967
D25	-162.87204746
D26	-178.77603551
D27	-0.16992303
D28	18.85110434
D29	-179.35636720
D30	179.07420053
D31	-0.07293485
D32	0.16295134
D33	24.24808042
D34	139.33546908
D35	53.46622916
D36	-179.80963831
D37	89.03589038
D38	-150.21016721
D39	-179.74990631
D40	178.97476058
D41	-0.61995562
D42	179.59067271
D43	-5.04053067
D44	3.06295780
D45	-1.05976163
D46	179.81704661
D47	179.80647108
D48	179.39835027
D49	0.87097267
D50	179.46698495
D51	-178.83081550
D52	174.37668872

Number of immaginary frequency = 1 (eigenvalue=-451.9808)

Zero-point correction=	0.430512 (Hartree/Particle)
Thermal correction to Energy=	0.457515
Thermal correction to Enthalpy=	0.458459
Thermal correction to Gibbs Free Energy=	0.371173
Sum of electronic and zero-point Energies=	-1550.960249
Sum of electronic and thermal Energies=	-1550.933246
Sum of electronic and thermal Enthalpies=	-1550.932301
Sum of electronic and thermal Free Energies=	-1551.019588

Structure: Transition State of CPI (3) with Guanine

C							
C	1	B1					
C	2	B2	1	A1			
C	3	B3	2	A2	1	D1	
C	4	B4	3	A3	2	D2	
C	1	B5	2	A4	3	D3	
C	2	B6	1	A5	6	D4	
C	7	B7	2	A6	1	D5	
N	3	B8	2	A7	1	D6	
C	8	B9	7	A8	2	D7	
O	10	B10	8	A9	7	D8	
N	10	B11	8	A10	7	D9	
C	12	B12	10	A11	8	D10	
C	13	B13	12	A12	10	D11	
C	14	B14	13	A13	12	D12	
C	12	B15	10	A14	8	D13	
C	13	B16	12	A15	10	D14	

C	17	B17	13	A16	12	D15
C	18	B18	17	A17	13	D16
C	19	B19	18	A18	17	D17
N	19	B20	18	A19	17	D18
C	21	B21	19	A20	18	D19
C	22	B22	21	A21	19	D20
C	15	B23	14	A22	13	D21
O	18	B24	17	A23	13	D22
N	24	B25	15	A24	14	D23
C	26	B26	24	A25	15	D24
C	27	B27	26	A26	24	D25
C	28	B28	27	A27	26	D26
N	29	B29	28	A28	27	D27
C	26	B30	24	A29	15	D28
N	27	B31	26	A30	24	D29
C	32	B32	27	A31	26	D30
N	33	B33	32	A32	27	D31
O	29	B34	28	A33	27	D32
N	31	B35	26	A34	24	D33
H	24	B36	15	A35	14	D34
H	24	B37	15	A36	14	D35
H	15	B38	14	A37	13	D36
H	17	B39	13	A38	12	D37
H	16	B40	12	A39	10	D38
H	16	B41	12	A40	10	D39
H	30	B42	29	A41	28	D40
H	21	B43	19	A42	18	D41
H	23	B44	22	A43	21	D42
H	22	B45	21	A44	19	D43
H	9	B46	3	A45	2	D44
H	7	B47	2	A46	1	D45
H	4	B48	3	A47	2	D46
H	5	B49	4	A48	3	D47
H	6	B50	1	A49	2	D48
H	1	B51	6	A50	5	D49
H	33	B52	32	A51	27	D50
H	32	B53	27	A52	26	D51
H	36	B54	31	A53	26	D52
H	36	B55	31	A54	26	D53

B1	1.40593593
B2	1.42110339
B3	1.39909785
B4	1.38334078
B5	1.38202456
B6	1.42727064
B7	1.38294605
B8	1.36306041
B9	1.48901551
B10	1.22986351
B11	1.36405444
B12	1.42920299
B13	1.42096356
B14	1.48519023
B15	1.46457013
B16	1.37604084
B17	1.45164107
B18	1.45033064
B19	1.39664545
B20	1.36498880
B21	1.36148012
B22	1.38153276
B23	1.49668854
B24	1.24338535

