SUPPORTING INFORMATION (Tables 1S-12S)

Modeling Substituent and Conformational Effects on the Reactivity of Antitumors Containing Cyclopropylcyclohexadienone Subunit.

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Table of CONTENTS

Table 1S. Cartesian coordinates and energies of the reactants **6** and **7** in gas phase and water at B3LYP/6-31G(d) and B3LYP-C-PCM-/6-31G(d) level of theory. (S2)

Table 2S. Cartesian coordinates and energies of the reactants **6** and **7** in gas phase and water at B3LYP/6-31+G(d,p) and B3LYP-C-PCM-/6-31G+(d,p) level of theory. (S3)

Table 3S. Cartesian coordinates and energies the reactants **6** and **7** in gas phase and water at B3LYP/6-311+G(d,p) and B3LYP-C-PCM-/6-311G+(d,p) level of theory. (S4)

Table 4S. Cartesian coordinates and energies of all the TSs located for the alkylation reaction of ammonia by **6** and **7** in gas phase, and water at B3LYP/6-31G(d) and B3LYP-C-PCM-/6-31G(d) level of theory (S5)

Table 5S. Cartesian coordinates and energies of the TSs **S6** and **S7** located for the alkylation reaction of ammonia by **6** and **7** in gas phase, and water at B3LYP/6-31+G(d,p) and B3LYP-C-PCM-/6-31+G(d,p) level of theory (S7)

Table 6S. Cartesian coordinates and energies of the TSs **S6** and **S7** located for the alkylation reaction of ammonia by **6** and **7** in gas phase, and water at B3LYP/6-311+G(d,p) and B3LYP-C-PCM-/6-311+G(d,p) level of theory (S9)

Table 7S. Cartesian coordinates and energies (in Hartee) of all stationary points (reactants and TSs) located for the alkylation reaction of ammonia by **8-12** in gas phase at B3LYP/6-31G(d) level of theory. (S10)

Table 8S. Cartesian coordinates and energies (in Hartee) of all stationary points (reactants and TSs) located for the alkylation reaction of ammonia by **8-12** in gas phase at B3LYP/6-31+G(d,p) level of theory (S14)

Table 9S. Cartesian coordinates of all stationary points (reactants and TSs) located for the alkylation reaction of ammonia by **8-12** in water solution at B3LYP-C-PCM-/6-31G(d) level of theory (S17)

Table 10S. Cartesian coordinates of all stationary points (reactants and TSs) located for the alkylation reaction of ammonia by **8-12** in water solution at B3LYP-C-PCM-/6-31+G(d,p) level of theory (S22)

Table 11S. Cartesian coordinates of the conformational TSs **TS-0°**, **TS-120°**, **TS-300°**, **TS-syn** and **TS-anti** in gas phase and in water at B3LYP/6-31G(d) (S26)

Table 12S. Cartesian coordinates of the conformational TSs **TS-0°**, **TS-120°**, **TS-300°**, **TS-syn**, **TS-anti**, **S9-syn** and **S9-anti** in gas phase and in water at B3LYP/6-31+G(d,p). (S29)

Table 1S. Cartesian coordinates and energies of the reactants **6** and **7** in gas phase and water at B3LYP/6-31G(d) and B3LYP-C-PCM-/6-31G(d) level of theory.

6 in gas phase

E = -384.8353292

Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
1	6	-1.249648	-0.004622	-0.282852
2	6	-1.245512	-0.002830	1.062572
3	6	0.011552	0.001986	1.839602
4	6	1.258765	-0.000085	1.046848
5	6	1.246007	-0.002071	-0.298522
6	6	-0.006735	-0.002184	-1.073290
7	1	-2.189446	-0.007475	-0.833702
8	1	-2.166191	-0.004216	1.638801
9	1	2.186615	0.000655	1.611461
10	1	2.178815	-0.003030	-0.861135
11	8	0.019267	0.007479	3.069506
12	6	-0.014603	-0.740904	-2.428560
13	1	0.897344	-1.265749	-2.697303
14	6	-0.015887	0.742171	-2.425313
15	1	0.895145	1.270051	-2.691366
16	1	-0.931087	1.268479	-2.679922
17	1	-0.928963	-1.267319	-2.685790

6 in water

<Psi(f)| H |Psi(f)> (a.u.) = -384.830331
 <Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -384.849689
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -384.847371

(Polar.Solute)-Solvent (kcal/mol) = -12.15

Cavitation energy (kcal/mol) = 16.93
 Dispersion energy (kcal/mol) = -19.59
 Repulsion energy (kcal/mol) = 4.12
 Total non electr. (kcal/mol) = 1.45

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.292731	1.243626	-0.009284
2	6	0	1.057039	1.247224	-0.005950
3	6	0	1.832359	-0.000129	0.002146
4	6	0	1.056689	-1.247258	-0.001632
5	6	0	-0.293066	-1.243395	-0.004317
6	6	0	-1.066083	0.000226	-0.005162
7	1	0	-0.848981	2.180944	-0.013847
8	1	0	1.621853	2.177023	-0.007344
9	1	0	1.621786	-2.176961	0.000928
10	1	0	-0.849298	-2.180803	-0.004537
11	8	0	3.074310	-0.000443	0.010177
12	6	0	-2.426710	0.000964	0.741869

13	1	0	-2.670591	-0.915275	1.273712
14	6	0	-2.437012	-0.000739	-0.731826
15	1	0	-2.690026	-0.918233	-1.257134
16	1	0	-2.690672	0.915336	-1.259447
17	1	0	-2.671462	0.918392	1.271179

7 in gas phase

E = -440.1925555

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	.000000	.000000	.000000
2	7	0	.000000	.000000	1.012428
3	6	0	1.240017	.000000	1.639593
4	6	0	2.326499	.809165	1.016593
5	1	0	-.657472	-.674144	1.385798
6	6	0	3.607720	.839491	1.753122
7	6	0	3.790366	.210531	2.923159
8	6	0	2.707252	-.578151	3.556315
9	6	0	1.445008	-.634874	2.825004
10	6	0	1.936374	2.092429	.261349
11	6	0	2.417153	.918746	-.515293
12	1	0	2.594863	2.947666	.381221
13	1	0	.877277	2.330365	.251754
14	1	0	1.712373	.345679	-1.112625
15	1	0	3.418672	.939744	-.935067
16	1	0	4.412430	1.413109	1.295268
17	1	0	4.736012	.247224	3.455883
18	8	0	2.881251	-1.157200	4.630789
19	1	0	.652492	-1.222307	3.282423

7 in water

<Psi(f)| H |Psi(f)> (a.u.) = -440.183068
 <Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -440.217145
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -440.214882

(Polar.Solute)-Solvent (kcal/mol) = -21.38

Cavitation energy (kcal/mol) = 18.32
 Dispersion energy (kcal/mol) = -21.51
 Repulsion energy (kcal/mol) = 4.61
 Total non electr. (kcal/mol) = 1.42

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-2.157178	-.123213	-1.933225
2	7	0	-2.147711	-.127975	-.916194
3	6	0	-.973239	-.146790	-.225485

4	6	0	.263135	.314243	-.911575
5	1	0	-2.952936	-.583823	-.492325
6	6	0	1.486344	.344113	-.093651
7	6	0	1.505017	-.022465	1.198542
8	6	0	.281965	-.484846	1.884272
9	6	0	-.923985	-.526719	1.095350
10	6	0	.452848	.003861	-2.411217
11	6	0	.142787	1.393824	-2.006979
12	1	0	-.318939	-.598654	-2.885832

13	1	0	1.466185	-.239917	-2.720921
14	1	0	-.856573	1.785302	-2.181424
15	1	0	.935332	2.137728	-2.033868
16	1	0	2.393647	.683174	-.592983
17	1	0	2.419408	.007514	1.787082
18	8	0	.315941	-.819710	3.087516
19	1	0	-1.831727	-.865929	1.591195

Table 2S. Cartesian coordinates and energies of the reactants **6** and **7** in gas phase and water at B3LYP/6-31+G(d,p) and B3LYP-C-PCM-/6-31G+(d,p) level of theory.

6 in gas phase

E = -384.8649799

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.291559	-1.247788	0.000556
2	6	0	1.056362	-1.253098	-0.001191
3	6	0	1.837699	0.000000	-0.002124
4	6	0	1.056362	1.253098	-0.001338
5	6	0	-0.291559	1.247789	0.000365
6	6	0	-1.073531	0.000000	0.001676
7	1	0	-0.845582	-2.185165	0.001075
8	1	0	1.625259	-2.177899	-0.002136
9	1	0	1.625258	2.177900	-0.002343
10	1	0	-0.845583	2.185165	0.000765
11	8	0	3.071448	0.000000	-0.003774
12	6	0	-2.429008	-0.000132	-0.739273
13	1	0	-2.689457	0.913112	-1.265138
14	6	0	-2.427673	0.000130	0.744812
15	1	0	-2.687293	0.913571	1.270761
16	1	0	-2.687251	-0.913120	1.271108
17	1	0	-2.689493	-0.913567	-1.264794

6 in water

<Psi(f)| H |Psi(f)> (a.u.) = -384.857641
 <Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -384.882792
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -384.880459

(Polar.Solute)-Solvent (kcal/mol) = -15.78

Cavitation energy (kcal/mol) = 16.93
 Dispersion energy (kcal/mol) = -19.59
 Repulsion energy (kcal/mol) = 4.12
 Total non electr. (kcal/mol) = 1.46

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

1	6	0	-0.294409	1.243401	-0.001517
2	6	0	1.059564	1.247252	-0.006920
3	6	0	1.827406	-0.000103	-0.004486
4	6	0	1.059185	-1.247262	0.003051
5	6	0	-0.294746	-1.243400	0.005238
6	6	0	-1.064153	0.000114	0.002783
7	1	0	-0.848441	2.182311	-0.003133
8	1	0	1.621605	2.179198	-0.012757
9	1	0	1.622124	-2.178765	0.008819
10	1	0	-0.848530	-2.182542	0.012076
11	8	0	3.078150	-0.000416	-0.007555
12	6	0	-2.433886	-0.001904	0.740568
13	1	0	-2.675747	-0.922963	1.265409
14	6	0	-2.435265	0.002259	-0.732355
15	1	0	-2.680936	-0.913748	-1.264002
16	1	0	-2.679172	0.923266	-1.256400
17	1	0	-2.678278	0.914428	1.272266

7 in gas

E = -440.2313297

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	.000000	.000000	.000000
2	7	0	.000000	.000000	1.010080
3	6	0	1.222552	.000000	1.664800
4	6	0	2.352540	.732661	1.024733
5	1	0	-.704463	-.610354	1.401408
6	6	0	3.620907	.745830	1.784225
7	6	0	3.755225	.174039	2.991960
8	6	0	2.624807	-.528662	3.641115
9	6	0	1.376303	-.575306	2.890934
10	6	0	2.034461	1.998905	.206918
11	6	0	2.473846	.768797	-.508050
12	1	0	2.731590	2.825249	.303781
13	1	0	.988894	2.286591	.165094
14	1	0	1.752503	.202627	-1.090692
15	1	0	3.481833	.725953	-.908804
16	1	0	4.459669	1.257923	1.316004
17	1	0	4.691895	.199189	3.540056
18	8	0	2.752727	-1.052610	4.754884
19	1	0	.551483	-1.104094	3.361288

7 in water

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -440.218005
 $\langle \Psi(f) | H + V(f) / 2 | \Psi(f) \rangle$ (a.u.) = -440.260875
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -440.258537

(Polar.Solute)-Solvent (kcal/mol) = -26.90

Cavitation energy (kcal/mol) = 18.33
 Dispersion energy (kcal/mol) = -21.53
 Repulsion energy (kcal/mol) = 4.66
 Total non electr. (kcal/mol) = 1.47

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

1	6	0	.033089	-1.528272	-.002425
2	6	0	1.368592	-1.353425	.004460
3	6	0	1.959439	-.003416	.004935
4	6	0	1.052577	1.108609	.004593
5	6	0	-.321522	.959293	-.005494
6	6	0	-.915044	-.403410	-.006042
7	1	0	-.398179	-2.529337	-.007603
8	1	0	2.053562	-2.199112	.003538
9	1	0	1.481229	2.109730	.009163
10	8	0	3.211783	.143906	-.003025
11	6	0	-2.254774	-.649840	-.735513
12	1	0	-2.676680	.194471	-1.277490
13	6	0	-2.246824	-.629092	.744530
14	1	0	-2.649754	.239205	1.261167
15	1	0	-2.334356	-1.568325	1.285797
16	1	0	-2.342598	-1.606148	-1.245699
17	7	0	-1.143436	2.038232	.026721
18	1	0	-.738244	2.966917	-.072789
19	1	0	-2.138393	1.971041	-.173193

Table 3S. Cartesian coordinates and energies the reactants **6** and **7** in gas phase and water at B3LYP/6-311+G(d,p) and B3LYP-C-PCM-/6-311G+(d,p) level of theory.

6 in gas phase

E = -384.942146

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.289994	-1.245653	0.000318
2	6	0	1.053293	-1.250984	-0.001078
3	6	0	1.835735	0.000002	-0.002254
4	6	0	1.053287	1.250985	-0.001419
5	6	0	-0.289999	1.245651	0.000072
6	6	0	-1.069570	-0.000003	0.000781
7	1	0	-0.843543	-2.181150	0.001113
8	1	0	1.620966	-2.174514	-0.001023
9	1	0	1.620958	2.174518	-0.001705
10	1	0	-0.843550	2.181147	0.000654
11	8	0	3.062395	0.000003	-0.003188
12	6	0	-2.424641	-0.000029	-0.738272
13	1	0	-2.683270	0.911701	-1.262202
14	6	0	-2.422690	0.000026	0.744096
15	1	0	-2.679983	0.911784	1.268632
16	1	0	-2.679978	-0.911686	1.268706
17	1	0	-2.683275	-0.911800	-1.262132

6 in water

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -384.934986
 $\langle \Psi(f) | H + V(f) / 2 | \Psi(f) \rangle$ (a.u.) = -384.959731
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -384.957459

(Polar.Solute)-Solvent (kcal/mol) = -15.53

Cavitation energy (kcal/mol) = 16.90
 Dispersion energy (kcal/mol) = -19.58
 Repulsion energy (kcal/mol) = 4.10
 Total non electr. (kcal/mol) = 1.43

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.292352	1.240731	-0.004850
2	6	0	1.056681	1.244793	-0.006891
3	6	0	1.825655	-0.000103	-0.001983
4	6	0	1.056213	-1.244801	0.001519
5	6	0	-0.292775	-1.240705	0.000915
6	6	0	-1.061044	0.000168	-0.001078
7	1	0	-0.845733	2.177972	-0.007463
8	1	0	1.617107	2.175805	-0.011161
9	1	0	1.617693	-2.175261	0.007253
10	1	0	-0.845931	-2.178198	0.005346
11	8	0	3.069254	-0.000512	0.000473
12	6	0	-2.427459	-0.001213	0.740168
13	1	0	-2.666323	-0.919686	1.265530
14	6	0	-2.432691	0.001594	-0.731106
15	1	0	-2.678375	-0.913541	-1.258980
16	1	0	-2.677355	0.919962	-1.254094
17	1	0	-2.668483	0.914256	1.269616

7 in gas

E = -440.322143

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	.000000	.000000	.000000
2	7	0	.000000	.000000	1.008643
3	6	0	1.224142	.000000	1.657879
4	6	0	2.348705	.732819	1.014784
5	1	0	-.699251	-.614584	1.398937
6	6	0	3.619097	.746462	1.765378
7	6	0	3.760046	.174820	2.967127
8	6	0	2.635930	-.530059	3.622616
9	6	0	1.385191	-.575203	2.878405
10	6	0	2.027284	1.998445	.199506
11	6	0	2.462161	.769969	-.517530
12	1	0	2.724137	2.821762	.294331
13	1	0	.983908	2.284731	.162624
14	1	0	1.738264	.205569	-1.093815
15	1	0	3.466122	.726753	-.921152
16	1	0	4.453100	1.259668	1.294101
17	1	0	4.698261	.200117	3.509194
18	8	0	2.769625	-1.052780	4.728272
19	1	0	.564608	-1.104909	3.351422

7 in water

<Psi(f)| H |Psi(f)> (a.u.) = -440.309066
 <Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -440.351292
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -440.349026

(Polar.Solute)-Solvent (kcal/mol) = -26.50

Cavitation energy (kcal/mol) = 18.30
 Dispersion energy (kcal/mol) = -21.51
 Repulsion energy (kcal/mol) = 4.64
 Total non electr. (kcal/mol) = 1.42

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.034080	-1.524677	.002647
2	6	0	1.364464	-1.350763	.009115
3	6	0	1.957371	-.003407	.002756
4	6	0	1.050819	1.106471	-.003368
5	6	0	-.318909	.958180	-.005050
6	6	0	-.912318	-.401868	-.002977
7	1	0	-.397120	-2.523854	.002451
8	1	0	2.047200	-2.196195	.014206
9	1	0	1.478729	2.106203	-.010313
10	8	0	3.202893	.141380	-.004639
11	6	0	-2.249117	-.644246	-.735891
12	1	0	-2.667142	.202961	-1.271360
13	6	0	-2.244924	-.632267	.742537
14	1	0	-2.649504	.230055	1.262347
15	1	0	-2.331287	-1.573774	1.274768
16	1	0	-2.335085	-1.594304	-1.252285
17	7	0	-1.141107	2.035279	.030423
18	1	0	-.737071	2.961873	-.077204
19	1	0	-2.132910	1.964496	-.177076

Table 4S. Cartesian coordinates and energies of all the TSs located for the alkylation reaction of ammonia by **6** and **7** in gas phase, and water at B3LYP/6-31G(d) and B3LYP-C-PCM-/6-31G(d) level of theory.

