

**Mechanism of the Acid Promoted Intramolecular Schmidt Reaction.
Theoretical Assessment of the Importance of Lone Pair–Cation, Cation– π and Steric Effects in Controlling Regioselectivity**

Osvaldo Gutierrez,[‡] Jeffrey Aubé,[†] and Dean J. Tantillo^{*‡}

[‡]Department of Chemistry, University of California at Davis, Davis, CA 95616.

[†]Department of Medicinal Chemistry, University of Kansas, Lawrence, Kansas 66045

tantillo@chem.ucdavis.edu

Supporting Information

Full authorship of reference 10	S2
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Transition states with explicit DCM molecule	S5
DFT Energies and Cartesian coordinates	S6
Selected IRCs	S84

Full authorship of *Gaussian 09*:

Gaussian 09, Revision B.01,

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

As shown in figure S1, for the parent system the transition state leading to the formation of the intermediates i.e., **I-1eq** to **1a-d**, is sensitive to the radii used. However, the barrier in all cases is predicted to be very small and in some cases the reaction is predicted to be barrierless. Also, the interconversion from **1c** to **1d** is found to be sensitive to the level of theory and solvent used. In some cases this transition state structure cannot be found and if found the barrier is also very small.

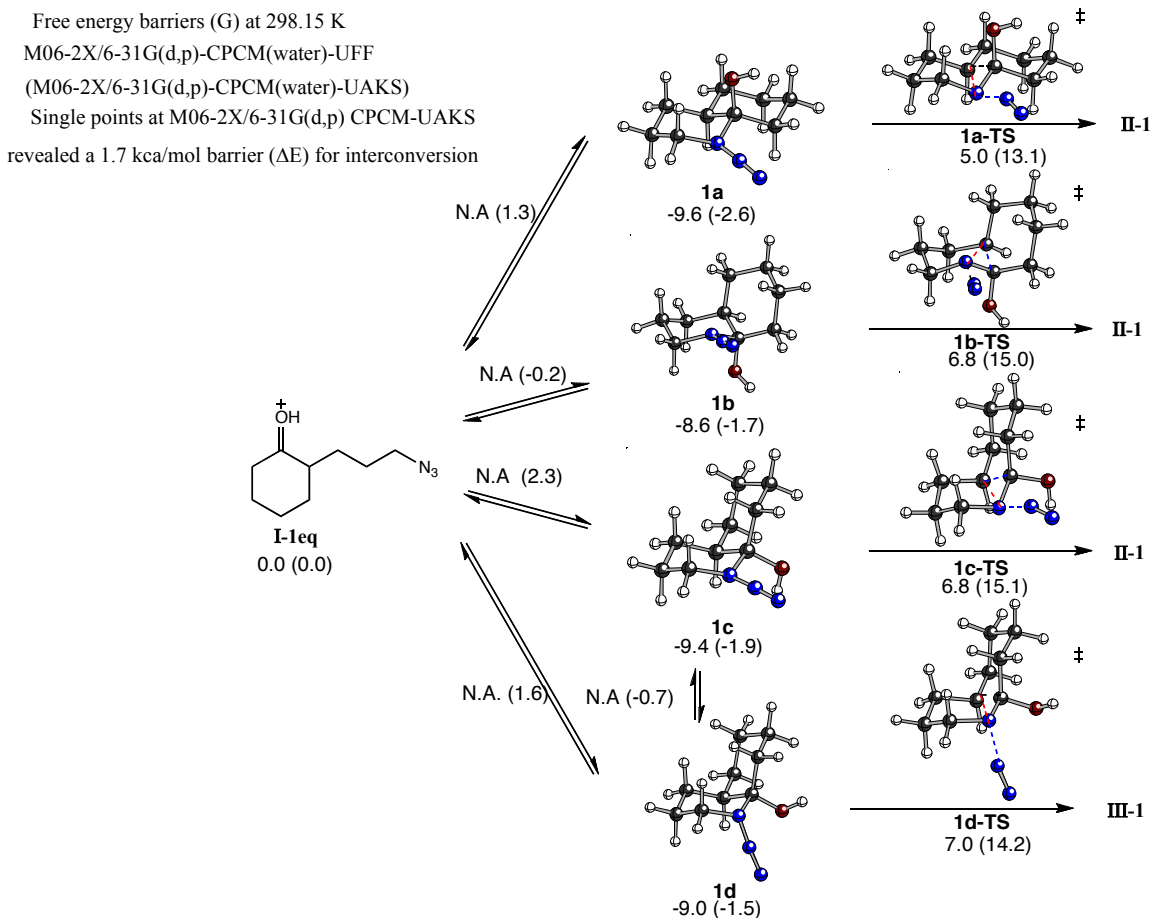
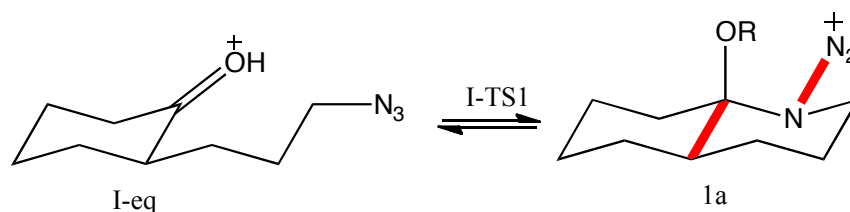