B25	1.82624017
B26	1.37141928
B27	1.38679042
B28	1.43727318
B29	1.43796862
B30	1.33105014
B31	1.36020437
B32	1.37806471
B33	1.30268112
B34	1.20831352
B35	1.35198842
B36	1.08456119
B37	1.08755108
B38	1.09461716
B39	1.08076909
B40	1.09775154
B41	1.08997421
B42	1.01356809
B43	1.00875611
B44	1.08345005
B45	1.08147306
B46	1.01123712
B47	1.07981298
B48	1.08634304
B49	1.08645816
B50	1.08625982
B51	1.08677384
B52	1.08176635
B53	1.01025595
B54	1.00725075
B55	1.00728457
A1	119.11098550
A2	122.10100108
A3	117.29997317
A4	118.79089919
A5	133.99890357
A6	107.16002737
A7	107.16900429
A8	138.63422197
A9	117.11998705
A10	119.92602084
A11	124.96500561
A12	107.20297993
A13	109.87601284
A14	126.13352930
A15	128.26856507
A16	119.98198717
A17	113.53601312
A18	126.93202682
A19	125.05267097
A20	109.67100498
A21	108.83897780
A22	92.97499797
A23	125.21869872
A24	115.68099993
A25	118.41796029
A26	127.77197206
A27	119.40297590
A28	109.43302007
A29	119.11725105
A30	127.04444410
A31	106.50603953
A32	112.80600193
A33	131.74096558

A34	120.03745281
A35	114.39400787
A36	114.81800863
A37	118.04373259
A38	121.72301274
A39	110.39211941
A40	110.87268913
A41	112.58903197
A42	121.86997635
A43	125.43815509
A44	121.22485256
A45	129.21655423
A46	125.46766355
A47	121.33101257
A48	119.26599429
A49	119.70006110
A50	120.75510624
A51	121.21053700
A52	127.52897009
A53	119.98800305
A54	119.14503087
D1	0.36296618
D2	-0.12194244
D3	-0.28609187
D4	-179.83914324
D5	179.25993488
D6	-179.09768147
D7	177.48644104
D8	-165.43419867
D9	16.86275146
D10	179.60400864
D11	-162.79098158
D12	5.26199438
D13	3.74360286
D14	17.76305979
D15	-179.67444111
D16	-0.50795136
D17	0.06793790
D18	-179.69895060
D19	179.93409752
D20	-0.01302725
D21	94.15600116
D22	179.68662590
D23	174.03197781
D24	70.21103141
D25	-146.27501474
D26	-0.32098405
D27	-0.52701218
D28	-75.49542044
D29	34.05507836
D30	-179.42837635
D31	-1.07100058
D32	179.71857652
D33	-31.83511883
D34	59.31597823
D35	-71.36196941
D36	-145.96089703
D37	-0.36738357
D38	-92.66693825
D39	28.15163909
D40	-178.71994869
D41	1.00404935
D42	-177.95715797
D43	-179.34309551

D44	-171.63632970
D45	-3.72952980
D46	179.70494365
D47	179.82399865
D48	-179.95900365
D49	179.94893852
D50	177.87336892
D51	-4.46935627
D52	-171.92179857
D53	-17.47970394

Number of immaginary frequency : 1 (eigenvalue=-464.5134)

Zero-point correction=	0.434555 (Hartree/Particle)
Thermal correction to Energy=	0.462978
Thermal correction to Enthalpy=	0.463922
Thermal correction to Gibbs Free Energy=	0.372153
Sum of electronic and zero-point Energies=	-1626.103829
Sum of electronic and thermal Energies=	-1626.075406
Sum of electronic and thermal Enthalpies=	-1626.074461
Sum of electronic and thermal Free Energies=	-1626.166231

Structure: Transition State of DSI (2) with Pyridine

C							
C	1	B1					
C	2	B2	1	A1			
N	3	B3	2	A2	1	D1	
C	4	B4	3	A3	2	D2	
C	1	B5	5	A4	4	D3	
C	6	B6	1	A5	5	D4	
C	7	B7	6	A6	1	D5	
C	8	B8	7	A7	6	D6	
C	3	B9	2	A8	1	D7	
N	10	B10	3	A9	2	D8	
C	11	B11	10	A10	3	D9	
C	12	B12	11	A11	10	D10	
C	13	B13	12	A12	11	D11	
C	11	B14	10	A13	3	D12	
C	13	B15	12	A14	11	D13	
C	16	B16	13	A15	12	D14	
C	17	B17	16	A16	13	D15	
C	12	B18	11	A17	10	D16	
C	16	B19	13	A18	12	D17	
C	20	B20	16	A19	13	D18	
N	17	B21	16	A20	13	D19	
C	14	B22	13	A21	12	D20	
O	18	B23	17	A22	16	D21	
O	10	B24	3	A23	2	D22	
N	23	B25	14	A24	13	D23	
C	26	B26	23	A25	14	D24	
C	27	B27	26	A26	23	D25	
C	28	B28	27	A27	26	D26	
C	29	B29	28	A28	27	D27	
C	26	B30	23	A29	14	D28	
H	23	B31	14	A30	13	D29	
H	23	B32	14	A31	13	D30	
H	14	B33	13	A32	12	D31	
H	19	B34	12	A33	11	D32	
H	15	B35	11	A34	10	D33	
H	15	B36	11	A35	10	D34	
H	27	B37	26	A36	23	D35	
H	28	B38	27	A37	26	D36	
H	29	B39	28	A38	27	D37	