S6i in gas phase

E = -441.3188079

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-.018974	-.432817	1.292997
2	6	0	-1.329990	-.015282	1.250063
3	6	0	-2.082269	.064104	-.000149
4	6	0	-1.341020	-.373957	-1.180779
5	6	0	-.029867	-.787732	-1.112939
6	6	0	.667868	-.844729	.121477
7	1	0	.502595	-.479570	2.250464
8	1	0	-1.864015	.248739	2.159290
9	1	0	-1.883446	-.383128	-2.122729
10	1	0	.483254	-1.109687	-2.020692
11	8	0	-3.261431	.469247	-.054575
12	6	0	2.729207	.238662	-.047204
13	1	0	3.139572	.509239	-1.013027
14	6	0	2.165867	-1.117659	.154938

15	1	0	2.465048	-1.801599	-.647892
16	1	0	2.473040	-1.541755	1.118070
17	1	0	3.147264	.775648	.796183
18	7	0	1.387336	1.899271	-.286108
19	1	0	1.767241	2.836564	-.425303
20	1	0	.789008	1.638120	-1.069392
21	1	0	.795598	1.875004	.543952

S6 in water

<Psi(f)| H |Psi(f)> (a.u.) = -441.336735
 <Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -441.384590
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -441.381663

(Polar.Solute)-Solvent (kcal/mol) = -30.03

Cavitation energy (kcal/mol) = 20.08
 Dispersion energy (kcal/mol) = -23.49
 Repulsion energy (kcal/mol) = 5.25

Total non electr. (kcal/mol) = 1.84

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.32364	-1.223057	.308989
2	6	0	-1.758680	-1.226148	-.032065
3	6	0	-2.514166	.003264	-.210216
4	6	0	-1.758994	1.228286	-.002710
5	6	0	-.432547	1.217385	.337560
6	6	0	.283618	-.005049	.516616
7	1	0	.097700	-2.167187	.439672
8	1	0	-2.291799	-2.163842	-.179501
9	1	0	-2.292406	2.169110	-.127400
10	1	0	.097372	2.158215	.490668
11	8	0	-3.735189	.006905	-.523798
12	6	0	1.717281	-.010517	1.020829
13	1	0	1.998036	.888118	1.572437
14	6	0	2.002228	.003899	-.405819
15	1	0	1.997800	-.920357	1.553939
16	7	0	4.254269	.004070	-.672582
17	1	0	4.544073	-.155769	-1.640101
18	1	0	4.664966	.891751	-.376028
19	1	0	4.679278	-.730874	-.103646
20	1	0	1.983984	-.916669	-.974406
21	1	0	1.984367	.935393	-.956278

S6i in water

<Psi(f)| H |Psi(f)> (a.u.) = -441.306510
<Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -441.353379
Total free energy in sol.
(with non electrost.terms) (a.u.) = -441.349702

(Polar.Solute)-Solvent (kcal/mol) = -29.41

Cavitation energy (kcal/mol) = 19.62
Dispersion energy (kcal/mol) = -22.86
Repulsion energy (kcal/mol) = 5.55
Total non electr. (kcal/mol) = 2.31

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-.123820	-.594371	-1.205599
2	6	0	-1.352097	-.984290	-.717781
3	6	0	-2.041520	-.244927	.321227
4	6	0	-1.337680	.926965	.803436
5	6	0	-.108700	1.303004	.307511
6	6	0	.520896	.572341	-.728732
7	1	0	.354631	-1.175754	-1.994084
8	1	0	-1.853178	-1.862378	-1.122484
9	1	0	-1.826780	1.521206	1.573800
10	1	0	.381431	2.195940	.695841
11	8	0	-3.174594	-.592805	.769151
12	6	0	2.661922	.204383	-.299342

13	1	0	3.109878	.684423	.562385
14	6	0	1.888094	.987052	-1.263788
15	1	0	2.049070	2.067511	-1.171725
16	1	0	2.032456	.658938	-2.300654
17	1	0	3.059896	-.763904	-.578681
18	7	0	1.790121	-1.100667	1.411422
19	1	0	2.500724	-1.662767	1.886381
20	1	0	1.325384	-.510679	2.102822
21	1	0	1.089826	-1.726363	1.011639

S7 in gas phase

E = -496.6902448

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	.000000	.000000	.000000
2	7	0	.000000	.000000	1.020796
3	6	0	1.352850	.000000	1.524749
4	6	0	2.145907	1.160899	1.287851
5	1	0	-.460140	-.862530	1.305247
6	6	0	3.453631	1.181205	1.838995
7	6	0	3.958915	.135729	2.570718
8	6	0	3.174649	-1.063607	2.850313
9	6	0	1.843224	-1.056719	2.257968
10	6	0	1.557393	2.383999	.635032
11	6	0	.753043	2.911429	1.791734
12	1	0	2.339272	3.088282	.326254
13	1	0	.920460	2.177502	-.237110
14	1	0	-.011451	2.207068	2.113722
15	1	0	1.355165	3.299542	2.611159
16	1	0	4.075576	2.060618	1.656243
17	1	0	4.971171	.164955	2.965849
18	8	0	3.610402	-2.020111	3.526324
19	1	0	1.235833	-1.947790	2.412075
20	7	0	-.211431	4.276426	1.380439
21	1	0	-.865079	4.006628	.642228
22	1	0	-.752574	4.629326	2.174849
23	1	0	.375062	5.034708	1.025310

S7i in gas phase

E = -496.674075

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-.925323	.339493	.053369
2	6	0	-.904997	.133538	1.414840
3	6	0	.311391	.199781	2.211597
4	6	0	1.517463	.533838	1.457803
5	6	0	1.475981	.757445	.106739
6	6	0	.272206	.688640	-.645843
7	1	0	-1.824990	-.092422	1.950961
8	1	0	2.442510	.627642	2.019155
9	1	0	2.390941	1.027063	-.421861

10	8	0	.321100	-.009628	3.441134
11	6	0	.583094	-.504875	-2.603974
12	1	0	1.577503	-.911526	-2.466356
13	6	0	.326567	.876546	-2.155308
14	1	0	1.153961	1.548099	-2.427834
15	1	0	-.588864	1.294663	-2.586160
16	1	0	-.028747	-.986651	-3.354525
17	7	0	-.300815	-2.175253	-1.371750
18	1	0	-.356421	-3.127529	-1.730802
19	1	0	.198437	-2.164457	-.485651
20	1	0	-1.234498	-1.786951	-1.214999
21	7	0	-2.129541	.114520	-.683186
22	1	0	-2.933929	.110175	-.061326
23	1	0	-2.290501	.817615	-1.400475

S7 in water

$\langle \text{Psi(f)} | \text{H} | \text{Psi(f)} \rangle$ (a.u.) = -496.684982
 $\langle \text{Psi(f)} | \text{H} + \text{V(f)}/2 | \text{Psi(f)} \rangle$ (a.u.) = -496.745958
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -496.742837

(Polar.Solute)-Solvent (kcal/mol) = -38.26

Cavitation energy (kcal/mol) = 21.42
 Dispersion energy (kcal/mol) = -25.27
 Repulsion energy (kcal/mol) = 5.80
 Total non electr. (kcal/mol) = 1.96

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.264985
3	6	0	1.209831	0.000000	2.047057
4	6	0	1.221304	0.013603	3.432582
5	6	0	-0.025787	0.024801	4.157552
6	6	0	-1.234270	0.010909	3.394072
7	6	0	-1.240118	-0.002639	2.028649
8	7	0	2.423763	0.084913	4.133529
9	1	0	3.241531	-0.140647	3.569498
10	1	0	2.450833	-0.420557	5.018332
11	1	0	2.155433	-0.015035	1.506101
12	1	0	-2.174613	-0.016393	1.471256
13	1	0	-2.176830	0.005772	3.942480
14	6	0	-0.090459	-0.033691	5.671691
15	1	0	-1.027476	-0.447936	6.048582
16	1	0	0.765983	-0.498361	6.165671
17	6	0	-0.051774	1.419519	5.548207

18	1	0	0.892070	1.911522	5.353511
19	1	0	-0.963047	1.963076	5.335958
20	7	0	-0.053713	2.295705	7.568882
21	1	0	-0.746138	1.825237	8.155405
22	1	0	0.856270	2.183823	8.020877
23	1	0	-0.276924	3.293448	7.570255

S7i in water

$\langle \text{Psi(f)} | \text{H} | \text{Psi(f)} \rangle$ (a.u.) = -496.657516
 $\langle \text{Psi(f)} | \text{H} + \text{V(f)}/2 | \text{Psi(f)} \rangle$ (a.u.) = -496.711186
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -496.707018

(Polar.Solute)-Solvent (kcal/mol) = -33.68

Cavitation energy (kcal/mol) = 21.20
 Dispersion energy (kcal/mol) = -24.35
 Repulsion energy (kcal/mol) = 5.77
 Total non electr. (kcal/mol) = 2.62

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-.999106	.487695	-.006927
2	6	0	-1.015953	.221854	1.356218
3	6	0	.176764	.099069	2.153284
4	6	0	1.424371	.282193	1.433789
5	6	0	1.439485	.551368	.085802
6	6	0	.251150	.686998	-.672187
7	1	0	-1.972327	.106433	1.865797
8	1	0	2.350152	.222337	2.002651
9	1	0	2.390702	.695945	-.426910
10	8	0	.145631	-.141883	3.399337
11	6	0	.277251	-.461893	-2.568557
12	1	0	1.157126	-.956663	-2.961964
13	6	0	.332172	.947185	-2.171584
14	1	0	1.277912	1.432567	-2.437691
15	1	0	-.510449	1.541263	-2.552890
16	1	0	-.679061	-.916591	-2.795169
17	7	0	.402549	-2.248724	-1.139382
18	1	0	.520096	-3.146483	-1.616828
19	1	0	1.182299	-2.112756	-.495677
20	1	0	-.456623	-2.280846	-.588987
21	7	0	-2.191026	.513763	-.740790
22	1	0	-3.018760	.641714	-.162754
23	1	0	-2.203588	1.166064	-1.522100

Table 5S. Cartesian coordinates and energies of the TSs **S6** and **S7** located for the alkylation reaction of ammonia by **6** and **7** in gas phase, and water at B3LYP/6-31+G(d,p) and B3LYP-C-PCM-/6-31+G(d,p) level of theory.

S6 in gas phase
 E = -441.3828484

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

1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.377300
3	6	0	1.234071	.000000	2.153347
4	6	0	2.453272	-.025753	1.354557
5	6	0	2.427709	-.027418	-.022504
6	6	0	1.206870	-.021498	-.746982
7	1	0	-.952729	-.009279	-.533765
8	1	0	-.932596	-.008871	1.934871
9	1	0	3.395628	-.054814	1.894761
10	1	0	3.369933	-.058046	-.573829
11	8	0	1.245874	.015055	3.409302
12	6	0	1.193770	.053136	-2.252075
13	1	0	2.075526	-.420923	-2.701344
14	6	0	1.209037	1.545819	-2.429770
15	1	0	.293365	-.400743	-2.684893
16	7	0	1.199015	2.038191	-4.111131
17	1	0	1.209584	3.055612	-4.215357
18	1	0	2.016848	1.657213	-4.589304
19	1	0	.364027	1.675953	-4.573975
20	1	0	.317028	2.048402	-2.060521
21	1	0	2.118897	2.027991	-2.077237

S6 in water

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -441.379468
 $\langle \Psi(f) | H + V(f)/2 | \Psi(f) \rangle$ (a.u.) = -441.436331
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -441.433210

(Polar.Solute)-Solvent (kcal/mol) = -35.68

Cavitation energy (kcal/mol) = 20.14
 Dispersion energy (kcal/mol) = -23.48
 Repulsion energy (kcal/mol) = 5.30
 Total non electr. (kcal/mol) = 1.96

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.433396	-1.223107	0.302685
2	6	0	-1.766572	-1.225880	-0.031105
3	6	0	-2.513523	0.003212	-0.200554
4	6	0	-1.768294	1.228201	0.003883
5	6	0	-0.434865	1.218110	0.336496
6	6	0	0.280200	-0.004738	0.509250
7	1	0	0.095501	-2.168662	0.426253
8	1	0	-2.298161	-2.165180	-0.175324
9	1	0	-2.301539	2.170121	-0.112607
10	1	0	0.092097	2.160649	0.488403
11	8	0	-3.748694	0.007344	-0.512624
12	6	0	1.718016	-0.010782	1.011457
13	1	0	1.994259	0.889466	1.562724
14	6	0	1.999673	0.003812	-0.414443
15	1	0	1.993178	-0.922779	1.543913
16	7	0	4.285509	0.003439	-0.670982
17	1	0	4.576218	-0.180612	-1.632866
18	1	0	4.679635	0.902279	-0.388793

19	1	0	4.690895	-0.719547	-0.074553
20	1	0	1.990722	-0.918792	-0.981819
21	1	0	1.990755	0.937261	-0.963486

S7 in gas phase
 E = -496.7471025

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	.000000	.000000	.000000
2	7	0	.000000	.000000	1.017662
3	6	0	1.333845	.000000	1.551102
4	6	0	2.172871	1.116755	1.254928
5	1	0	-.502314	-.828013	1.323122
6	6	0	3.472283	1.130920	1.832004
7	6	0	3.926434	.124033	2.649003
8	6	0	3.087693	-1.019059	2.992672
9	6	0	1.772425	-1.017400	2.372490
10	6	0	1.647732	2.315160	.504801
11	6	0	.917738	2.942084	1.653402
12	1	0	2.463031	2.944595	.132288
13	1	0	.983007	2.075702	-.333903
14	1	0	.109038	2.325887	2.038873
15	1	0	1.558749	3.358855	2.426773
16	1	0	4.130677	1.969797	1.600049
17	1	0	4.930627	.145274	3.062423
18	8	0	3.476402	-1.940215	3.752165
19	1	0	1.134921	-1.876150	2.573463
20	7	0	-.012402	4.393140	1.185877
21	1	0	-.714417	4.128799	.494255
22	1	0	-.489709	4.808295	1.988046
23	1	0	.601167	5.095656	.772296

S7 in water

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -496.735455
 $\langle \Psi(f) | H + V(f)/2 | \Psi(f) \rangle$ (a.u.) = -496.807818
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -496.804623

(Polar.Solute)-Solvent (kcal/mol) = -45.41

Cavitation energy (kcal/mol) = 21.47
 Dispersion energy (kcal/mol) = -25.27
 Repulsion energy (kcal/mol) = 5.80
 Total non electr. (kcal/mol) = 2.01

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.280328
3	6	0	1.209806	0.000000	2.048019

4	6	0	1.224786	0.036433	3.439598
5	6	0	-0.020897	0.081325	4.163950
6	6	0	-1.231805	0.054203	3.404387
7	6	0	-1.239881	0.009842	2.035105
8	7	0	2.428775	0.089611	4.124418
9	1	0	3.254415	-0.142620	3.576297
10	1	0	2.462016	-0.313671	5.058552
11	1	0	2.155431	-0.032838	1.507540
12	1	0	-2.176943	-0.009208	1.481857
13	1	0	-2.174937	0.069698	3.951391
14	6	0	-0.081135	0.075150	5.680398

15	1	0	-1.017074	-0.327696	6.072147
16	1	0	0.779308	-0.371585	6.184035
17	6	0	-0.046589	1.522770	5.505421
18	1	0	0.894698	2.017722	5.299251
19	1	0	-0.962796	2.057227	5.286580
20	7	0	-0.049976	2.472929	7.521185
21	1	0	-0.727760	1.999998	8.121475
22	1	0	0.869650	2.397151	7.959024
23	1	0	-0.301184	3.461990	7.474744

Table 6S. Cartesian coordinates and energies of the TSs **S6** and **S7** located for the alkylation reaction of ammonia by **6** and **7** in gas phase, and water at B3LYP/6-311+G(d,p) and B3LYP-C-PCM-/6-311+G(d,p) level of theory.