Figure S1. Free energies (298.15 K) for parent system calculated using M06-2X/6-31G(d,p) in water (CPCM;UFF radii). Free energies in parenthesis are calculated using M06-2X/6-31G(d,p) in water (CPCM-UAKS radii). N.A. refers that no transition state structure was found connecting the two stationary points at that level of theory. Note: TS connecting **1c** and **1d** at M06-2X/6-31G(d,p) in water (CPCM;UFF radii) was not found but a single point calculation at the same level revealed a ΔE of only 1.7 kcal/mol.

Therefore we conclude that although the formation of intermediates (see Figure S2 for a representative example on effect of method on barriers and free energies) and interconversion of **1c** and **1d** is sensitive to level of theory, the barriers are very small. With all methods, however, the transition states leading from the intermediates to the products were found to be highest in energy.



Method	$\Delta G^\ddagger$ (ΔG)
B3LYP-SMD-UAKS	4.6 (5.4)
M06-2X-SMD-UAKS	1.8 (-2.7)
M06-2X-SMD-UFF	0.8 (-5.8)
M06-2X-SMD-UFF-6-311+G(d,p)	1.1 (-5.6)
M06-2X-CPCM-UAKS	1.3 (-2.6)
M06-2X-CPCM-UFF	N.A. (-9.6)

Figure S2. Free energies and enthalpies for parent system for the formation of intermediate **1a** at different levels of theory.

Table S1 shows a DFT method comparison; in all cases the free energy barriers from the intermediates are ca. 13-15 kcal/mol. Although all methods explored predict similar experimental ratios, M06-2X/6-31G(d,p) in water (CPCM-UA0) was shown to best correlate with experimental data and therefore was used for other systems. As shown in the main text, this methodology makes predictions that are in excellent agreement with experimental data.

Table S1. Method comparison for parent reaction. All relative free energies are with respect to lowest energy intermediate **1a** (except for those in brackets, which are relative to **1a-TS**).

method	1a	1b	1c	1d	1a-TS	1b-TS	1c-TS	1d-TS
M06-2X/6-31G(d,p)-water(SMD-UAKS)	0.0	1.6	1.1	1.0	15.2	17.8	18.4	16.0
B3LYP/6-31G(d,p)-water(SMD-UAKS)	0.0	1.4	1.2	1.2	14.7	17.8	16.7	15.6
M06-2X/6-31G(d,p)-water(SMD-UFF)	0.0	1.7	0.6	0.8	14.2	16.7	16.0	15.3
M06-2X/6-311G+(d,p)-water(SMD-UFF)	0.0	1.6	0.7	0.6	13.5	16.1	14.2	14.5
M06-2X/6-31G(d,p)-water(CPCM-UFF)	0.0	0.9	0.2	0.6	14.6	16.4	16.4	16.6
M06-2X/6-31G(d,p)-water(CPCM-UAKS) [brackets in DCM]* {using Sn CL4 lewis acid: B3LYP/6-	0.0	0.9	0.7	1.1	15.7[0.0] {0.0} {{0.0}}	17.6[1.7] {0.7} {{1.2}}	17.7[1.8] {1.5} {{3.6}}	16.8[2.0] {2.4} {{2.6}}

31G(d,p)-SDD for Sn; DCM(CPCM;UFF)} using Sn CL4 lewis acid: M06/6- 31G(d,p)-SDD for Sn; DCM(CPCM;UFF) in {}.								
B3LYP/6-31G(d,p)- water(CPCM-UAKS)	0.0	1.5	0.6	1.3	15.7	17.9	17.4	16.8