H	30	B40	29	A39	28	D38
H	31	B41	26	A40	23	D39
H	22	B42	17	A41	16	D40
H	20	B43	16	A42	13	D41
C	21	B44	20	A43	16	D42
H	4	B45	3	A44	2	D43
H	2	B46	1	A45	6	D44
H	9	B47	8	A46	7	D45
H	8	B48	7	A47	6	D46
H	7	B49	6	A48	1	D47
H	6	B50	1	A49	5	D48
O	45	B51	21	A50	20	D49
O	45	B52	21	A51	20	D50
C	52	B53	45	A52	21	D51
H	54	B54	52	A53	45	D52
H	54	B55	52	A54	45	D53
H	54	B56	52	A55	45	D54

B1	1.42619837
B2	1.38241686
B3	1.37485327
B4	1.36237605
B5	1.40539900
B6	1.38199150
B7	1.41024540
B8	1.38322920
B9	1.48491877
B10	1.36768467
B11	1.42288788
B12	1.42619159
B13	1.48547592
B14	1.46445442
B15	1.42376705
B16	1.40421907
B17	1.45771349
B18	1.37396338
B19	1.41713088
B20	1.38985365
B21	1.35345369
B22	1.48544913
B23	1.23905533
B24	1.22842503
B25	1.90997740
B26	1.33861022
B27	1.38675862
B28	1.39271562
B29	1.39330058
B30	1.33906904
B31	1.08555119
B32	1.08613587
B33	1.09372194
B34	1.08077952
B35	1.09811262
B36	1.09239846
B37	1.08773253
B38	1.08531070
B39	1.08574435
B40	1.08520916
B41	1.08786374
B42	1.01044199
B43	1.08176655
B44	1.45559844
B45	1.01067767
B46	1.07960451

B47	1.08636603
B48	1.08651890
B49	1.08642260
B50	1.08708062
B51	1.34728488
B52	1.21520610
B53	1.42276490
B54	1.09063727
B55	1.09363685
B56	1.09357896
A1	107.12948922
A2	108.54821524
A3	110.26336177
A4	119.05937690
A5	118.87181880
A6	121.11521775
A7	121.51232487
A8	137.93794556
A9	119.52464794
A10	125.05472728
A11	107.41986560
A12	109.52080948
A13	125.41981785
A14	118.27374947
A15	116.83233664
A16	126.39549125
A17	128.03991447
A18	136.40205892
A19	106.68812650
A20	108.28983965
A21	89.20544634
A22	121.11343210
A23	117.67221109
A24	111.65876145
A25	117.48347431
A26	122.16096023
A27	118.77419387
A28	118.84576058
A29	118.07824832
A30	116.63031321
A31	116.31944241
A32	118.47648794
A33	121.65358944
A34	110.59871423
A35	110.56413075
A36	115.98592821
A37	119.86863950
A38	120.58257230
A39	121.45505853
A40	116.08349779
A41	124.70115096
A42	128.56360763
A43	132.18662935
A44	120.26617009
A45	125.63769621
A46	121.34499743
A47	119.20984821
A48	119.75193173
A49	120.43107929
A50	112.21052583
A51	124.16407540
A52	114.35589605
A53	105.71805558
A54	110.81362648

A55	110.79680977
D1	-0.19781392
D2	0.33777130
D3	-179.89022516
D4	0.00625129
D5	0.02853913
D6	0.01336872
D7	175.57348846
D8	16.58868523
D9	-175.15048965
D10	-165.42543292
D11	4.47774541
D12	7.29982690
D13	-176.73011985
D14	-1.66713103
D15	0.54518486
D16	16.27246545
D17	178.10379324
D18	-179.78106348
D19	179.78203080
D20	95.64115910
D21	179.90970919
D22	-164.25887874
D23	178.41019745
D24	-72.06545012
D25	154.63119702
D26	-0.18352218
D27	0.12620082
D28	82.43440125
D29	68.82239536
D30	-72.48091013
D31	-145.62406336
D32	-2.11115102
D33	-87.97880059
D34	32.73773379
D35	-25.82946916
D36	179.44597224
D37	-179.73328452
D38	179.53329506
D39	25.43503668
D40	-179.10652017
D41	-0.54799499
D42	179.54624651
D43	173.54316231
D44	-2.92854989
D45	-179.85321696
D46	-179.82385303
D47	-179.81061906
D48	-179.70911061
D49	0.65627068
D50	-179.36352283
D51	-179.61322947
D52	179.80717485
D53	-60.49688942
D54	60.15529889

Number of immaginary frequency:1

Energy=-1560.2200443(a.u.)