S6 in gas phase
E = -441.4748043

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.373300
3	6	0	1.231535	.000000	2.150371
4	6	0	2.447917	-.028312	1.350288
5	6	0	2.422066	-.030046	-.022768
6	6	0	1.204054	-.022669	-.745226
7	1	0	-.951268	-.009331	-.532482
8	1	0	-.931278	-.008334	1.929771
9	1	0	3.389024	-.058837	1.889169
10	1	0	3.362637	-.062809	-.573030
11	8	0	1.243477	.016550	3.399504
12	6	0	1.190803	.048913	-2.249366
13	1	0	2.070198	-.428702	-2.694598
14	6	0	1.207393	1.538797	-2.435841
15	1	0	.291771	-.406828	-2.677995
16	7	0	1.197450	2.019073	-4.118409
17	1	0	1.208968	3.034207	-4.228025
18	1	0	2.014217	1.634079	-4.591965
19	1	0	.362634	1.654500	-4.576398
20	1	0	.317334	2.042251	-2.068676
21	1	0	2.116333	2.020110	-2.085628

S6 in water

<Psi(f)| H |Psi(f)> (a.u.) = -441.471813
 <Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -441.528499
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -441.525445

(Polar.Solute)-Solvent (kcal/mol) = -35.57

Cavitation energy (kcal/mol) = 20.11
 Dispersion energy (kcal/mol) = -23.48
 Repulsion energy (kcal/mol) = 5.28
 Total non electr. (kcal/mol) = 1.92

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.436789	-1.219909	0.306956
2	6	0	-1.764634	-1.222807	-0.030826
3	6	0	-2.510635	0.003702	-0.205204
4	6	0	-1.765874	1.225379	0.005518
5	6	0	-0.437839	1.214068	0.342418
6	6	0	0.274606	-0.005471	0.518095
7	1	0	0.090623	-2.164118	0.431308
8	1	0	-2.294326	-2.160883	-0.177254
9	1	0	-2.296821	2.166511	-0.111851
10	1	0	0.087861	2.154848	0.496704
11	8	0	-3.736875	0.008288	-0.526212
12	6	0	1.714411	-0.012172	1.011845
13	1	0	1.990528	0.885232	1.563463
14	6	0	1.998932	0.004058	-0.411815
15	1	0	1.989048	-0.922847	1.542373
16	7	0	4.283459	0.004167	-0.672609
17	1	0	4.566324	-0.191191	-1.633507
18	1	0	4.679767	0.905670	-0.405957
19	1	0	4.695899	-0.710051	-0.072153
20	1	0	1.984336	-0.916083	-0.978807
21	1	0	1.984482	0.936351	-0.958288

S7 in gas phase
E = -496.8527514

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	.000000	.000000	.000000
2	7	0	.000000	.000000	1.015821
3	6	0	1.334227	.000000	1.546315
4	6	0	2.174449	1.109641	1.242284
5	1	0	-.500814	-.826907	1.321208
6	6	0	3.472717	1.123109	1.814296
7	6	0	3.924055	.123500	2.634916
8	6	0	3.084829	-1.013956	2.989410
9	6	0	1.770558	-1.010779	2.370642
10	6	0	1.652745	2.303564	.484522

11	6	0	.925463	2.946100	1.624193
12	1	0	2.470004	2.923395	.106269
13	1	0	.989330	2.058233	-.350881
14	1	0	.117389	2.336998	2.016768
15	1	0	1.567970	3.367582	2.391112
16	1	0	4.132589	1.956315	1.575147
17	1	0	4.927947	.144087	3.044501
18	8	0	3.469448	-1.925708	3.751140
19	1	0	1.131473	-1.864890	2.577206
20	7	0	.000747	4.392795	1.139615
21	1	0	-.700103	4.121897	.451568
22	1	0	-.474892	4.816280	1.936370
23	1	0	.616526	5.087569	.720003

S7 in water

<Psi(f) H Psi(f)>		(a.u.) = -496.841391
<Psi(f) H+V(f)/2 Psi(f)>		(a.u.) = -496.913485
Total free energy in sol.		
(with non electrost.terms) (a.u.) =		-496.910356
(Polar.Solute)-Solvent (kcal/mol) =		-45.24
Cavitation energy (kcal/mol) =		21.45
Dispersion energy (kcal/mol) =		-25.26
Repulsion energy (kcal/mol) =		5.77
Total non electr. (kcal/mol) =		1.96

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.274086
3	6	0	1.206984	0.000000	2.042022
4	6	0	1.221311	0.037082	3.429879
5	6	0	-0.021466	0.075981	4.153147
6	6	0	-1.228503	0.049931	3.394601
7	6	0	-1.236925	0.006764	2.029499
8	7	0	2.423819	0.090730	4.114803
9	1	0	3.248306	-0.141446	3.567670
10	1	0	2.455207	-0.314635	5.046492
11	1	0	2.151811	-0.031866	1.503336
12	1	0	-2.172949	-0.013625	1.477919
13	1	0	-2.170498	0.062808	3.940075
14	6	0	-0.080991	0.070932	5.669086
15	1	0	-1.012004	-0.339130	6.058959
16	1	0	0.780989	-0.371968	6.168811
17	6	0	-0.055385	1.518113	5.504055
18	1	0	0.880923	2.017103	5.296821
19	1	0	-0.972844	2.045187	5.283618
20	7	0	-0.064572	2.461655	7.523212
21	1	0	-0.733010	1.982361	8.127206
22	1	0	0.856288	2.400110	7.958216
23	1	0	-0.329081	3.446106	7.476105

Table 7S. Cartesian coordinates and energies (in Hartree) of all stationary points (reactants and TSs) located for the alkylation reaction of ammonia by **8-12** in gas phase at B3LYP/6-31G(d) level of theory.

8

E = -478.2972539

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.549528	1.567942	-.375630
2	6	0	1.805221	1.098809	-.469015
3	6	0	2.157857	-.324605	-.192973
4	6	0	1.047985	-1.236050	.090328
5	6	0	-.218971	-.760850	.177317
6	6	0	-.532590	.685302	.081741
7	1	0	1.276845	-2.296856	.137800
8	8	0	3.328630	-.702164	-.269038
9	6	0	-1.543641	1.194527	1.125278
10	1	0	-1.720593	.570623	1.997257
11	6	0	-2.041590	.753248	-.205994
12	1	0	-2.450011	1.476710	-.904670
13	1	0	-1.506040	2.262459	1.320896
14	6	0	-2.520186	-.692766	-.287416
15	7	0	-1.409725	-1.452519	.307401
16	1	0	-3.448110	-.859371	.272660
17	1	0	-1.393352	-2.454920	.168288
18	1	0	-2.694065	-.978660	-1.335778
19	1	0	2.636691	1.737459	-.752631
20	1	0	.315997	2.614150	-.565138

9Z

E = -591.632468

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.513884	-1.630573	-.265431
2	6	0	-2.487091	-.710578	-.377502
3	6	0	-2.230080	.747645	-.224460
4	6	0	-.826081	1.171634	-.075428
5	6	0	.143109	.236096	.013941
6	6	0	-.147928	-1.215106	.078952
7	1	0	-.608672	2.230447	-1.09800
8	8	0	-3.153520	1.557732	-.282927
9	6	0	.608087	-1.977051	1.187123
10	1	0	1.070016	-1.391803	1.978416
11	6	0	1.178366	-1.937397	-.186237
12	1	0	1.215046	-2.835954	-.793872
13	1	0	.137872	-2.899200	1.515165
14	6	0	2.215644	-.854238	-.436294
15	7	0	1.541958	.394652	-.015078
16	1	0	3.133723	-1.004160	.141944
17	6	0	2.232306	1.577006	.137063
18	8	0	1.736167	2.661641	.365891

19	1	0	3.324122	1.425304	.033660
20	1	0	2.478247	-.805413	-1.500834
21	1	0	-3.517888	-.986350	-.579047
22	1	0	-1.722033	-2.695038	-.354157

9E

E =-591.6358397

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.747637	1.441365	-.209314
2	6	0	2.672927	.465854	-.204779
3	6	0	2.322848	-.966784	-.012515
4	6	0	.888240	-1.298155	.040146
5	6	0	-.031828	-.309330	.043823
6	6	0	.338825	1.122664	.053870
7	1	0	.631934	-2.350817	-.013976
8	8	0	3.194196	-1.833475	.028637
9	6	0	-.452663	1.997808	1.049115
10	1	0	-1.002686	1.494439	1.840542
11	6	0	-.928844	1.892393	-.354452
12	1	0	-.868375	2.746628	-1.021190
13	1	0	.048854	2.912193	1.351687
14	6	0	-2.012675	.851464	-.599406
15	7	0	-1.428206	-.394989	-.065329
16	1	0	-2.951825	1.066091	-.082841
17	6	0	-2.211917	-1.495940	.189902
18	8	0	-3.411255	-1.524834	-.011572
19	1	0	-1.643209	-2.340823	.613102
20	1	0	-2.229524	.733637	-1.667757
21	1	0	3.729379	.675688	-.342097
22	1	0	2.024054	2.486324	-.335029

10Z

E = -723.2161123

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.366904	-.748172	-.010742
2	6	0	-1.833306	.558604	-.062065
3	6	0	-1.025928	1.773678	-.023582
4	6	0	.430183	1.534704	-.021582
5	6	0	.916243	.271408	.022582
6	6	0	.075495	-.948703	.190837
7	1	0	1.081308	2.391368	-.130139
8	8	0	-1.533345	2.898454	-.057462
9	6	0	.588307	-1.928439	1.260063
10	1	0	1.339730	-1.579589	1.964620
11	6	0	.966839	-2.139673	-.166414
12	1	0	.574383	-2.983095	-.725443
13	1	0	-.175503	-2.572906	1.684034
14	6	0	2.316191	-1.570432	-.569820
15	7	0	2.249544	-.153127	-.146778

16	1	0	3.155954	-2.072819	-.077315
17	1	0	2.459310	-1.636080	-1.656175
18	7	0	-3.199373	.519002	-.163852
19	6	0	-2.498660	-1.603006	-.077260
20	6	0	-3.613449	-.783399	-.178176
21	1	0	-3.768377	1.351563	-.225252
22	1	0	-4.659665	-1.039068	-.266672
23	1	0	-2.514525	-2.684840	-.062401
24	6	0	3.373673	.640964	-.110432
25	8	0	3.395051	1.834908	.114482
26	1	0	4.290448	.052239	-.307451

10E

E = -723.219355

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.389394
3	6	0	1.169818	.000000	2.259472
4	6	0	2.451825	.099035	1.537328
5	6	0	2.490521	.074681	.183041
6	6	0	1.296014	-.114576	-.684511
7	1	0	3.330294	.288172	2.144984
8	8	0	1.079208	-.007324	3.490654
9	6	0	1.490188	-1.117997	-1.834785
10	1	0	2.341920	-1.793290	-1.796148
11	6	0	1.722248	.330996	-2.089652
12	1	0	1.042985	.897335	-2.718666
13	1	0	.569477	-1.561367	-2.201231
14	6	0	3.173606	.777281	-1.993917
15	7	0	3.591777	.315594	-.654976
16	1	0	3.823156	.331804	-2.751951
17	1	0	3.271097	1.867681	-2.058218
18	7	0	-1.302800	.023100	1.815181
19	6	0	-1.355609	.016867	-.420762
20	6	0	-2.131734	.037625	.728957
21	1	0	-1.561089	.041461	2.791695
22	1	0	-3.205883	.069132	.842980
23	1	0	-1.734995	.020401	-1.434010
24	6	0	4.921597	.222288	-.319631
25	8	0	5.826807	.527091	-1.073830
26	1	0	5.083148	-.175026	.696584

11

E = -462.2599355

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.554273	1.598899	-1.76028
2	6	0	1.814357	1.164328	-.368166
3	6	0	2.180104	-.269084	-.270944
4	6	0	1.069160	-1.214192	-.035071
5	6	0	-1.86257	-.779591	.180633

6	6	0	-.513116	.662552	.186381
7	1	0	1.313924	-2.271342	-.099983
8	8	0	3.340396	-.648994	-.425454
9	6	0	-1.595318	1.115206	1.192771
10	1	0	-1.830619	.455049	2.023581
11	6	0	-2.013540	.763504	-.186458
12	1	0	-2.345899	1.554870	-.852982
13	1	0	-1.554882	2.167682	1.458983
14	6	0	-2.517978	-.660505	-.419003
15	6	0	-1.466440	-1.582607	.256763
16	1	0	-3.528952	-.814323	-.024022
17	1	0	-2.549628	-.859055	-1.496457
18	1	0	2.627525	1.845519	-.601510
19	1	0	.310807	2.658659	-.236634
20	1	0	-1.378177	-2.555315	-.235277
21	1	0	-1.738745	-1.780847	1.302657

12

E = -556.9170988

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.869564	-.488081	.479767
2	6	0	-1.850804	-.355512	1.816957
3	6	0	-.585317	-.166236	2.554664
4	6	0	.623271	-.071688	1.727425
5	6	0	.616029	-.178643	.375111
6	6	0	-.647866	-.487793	-.347686
7	1	0	1.550739	.121534	2.262064
8	8	0	-.554284	-.061716	3.782146
9	6	0	-.577654	-1.603044	-1.420594
10	1	0	.418808	-2.003587	-1.582059
11	6	0	-.831567	-.209801	-1.861403
12	1	0	-1.870953	.017207	-2.090686
13	1	0	-1.383666	-2.331329	-1.423915
14	7	0	1.807026	-.143275	-.385526
15	1	0	2.595623	-.367325	.216201
16	1	0	-2.759828	-.382664	2.410749
17	1	0	-2.812280	-.636061	-.045475
18	6	0	.163054	.595600	-2.700040
19	1	0	.873520	-.078595	-3.194042
20	1	0	-.403125	1.085011	-3.500899
21	6	0	.934379	1.662319	-1.910439
22	1	0	.247403	2.178436	-1.228335
23	1	0	1.326578	2.427164	-2.591984
24	6	0	2.121027	1.094139	-1.131624
25	1	0	2.930372	.843705	-1.828883
26	1	0	2.501960	1.875599	-.454048

S8'

E = -534.7903487

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

1	6	0	-1.749231	-.414892	.794798
2	6	0	-1.579161	-.229577	2.144690
3	6	0	-.264603	-.010076	2.751249
4	6	0	.841949	.038893	1.801441
5	6	0	.640091	-.157291	.457499
6	6	0	-.643539	-.411358	-.089183
7	1	0	1.830553	.263641	2.198085
8	8	0	-.108647	.157553	3.978753
9	6	0	-.695085	-.743273	-1.551109
10	1	0	-.113305	-1.643489	-1.824705
11	6	0	-.073555	.493655	-2.139274
12	1	0	-.765231	1.328824	-2.237234
13	1	0	-1.724829	-.875010	-1.903222
14	6	0	1.296174	.888551	-1.559197
15	7	0	1.678524	-.072971	-.529402
16	1	0	2.068832	.901858	-2.344609
17	1	0	2.566650	.186314	-.108123
18	1	0	1.213421	1.919234	-1.174527
19	1	0	-2.427732	-.250297	2.823446
20	1	0	-2.745699	-.598704	.389834
21	7	0	.238616	.156498	-3.860967
22	1	0	.878676	-.638880	-3.893863
23	1	0	-.630389	-.107857	-4.327556
24	1	0	.660011	.941452	-4.360459

S9E

E = -648.1396704

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.396182	-1.750955	.465041
2	6	0	2.645800	-1.304218	.111115
3	6	0	2.923550	.092029	-.243934
4	6	0	1.777830	1.002592	-1.65550
5	6	0	.547090	.515550	.181805
6	6	0	.312063	-.845007	.510969
7	1	0	1.964378	2.053402	-.363853
8	8	0	4.059791	.483107	-.571961
9	6	0	-1.525752	-1.567584	-.620283
10	6	0	-1.163635	-1.053044	.744780
11	1	0	-1.435915	-1.751668	1.545676
12	6	0	-1.666294	.380517	1.008076
13	7	0	-.693518	1.218926	.302579
14	1	0	-2.672569	.611208	.640552
15	1	0	-1.646319	.592767	2.084333
16	1	0	3.496202	-1.979904	.092286
17	1	0	1.240659	-2.798219	.727605
18	7	0	-3.257692	-1.888817	-.815867
19	1	0	-3.566655	-2.610734	-.161989
20	1	0	-3.773325	-1.029756	-.612222
21	1	0	-3.492776	-2.188626	-1.765549
22	1	0	-1.379134	-.840273	-1.416109
23	1	0	-1.112136	-2.543629	-.864943
24	6	0	-1.051074	2.408763	-.253016
25	8	0	-2.174222	2.893591	-.171370
26	1	0	-.223042	2.889233	-.800123

S10

E = -779.7171418

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.586546	.202781	.248956
2	6	0	-1.593609	.043049	1.644229
3	6	0	-.444309	.022341	2.534366
4	6	0	.816727	.199963	1.836184
5	6	0	.832938	.335345	.459924
6	6	0	-.312059	.357205	-.369700
7	1	0	1.719361	.249430	2.436099
8	8	0	-.577795	-.120649	3.770372
9	6	0	.018929	-1.072698	-2.113095
10	1	0	-.986035	-1.483388	-2.037301
11	6	0	.111037	.399230	-1.813566
12	1	0	-.508055	1.009105	-2.484395
13	1	0	.754756	-1.669733	-1.577586
14	6	0	1.562155	.907317	-1.718983
15	7	0	1.983558	.485501	-.380667
16	1	0	2.261034	.502716	-2.460187
17	1	0	1.582675	2.001400	-1.799528
18	7	0	-2.900512	-.075730	2.050945
19	6	0	-2.956971	.171229	-.173384
20	6	0	-3.727840	.000666	.963407
21	1	0	-3.147003	-.179580	3.024693
22	1	0	-4.801924	-.065718	1.070092
23	1	0	-3.343402	.279326	-1.179704
24	6	0	3.280878	.179905	-.109808
25	8	0	4.192448	.269440	-.926366
26	1	0	3.429807	-.171578	.924487
27	7	0	.425703	-1.479406	-3.767203
28	1	0	.401196	-2.488063	-3.941121
29	1	0	-.219468	-1.023455	-4.415808
30	1	0	1.370614	-1.141361	-3.964494

S11

E = -518.759176

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.792747	-1.427587	.657703
2	6	0	2.129865	-1.343868	.341871
3	6	0	2.748456	-.129072	-.195116
4	6	0	1.837868	1.002311	-.356790
5	6	0	.506616	.897049	-.036854
6	6	0	-.042239	-.303191	.478647
7	1	0	2.266238	1.930749	-.728926
8	8	0	3.962819	-.068104	-.484832
9	6	0	-2.055964	-.839930	-.574831
10	6	0	-1.531188	-.168325	.674248
11	1	0	-1.933753	-.662142	1.572975

12	6	0	-1.742028	1.365975	.692070
13	6	0	-.583598	1.948713	-.158266
14	1	0	-2.737560	1.690710	.341221
15	1	0	-1.651513	1.705284	1.729218
16	1	0	2.792358	-2.192643	.492871
17	1	0	.384096	-2.355478	1.064538
18	1	0	-.274928	2.937249	.199901
19	1	0	-.894392	2.087773	-1.206108
20	7	0	-3.733778	-.842425	-.659029
21	1	0	-4.122382	-1.369595	.127301
22	1	0	-4.064029	.123786	-.581184
23	1	0	-4.101152	-1.243334	-1.528690
24	1	0	-1.775971	-.321711	-1.491692
25	1	0	-1.816318	-1.901287	-.635660

S11'

E = -518.7618195

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.676290	-.569208	.795849
2	6	0	-1.591376	-.219201	2.122313
3	6	0	-.338167	.199765	2.746632
4	6	0	.803233	.230646	1.837905
5	6	0	.702635	-.134331	.516097
6	6	0	-.533111	-.565568	-.038445
7	1	0	1.749326	.576647	2.249874
8	8	0	-.255652	.524272	3.950345
9	6	0	-.575645	-.928784	-1.499608
10	1	0	.056295	-1.788563	-1.790080
11	6	0	-.064981	.354817	-2.092747
12	1	0	-.789344	1.162838	-2.009425
13	1	0	-1.602383	-1.142258	-1.819800
14	6	0	1.375296	.739399	-1.717967
15	6	0	1.849610	-.036535	-.463855
16	1	0	2.058840	.544007	-2.559868
17	1	0	1.416705	1.816215	-1.523004
18	1	0	-2.468866	-.246833	2.763676
19	1	0	-2.634480	-.883278	.377084
20	1	0	2.715474	.469469	-.026341
21	1	0	2.191299	-1.036995	-.770456
22	7	0	-.037072	.204172	-3.867642
23	1	0	-.977849	.005336	-4.212131
24	1	0	.310952	1.049702	-4.324469
25	1	0	.571525	-.575670	-4.121372

S12

E = -613.4179823

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.697222	.344063	1.022070
2	6	0	-1.647665	-.117651	2.313753

3	6	0	-.454086	-.752403	2.865879
4	6	0	.670163	-.810828	1.939455
5	6	0	.599959	-.348077	.645028
6	6	0	-.592032	.246919	.135771
7	1	0	1.596675	-1.238902	2.320146
8	8	0	-.394124	-1.191363	4.033780
9	6	0	-.952732	-.787660	-1.848561
10	1	0	-.073846	-1.417467	-1.720956
11	6	0	-.735203	.608093	-1.327299
12	1	0	-1.662462	1.184556	-1.441421
13	1	0	-1.877918	-1.255058	-1.519412
14	7	0	1.711458	-.474337	-.262295
15	1	0	2.371507	-1.144408	.126955
16	1	0	-2.503266	-.019400	2.977089
17	1	0	-2.614467	.808822	.653009

18	6	0	.432688	1.388873	-2.011545
19	1	0	.938608	.754532	-2.758113
20	1	0	.016657	2.242460	-2.563049
21	6	0	1.498214	1.896407	-1.030678
22	1	0	.997181	2.367411	-1.79169
23	1	0	2.107719	2.672391	-1.510993
24	6	0	2.432765	.782725	-.537848
25	1	0	3.178013	.561069	-1.314794
26	1	0	2.980986	1.150517	.345510
27	7	0	-1.150762	-.851960	-3.577668
28	1	0	-1.221546	-1.810775	-3.929019
29	1	0	-1.990945	-.340998	-3.856528
30	1	0	-.343863	-.402528	-4.015894

Table 8S. Cartesian coordinates and energies (in Hartee) of all stationary points (reactants and TSs) located for the alkylation reaction of ammonia by **8-12** in gas phase at B3LYP/6-31+G(d,p) level of theory.