Structure: Transition State of DSI (2) with Adenine

N
C 1 B1

C	2	B2	1	A1			
N	3	B3	2	A2	1	D1	
C	1	B4	2	A3	3	D2	
C	2	B5	1	A4	5	D3	
N	6	B6	2	A5	1	D4	
C	7	B7	6	A6	2	D5	
N	8	B8	7	A7	6	D6	
N	6	B9	2	A8	1	D7	
C	9	B10	8	A9	7	D8	
C	11	B11	9	A10	8	D9	
C	12	B12	11	A11	9	D10	
C	13	B13	12	A12	11	D11	
N	14	B14	13	A13	12	D12	
C	15	B15	14	A14	13	D13	
C	13	B16	12	A15	11	D14	
C	17	B17	13	A16	12	D15	
C	18	B18	17	A17	13	D16	
C	14	B19	13	A18	12	D17	
C	17	B20	13	A19	12	D18	
C	21	B21	17	A20	13	D19	
N	18	B22	17	A21	13	D20	
C	15	B23	14	A22	13	D21	
O	24	B24	15	A23	14	D22	
O	19	B25	18	A24	17	D23	
C	22	B26	21	A25	17	D24	
O	27	B27	22	A26	21	D25	
C	24	B28	15	A27	14	D26	
N	29	B29	24	A28	15	D27	
C	30	B30	29	A29	24	D28	
C	31	B31	30	A30	29	D29	
C	29	B32	24	A31	15	D30	
C	31	B33	30	A32	29	D31	
C	34	B34	31	A33	30	D32	
C	35	B35	34	A34	31	D33	
C	36	B36	35	A35	34	D34	
O	27	B37	22	A36	21	D35	
C	38	B38	27	A37	22	D36	
H	11	B39	9	A38	8	D37	
H	11	B40	9	A39	8	D38	
H	12	B41	11	A40	9	D39	
H	20	B42	14	A41	13	D40	
H	16	B43	15	A42	14	D41	
H	16	B44	15	A43	14	D42	
H	8	B45	7	A44	6	D43	
H	23	B46	18	A45	17	D44	
H	21	B47	17	A46	13	D45	
H	30	B48	29	A47	24	D46	
H	33	B49	29	A48	24	D47	
H	34	B50	31	A49	30	D48	
H	35	B51	34	A50	31	D49	
H	36	B52	35	A51	34	D50	
H	37	B53	36	A52	35	D51	
H	10	B54	6	A53	2	D52	
H	10	B55	6	A54	2	D53	
H	5	B56	1	A55	2	D54	
H	4	B57	3	A56	2	D55	
H	39	B58	38	A57	27	D56	
H	39	B59	38	A58	27	D57	
H	39	B60	38	A59	27	D58	

B1	1.37285209
B2	1.39480508
B3	1.36403074
B4	1.30597703

B5	1.40930038
B6	1.34641825
B7	1.32231603
B8	1.33688139
B9	1.33616682
B10	1.90756052
B11	1.48239475
B12	1.49154047
B13	1.42069587
B14	1.43081634
B15	1.46486492
B16	1.42262059
B17	1.40599930
B18	1.45667152
B19	1.37526626
B20	1.41754511
B21	1.38997413
B22	1.35440759
B23	1.36217612
B24	1.22811774
B25	1.24051470
B26	1.45521925
B27	1.21542611
B28	1.49369881
B29	1.37417726
B30	1.36314082
B31	1.42079245
B32	1.38596395
B33	1.39904213
B34	1.38321987
B35	1.41042155
B36	1.38254004
B37	1.34783312
B38	1.42232991
B39	1.08580894
B40	1.08630025
B41	1.09302146
B42	1.08093168
B43	1.09742510
B44	1.08894110
B45	1.08834183
B46	1.01025212
B47	1.08184190
B48	1.01185535
B49	1.08040790
B50	1.08617003
B51	1.08630730
B52	1.08623886
B53	1.08698346
B54	1.00771758
B55	1.00783806
B56	1.08267111
B57	1.01606197
B58	1.09069243
B59	1.09371076
B60	1.09364981
A1	111.36698620
A2	104.77501998
A3	103.88008425
A4	131.64031223
A5	119.02296405
A6	118.50102963
A7	127.90300192
A8	122.15503187

A9	118.55779204
A10	115.23100807
A11	90.76701142
A12	109.70198314
A13	107.24902762
A14	108.26698855
A15	132.30097094
A16	116.79098410
A17	126.65998942
A18	125.04003243
A19	136.47697997
A20	106.71195865
A21	108.24689389
A22	124.33199635
A23	123.31300659
A24	121.18749601
A25	132.09754055
A26	124.24898782
A27	119.87498683
A28	112.79898867
A29	110.49301249
A30	107.17900736
A31	138.83893426
A32	130.71602291
A33	117.30101852
A34	121.55600460
A35	121.15099839
A36	112.20603196
A37	114.35600696
A38	94.39234949
A39	96.89563035
A40	115.62485474
A41	121.72897563
A42	110.10396065
A43	111.50803692
A44	116.59773207
A45	124.57103236
A46	128.53803011
A47	119.84655061
A48	127.10977256
A49	121.33399862
A50	119.26499340
A51	119.13809315
A52	120.76757998
A53	120.25495255
A54	119.43501487
A55	125.82719915
A56	128.84300428
A57	105.72195367
A58	110.83299100
A59	110.81399469
D1	-0.32099629
D2	-0.09738653
D3	179.40665026
D4	-179.30166232
D5	-0.37597699
D6	0.10895730
D7	0.47033808
D8	177.51459936
D9	-99.10724738
D10	175.97401585
D11	94.53598840
D12	2.69402894
D13	16.60394723

D14	-83.48282589
D15	177.12407330
D16	0.50496630
D17	-177.98927286
D18	-2.95516519
D19	-179.95513196
D20	179.88330627
D21	-154.13497574
D22	-4.57708260
D23	179.65929995
D24	179.86431657
D25	-179.57675873
D26	171.83698004
D27	-162.08304958
D28	-178.90097505
D29	-0.08501488
D30	19.57992723
D31	-179.18748854
D32	179.01279011
D33	-0.06300976
D34	0.14301349
D35	0.49519627
D36	-179.75899315
D37	22.52769238
D38	137.70797906
D39	53.90257037
D40	-179.90115908
D41	89.07579932
D42	-150.14225620
D43	-179.68300198
D44	-179.25451581
D45	-0.71903836
D46	-5.00060819
D47	3.26302499
D48	-1.12120348
D49	179.81102152
D50	179.79126358
D51	179.46051363
D52	0.90198556
D53	179.40600132
D54	-178.93972097
D55	174.78225681
D56	179.95500105
D57	-60.34204886
D58	60.30202471

Number of immaginary frequency:1

Energy= -1779.0340364(a.u.)

Structure: Transition State of DSA (1) with Pyridine

C						
C	1	B1				
C	2	B2	1	A1		
C	3	B3	2	A2	1	D1
C	4	B4	3	A3	2	D2
H	5	B5	4	A4	3	D3
H	4	B6	3	A5	2	D4
H	3	B7	2	A6	1	D5
H	2	B8	1	A7	5	D6
H	1	B9	2	A8	3	D7
N	1	B10	2	A9	3	D8
C	11	B11	1	A10	2	D9

C	12	B12	11	A11	1	D10
C	12	B13	11	A12	1	D11
C	14	B14	12	A13	11	D12
N	15	B15	14	A14	12	D13
C	16	B16	15	A15	14	D14
C	17	B17	16	A16	15	D15
C	18	B18	17	A17	16	D16
C	19	B19	18	A18	17	D17
C	20	B20	19	A19	18	D18
H	15	B21	14	A20	12	D19
H	15	B22	14	A21	12	D20
H	14	B23	12	A22	11	D21
H	18	B24	17	A23	16	D22
O	19	B25	18	A24	17	D23
H	12	B26	11	A25	1	D24
H	12	B27	11	A26	1	D25
C	21	B28	20	A27	19	D26
C	29	B29	21	A28	20	D27
N	20	B30	19	A29	18	D28
H	31	B31	20	A30	19	D29
H	29	B32	21	A31	20	D30
C	30	B33	29	A32	21	D31
O	34	B34	30	A33	29	D32
O	34	B35	30	A34	29	D33
C	36	B36	34	A35	30	D34
H	37	B37	36	A36	34	D35
H	37	B38	36	A37	34	D36
H	37	B39	36	A38	34	D37
C	16	B40	15	A39	14	D38
O	41	B41	16	A40	15	D39
C	41	B42	16	A41	15	D40
C	43	B43	41	A42	16	D41
H	44	B44	43	A43	41	D42
C	44	B45	43	A44	41	D43
C	46	B46	44	A45	43	D44
N	47	B47	46	A46	44	D45
H	48	B48	47	A47	46	D46
C	47	B49	46	A48	44	D47
C	50	B50	47	A49	46	D48
C	51	B51	50	A50	47	D49
C	52	B52	51	A51	50	D50
H	53	B53	52	A52	51	D51
O	50	B54	47	A53	46	D52
C	55	B55	50	A54	47	D53
H	56	B56	55	A55	50	D54
H	56	B57	55	A56	50	D55
H	56	B58	55	A57	50	D56
O	51	B59	50	A58	47	D57
O	52	B60	51	A59	50	D58
C	61	B61	52	A60	51	D59
H	62	B62	61	A61	52	D60
H	62	B63	61	A62	52	D61
H	62	B64	61	A63	52	D62
C	60	B65	51	A64	50	D63
H	66	B66	60	A65	51	D64
H	66	B67	60	A66	51	D65
H	66	B68	60	A67	51	D66