8
E = -478.332968

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.522305	1.591968	-.303554
2	6	0	1.800588	1.171133	-.279940
3	6	0	2.174719	-.241312	.018239
4	6	0	1.082917	-1.199374	.179528
5	6	0	-.206882	-.772192	.142293
6	6	0	-.563911	.662729	.036376
7	1	0	1.347243	-2.250886	.237646
8	8	0	3.365653	-.573743	.059174
9	6	0	-1.687852	1.119005	.986153
10	1	0	-1.921969	.472116	1.827091
11	6	0	-2.040366	.682761	-.393596
12	1	0	-2.403466	1.403756	-1.118726
13	1	0	-1.705685	2.183583	1.198674
14	6	0	-2.457820	-.777453	-.540556
15	7	0	-1.374490	-1.510236	.136043
16	1	0	-3.423107	-.986447	-.065791
17	1	0	-1.314125	-2.510951	.008595
18	1	0	-2.525024	-1.049171	-1.604009
19	1	0	2.629474	1.844599	-.475155
20	1	0	.270674	2.631405	-.503671

9Z
E = -591.6698551

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.513372	-1.631223	-0.264843
2	6	0	-2.489252	-0.711148	-0.380087
3	6	0	-2.229452	0.745475	-0.227266
4	6	0	-0.827455	1.173640	-0.079242
5	6	0	0.143149	0.236466	0.011719
6	6	0	-0.147895	-1.214458	0.078756
7	1	0	-0.612201	2.233002	-0.116158

8	8	0	-3.155909	1.557609	-0.283960
9	6	0	0.608740	-1.975511	1.188286
10	1	0	1.069728	-1.386487	1.976871
11	6	0	1.177919	-1.937197	-0.186891
12	1	0	1.212057	-2.836235	-0.793297
13	1	0	0.137492	-2.896289	1.516858
14	6	0	2.215660	-0.855008	-0.440840
15	7	0	1.542238	0.396276	-0.017703
16	1	0	3.134172	-1.005472	0.135429
17	6	0	2.235853	1.574817	0.141262
18	8	0	1.738913	2.660288	0.379757
19	1	0	3.326528	1.428270	0.033529
20	1	0	2.471294	-0.805079	-1.506477
21	1	0	-3.519060	-0.988820	-0.581961
22	1	0	-1.723069	-2.695116	-0.352366

9E
E = -591.6736753

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.746567	1.442044	-0.210988
2	6	0	2.673880	0.465433	-0.208527
3	6	0	2.319905	-0.964295	-0.010492
4	6	0	0.887407	-1.298292	0.042770
5	6	0	-0.033345	-0.307154	0.046544
6	6	0	0.338405	1.123760	0.055054
7	1	0	0.632212	-2.350860	-0.009909
8	8	0	3.193539	-1.833960	0.035299
9	6	0	-0.451557	2.002006	1.050738
10	1	0	-1.000742	1.497478	1.841481
11	6	0	-0.928141	1.894557	-0.353469
12	1	0	-0.864618	2.747114	-1.021439
13	1	0	0.053145	2.914688	1.351195
14	6	0	-2.014667	0.855856	-0.598010
15	7	0	-1.430996	-0.393913	-0.064444
16	1	0	-2.952334	1.073347	-0.080650
17	6	0	-2.206896	-1.499637	0.185791
18	8	0	-3.408853	-1.536458	-0.020150

19	1	0	-1.640847	-2.345255	0.607509
20	1	0	-2.230801	0.737152	-1.665919
21	1	0	3.729383	0.675673	-0.349461
22	1	0	2.024738	2.485737	-0.339355

11

E = -462.2927887

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.552874	1.598574	-.180216
2	6	0	1.815768	1.164433	-.371331
3	6	0	2.178849	-.268160	-.266088
4	6	0	1.070970	-1.215372	-.034106
5	6	0	-.187414	-.779368	.177754
6	6	0	-.513646	.662265	.183908
7	1	0	1.315273	-2.272288	-.098335
8	8	0	3.344334	-.648131	-.412544
9	6	0	-1.595062	1.115581	1.192533
10	1	0	-1.827300	.452832	2.021576
11	6	0	-2.014917	.764109	-.187213
12	1	0	-2.344984	1.556005	-.853679
13	1	0	-1.551648	2.167270	1.459161
14	6	0	-2.521531	-.660117	-.418434
15	6	0	-1.466704	-1.584055	.250844
16	1	0	-3.529484	-.811807	-.016117
17	1	0	-2.560391	-.857674	-1.495385
18	1	0	2.627425	1.845966	-.607113
19	1	0	.311008	2.657947	-.245362
20	1	0	-1.375579	-2.553006	-.246516
21	1	0	-1.734107	-1.787535	1.296212

S8

E = -534.8448205

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.833431	-1.464689	.652865
2	6	0	2.154907	-1.330225	.289153
3	6	0	2.701295	-.083728	-.257415
4	6	0	1.760439	1.024194	-.385981
5	6	0	.449631	.854795	-.013750
6	6	0	-.044105	-.364714	.520834
7	1	0	2.138708	1.967012	-.771554
8	8	0	3.907936	.020750	-.586288
9	6	0	-1.997240	-.796980	-.561325
10	6	0	-1.527813	-.210911	.744586
11	1	0	-1.947080	-.724230	1.617951
12	6	0	-1.665055	1.324224	.821270
13	7	0	-.623552	1.791258	-.106302
14	1	0	-2.654101	1.705799	.526054
15	1	0	-1.478992	1.633153	1.862133
16	1	0	2.853835	-2.153055	.405763
17	1	0	.472337	-2.407601	1.064590
18	1	0	-.352511	2.760915	.010137
19	7	0	-3.737065	-.717345	-.792315

20	1	0	-4.226915	-1.220381	-.050617
21	1	0	-4.030221	.260749	-.765487
22	1	0	-4.019521	-1.112668	-1.692646
23	1	0	-1.657558	-.236978	-1.429932
24	1	0	-1.830077	-1.867911	-.657195

S8'

E = -534.8442314

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.749950	-.407602	.790855
2	6	0	-1.586433	-.232286	2.145396
3	6	0	-.273431	-.014908	2.752311
4	6	0	.838998	.043056	1.814514
5	6	0	.643358	-.144958	.464942
6	6	0	-.637887	-.402310	-.087642
7	1	0	1.824019	.267887	2.217498
8	8	0	-.123413	.144554	3.988025
9	6	0	-.681496	-.751848	-1.547947
10	1	0	-.089835	-1.649686	-1.799404
11	6	0	-.067588	.488699	-2.127821
12	1	0	-.760054	1.322895	-2.224771
13	1	0	-1.709303	-.893075	-1.898539
14	6	0	1.310217	.877891	-1.568811
15	7	0	1.684445	-.058443	-.511970
16	1	0	2.079204	.856023	-2.354870
17	1	0	2.578370	.183651	-.097276
18	1	0	1.246043	1.917172	-1.205621
19	1	0	-2.437193	-.260903	2.819920
20	1	0	-2.744022	-.592453	.383301
21	7	0	.226439	.161512	-3.897154
22	1	0	.876941	-.621479	-3.960299
23	1	0	-.649327	-.104984	-4.345972
24	1	0	.621543	.962632	-4.389079

S9Z

E = -648.1849217

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.422929
3	6	0	1.147218	0.000000	2.174457
4	6	0	2.444565	0.004469	1.496244
5	6	0	2.411617	-0.009107	0.031792
6	6	0	1.235106	0.002361	-0.683617
7	7	0	-1.364772	-0.016784	1.860742
8	6	0	-1.855167	0.097622	3.130659
9	8	0	-1.205310	0.296731	4.144536
10	1	0	1.128170	-0.014325	3.255984
11	8	0	3.523545	0.008960	2.131890
12	6	0	-1.431121	1.636095	-0.702382
13	7	0	-2.957262	2.274574	-1.269606
14	6	0	-1.414063	0.141634	-0.500780
15	1	0	-1.659985	-0.411580	-1.415028

16	6	0	-2.228025	-0.340852	0.713306
17	1	0	-3.212242	0.133014	0.826940
18	1	0	-2.377495	-1.425582	0.632944
19	1	0	3.372670	-0.033358	-0.472905
20	1	0	1.256454	-0.008201	-1.773650
21	1	0	-3.209970	1.859665	-2.168343
22	1	0	-3.698162	2.060567	-0.599295
23	1	0	-2.917235	3.290660	-1.385598
24	1	0	-1.301940	2.199629	0.220219
25	1	0	-0.764924	1.981176	-1.490287
26	1	0	-2.960274	-0.001287	3.151430

S9E

E = -648.195104

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.394962	-1.752518	0.467258
2	6	0	2.647056	-1.307336	0.112248
3	6	0	2.916084	0.086460	-0.252694
4	6	0	1.775319	1.000079	-0.181889
5	6	0	0.542498	0.514409	0.168331
6	6	0	0.309053	-0.846345	0.501561
7	1	0	1.964872	2.048711	-0.384887
8	8	0	4.056939	0.477909	-0.585621
9	6	0	-1.503743	-1.567105	-0.613375
10	6	0	-1.165534	-1.051043	0.752686
11	1	0	-1.427487	-1.748924	1.555638
12	6	0	-1.666461	0.381911	1.014052
13	7	0	-0.696045	1.218636	0.295772
14	1	0	-2.675796	0.605519	0.655116
15	1	0	-1.634032	0.602034	2.088047
16	1	0	3.497994	-1.981405	0.100737
17	1	0	1.242169	-2.796856	0.738713
18	7	0	-3.284310	-1.911507	-0.833838
19	1	0	-3.602524	-2.605600	-0.157627
20	1	0	-3.811314	-1.049983	-0.687369
21	1	0	-3.483601	-2.256306	-1.774069
22	1	0	-1.372642	-0.844490	-1.415240
23	1	0	-1.102933	-2.548851	-0.852352
24	6	0	-1.037269	2.423874	-0.232904
25	8	0	-2.155895	2.924913	-0.131276
26	1	0	-0.212361	2.909354	-0.776710

S11

E = -518.8100213

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.792479	-1.448243	.619973
2	6	0	2.128473	-1.363988	.293337
3	6	0	2.737514	-.138798	-.226224

4	6	0	1.837253	1.003194	-.355414
5	6	0	.507234	.896640	-.025990
6	6	0	-.040826	-.315607	.469245
7	1	0	2.269088	1.937824	-.705087
8	8	0	3.954208	-.075797	-.529165
9	6	0	-2.010959	-.806360	-.563062
10	6	0	-1.525157	-.168856	.707549
11	1	0	-1.910963	-.689490	1.594874
12	6	0	-1.722410	1.364937	.766935
13	6	0	-.575643	1.960696	-.092622
14	1	0	-2.720050	1.698585	.441601
15	1	0	-1.607003	1.678936	1.809340
16	1	0	2.789829	-2.216106	.422397
17	1	0	.386709	-2.381183	1.014137
18	1	0	-.243733	2.932607	.286530
19	1	0	-.901831	2.129507	-1.130120
20	7	0	-3.783626	-.827238	-.689595
21	1	0	-4.184015	-1.378227	.070974
22	1	0	-4.130681	.129563	-.607567
23	1	0	-4.107425	-1.216675	-1.577803
24	1	0	-1.756352	-.259853	-1.469228
25	1	0	-1.799604	-1.870144	-.651930

S11'

E = -518.8123542

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.677546	-.559092	.792795
2	6	0	-1.595416	-.214556	2.123463
3	6	0	-.340452	.195492	2.745718
4	6	0	.804954	.229294	1.845912
5	6	0	.706287	-.131256	.519811
6	6	0	-.529356	-.561074	-.037257
7	1	0	1.749134	.573943	2.261421
8	8	0	-.259714	.514763	3.957459
9	6	0	-.566337	-.937343	-1.497585
10	1	0	.076725	-1.791793	-1.770791
11	6	0	-.064767	.352117	-2.075008
12	1	0	-.792254	1.158015	-2.003613
13	1	0	-1.590148	-1.161344	-1.815592
14	6	0	1.376799	.735376	-1.716537
15	6	0	1.855307	-.031636	-.457824
16	1	0	2.053895	.525636	-2.558326
17	1	0	1.425400	1.813462	-1.531573
18	1	0	-2.473651	-.242873	2.762444
19	1	0	-2.635667	-.869038	.373652
20	1	0	2.716033	.479814	-.018245
21	1	0	2.199829	-1.033735	-.752646
22	7	0	-.047392	.207975	-3.901874
23	1	0	-.991994	.025971	-4.239622
24	1	0	.304628	1.057111	-4.344483
25	1	0	.550692	-.573027	-4.170100

Table 9S. Cartesian coordinates of all stationary points (reactants and TSs) located for the alkylation reaction of ammonia by **8-12** in water solution at B3LYP-C-PCM-/6-31G(d) level of theory

8

<hr/>						
<Psi(f) H Psi(f)> (a.u.) = -478.287532						
<Psi(f) H+V(f)/2 Psi(f)> (a.u.) = -478.322213						
Total free energy in sol.						
(with non electrost.terms) (a.u.) = -478.320427						
<hr/>						
(Polar.Solute)-Solvent (kcal/mol) = -21.76						
<hr/>						
Cavitation energy		(kcal/mol)	=	18.53		
Dispersion energy		(kcal/mol)	=	-23.89		
Repulsion energy		(kcal/mol)	=	6.48		
Total non electr.		(kcal/mol)	=	1.12		
<hr/>						
<hr/>						
Center	Atomic	Atomic	Coordinates (Angstroms)			
Number	Number	Type	X	Y	Z	
<hr/>						
1	6	0	0.520053	1.588222	-0.305662	
2	6	0	1.798830	1.168292	-0.257764	
3	6	0	2.168210	-0.239593	0.039139	
4	6	0	1.091272	-1.193759	0.189108	
5	6	0	-0.211181	-0.775805	0.114777	
6	6	0	-0.563897	0.657014	0.008111	
7	1	0	1.347373	-2.248370	0.261031	
8	8	0	3.373068	-0.565672	0.094297	
9	6	0	-1.680362	1.116990	0.972789	
10	1	0	-1.897293	0.469515	1.819940	
11	6	0	-2.053029	0.685445	-0.394575	
12	1	0	-2.421199	1.412723	-1.123664	
13	1	0	-1.684311	2.182730	1.189719	
14	6	0	-2.472282	-0.774601	-0.524761	
15	7	0	-1.354367	-1.513325	0.080951	
16	1	0	-3.409631	-0.983967	0.006604	
17	1	0	-1.317243	-2.532070	-0.008827	
18	1	0	-2.603499	-1.056468	-1.579843	
19	1	0	2.627850	1.851654	-0.430386	
20	1	0	0.268294	2.629672	-0.502584	
<hr/>						

9Z

<hr/>		
$\langle \Psi(f) H \Psi(f) \rangle$	(a.u.) =	-591.622530
$\langle \Psi(f) H + V(f)/2 \Psi(f) \rangle$	(a.u.) =	-591.657524
Total free energy in sol.		
(with non electrost.terms)		(a.u.) = -591.653576
<hr/>		
(Polar.Solute)-Solvent		(kcal/mol) = -21.96
<hr/>		
Cavitation energy	(kcal/mol) =	21.61
Dispersion energy	(kcal/mol) =	-24.86
Repulsion energy	(kcal/mol) =	5.73
Total non electr.	(kcal/mol) =	2.48
<hr/>		