B1	1.38673302
B2	1.39277209
B3	1.39327234
B4	1.38647550
B5	1.08786561
B6	1.08519887

B7	1.08573682
B8	1.08531076
B9	1.08774927
B10	1.33851491
B11	1.91006022
B12	2.08523772
B13	1.48532519
B14	1.52261201
B15	1.46380744
B16	1.42256310
B17	1.37406323
B18	1.45095144
B19	1.45785132
B20	1.40431265
B21	1.09233893
B22	1.09826328
B23	1.09367373
B24	1.08085231
B25	1.23918295
B26	1.08609680
B27	1.08553658
B28	1.41706086
B29	1.38988709
B30	1.35351536
B31	1.01041021
B32	1.08174347
B33	1.45542976
B34	1.21525172
B35	1.34740934
B36	1.42269911
B37	1.09365453
B38	1.09065281
B39	1.09359813
B40	1.36883988
B41	1.22782013
B42	1.48459449
B43	1.38497576
B44	1.07953919
B45	1.42574349
B46	1.41569647
B47	1.35918035
B48	1.00994018
B49	1.40215344
B50	1.38931308
B51	1.42425782
B52	1.37935666
B53	1.08560853
B54	1.36318820
B55	1.42381554
B56	1.09307635
B57	1.09713873
B58	1.09201349
B59	1.37071381
B60	1.37173162
B61	1.41991152
B62	1.09260599
B63	1.09517475
B64	1.09787685
B65	1.42219864
B66	1.09677545
B67	1.09527206
B68	1.09248455
A1	118.76646070
A2	118.84977285

A3	118.74303715
A4	121.74699256
A5	121.45533241
A6	120.58586858
A7	119.87571616
A8	121.85897127
A9	122.16070305
A10	117.50649799
A11	157.09908489
A12	111.69823842
A13	113.71010749
A14	103.84498058
A15	109.48711942
A16	128.05341839
A17	120.22660492
A18	113.73958248
A19	126.39139274
A20	113.07783739
A21	109.77970621
A22	115.44196852
A23	121.63679006
A24	125.16447047
A25	96.21959030
A26	96.43100889
A27	106.76746550
A28	106.69202397
A29	125.31898187
A30	124.69603207
A31	128.55333374
A32	132.17026029
A33	124.19409583
A34	112.19738487
A35	114.35868429
A36	110.82345412
A37	105.71922706
A38	110.80098855
A39	125.40674417
A40	122.77139157
A41	119.42864999
A42	137.76871198
A43	127.08328572
A44	107.31935564
A45	106.32528284
A46	108.02482429
A47	128.05606780
A48	122.62348442
A49	117.14573392
A50	120.79766503
A51	121.61446912
A52	119.17207562
A53	118.46041018
A54	115.51110782
A55	111.19607415
A56	110.65379438
A57	105.95113446
A58	119.57975956
A59	118.79387756
A60	114.04048331
A61	106.35304582
A62	111.31493108
A63	110.74563256
A64	113.27407941
A65	110.66945252
A66	110.80385680

A67	106.35811844
D1	0.15707595
D2	-0.32386195
D3	-179.58099039
D4	179.55744910
D5	-179.69005562
D6	179.66877942
D7	-179.74034469
D8	-0.22580376
D9	154.80524738
D10	-69.34580240
D11	-72.24673978
D12	-77.59326700
D13	-69.93013912
D14	-23.74734783
D15	-165.83715663
D16	177.73185526
D17	-0.75350572
D18	0.63572943
D19	49.94078247
D20	171.74626038
D21	57.01184597
D22	-2.13866484
D23	-179.93857969
D24	166.17113579
D25	49.78100592
D26	-179.31991663
D27	-0.01391867
D28	-178.53458081
D29	0.15605957
D30	179.21659697
D31	179.62678470
D32	-179.51575377
D33	0.50880192
D34	-179.69003912
D35	-60.44852154
D36	179.85544711
D37	60.20260953
D38	154.05535529
D39	-171.56816123
D40	7.53953760
D41	16.81004421
D42	-1.02968033
D43	175.91224941
D44	-0.17968876
D45	0.22480398
D46	-175.26326088
D47	179.48463184
D48	0.22310638
D49	0.94493049
D50	-1.14944258
D51	-179.55021608
D52	-176.88123163
D53	-120.64768186
D54	-63.73487294
D55	58.37908552
D56	176.75039840
D57	-179.79696287
D58	-178.20065316
D59	-74.67109765
D60	-179.65230153
D61	61.07944682
D62	-61.04360736
D63	101.67099074

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   D64          -61.09477849
   D65           61.06552954
   D66         -179.86763091

  Number of immaginary frequency:1 (eigenvalue=-531.3034)

  Zero-point correction=                           0.547998 (Hartree/Particle)
  Thermal correction to Energy=                    0.585309
  Thermal correction to Enthalpy=                  0.586253
  Thermal correction to Gibbs Free Energy=         0.473554
  Sum of electronic and zero-point Energies=         -1902.849700
  Sum of electronic and thermal Energies=            -1902.812388
  Sum of electronic and thermal Enthalpies=          -1902.811444
  Sum of electronic and thermal Free Energies=       -1902.924144
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Structure: Transition State of DSA (1) with Adenine

```
 C
 c   1 cc2
 c   2 cc3        1 ccc3
 c   3 cc4        2 ccc4         1 dih4
 c   4 cc5        3 ccc5         2 dih5
 c   5 cc6        4 ccc6         3 dih6
 n   3 nc7        2 ncc7         1 dih7
 c   7 cn8        3 cnc8         2 dih8
 c   8 cc9        7 ccn9         3 dih9
 c   8 cc10       9 ccc10        2 dih10
 o  10 oc11       8 occ11        9 dih11
 o   4 oc12       3 occ12        2 dih12
 c  12 co13       4 coc13        3 dih13
 o   5 oc14       4 occ14        3 dih14
 c  14 co15       5 coc15        4 dih15
 o   6 oc16       5 occ16        4 dih16
 c  16 co17       6 coc17        5 dih17
 n  10 nc18       8 ncc18        9 dih18
 c  18 cn19      10 cnc19        8 dih19
 c  19 cc20      18 ccn20       10 dih20
 c  20 cc21      19 ccc21       18 dih21
 c  21 cc22      20 ccc22       19 dih22
 c  19 cc23      20 ccc23       21 dih23
 c  23 cc24      19 ccc24       20 dih24
 c  24 cc25      23 ccc25       19 dih25
 c  25 cc26      24 ccc26       23 dih26
 n  25 nc27      26 ncc27       20 dih27
 c  27 cn28      25 cnc28       26 dih28
 c  28 cc29      27 ccn29       25 dih29
 c  21 cc30      20 ccc30       19 dih30
 n  30 nc31      21 ncc31       20 dih31
 c  31 cn32      30 cnc32       21 dih32
 c  32 cc33      31 ccn33       30 dih33
 c  33 cc34      32 ccc34       31 dih34
 n  34 nc35      33 ncc35       32 dih35
 c  35 cn36      34 cnc36       33 dih36
 n  32 nc37      33 ncc37       34 dih37
 c  37 cn38      32 cnc38       33 dih38
 n  38 nc39      37 ncn39       32 dih39
 n  34 nc40      33 ncc40       39 dih40
 o  24 oc41      25 occ41       26 dih41
 c  28 cc42      29 ccc42       26 dih42
 o  42 oc43      28 occ43       29 dih43
 c  43 co44      42 coc44       28 dih44
 o  42 oc45      28 occ45       29 dih45
 h  30 hc46      31 hcn46       32 dih46
 h  30 hc47      31 hcn47       32 dih47
```

```
 h  21 hc48      30 hcc48       31 dih48
 h  23 hc49      19 hcc49       20 dih49
 h  22 hc50      21 hcc50       30 dih50
 h  22 hc51      21 hcc51       30 dih51
 h  36 hc52      35 hcn52       34 dih52
 h  27 hn53      25 hnc53       26 dih53
 h  29 hc54      26 hcc54       20 dih54
 h   7 hn55       8 hnc55       10 dih55
 h   9 hc56       8 hcc56       10 dih56
 h   1 hc57       2 hcc57        9 dih57
 h  40 hn58      34 hnc58       33 dih58
 h  40 hn59      34 hnc59       33 dih59
 h  38 hc60      39 hcn60       33 dih60
 h  37 hn61      32 hnc61       33 dih61
 h  44 hc62      43 hco62       42 dih62
 h  44 hc63      43 hco63       42 dih63
 h  44 hc64      43 hco64       42 dih64
 h  17 hc65      16 hco65        6 dih65
 h  17 hc66      16 hco66        6 dih66
 h  17 hc67      16 hco67        6 dih67
 h  15 hc68      14 hco68        5 dih68
 h  15 hc69      14 hco69        5 dih69
 h  15 hc70      14 hco70        5 dih70
 h  13 hc71      12 hco71        4 dih71
 h  13 hc72      12 hco72        4 dih72
 h  13 hc73      12 hco73        4 dih73

cc2          1.409847
cc3          1.408365
ccc3         119.364
cc4          1.405823
ccc4         123.090
dih4           1.058
cc5          1.392138
ccc5         117.088
dih5          -0.804
cc6          1.433297
ccc6         120.185
dih6          -0.117
nc7          1.367746
ncc7         108.327
dih7        -177.855
cn8          1.378840
cnc8         109.183
dih8          -1.840
cc9          1.380990
ccn9         108.695
dih9           1.811
cc10         1.490533