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

1	6	0	-1.561119	-1.586212	-0.174639	
2	6	0	-2.522847	-0.641358	-0.182510	
3	6	0	-2.215813	0.795936	-0.030919	
4	6	0	-0.806033	1.185938	0.019310	
5	6	0	0.152839	0.226889	0.002097	
6	6	0	-0.167199	-1.210313	0.043780	
7	1	0	-0.568368	2.241876	-0.005238	
8	8	0	-3.125608	1.642308	-0.004024	
9	6	0	0.659458	-2.025373	1.075287	
10	1	0	1.180516	-1.460473	1.846337	
11	6	0	1.125500	-1.961705	-0.326163	
12	1	0	1.093017	-2.849608	-0.965955	
13	1	0	0.178191	-2.939083	1.414058	
14	6	0	2.164574	-0.893001	-0.619672	
15	7	0	1.539451	0.365488	-0.136710	
16	1	0	3.110247	-1.069148	-0.095027	
17	6	0	2.260179	1.521946	0.000402	
18	8	0	1.796855	2.613149	0.298776	
19	1	0	3.336739	1.359855	-0.185539	
20	1	0	2.362532	-0.817200	-1.696195	
21	1	0	-3.573527	-0.900341	-0.293259	
22	1	0	-1.802727	-2.644430	-0.262063	

9E

$\langle \Psi(f) H \Psi(f) \rangle$		(a.u.) =	-591.628953
$\langle \Psi(f) H + V(f)/2 \Psi(f) \rangle$		(a.u.) =	-591.658657
Total free energy in sol.			
(with non electrost.terms)		(a.u.) =	-591.654567

(Polar.Solute)-Solvent		(kcal/mol) =	-18.64

Cavitation energy	(kcal/mol)	=	21.73
Dispersion energy	(kcal/mol)	=	-24.90
Repulsion energy	(kcal/mol)	=	5.74
Total non electr.	(kcal/mol)	=	2.57

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

1	6	0	1.725507	1.455450	-0.224937	
2	6	0	2.661797	0.485377	-0.208726	
3	6	0	2.320430	-0.938099	-0.006106	
4	6	0	0.900139	-1.284350	0.060026	
5	6	0	-0.031578	-0.299972	0.046296	
6	6	0	0.325424	1.126921	0.028307	
7	1	0	0.644297	-2.340218	0.029109	
8	8	0	3.207161	-1.806757	0.041553	
9	6	0	-0.470739	2.013140	1.022548	
10	1	0	-0.996295	1.504862	1.829423	
11	6	0	-0.957353	1.888637	-0.367556	
12	1	0	-0.909337	2.744637	-1.047543	

13	1	0	0.036602	2.932165	1.305760
14	6	0	-2.030872	0.833877	-0.587535
15	7	0	-1.423011	-0.408588	-0.061411
16	1	0	-2.958303	1.047828	-0.045928
17	6	0	-2.170318	-1.524383	0.194681
18	8	0	-3.376504	-1.584746	0.002982
19	1	0	-1.581227	-2.361844	0.605524
20	1	0	-2.266052	0.706731	-1.651769
21	1	0	3.716909	0.713663	-0.339721
22	1	0	1.994003	2.502685	-0.352687

10E

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -723.213595
 $\langle \Psi(f) | H + V(f) / 2 | \Psi(f) \rangle$ (a.u.) = -723.244342
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -723.238784

(Polar.Solute)-Solvent (kcal/mol) = -19.29

Cavitation energy (kcal/mol) = 25.61
 Dispersion energy (kcal/mol) = -28.20
 Repulsion energy (kcal/mol) = 6.07
 Total non electr. (kcal/mol) = 3.49

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.395517
3	6	0	1.176224	0.000000	2.245088
4	6	0	2.450029	0.081390	1.519906
5	6	0	2.483126	0.057725	0.162665
6	6	0	1.287589	-0.111190	-0.692995
7	1	0	3.339448	0.257277	2.119156
8	8	0	1.110151	-0.001361	3.488391
9	6	0	1.457601	-1.105929	-1.860337
10	1	0	2.298782	-1.796955	-1.826594
11	6	0	1.708152	0.335094	-2.105103
12	1	0	1.025224	0.930740	-2.718409
13	1	0	0.522625	-1.531485	-2.215908
14	6	0	3.167207	0.753083	-2.016352
15	7	0	3.584679	0.297240	-0.671978
16	1	0	3.797905	0.279143	-2.775492
17	1	0	3.287141	1.841087	-2.090370
18	7	0	-1.307879	0.020898	1.817330
19	6	0	-1.352036	0.012487	-0.422026
20	6	0	-2.128772	0.032990	0.728801
21	1	0	-1.599145	0.042876	2.793052
22	1	0	-3.204698	0.061058	0.842957
23	1	0	-1.726920	0.012811	-1.437844
24	6	0	4.901437	0.220604	-0.316875
25	8	0	5.819884	0.533565	-1.062339
26	1	0	5.059907	-0.165361	0.704243

10Z

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -723.207536
 $\langle \Psi(f) | H + V(f) / 2 | \Psi(f) \rangle$ (a.u.) = -723.243027
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -723.237576

(Polar.Solute)-Solvent (kcal/mol) = -22.27

Cavitation energy (kcal/mol) = 25.62
 Dispersion energy (kcal/mol) = -28.34
 Repulsion energy (kcal/mol) = 6.14
 Total non electr. (kcal/mol) = 3.42

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.395210
3	6	0	1.177442	0.000000	2.243021
4	6	0	2.454700	0.053610	1.521354
5	6	0	2.485991	0.046928	0.162905
6	6	0	1.287019	-0.118509	-0.692526
7	1	0	3.355522	0.180639	2.108371
8	8	0	1.109709	0.009627	3.486799
9	6	0	1.450926	-1.134472	-1.843452
10	1	0	2.291135	-1.826073	-1.801709
11	6	0	1.703677	0.302116	-2.110745
12	1	0	1.026192	0.891968	-2.734471
13	1	0	0.514494	-1.563300	-2.191309
14	6	0	3.160161	0.722560	-2.026928
15	7	0	3.587725	0.278493	-0.674805
16	1	0	3.784640	0.245934	-2.791139
17	1	0	3.265448	1.811447	-2.109534
18	7	0	-1.307303	0.023366	1.817592
19	6	0	-1.352622	0.013191	-0.421430
20	6	0	-2.129078	0.035488	0.729782
21	1	0	-1.596351	0.044014	2.793780
22	1	0	-3.204874	0.065865	0.844270
23	1	0	-1.728249	0.013628	-1.436950
24	6	0	4.907289	0.253386	-0.313758
25	8	0	5.333864	-0.012808	0.801242
26	1	0	5.570358	0.498684	-1.162676

11

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -462.254599
 $\langle \Psi(f) | H + V(f) / 2 | \Psi(f) \rangle$ (a.u.) = -462.274930
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -462.273229

(Polar.Solute)-Solvent (kcal/mol) = -12.76

Cavitation energy (kcal/mol) = 19.14
 Dispersion energy (kcal/mol) = -23.14
 Repulsion energy (kcal/mol) = 5.07

Total non electr. (kcal/mol) = 1.07

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.552772	1.595435	-0.168493
2	6	0	1.817042	1.159149	-0.359565
3	6	0	2.173282	-0.267397	-0.269945
4	6	0	1.073558	-1.210312	-0.035121
5	6	0	-0.187891	-0.775226	0.175463
6	6	0	-0.508506	0.659632	0.179468
7	1	0	1.312343	-2.271076	-0.091859
8	8	0	3.344695	-0.651945	-0.430602
9	6	0	-1.601969	1.116971	1.183748
10	1	0	-1.823876	0.451103	2.015134
11	6	0	-2.020823	0.764701	-0.185290
12	1	0	-2.340434	1.555685	-0.861179
13	1	0	-1.547753	2.170722	1.447430
14	6	0	-2.519355	-0.660949	-0.412565
15	6	0	-1.463267	-1.580126	0.254671
16	1	0	-3.525414	-0.814727	-0.004705
17	1	0	-2.562933	-0.861176	-1.489714
18	1	0	2.628298	1.848229	-0.585260
19	1	0	0.311640	2.656785	-0.223498
20	1	0	-1.374496	-2.552206	-0.240012
21	1	0	-1.723989	-1.779055	1.304242

12

<Psi(f)| H |Psi(f)> (a.u.) = -556.909844
 <Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -556.937202
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -556.935091

(Polar.Solute)-Solvent (kcal/mol) = -17.17

Cavitation energy (kcal/mol) = 22.07
 Dispersion energy (kcal/mol) = -26.98
 Repulsion energy (kcal/mol) = 6.24
 Total non electr. (kcal/mol) = 1.32

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.862992	-0.475355	0.465880
2	6	0	-1.860098	-0.392677	1.809634
3	6	0	-0.606757	-0.221680	2.557727
4	6	0	0.599046	-0.084754	1.762420
5	6	0	0.617837	-0.130421	0.394493
6	6	0	-0.636609	-0.434669	-0.344459
7	1	0	1.524685	0.099421	2.305381
8	8	0	-0.596599	-0.165353	3.803936
9	6	0	-0.546796	-1.567918	-1.408606
10	1	0	0.459269	-1.952740	-1.560302
11	6	0	-0.832005	-0.192756	-1.866134
12	1	0	-1.879822	0.007949	-2.087034

13	1	0	-1.337902	-2.313784	-1.390194
14	7	0	1.821088	-0.068490	-0.304452
15	1	0	2.606414	-0.213078	0.338761
16	1	0	-2.780750	-0.452590	2.386293
17	1	0	-2.799386	-0.613376	-0.074396
18	6	0	0.139609	0.616132	-2.721683
19	1	0	0.820218	-0.058184	-3.258428
20	1	0	-0.451196	1.128184	-3.490492
21	6	0	0.958261	1.655086	-1.950830
22	1	0	0.302607	2.201415	-1.259367
23	1	0	1.362230	2.399633	-2.648538
24	6	0	2.144910	1.063224	-1.202086
25	1	0	2.888989	0.700409	-1.923117
26	1	0	2.623387	1.863725	-0.617025

S8

<Psi(f)| H |Psi(f)> (a.u.) = -534.784200
 <Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -534.851086
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -534.847803

(Polar.Solute)-Solvent (kcal/mol) = -41.97

Cavitation energy (kcal/mol) = 21.65
 Dispersion energy (kcal/mol) = -27.44
 Repulsion energy (kcal/mol) = 7.85
 Total non electr. (kcal/mol) = 2.06

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.793504	-1.443840	.660927
2	6	0	2.118142	-1.343261	.317771
3	6	0	2.692011	-1.222020	-.243733
4	6	0	1.791609	.999966	-.407760
5	6	0	.463366	.883751	-.059614
6	6	0	-.070302	-.337530	.465893
7	1	0	2.202119	1.936748	-.780279
8	8	0	3.917923	-.054393	-.550529
9	6	0	-1.762872	-.780425	-.453577
10	6	0	-1.530152	-.093828	.816016
11	1	0	-1.933574	-.604840	1.715428
12	6	0	-1.653810	1.435481	.761786
13	7	0	-.547223	1.837916	-.129301
14	1	0	-2.622258	1.756024	.355461
15	1	0	-1.538908	1.857502	1.772544
16	1	0	2.795197	-2.183653	.456866
17	1	0	.397405	-2.368706	1.079976
18	1	0	-.267089	2.816730	-.095814
19	7	0	-3.912796	-.867577	-.829615
20	1	0	-4.392751	-1.353937	-.068959
21	1	0	-4.314574	.069705	-.898332
22	1	0	-4.130444	-1.362196	-1.697987
23	1	0	-1.633585	-.247639	-1.387354
24	1	0	-1.733753	-1.862734	-.481161

S8'

$\langle \text{Psi(f)} | \text{H} | \text{Psi(f)} \rangle$ (a.u.) = -534.785171
 $\langle \text{Psi(f)} | \text{H} + \text{V(f)} / 2 | \text{Psi(f)} \rangle$ (a.u.) = -534.849869
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -534.846837

(Polar.Solute)-Solvent (kcal/mol) = -40.60

Cavitation energy (kcal/mol) = 21.54
 Dispersion energy (kcal/mol) = -27.88
 Repulsion energy (kcal/mol) = 8.24
 Total non electr. (kcal/mol) = 1.90

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.716789	-.423921	.677345
2	6	0	-1.670153	-.210380	2.029490
3	6	0	-.413963	.024751	2.736171
4	6	0	.769790	.083133	1.910876
5	6	0	.707516	-.119444	.546804
6	6	0	-.525023	-.454476	-.099496
7	1	0	1.708281	.369526	2.383457
8	8	0	-.384773	.214426	3.986256
9	6	0	-.467408	-.986883	-1.520565
10	1	0	.283521	-1.769104	-1.681947
11	6	0	-.054303	.363106	-1.883754
12	1	0	-.810926	1.118862	-2.067591
13	1	0	-1.452666	-1.280809	-1.892669
14	6	0	1.362782	.774359	-1.537722
15	7	0	1.777454	.026637	-.341030
16	1	0	2.032655	.537965	-2.378612
17	1	0	2.630655	.394898	.078963
18	1	0	1.403545	1.866019	-1.363286
19	1	0	-2.578396	-.228489	2.629079
20	1	0	-2.666163	-.637128	.186390
21	7	0	.202671	.348175	-4.142682
22	1	0	.800773	-.430610	-4.427315
23	1	0	-.703136	.216696	-4.598072
24	1	0	.614472	1.201621	-4.527358

S9Z

$\langle \text{Psi(f)} | \text{H} | \text{Psi(f)} \rangle$ (a.u.) = -648.118177
 $\langle \text{Psi(f)} | \text{H} + \text{V(f)} / 2 | \text{Psi(f)} \rangle$ (a.u.) = -648.199668
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -648.194969

(Polar.Solute)-Solvent (kcal/mol) = -51.14

Cavitation energy (kcal/mol) = 24.33
 Dispersion energy (kcal/mol) = -29.42
 Repulsion energy (kcal/mol) = 8.04
 Total non electr. (kcal/mol) = 2.95

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.370996
3	6	0	1.228020	.000000	2.149546
4	6	0	2.477660	.020913	1.414854
5	6	0	2.454894	.019978	.043053
6	6	0	1.233012	-.018016	-.702058
7	1	0	3.407088	.063987	1.968569
8	8	0	1.205080	-.003151	3.417160
9	6	0	1.284797	-1.392941	-2.048784
10	6	0	1.558766	.030712	-2.188123
11	1	0	.896652	.611669	-2.844830
12	6	0	3.038109	.413260	-2.232667
13	7	0	3.531154	.108578	-.864576
14	1	0	3.599993	-.164763	-2.977019
15	1	0	3.151621	1.486106	-2.439292
16	1	0	-.935285	.002091	1.926522
17	1	0	-.935722	-.005875	-.557149
18	7	0	1.544181	-2.367854	-4.084383
19	1	0	1.248522	-3.346505	-4.069936
20	1	0	.981265	-1.891820	-4.792633
21	1	0	2.514231	-2.348483	-4.405663
22	1	0	2.052345	-2.068596	-1.689469
23	1	0	.262747	-1.750069	-2.075977
24	6	0	4.859408	.025334	-.574839
25	8	0	5.339834	-.154856	.538846
26	1	0	5.485824	.135221	-1.479180

S9E

$\langle \text{Psi(f)} | \text{H} | \text{Psi(f)} \rangle$ (a.u.) = -648.130975
 $\langle \text{Psi(f)} | \text{H} + \text{V(f)} / 2 | \text{Psi(f)} \rangle$ (a.u.) = -648.201045
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -648.196215

(Polar.Solute)-Solvent (kcal/mol) = -43.97

Cavitation energy (kcal/mol) = 24.47
 Dispersion energy (kcal/mol) = -29.43
 Repulsion energy (kcal/mol) = 7.99
 Total non electr. (kcal/mol) = 3.03

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.338942	-1.763330	.425902
2	6	0	2.590931	-1.336664	.068345
3	6	0	2.861861	.039922	-.317337
4	6	0	1.749345	.967880	-.272055
5	6	0	.503694	.517174	.082215
6	6	0	.250967	-.850963	.411234
7	1	0	1.955428	2.013111	-.487134
8	8	0	4.023957	.416413	-.653960

9	6	0	-1.273952	-1.536430	-.533852
10	6	0	-1.209609	-.996501	.817259
11	1	0	-1.454151	-1.675639	1.644982
12	6	0	-1.705530	.443252	.971154
13	7	0	-.686982	1.250047	.263483
14	1	0	-2.693213	.604579	.522884
15	1	0	-1.742554	.738794	2.028835
16	1	0	3.432921	-2.025115	.061000
17	1	0	1.163929	-2.801549	.704540
18	7	0	-3.426451	-2.164746	-.932648
19	1	0	-3.749045	-2.821820	-.219163
20	1	0	-4.070417	-1.371030	-.925593
21	1	0	-3.526762	-2.627713	-1.838924
22	1	0	-1.366945	-.876784	-1.389747
23	1	0	-1.008253	-2.571119	-.714988
24	6	0	-.902391	2.552336	-.062067
25	8	0	-1.938567	3.155834	.197185
26	1	0	-.055564	3.019148	-.593121

S10

<hr/>					
<Psi(f) H Psi(f)> (a.u.) = -779.714585					
<Psi(f) H+V(f)/2 Psi(f)> (a.u.) = -779.772097					
Total free energy in sol.					
(with non electrost.terms) (a.u.) = -779.765035					
<hr/>					
(Polar.Solute)-Solvent (kcal/mol) = -36.09					
<hr/>					
Cavitation energy (kcal/mol) = 28.94					
Dispersion energy (kcal/mol) = -31.54					
Repulsion energy (kcal/mol) = 7.03					
Total non electr. (kcal/mol) = 4.43					
<hr/>					
<hr/>					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
<hr/>					
1	6	0	-1.573532	0.149738	0.237816
2	6	0	-1.600390	-0.001790	1.636101
3	6	0	-0.447641	-0.053023	2.509293
4	6	0	0.819186	0.091571	1.820594
5	6	0	0.860595	0.223885	0.447336
6	6	0	-0.290210	0.226206	-0.392868
7	1	0	1.716356	0.136301	2.431760
8	8	0	-0.557566	-0.183027	3.759139
9	6	0	-0.050903	-0.988062	-1.928375
10	1	0	-1.052906	-1.389897	-2.008794
11	6	0	0.139212	0.458357	-1.828805
12	1	0	-0.501377	1.094493	-2.452498
13	1	0	0.736309	-1.655040	-1.597824
14	6	0	1.601033	0.899951	-1.715468
15	7	0	1.999966	0.455154	-0.362862
16	1	0	2.252275	0.442147	-2.466190
17	1	0	1.691176	1.991094	-1.787661
18	7	0	-2.920086	-0.071601	2.025542
19	6	0	-2.931121	0.165624	-0.204280
20	6	0	-3.722026	0.029047	0.923018
21	1	0	-3.224811	-0.173592	2.990170

22	1	0	-4.800226	0.000943	1.016548
23	1	0	-3.291464	0.268358	-1.220303
24	6	0	3.301144	0.367724	0.009323
25	8	0	4.244644	0.653241	-0.724464
26	1	0	3.439069	0.005087	1.041893
27	7	0	0.317839	-1.625951	-3.989103
28	1	0	0.209882	-2.637644	-4.091482
29	1	0	-0.346005	-1.178991	-4.624995
30	1	0	1.258972	-1.383557	-4.305183

S11

 <Psi(f)| H |Psi(f)> (a.u.) = -518.758846
 <Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -518.808839
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -518.805996

(Polar.Solute)-Solvent (kcal/mol) = -31.37

Cavitation energy (kcal/mol) = 22.31
 Dispersion energy (kcal/mol) = -26.62
 Repulsion energy (kcal/mol) = 6.10
 Total non electr. (kcal/mol) = 1.78

<hr/>					
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
<hr/>					
1	6	0	.771300	-1.435634	.651144
2	6	0	2.104016	-1.373920	.330660
3	6	0	2.721413	-.176942	-.225858
4	6	0	1.839094	.965123	-.414452
5	6	0	.509036	.894505	-.098887
6	6	0	-.058187	-.303974	.435355
7	1	0	2.285753	1.884363	-.791163
8	8	0	3.949481	-.131706	-.512279
9	6	0	-1.750371	-.764809	-.434398
10	6	0	-1.515449	-.059644	.817787
11	1	0	-1.879483	-.558489	1.719162
12	6	0	-1.670349	1.468396	.773729
13	6	0	-.551801	1.974468	-.174024
14	1	0	-2.672651	1.772737	.451637
15	1	0	-1.510679	1.860947	1.784780
16	1	0	2.753624	-2.232443	.490155
17	1	0	.346256	-2.348100	1.069006
18	1	0	-.172684	2.960003	.118185
19	1	0	-.922749	2.077010	-1.204580
20	7	0	-3.969234	-.932034	-.752870
21	1	0	-4.405733	-1.450435	.012430
22	1	0	-4.408506	-.009841	-.784661
23	1	0	-4.207590	-1.414288	-1.622392
24	1	0	-1.694564	-.242334	-1.381578
25	1	0	-1.714414	-1.846661	-.458998

S11'

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -518.755825
 $\langle \Psi(f) | H + V(f)/2 | \Psi(f) \rangle$ (a.u.) = -518.817238
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -518.815404

(Polar.Solute)-Solvent (kcal/mol) = -38.54

Cavitation energy (kcal/mol) = 21.67
 Dispersion energy (kcal/mol) = -27.94
 Repulsion energy (kcal/mol) = 7.42
 Total non electr. (kcal/mol) = 1.15

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.662396	-0.423352	0.734949
2	6	0	-1.609691	-0.083163	2.062218
3	6	0	-0.355847	0.212958	2.729445
4	6	0	0.828364	0.161437	1.900532
5	6	0	0.772741	-0.190958	0.574681
6	6	0	-0.472182	-0.540733	-0.035719
7	1	0	1.770156	0.471623	2.350920
8	8	0	-0.312113	0.540705	3.956099
9	6	0	-0.485536	-1.097005	-1.456793
10	1	0	0.258679	-1.873841	-1.658483
11	6	0	-0.110605	0.265580	-1.800951
12	1	0	-0.892257	1.003861	-1.940478
13	1	0	-1.486678	-1.403850	-1.765543
14	6	0	1.335639	0.681970	-1.621205
15	6	0	1.917313	-0.073551	-0.403103
16	1	0	1.896919	0.460444	-2.537306
17	1	0	1.389606	1.763951	-1.453822
18	1	0	-2.518563	-0.026592	2.658141
19	1	0	-2.618487	-0.657866	0.267811
20	1	0	2.773178	0.458474	0.023435
21	1	0	2.275230	-1.069059	-0.703871
22	7	0	-0.124877	0.306549	-4.184400
23	1	0	-1.004099	-0.083678	-4.530500
24	1	0	-0.047981	1.250140	-4.571236
25	1	0	0.628538	-0.244187	-4.601380

S12

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -613.409200
 $\langle \Psi(f) | H + V(f)/2 | \Psi(f) \rangle$ (a.u.) = -613.476207
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -613.474051

(Polar.Solute)-Solvent (kcal/mol) = -42.05

Cavitation energy (kcal/mol) = 24.52
 Dispersion energy (kcal/mol) = -31.62
 Repulsion energy (kcal/mol) = 8.46
 Total non electr. (kcal/mol) = 1.35

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.704929	0.240817	0.967102
2	6	0	-1.691916	-0.247505	2.245427
3	6	0	-0.493419	-0.827104	2.814875
4	6	0	0.669130	-0.809750	1.967416
5	6	0	0.664010	-0.307933	0.677664
6	6	0	-0.556567	0.213796	0.116614
7	1	0	1.597742	-1.199434	2.383536
8	8	0	-0.468519	-1.300692	3.996274
9	6	0	-0.987520	-0.670971	-1.556776
10	1	0	-0.168099	-1.376118	-1.640377
11	6	0	-0.684971	0.735786	-1.318108
12	1	0	-1.571232	1.374882	-1.386306
13	1	0	-1.986669	-1.058572	-1.397598
14	7	0	1.819460	-0.375414	-0.125787
15	1	0	2.505054	-0.994991	0.310079
16	1	0	-2.586239	-0.218256	2.864875
17	1	0	-2.625624	0.659469	0.559969
18	6	0	0.521567	1.375133	-2.027647
19	1	0	1.001741	0.639940	-2.685440
20	1	0	0.141373	2.171657	-2.678356
21	6	0	1.560241	1.950795	-1.062604
22	1	0	1.048986	2.475899	-0.245191
23	1	0	2.177887	2.701484	-1.571600
24	6	0	2.499973	0.881214	-0.504534
25	1	0	3.238271	0.612339	-1.270949
26	1	0	3.056742	1.301838	0.349354
27	7	0	-1.339048	-0.914244	-3.750862
28	1	0	-1.534424	-1.884870	-4.007552
29	1	0	-2.141511	-0.353281	-4.045014
30	1	0	-0.536076	-0.609102	-4.304866

Table 10S. Cartesian coordinates of all stationary points (reactants and TSs) located for the alkylation reaction of ammonia by **8-12** in water solution at B3LYP-C-PCM-/6-31+G(d,p) level of theory

8

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -478.319651
 $\langle \Psi(f) | H + V(f)/2 | \Psi(f) \rangle$ (a.u.) = -478.362605
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -478.360916

(Polar.Solute)-Solvent (kcal/mol) = -26.95

Cavitation energy (kcal/mol) = 18.55

Dispersion energy (kcal/mol) = -23.92
 Repulsion energy (kcal/mol) = 6.43
 Total non electr. (kcal/mol) = 1.06

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.517677	1.586927	-.315566
2	6	0	1.799442	1.162932	-.272434
3	6	0	2.160803	-.239745	.044824

S22

4	6	0	1.092967	-1.192974	.202750
5	6	0	-.214978	-.771947	.117597
6	6	0	-.564640	.659270	.006888
7	1	0	1.345881	-2.248011	.284882
8	8	0	3.376416	-.565977	.111817
9	6	0	-1.679375	1.114913	.979072
10	1	0	-1.884695	.462830	1.826707
11	6	0	-2.056434	.687256	-.389217
12	1	0	-2.430673	1.428425	-1.103728
13	1	0	-1.684901	2.180927	1.195017
14	6	0	-2.472348	-.772056	-.531388
15	7	0	-1.349826	-1.515459	.065834
16	1	0	-3.408533	-.987545	-.001928
17	1	0	-1.299490	-2.532556	-.039196
18	1	0	-2.595871	-1.047003	-1.588467
19	1	0	2.627341	1.843972	-.461415
20	1	0	.269711	2.627521	-.522401

9Z

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -591.656168
 $\langle \Psi(f) | H + V(f)/2 | \Psi(f) \rangle$ (a.u.) = -591.700309
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -591.696381

(Polar.Solute)-Solvent (kcal/mol) = -27.70

Cavitation energy (kcal/mol) = 21.63
 Dispersion energy (kcal/mol) = -24.89
 Repulsion energy (kcal/mol) = 5.72
 Total non electr. (kcal/mol) = 2.46

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.558478	-1.586905	-0.168914
2	6	0	-2.524014	-0.640525	-0.187049
3	6	0	-2.213148	0.792788	-0.043517
4	6	0	-0.808757	1.190107	0.013260
5	6	0	0.153230	0.228213	0.005736
6	6	0	-0.167973	-1.207663	0.046428
7	1	0	-0.572916	2.247180	-0.018004
8	8	0	-3.129538	1.644628	-0.025628
9	6	0	0.663703	-2.026640	1.074930
10	1	0	1.183836	-1.459546	1.845882
11	6	0	1.124593	-1.960240	-0.327591
12	1	0	1.074477	-2.846329	-0.966825
13	1	0	0.181327	-2.941976	1.408749
14	6	0	2.162612	-0.892740	-0.626940
15	7	0	1.539224	0.367926	-0.137521
16	1	0	3.110913	-1.068703	-0.105796
17	6	0	2.263595	1.517635	0.007821
18	8	0	1.800088	2.606205	0.335757
19	1	0	3.337393	1.368228	-0.200650
20	1	0	2.349555	-0.815311	-1.705075
21	1	0	-3.573995	-0.904016	-0.296463
22	1	0	-1.801740	-2.645852	-0.245191

9E

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -591.663566
 $\langle \Psi(f) | H + V(f)/2 | \Psi(f) \rangle$ (a.u.) = -591.701874
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -591.697734

(Polar.Solute)-Solvent (kcal/mol) = -24.04

Cavitation energy (kcal/mol) = 21.75
 Dispersion energy (kcal/mol) = -24.89
 Repulsion energy (kcal/mol) = 5.74
 Total non electr. (kcal/mol) = 2.60

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.723267	1.458763	-0.205659
2	6	0	2.661475	0.484838	-0.205974
3	6	0	2.313961	-0.935866	-0.023483
4	6	0	0.899806	-1.285856	0.059695
5	6	0	-0.032352	-0.296299	0.059398
6	6	0	0.325434	1.127569	0.040626
7	1	0	0.639533	-2.341114	0.027127
8	8	0	3.204973	-1.813878	-0.006405
9	6	0	-0.480881	2.024026	1.023608
10	1	0	-1.012005	1.513403	1.826089
11	6	0	-0.955495	1.891472	-0.368413
12	1	0	-0.877903	2.731597	-1.064517
13	1	0	0.031184	2.940409	1.307330
14	6	0	-2.028274	0.835771	-0.591581
15	7	0	-1.425056	-0.406272	-0.050252
16	1	0	-2.959947	1.056636	-0.059413
17	6	0	-2.160859	-1.524393	0.208819
18	8	0	-3.371062	-1.598611	0.008916
19	1	0	-1.575553	-2.358546	0.629112
20	1	0	-2.250363	0.699219	-1.657396
21	1	0	3.716434	0.715141	-0.337923
22	1	0	1.996228	2.506922	-0.320953

11

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -462.284940
 $\langle \Psi(f) | H + V(f)/2 | \Psi(f) \rangle$ (a.u.) = -462.311456
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -462.309824

(Polar.Solute)-Solvent (kcal/mol) = -16.64

Cavitation energy (kcal/mol) = 19.14
 Dispersion energy (kcal/mol) = -23.18
 Repulsion energy (kcal/mol) = 5.07
 Total non electr. (kcal/mol) = 1.02

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.551238	1.595053	-.168113
2	6	0	1.818503	1.156801	-.363565
3	6	0	2.167660	-.267413	-.268150
4	6	0	1.075534	-1.212476	-.036177
5	6	0	-.189243	-.773949	.177255
6	6	0	-.506561	.660827	.181048
7	1	0	1.311455	-2.273843	-.099497
8	8	0	3.349264	-.654119	-.424725
9	6	0	-1.607445	1.120382	1.183776
10	1	0	-1.825020	.451638	2.014812
11	6	0	-2.022570	.765822	-.184688
12	1	0	-2.337025	1.557751	-.862370
13	1	0	-1.552043	2.174695	1.444828
14	6	0	-2.518890	-.661111	-.413220
15	6	0	-1.461411	-1.580095	.251684
16	1	0	-3.524894	-.812803	-.004145
17	1	0	-2.562385	-.860300	-1.490633
18	1	0	2.627634	1.846966	-.595136
19	1	0	.313253	2.657243	-.224521
20	1	0	-1.366494	-2.550209	-.246082
21	1	0	-1.719482	-1.781236	1.301435

S8

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -534.833257
 $\langle \Psi(f) | H + V(f)/2 | \Psi(f) \rangle$ (a.u.) = -534.909322
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -534.906433

(Polar.Solute)-Solvent (kcal/mol) = -47.73

Cavitation energy (kcal/mol) = 21.74
 Dispersion energy (kcal/mol) = -27.26
 Repulsion energy (kcal/mol) = 7.34
 Total non electr. (kcal/mol) = 1.81

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.791217	-1.440875	.670473
2	6	0	2.118775	-1.342536	.318449
3	6	0	2.681855	-.125016	-.250122
4	6	0	1.794662	.996881	-.418123
5	6	0	.463639	.886606	-.055883
6	6	0	-.069065	-.332444	.475381
7	1	0	2.202277	1.932622	-.796904
8	8	0	3.920093	-.060999	-.568537
9	6	0	-1.752760	-.782519	-.446822
10	6	0	-1.530590	-.088940	.819917
11	1	0	-1.932553	-.581825	1.716517
12	6	0	-1.650561	1.440730	.767930
13	7	0	-.536298	1.847239	-.113331
14	1	0	-2.614948	1.767121	.361036
15	1	0	-1.533435	1.856803	1.780104

16	1	0	2.792527	-2.186106	.455619
17	1	0	.397838	-2.366980	1.089008
18	1	0	-.253492	2.831143	-.083687
19	7	0	-3.932170	-.879653	-.843362
20	1	0	-4.402603	-1.397586	-.098799
21	1	0	-4.335325	.057808	-.884662
22	1	0	-4.123478	-1.350264	-1.729922
23	1	0	-1.626745	-.253455	-1.384359
24	1	0	-1.734571	-1.865724	-.466009

S8'

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -534.832861
 $\langle \Psi(f) | H + V(f)/2 | \Psi(f) \rangle$ (a.u.) = -534.910017
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -534.906834

(Polar.Solute)-Solvent (kcal/mol) = -48.42

Cavitation energy (kcal/mol) = 21.63
 Dispersion energy (kcal/mol) = -27.89
 Repulsion energy (kcal/mol) = 8.26
 Total non electr. (kcal/mol) = 2.00

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.723805	-.404544	.684712
2	6	0	-1.665087	-.219620	2.045836
3	6	0	-.402791	-.009749	2.739098
4	6	0	.776762	.051261	1.920994
5	6	0	.702857	-.114362	.545438
6	6	0	-.536441	-.425161	-.097423
7	1	0	1.722745	.315755	2.392185
8	8	0	-.365057	.160373	4.006964
9	6	0	-.480479	-.949467	-1.523038
10	1	0	.268401	-1.737070	-1.674096
11	6	0	-.059886	.395413	-1.886680
12	1	0	-.811318	1.150042	-2.108110
13	1	0	-1.467830	-1.236906	-1.896799
14	6	0	1.347322	.814862	-1.527987
15	7	0	1.765978	.056189	-.340689
16	1	0	2.020854	.606335	-2.376104
17	1	0	2.630887	.400719	.076244
18	1	0	1.373341	1.905364	-1.328044
19	1	0	-2.571271	-.244169	2.648837
20	1	0	-2.678755	-.602045	.198497
21	7	0	.220471	.304034	-4.192017
22	1	0	.830525	-.482388	-4.421849
23	1	0	-.681429	.143092	-4.643685
24	1	0	.628814	1.147850	-4.598190

S9Z

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -648.172377
 $\langle \Psi(f) | H + V(f)/2 | \Psi(f) \rangle$ (a.u.) = -648.253800

Total free energy in sol.
(with non electrost.terms) (a.u.) = -648.248347

(Polar.Solute)-Solvent (kcal/mol) = -51.09

Cavitation energy (kcal/mol) = 24.88
Dispersion energy (kcal/mol) = -28.19
Repulsion energy (kcal/mol) = 6.74
Total non electr. (kcal/mol) = 3.42