ccc10        137.528
dih10        176.654
oc11         1.228217
occ11        117.236
dih11       -151.138
oc12         1.354507
occ12        115.023
dih12       -178.147
co13         1.419630
coc13        120.251
dih13       -151.254
oc14         1.366736
occ14        119.857
dih14       -175.288
co15         1.421966
```

```
coc15       115.828
dih15      -114.727
oc16        1.358951
occ16       113.639
dih16      -177.816
co17        1.407699
coc17       117.455
dih17       178.465
nc18        1.361453
ncc18       118.410
dih18        32.042
cn19        1.434721
cnc19       124.325
dih19       172.269
cc20        1.406155
ccn20       107.413
dih20      -146.720
cc21        1.482331
ccc21       109.970
dih21         6.685
cc22        1.530560
ccc22       100.874
dih22       -24.439
cc23        1.384612
ccc23       125.648
dih23      -172.539
cc24        1.441709
ccc24       119.953
dih24         1.634
cc25        1.456513
ccc25       112.997
dih25         0.267
cc26        1.411093
ccc26       126.770
dih26        -0.488
nc27        1.353479
ncc27       108.234
dih27       179.356
cn28        1.367546
cnc28       109.720
dih28         0.323
cc29        1.389219
ccn29       108.672
dih29        -0.280
cc30        1.554570
ccc30       108.028
dih30        93.171
nc31        1.469994
ncc31       114.928
dih31       175.086
cn32        1.362923
cnc32       124.931
dih32        92.356
cc33        1.389674
ccn33       122.500
dih33      -173.502
cc34        1.412767
ccc34       118.048
dih34         1.434
nc35        1.346113
ncc35       118.780
dih35        -0.062
cn36        1.310488
cnc36       119.679
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dih36        -0.575
nc37        1.357323
ncc37        105.512
dih37       -179.983
cn38        1.378749
cnc38        106.156
dih38          0.950
nc39        1.305638
ncn39        113.189
dih39         -1.174
nc40        1.335565
ncc40        122.084
dih40          0.283
oc41        1.245821
occ41        120.838
dih41        179.766
cc42        1.452998
ccc42        132.022
dih42       -180.000
oc43        1.350485
occ43        112.213
dih43          0.483
co44        1.421189
coc44        114.275
dih44       -179.746
oc45        1.215948
occ45        124.515
dih45       -179.596
hc46        1.093187
hcn46        106.955
dih46       -146.600
hc47        1.093623
hcn47        108.333
dih47        -30.962
hc48        1.100153
hcc48        108.411
dih48         48.790
hc49        1.081676
hcc49        121.577
dih49        179.885
hc50        1.096966
hcc50        109.428
dih50        160.571
hc51        1.091403
hcc51        114.526
dih51         38.534
hc52        1.085888
hcn52        118.763
dih52       -178.986
hn53        1.010230
hnc53        124.198
dih53       -179.571
hc54        1.082141
hcc54        128.535
dih54         -0.547
hn55        1.011834
hnc55        121.011
dih55        -14.153
hc56        1.081304
hcc56        126.191
dih56         -1.796
hc57        1.083565
hcc57        120.382
dih57          0.465
```

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hn58        1.008097
hnc58       120.110
dih58         1.118
hn59        1.008013
hnc59       119.639
dih59       179.396
hc60        1.082032
hcn60       126.074
dih60      -178.448
hn61        1.015513
hnc61       128.699
dih61       171.514
hc62        1.090962
hco62       105.754
dih62       179.692
hc63        1.093911
hco63       110.903
dih63       -60.616
hc64        1.093785
hco64       110.893
dih64        60.026
hc65        1.091246
hco65       106.033
dih65      -179.288
hc66        1.097989
hco66       111.363
dih66       -60.481
hc67        1.098066
hco67       111.599
dih67        61.739
hc68        1.092191
hco68       106.020
dih68       177.862
hc69        1.092833
hco69       111.313
dih69       -62.987
hc70        1.097995
hco70       110.943
dih70        59.297
hc71        1.092023
hco71       105.339
dih71       165.912
hc72        1.091467
hco72       111.668
dih72       -74.589
hc73        1.096410
hco73       110.921
dih73        48.000

Number of immaginary frequency:1
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Complete reference 31:

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