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.375314
3	6	0	1.225925	0.000000	2.153950
4	6	0	2.477994	-0.014905	1.423478
5	6	0	2.455318	-0.036381	0.049053
6	6	0	1.233095	-0.050549	-0.698437
7	1	0	3.407834	0.020447	1.978419
8	8	0	1.203538	0.024708	3.426467
9	6	0	1.255759	-1.454468	-2.040210
10	6	0	1.560050	-0.036180	-2.184315
11	1	0	0.910924	0.553931	-2.850449
12	6	0	3.046028	0.318848	-2.231151
13	7	0	3.535495	0.014429	-0.859278
14	1	0	3.599908	-0.268409	-2.971705
15	1	0	3.175201	1.388546	-2.439500
16	1	0	-0.938169	0.024654	1.926157
17	1	0	-0.936969	0.007520	-0.555583
18	7	0	1.501629	-2.452935	-4.073201
19	1	0	1.176346	-3.420689	-4.041180
20	1	0	0.952247	-1.957128	-4.777217
21	1	0	2.476763	-2.455488	-4.376195
22	1	0	2.005146	-2.142500	-1.665746
23	1	0	0.225437	-1.786931	-2.067593
24	6	0	4.858557	-0.108177	-0.577244
25	8	0	5.336783	-0.297515	0.542620
26	1	0	5.490834	-0.023326	-1.478786

S9E

<Psi(f)| H |Psi(f)> (a.u.) = -648.186238
<Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -648.255688
Total free energy in sol.
(with non electrost.terms) (a.u.) = -648.250070

(Polar.Solute)-Solvent (kcal/mol) = -43.58

Cavitation energy (kcal/mol) = 24.98
Dispersion energy (kcal/mol) = -28.23
Repulsion energy (kcal/mol) = 6.77
Total non electr. (kcal/mol) = 3.53

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

1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.374516
3	6	0	1.223167	0.000000	2.159516
4	6	0	2.473467	0.001774	1.430206
5	6	0	2.452497	-0.015465	0.056553
6	6	0	1.237600	-0.034445	-0.696554
7	1	0	3.397355	0.061736	2.000187
8	8	0	1.194849	0.016256	3.430822
9	6	0	1.272265	-1.402651	-2.071539
10	6	0	1.577007	0.018346	-2.179336
11	1	0	0.933254	0.622031	-2.837610
12	6	0	3.067841	0.367061	-2.213445
13	7	0	3.539218	0.061970	-0.843129
14	1	0	3.628497	-0.223186	-2.945488
15	1	0	3.217257	1.433840	-2.425676
16	1	0	-0.939041	0.015768	1.924237
17	1	0	-0.936237	0.005976	-0.556709
18	7	0	1.522439	-2.336517	-4.137492
19	1	0	1.229212	-3.315153	-4.136930
20	1	0	0.946429	-1.832988	-4.814132
21	1	0	2.491965	-2.296795	-4.455650
22	1	0	2.020135	-2.102792	-1.715262
23	1	0	0.242202	-1.735133	-2.113667
24	6	0	4.853687	-0.040540	-0.530695
25	8	0	5.765161	0.114118	-1.347906
26	1	0	5.046524	-0.283733	0.526585

S11

<Psi(f)| H |Psi(f)> (a.u.) = -518.804461
<Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -518.864189
Total free energy in sol.
(with non electrost.terms) (a.u.) = -518.861254

(Polar.Solute)-Solvent (kcal/mol) = -37.48

Cavitation energy (kcal/mol) = 22.37
Dispersion energy (kcal/mol) = -26.63
Repulsion energy (kcal/mol) = 6.10
Total non electr. (kcal/mol) = 1.84

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.768962	-1.435177	.645774
2	6	0	2.108255	-1.372938	.330256
3	6	0	2.717790	-1.75620	-2.18966
4	6	0	1.848086	.967705	-.410204
5	6	0	.512147	.897077	-.100298
6	6	0	-.055349	-.302808	.432173
7	1	0	2.294698	1.888954	-.782872
8	8	0	3.960510	-1.130121	-.505109
9	6	0	-1.746977	-.767171	-.437043
10	6	0	-1.515423	-.058854	.812622
11	1	0	-1.872880	-.559069	1.716287
12	6	0	-1.669558	1.469996	.767010

13	6	0	-.544453	1.978578	-.172309
14	1	0	-2.669768	1.771910	.436465
15	1	0	-1.518192	1.861641	1.779736
16	1	0	2.754205	-2.234523	.489612
17	1	0	.344818	-2.350895	1.057316
18	1	0	-.161846	2.959798	.129388
19	1	0	-.907564	2.087387	-1.205088
20	7	0	-3.999032	-.941239	-.750741
21	1	0	-4.415821	-1.459446	.024497
22	1	0	-4.430517	-.016384	-.781674
23	1	0	-4.229620	-1.429105	-1.618027
24	1	0	-1.698487	-.245179	-1.386372
25	1	0	-1.720771	-1.850185	-.457290

S11'

<Psi(f)| H |Psi(f)> (a.u.) = -518.806901
<Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -518.865343
Total free energy in sol.
(with non electrost.terms) (a.u.) = -518.862557

(Polar.Solute)-Solvent (kcal/mol) = -36.67

Cavitation energy (kcal/mol) = 22.26
Dispersion energy (kcal/mol) = -26.58
Repulsion energy (kcal/mol) = 6.07
Total non electr. (kcal/mol) = 1.75

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.663751	-.433467	.744717
2	6	0	-1.604695	-.120319	2.083039
3	6	0	-.348060	.171662	2.745025
4	6	0	.829448	.162311	1.906325
5	6	0	.766312	-.158955	.568677
6	6	0	-.479189	-.521446	-.034930
7	1	0	1.773398	.472721	2.352984
8	8	0	-.293886	.459006	3.986881
9	6	0	-.489619	-1.058065	-1.463317
10	1	0	.253378	-1.835083	-1.667680
11	6	0	-.115700	.300879	-1.825750
12	1	0	-.900246	1.034279	-1.979584
13	1	0	-1.489491	-1.362478	-1.775771
14	6	0	1.320070	.735961	-1.629154
15	6	0	1.906217	-.011693	-.409319
16	1	0	1.894787	.527983	-2.540016
17	1	0	1.355136	1.818200	-1.460301
18	1	0	-2.511420	-.090383	2.685032
19	1	0	-2.622143	-.669633	.282306
20	1	0	2.749445	.537157	.021182
21	1	0	2.285065	-.999572	-.710126
22	7	0	-.114623	.256355	-4.210953
23	1	0	-1.072116	.225018	-4.564620
24	1	0	.347671	1.060385	-4.639103
25	1	0	.363792	-.586342	-4.534551

Table 11S. Cartesian coordinates of the conformational TSs **TS-0°**, **TS-120°**, **TS-300°**, **TS-syn** and **TS-anti** in gas phase and in water at B3LYP/6-31G(d).

TS-0° GAS

E = -440.1911996

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.339900
3	6	0	1.263660	0.000000	2.117796
4	6	0	2.493869	-0.001745	1.340499
5	6	0	2.516950	-0.002129	-0.023506
6	6	0	1.242978	-0.001063	-0.802265
7	1	0	-0.933302	0.000376	-0.561519
8	1	0	-0.920546	0.000737	1.916087
9	1	0	3.421607	-0.002265	1.907338
10	8	0	1.249011	0.001302	3.351608
11	6	0	1.191606	-0.745026	-2.146118
12	1	0	2.085935	-1.283453	-2.447371
13	6	0	1.193046	0.743974	-2.145956
14	1	0	2.088807	1.280524	-2.446305
15	1	0	0.269739	1.267552	-2.375665
16	1	0	0.267106	-1.266543	-2.376189
17	7	0	3.696271	-0.003395	-0.723267

18	1	0	3.737131	-0.003631	-1.727736
19	1	0	4.573297	-0.004533	-0.226999

TS-0° water

<Psi(f)| H |Psi(f)> (a.u.) = -440.181804
<Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -440.216850
Total free energy in sol.
(with non electrost.terms) (a.u.) = -440.214606

(Polar.Solute)-Solvent (kcal/mol) = -21.99

Cavitation energy (kcal/mol) = 18.31
Dispersion energy (kcal/mol) = -21.52
Repulsion energy (kcal/mol) = 4.62
Total non electr. (kcal/mol) = 1.41

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.342892
3	6	0	1.261759	.000000	2.111618
4	6	0	2.482687	.009583	1.349492

5	6	0	2.512233	.012371	-.028139
6	6	0	1.237812	.002935	-.797065
7	1	0	-.934548	-.003139	-.560442
8	1	0	-.925959	-.003293	1.913757
9	1	0	3.418226	.012502	1.905849
10	8	0	1.240752	-.008167	3.361803
11	6	0	1.184732	-.749356	-2.142554
12	1	0	2.089325	-1.277183	-2.436395
13	6	0	1.174870	.731619	-2.154392
14	1	0	2.071702	1.267103	-2.458059
15	1	0	.244203	1.248671	-2.375187
16	1	0	.261174	-1.282710	-2.354395
17	7	0	3.682229	.017301	-.709931
18	1	0	3.736974	.033803	-1.722798
19	1	0	4.564504	.023497	-.205475

TS-120° GAS

E = -440.1829281

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.345294
3	6	0	1.258216	.000000	2.115599
4	6	0	2.499108	-.000340	1.317513
5	6	0	2.505968	-.000377	-.032160
6	6	0	1.237250	-.000026	-.796151
7	1	0	-.939010	.000062	-.551686
8	1	0	-.920777	.000070	1.921130
9	1	0	3.427849	-.000516	1.883302
10	8	0	1.276510	.000217	3.346366
11	6	0	1.204432	-.739145	-2.153197
12	1	0	2.123712	-1.241268	-2.434444
13	6	0	1.204744	.739923	-2.152771
14	1	0	2.124290	1.241802	-2.433596
15	1	0	.287938	1.275253	-2.381545
16	1	0	.287363	-1.273899	-2.382291
17	7	0	3.714520	-.000658	-.824920
18	1	0	4.281278	.811885	-.585924
19	1	0	4.280428	-.813992	-.586594

TS-120° water

<Psi(f)| H |Psi(f)> (a.u.) = -440.177767
 <Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -440.201750
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -440.199302

(Polar.Solute)-Solvent (kcal/mol) = -15.05

Cavitation energy (kcal/mol) = 18.34
 Dispersion energy (kcal/mol) = -21.68
 Repulsion energy (kcal/mol) = 4.87
 Total non electr. (kcal/mol) = 1.54

Center	Atomic	Atomic	Coordinates (Angstroms)		
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Number	Number	Type	X	Y	Z
1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.348684
3	6	0	1.255230	.000000	2.109246
4	6	0	2.491349	.019517	1.323478
5	6	0	2.502067	.025624	-.031519
6	6	0	1.234629	.011147	-.785917
7	1	0	-.939594	-.007171	-.552078
8	1	0	-.926054	-.008084	1.919240
9	1	0	3.425725	.026278	1.882247
10	8	0	1.269279	-.015083	3.352414
11	6	0	1.211446	-.729589	-2.148988
12	1	0	2.137685	-1.230509	-2.413635
13	6	0	1.192499	.742392	-2.153185
14	1	0	2.105776	1.265174	-2.420166
15	1	0	.264693	1.262600	-2.377307
16	1	0	.297500	-1.275444	-2.369345
17	7	0	3.706035	.044840	-.817048
18	1	0	4.267180	.860527	-.551458
19	1	0	4.280907	-.768025	-.573104

TS-300° GAS

E = -440.1788026

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.343400
3	6	0	1.260395	0.000000	2.112462
4	6	0	2.502103	0.000433	1.316169
5	6	0	2.518496	0.000866	-0.032332
6	6	0	1.238990	0.000413	-0.802355
7	1	0	-0.939018	-0.000261	-0.552105
8	1	0	-0.920847	-0.000419	1.919106
9	1	0	3.438597	0.000477	1.863879
10	8	0	1.274504	-0.000457	3.342381
11	6	0	1.173188	-0.741782	-2.151814
12	1	0	2.073111	-1.257605	-2.473467
13	6	0	1.172580	0.742218	-2.151951
14	1	0	2.072072	1.258905	-2.473761
15	1	0	0.250917	1.273775	-2.368621
16	1	0	0.251889	-1.274078	-2.368221
17	7	0	3.790140	0.000211	-0.699858
18	1	0	3.901194	-0.821139	-1.292831
19	1	0	3.898814	0.817185	-1.299281

TS-300° in water

<Psi(f)| H |Psi(f)> (a.u.) = -440.171211
 <Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -440.201055
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -440.198442

(Polar.Solute)-Solvent (kcal/mol) = -18.73

Cavitation energy (kcal/mol) = 18.44

Dispersion energy (kcal/mol) = -21.40
 Repulsion energy (kcal/mol) = 4.61
 Total non electr. (kcal/mol) = 1.64

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.347752
3	6	0	1.256055	.000000	2.105697
4	6	0	2.490650	-.006723	1.317089
5	6	0	2.509276	-.013594	-.036828
6	6	0	1.233313	-.005839	-.794315
7	1	0	-.940182	.003073	-.551585
8	1	0	-.925806	.003429	1.918820
9	1	0	3.429612	-.011040	1.864916
10	8	0	1.274102	.002786	3.348230
11	6	0	1.159809	-.733418	-2.159918
12	1	0	2.058381	-1.261865	-2.469308
13	6	0	1.172612	.741095	-2.151356
14	1	0	2.082347	1.255961	-2.450234
15	1	0	.251674	1.282714	-2.351773
16	1	0	.229080	-1.255595	-2.365787
17	7	0	3.776391	-.026770	-.705232
18	1	0	3.835280	-.830780	-1.340032
19	1	0	3.876743	.804008	-1.299564

TS-syn GAS
 E = -591.606006

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.343920
3	6	0	1.254736	0.000000	2.146752
4	6	0	2.518297	0.101050	1.403503
5	6	0	2.507814	0.109640	0.049905
6	6	0	1.267542	-0.062450	-0.739740
7	1	0	3.423973	0.226614	1.988663
8	8	0	1.214395	-0.025824	3.376342
9	6	0	1.399984	-1.003009	-1.953779
10	1	0	2.256681	-1.670829	-1.980323
11	6	0	1.601299	0.458584	-2.144155
12	1	0	0.885192	1.043046	-2.713465
13	1	0	0.466955	-1.433232	-2.306361
14	6	0	3.043448	0.941552	-2.081694
15	7	0	3.572037	0.335136	-0.832428
16	1	0	3.643839	0.614547	-2.937054
17	6	0	4.752894	0.965161	-0.301724
18	8	0	5.816688	0.419299	-0.210620
19	1	0	4.595708	2.018593	0.012210
20	1	0	3.078662	2.042052	-2.031458
21	1	0	-0.921930	-0.005751	1.917650
22	1	0	-0.927372	-0.023080	-0.569129

TS-anti GAS
 E = -591.6048183

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.343535
3	6	0	1.255382	0.000000	2.145573
4	6	0	2.517570	0.112700	1.403093
5	6	0	2.509417	0.107268	0.050743
6	6	0	1.268461	-0.073334	-0.738195
7	1	0	3.414678	0.289463	1.986803
8	8	0	1.214211	-0.032895	3.375258
9	6	0	1.391143	-1.023560	-1.944012
10	1	0	2.244372	-1.696118	-1.969304
11	6	0	1.601292	0.434904	-2.148526
12	1	0	0.886458	1.020654	-2.717979
13	1	0	0.454819	-1.451717	-2.289957
14	6	0	3.045915	0.910379	-2.097988
15	7	0	3.566569	0.299730	-0.846986
16	1	0	3.635417	0.571853	-2.958023
17	6	0	4.846546	0.766407	-0.380517
18	8	0	5.032536	1.856441	0.092166
19	1	0	5.660767	0.032633	-0.512496
20	1	0	3.096719	2.006526	-2.042602
21	1	0	-0.921697	0.000079	1.917731
22	1	0	-0.926998	-0.016179	-0.570031

TS-syn water

<Psi(f)| H |Psi(f)> (a.u.) = -591.597922
 <Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -591.629123
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -591.625118

(Polar.Solute)-Solvent (kcal/mol) = -19.58

Cavitation energy (kcal/mol) = 21.67
 Dispersion energy (kcal/mol) = -25.05
 Repulsion energy (kcal/mol) = 5.89
 Total non electr. (kcal/mol) = 2.51

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.347482
3	6	0	1.251310	0.000000	2.139055
4	6	0	2.507430	0.103061	1.405817
5	6	0	2.496686	0.128660	0.045156
6	6	0	1.260473	-0.038323	-0.737756
7	1	0	3.419240	0.230462	1.985540
8	8	0	1.212749	-0.031974	3.382076
9	6	0	1.386356	-0.959807	-1.974967
10	1	0	2.242285	-1.631385	-2.003815
11	6	0	1.587279	0.495890	-2.146906
12	1	0	0.852916	1.097225	-2.688017
13	1	0	0.446984	-1.386382	-2.318828
14	6	0	3.028890	0.976720	-2.082202

15	7	0	3.557137	0.374975	-0.821324
16	1	0	3.630298	0.639526	-2.933943
17	6	0	4.720320	1.022178	-0.281108
18	8	0	5.795929	0.488053	-0.204609
19	1	0	4.548206	2.066091	0.050593
20	1	0	3.073200	2.075258	-2.028352
21	1	0	-0.926787	-0.016853	1.916180
22	1	0	-0.928682	-0.032217	-0.568009

TS-anti water

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -591.596501
 $\langle \Psi(f) | H + V(f)/2 | \Psi(f) \rangle$ (a.u.) = -591.627353
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -591.623147

(Polar.Solute)-Solvent (kcal/mol) = -19.36

Cavitation energy (kcal/mol) = 21.73
 Dispersion energy (kcal/mol) = -24.91
 Repulsion energy (kcal/mol) = 5.82
 Total non electr. (kcal/mol) = 2.64

Center Atomic Atomic Coordinates (Angstroms)

Table 12S. Cartesian coordinates of the conformational TSs **TS-0°**, **TS-120°**, **TS-300°**, **TS-syn**, **TS-anti**, **S9-syn** and **S9-anti** in gas phase and in water at B3LYP/6-31+G(d,p).

TS-0° GAS

E = -440.2305627

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.342201
3	6	0	1.265548	.000000	2.114066
4	6	0	2.495221	-.000101	1.338773
5	6	0	2.516110	-.000135	-.027177
6	6	0	1.241713	-.000046	-.804381
7	1	0	-.935293	.000028	-.556980
8	1	0	-.920263	.000015	1.918006
9	1	0	3.422944	-.000152	1.904632
10	8	0	1.254178	.000078	3.352278
11	6	0	1.183473	-.745239	-2.148414
12	1	0	2.076515	-1.281182	-2.455775
13	6	0	1.183580	.745238	-2.148377
14	1	0	2.076713	1.281054	-2.455700
15	1	0	.258116	1.267489	-2.370002
16	1	0	.257933	-1.267339	-2.370078
17	7	0	3.698792	-.000240	-.724353
18	1	0	3.743936	-.000315	-1.727939
19	1	0	4.573395	-.000313	-.225362

TS-120° GAS

E = -440.2215396

Number	Number	Type	X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.347120
3	6	0	1.249890	0.000000	2.141621
4	6	0	2.507328	0.064658	1.412214
5	6	0	2.502139	0.067972	0.050296
6	6	0	1.261902	-0.077370	-0.734619
7	1	0	3.416395	0.210056	1.990737
8	8	0	1.204013	0.002201	3.385887
9	6	0	1.357314	-1.021177	-1.956197
10	1	0	2.191125	-1.720229	-1.974715
11	6	0	1.608570	0.422786	-2.153548
12	1	0	0.903609	1.049143	-2.704513
13	1	0	0.404450	-1.422112	-2.293333
14	6	0	3.067553	0.850413	-2.100409
15	7	0	3.558453	0.258415	-0.825000
16	1	0	3.652229	0.466307	-2.944920
17	6	0	4.850494	0.669454	-0.350178
18	8	0	5.072102	1.768809	0.092738
19	1	0	5.633411	-0.102728	-0.439669
20	1	0	3.160765	1.944817	-2.067428
21	1	0	-0.927489	0.007979	1.915097
22	1	0	-0.928296	-0.010893	-0.569279

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.347526
3	6	0	1.260194	.000000	2.111841
4	6	0	2.500858	.000089	1.316080
5	6	0	2.506131	.000200	-.035963
6	6	0	1.235924	.000124	-.798035
7	1	0	-.940548	-.000036	-.548106
8	1	0	-.920519	-.000064	1.922917
9	1	0	3.430381	.000105	1.879459
10	8	0	1.280702	-.000053	3.346641
11	6	0	1.195582	-.740022	-2.155334
12	1	0	2.113510	-1.241123	-2.441923
13	6	0	1.195416	.740451	-2.155243
14	1	0	2.113207	1.241824	-2.441796
15	1	0	.276512	1.274231	-2.376522
16	1	0	.276805	-1.273982	-2.376702
17	7	0	3.714664	.000200	-.824459
18	1	0	4.281805	.816924	-.610820
19	1	0	4.281908	-.816381	-.610546

TS-120° water

$\langle \Psi(f) | H | \Psi(f) \rangle$ (a.u.) = -440.214021
 $\langle \Psi(f) | H + V(f)/2 | \Psi(f) \rangle$ (a.u.) = -440.243998
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -440.241527

(Polar.Solute)-Solvent (kcal/mol) = -18.81

Cavitation energy (kcal/mol) = 18.35
Dispersion energy (kcal/mol) = -21.68
Repulsion energy (kcal/mol) = 4.88
Total non electr. (kcal/mol) = 1.55

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.352724
3	6	0	1.253511	.000000	2.108003
4	6	0	2.490001	.024418	1.332124
5	6	0	2.502151	.032254	-.026786
6	6	0	1.236490	.013976	-.781202
7	1	0	-.940513	-.009123	-.550841
8	1	0	-.928563	-.009828	1.920155
9	1	0	3.425461	.032995	1.889837
10	8	0	1.265465	-.019207	3.360078
11	6	0	1.214207	-.727814	-2.147675
12	1	0	2.142088	-1.228318	-2.409018
13	6	0	1.190832	.743443	-2.153129
14	1	0	2.102730	1.270760	-2.417450
15	1	0	.259010	1.259051	-2.372198
16	1	0	.299404	-1.275257	-2.361559
17	7	0	3.709307	.057024	-.801916
18	1	0	4.267553	.878546	-.549912
19	1	0	4.286730	-.758981	-.576860

TS-300° GAS

E = -440.2174426

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.345686
3	6	0	1.262288	.000000	2.108652
4	6	0	2.503322	.000010	1.313763
5	6	0	2.517329	.000034	-.037054
6	6	0	1.237132	.000019	-.804986
7	1	0	-.940983	.000000	-.547821
8	1	0	-.920674	-.000006	1.920881
9	1	0	3.440291	.000010	1.860384
10	8	0	1.279429	-.000004	3.342468
11	6	0	1.162005	-.742579	-2.154921
12	1	0	2.058227	-1.259246	-2.483516
13	6	0	1.161953	.742650	-2.154903
14	1	0	2.058122	1.259407	-2.483503
15	1	0	.237591	1.272436	-2.361743
16	1	0	.237690	-1.272436	-2.361790
17	7	0	3.787288	.000022	-.703486
18	1	0	3.928296	-.823930	-1.281677
19	1	0	3.928219	.823860	-1.281858

TS-300° water

<Psi(f)| H |Psi(f)> (a.u.) = -440.206808
<Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -440.243652
Total free energy in sol.
(with non electrost.terms) (a.u.) = -440.241014

(Polar.Solute)-Solvent (kcal/mol) = -23.12

Cavitation energy (kcal/mol) = 18.45
Dispersion energy (kcal/mol) = -21.42
Repulsion energy (kcal/mol) = 4.63
Total non electr. (kcal/mol) = 1.66

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.351696
3	6	0	1.256969	.000000	2.100700
4	6	0	2.491155	-.007666	1.318345
5	6	0	2.508130	-.015046	-.039504
6	6	0	1.232659	-.007127	-.792329
7	1	0	-.941854	.003873	-.549343
8	1	0	-.927251	.003914	1.921280
9	1	0	3.430946	-.012022	1.866144
10	8	0	1.277137	.003630	3.351962
11	6	0	1.154072	-.734994	-2.161676
12	1	0	2.051587	-1.266598	-2.469806
13	6	0	1.167611	.738606	-2.154105
14	1	0	2.076763	1.255306	-2.452540
15	1	0	.243832	1.278797	-2.346751
16	1	0	.220122	-1.255093	-2.359225
17	7	0	3.772597	-.030210	-.707906
18	1	0	3.848596	-.839481	-1.333173
19	1	0	3.893369	.803994	-1.292586

TS-syn GAS

E = -591.6441762

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.346088
3	6	0	1.256824	0.000000	2.143861
4	6	0	2.519790	0.111344	1.404589
5	6	0	2.507393	0.124179	0.048003
6	6	0	1.267387	-0.056191	-0.740354
7	1	0	3.424183	0.238343	1.990607
8	8	0	1.217482	-0.036164	3.377290
9	6	0	1.403251	-0.999489	-1.953165
10	1	0	2.265084	-1.660263	-1.976372
11	6	0	1.595635	0.464239	-2.146095
12	1	0	0.873994	1.042822	-2.713680
13	1	0	0.471931	-1.435226	-2.301594
14	6	0	3.035070	0.957356	-2.088386
15	7	0	3.567302	0.360935	-0.833980
16	1	0	3.636202	0.627505	-2.941463

17	6	0	4.754539	0.981855	-0.311924
18	8	0	5.812771	0.420952	-0.219381
19	1	0	4.617783	2.039913	-0.006904
20	1	0	3.062465	2.057561	-2.041226
21	1	0	-0.921686	-0.009686	1.919376
22	1	0	-0.928500	-0.025720	-0.566258

TS-anti GAS

E = -591.6425196

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.345705
3	6	0	1.257472	0.000000	2.143217
4	6	0	2.518744	0.123299	1.405193
5	6	0	2.508841	0.120114	0.049707
6	6	0	1.268720	-0.071983	-0.738121
7	1	0	3.414029	0.306108	1.989064
8	8	0	1.216352	-0.041376	3.376892
9	6	0	1.394318	-1.034577	-1.934855
10	1	0	2.251628	-1.701807	-1.950834
11	6	0	1.597995	0.424121	-2.153424
12	1	0	0.878972	1.000548	-2.726386
13	1	0	0.459350	-1.469588	-2.273909
14	6	0	3.040734	0.908324	-2.111624
15	7	0	3.560975	0.324978	-0.846641
16	1	0	3.631929	0.553748	-2.963378
17	6	0	4.855929	0.758042	-0.394590
18	8	0	5.069510	1.841642	0.085773
19	1	0	5.656225	0.012646	-0.540575
20	1	0	3.084627	2.005157	-2.076655
21	1	0	-0.921572	-0.001345	1.919338
22	1	0	-0.928096	-0.017196	-0.567280

TS-syn water

<Psi(f)| H |Psi(f)> (a.u.) = -591.632593
 <Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -591.672846
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -591.668782

(Polar.Solute)-Solvent (kcal/mol) = -25.26

Cavitation energy (kcal/mol) = 21.69
 Dispersion energy (kcal/mol) = -25.04
 Repulsion energy (kcal/mol) = 5.90
 Total non electr. (kcal/mol) = 2.55

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.351338
3	6	0	1.250762	0.000000	2.137567
4	6	0	2.507808	0.099314	1.415386

5	6	0	2.497086	0.126464	0.049378
6	6	0	1.260542	-0.036340	-0.733988
7	1	0	3.419890	0.222801	1.996512
8	8	0	1.208712	-0.030640	3.389970
9	6	0	1.387049	-0.959633	-1.973692
10	1	0	2.243634	-1.631298	-1.994081
11	6	0	1.590098	0.495208	-2.145470
12	1	0	0.851975	1.099127	-2.682970
13	1	0	0.445995	-1.384690	-2.315273
14	6	0	3.031498	0.976383	-2.080035
15	7	0	3.555961	0.380615	-0.811863
16	1	0	3.634250	0.632196	-2.928592
17	6	0	4.726091	1.013450	-0.277347
18	8	0	5.795364	0.459388	-0.200547
19	1	0	4.578553	2.063196	0.048195
20	1	0	3.076338	2.074960	-2.027245
21	1	0	-0.928813	-0.017453	1.917441
22	1	0	-0.929941	-0.033233	-0.566353

TS-anti water

<Psi(f)| H |Psi(f)> (a.u.) = -591.630295
 <Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -591.670512
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -591.666251

(Polar.Solute)-Solvent (kcal/mol) = -25.24

Cavitation energy (kcal/mol) = 21.76
 Dispersion energy (kcal/mol) = -24.93
 Repulsion energy (kcal/mol) = 5.84
 Total non electr. (kcal/mol) = 2.67

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.350916
3	6	0	1.247342	0.000000	2.143240
4	6	0	2.505951	0.057604	1.429057
5	6	0	2.503199	0.066746	0.060451
6	6	0	1.264298	-0.076575	-0.728364
7	1	0	3.415389	0.196367	2.009639
8	8	0	1.193129	0.006673	3.397385
9	6	0	1.362755	-1.034008	-1.942819
10	1	0	2.196769	-1.733707	-1.944757
11	6	0	1.619009	0.406726	-2.152850
12	1	0	0.914860	1.033504	-2.707871
13	1	0	0.408956	-1.435857	-2.276542
14	6	0	3.079681	0.830263	-2.101321
15	7	0	3.556288	0.273118	-0.804290
16	1	0	3.667604	0.416540	-2.930216
17	6	0	4.871621	0.610579	-0.345276
18	8	0	5.150853	1.696100	0.106825
19	1	0	5.619778	-0.193865	-0.451209
20	1	0	3.178491	1.924719	-2.096830
21	1	0	-0.930302	0.007682	1.915115
22	1	0	-0.928952	-0.011562	-0.568454

S9-syn GAS

E = -648.1619123

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.375844
3	6	0	1.233725	.000000	2.167927
4	6	0	2.484080	.021002	1.408352
5	6	0	2.439861	.029213	.037690
6	6	0	1.228046	.030811	-.701669
7	1	0	3.414913	.026621	1.966567
8	8	0	1.217521	-.010331	3.419572
9	6	0	1.473504	-1.529752	-2.315445
10	6	0	1.566756	-.037224	-2.166090
11	1	0	.904440	.507355	-2.848662
12	6	0	3.009037	.499458	-2.170678
13	7	0	3.557713	.024330	-.879536
14	1	0	3.631335	.141221	-3.001552
15	1	0	2.973192	1.601170	-2.220267
16	1	0	-.930920	.001472	1.934489
17	1	0	-.942270	-.000242	-.547722
18	7	0	1.937124	-2.130332	-3.947736
19	1	0	1.847719	-3.146529	-4.007689
20	1	0	1.354807	-1.709517	-4.672431
21	1	0	2.910694	-1.882782	-4.128395
22	1	0	2.193346	-2.079141	-1.714116
23	1	0	.464212	-1.929682	-2.252214
24	6	0	4.693577	.782058	-.438908
25	8	0	5.749796	.290996	-.133890
26	1	0	4.529179	1.881180	-.410881

S9-anti GAS

E = 648.1571601

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	.000000	.000000	.000000
2	6	0	.000000	.000000	1.375864
3	6	0	1.235740	.000000	2.163501
4	6	0	2.481494	.027877	1.400173
5	6	0	2.439277	.031952	.029665
6	6	0	1.226281	.024330	-.704090
7	1	0	3.409073	.064597	1.962808
8	8	0	1.224280	-.017428	3.416354
9	6	0	1.419805	-1.533751	-2.339372
10	6	0	1.548445	-.044985	-2.171261
11	1	0	.890830	.521091	-2.841870
12	6	0	2.996624	.469045	-2.189175
13	7	0	3.556228	-.016652	-.895511
14	1	0	3.604455	.093960	-3.025090
15	1	0	2.983805	1.566145	-2.230017
16	1	0	-.930159	.006026	1.935803
17	1	0	-.942542	.007213	-.547621
18	7	0	1.804953	-2.103387	-3.981712

19	1	0	1.728565	-3.120167	-4.056232
20	1	0	1.177722	-1.680686	-4.667412
21	1	0	2.762506	-1.834930	-4.212652
22	1	0	2.146576	-2.102721	-1.764044
23	1	0	.405441	-1.913565	-2.239278
24	6	0	4.750359	.693319	-.502032
25	8	0	4.831857	1.892153	-.397439
26	1	0	5.602106	.032638	-.265036

S9-syn water

<Psi(f)| H |Psi(f)> (a.u.) = -648.151657
 <Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -648.224130
 Total free energy in sol.
 (with non electrost.terms) (a.u.) = -648.218683

(Polar.Solute)-Solvent (kcal/mol) = -45.48

Cavitation energy (kcal/mol) = 24.92
 Dispersion energy (kcal/mol) = -28.35
 Repulsion energy (kcal/mol) = 6.85
 Total non electr. (kcal/mol) = 3.42

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	.000000	.000000	.000000
2	6	0	.000000	.000000	2.273574
3	6	0	1.400413	.000000	2.676922
4	6	0	.779408	-.037702	4.061544
5	6	0	.854903	-1.380953	4.545889
6	7	0	1.402048	-2.224268	3.548499
7	6	0	2.198287	-3.313810	4.022570
8	8	0	1.875048	-4.472116	3.899272
9	1	0	3.160493	-3.021610	4.493071
10	6	0	.476744	-1.727989	5.822921
11	6	0	-.016917	-.706510	6.722860
12	6	0	-.073180	.656068	6.214414
13	6	0	.313411	.978607	4.935183
14	8	0	-.373529	-.983419	7.913132
15	6	0	2.121602	-1.345448	2.572516
16	1	0	.426226	-.855835	-.358499
17	1	0	-.943450	.069833	-.385322
18	1	0	.542280	.793648	-.345239
19	1	0	.554453	-2.748929	6.192682
20	1	0	-.438268	1.424850	6.892252
21	1	0	.257917	2.008377	4.583692
22	1	0	2.069487	-1.779427	1.568192
23	1	0	3.177999	-1.227744	2.864546
24	1	0	1.993355	.886070	2.400058
25	1	0	-.566243	-.923702	2.241302
26	1	0	-.544779	.936317	2.242667

S9-anti water

<Psi(f)| H |Psi(f)> (a.u.) = -648.147955
 <Psi(f)|H+V(f)/2|Psi(f)> (a.u.) = -648.220496
 Total free energy in sol.

(with non electrost.terms) (a.u.) = -648.214991

(Polar.Solute)-Solvent (kcal/mol) = -45.52

Cavitation energy (kcal/mol) = 24.95

Dispersion energy (kcal/mol) = -28.24

Repulsion energy (kcal/mol) = 6.74

Total non electr. (kcal/mol) = 3.45

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

1	7	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	2.250607
3	6	0	1.383702	0.000000	2.713346
4	6	0	0.707297	-0.042056	4.073192
5	6	0	0.755247	-1.387948	4.554725
6	7	0	1.324979	-2.219770	3.565262
7	6	0	1.977001	-3.427934	3.975503
8	8	0	3.049245	-3.452668	4.537745

9	1	0	1.414590	-4.353048	3.759064
10	6	0	0.307779	-1.735177	5.810277
11	6	0	-0.236254	-0.717236	6.681781
12	6	0	-0.257359	0.647947	6.179113
13	6	0	0.202198	0.973265	4.924687
14	8	0	-0.663449	-0.997483	7.849788
15	6	0	2.113315	-1.343181	2.642700
16	1	0	0.375264	-2.753116	6.189265
17	1	0	1.983616	0.888890	2.474088
18	1	0	2.118940	-1.770637	1.633528
19	1	0	3.145487	-1.229487	3.001529
20	1	0	-0.652458	1.416168	6.840512
21	1	0	0.177398	2.005449	4.577324
22	1	0	0.471714	0.830810	-0.361238
23	1	0	0.483161	-0.823804	-0.361312
24	1	0	-0.954847	-0.006030	-0.363321
25	1	0	-0.562242	-0.925104	2.208276
26	1	0	-0.544991	0.935587	2.213097