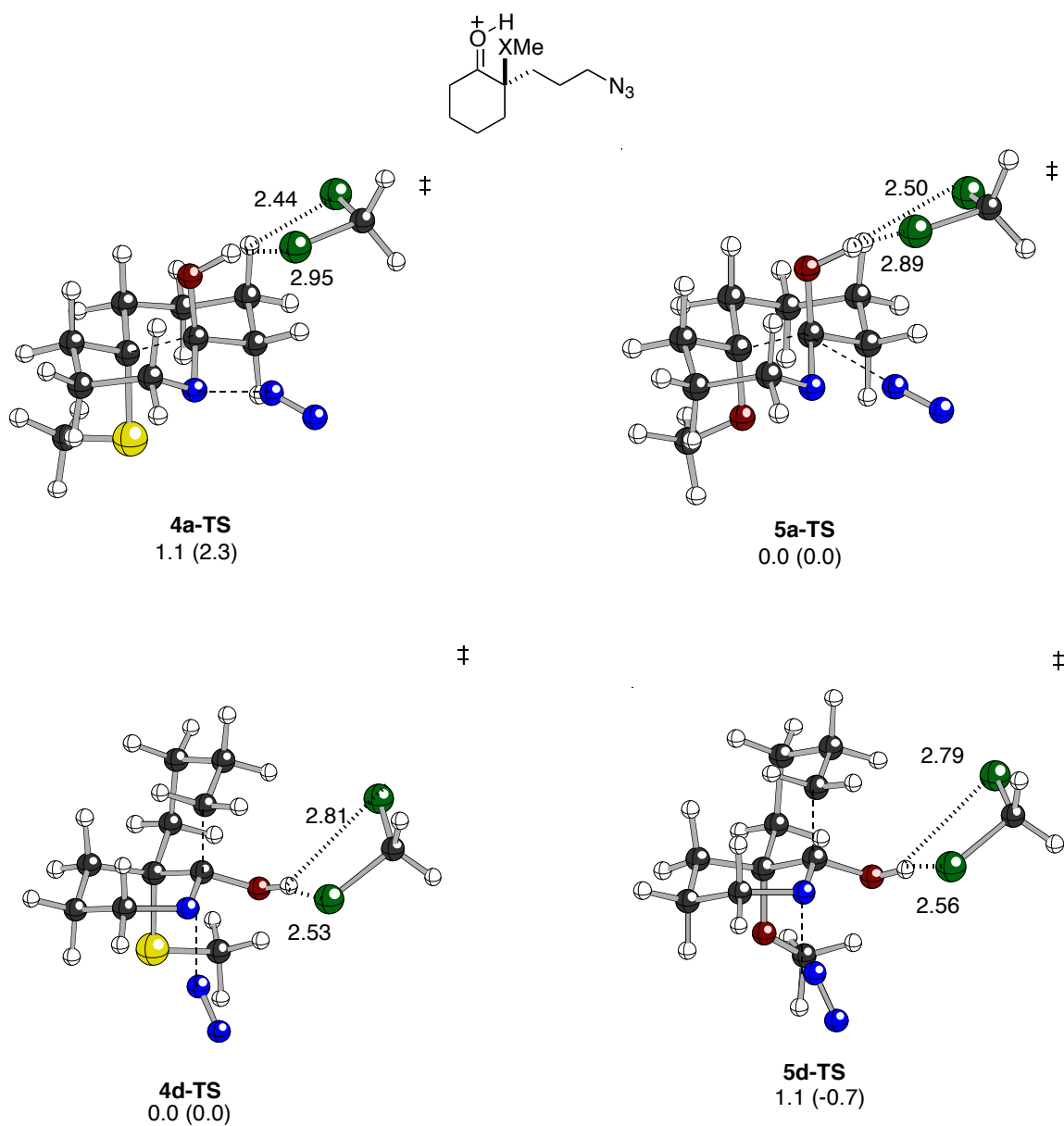


Figure S3. Selected transition state structures for the **4** and **5** systems with explicit DCM molecules calculated using M06-2X/6-31G(d,p) in DCM (CPCM-UFF). Relative free energies (298.15 K) (enthalpies are in parentheses) are with respect to the lowest free energy transition state structure.

Figure S3 shows that an explicit DCM (dichloromethane) molecule has the same effect as an explicit water molecule, namely that for the thiomethyl group the lowest energy transition state structure will yield the bridged lactam, while for the methoxy system the transition state structure leading to the bridged product is disfavored.

1-eq

G(298.15 K)= -591.370719

H(298.15 K)= -591.315737

C	2.30243600	3.73099600	-0.51621800		
C	2.47284600	2.29151300	-0.99493200		
C	2.49877400	1.27232200	0.18554000		
C	1.31194900	1.55381600	1.02598700		
C	1.05451600	2.91851000	1.52770800		
C	1.03602400	3.89154300	0.31846200		
H	1.65865400	2.01235200	-1.67399600		
H	3.41106400	2.17748000	-1.54137200		
H	3.17583200	4.02894800	0.07509200		
H	2.25726900	4.39625200	-1.38240800		
H	0.13032200	2.96108500	2.10716300		
H	1.89441900	3.18631500	2.17973500		
H	0.14948100	3.68723600	-0.28966900		
H	0.93924200	4.90391600	0.71412600		
H	3.36003800	1.54532100	0.81607000		
C	2.60367800	-0.18869300	-0.25121600		
H	1.74555100	-0.44037400	-0.88547100		
H	2.54704000	-0.83358500	0.63162500		
C	4.06777500	-1.97700800	-1.28027200		
N	4.11259300	-2.79229700	-0.04038200	C	3.90179600 -0.48577300 -0.99963700

H	3.92691400	0.03658700	-1.96110300
H	4.76258700	-0.12642400	-0.41978600
N	6.01201500	-2.50974400	1.33252700
N	5.12180400	-2.60775900	0.64113100
O	0.50745300	0.59209800	1.23406500
H	3.21045300	-2.35980900	-1.83646100
H	-0.26748900	0.83498400	1.77828900
H	4.96846500	-2.15698300	-1.87631200

1-a

G(298.15 K)= -591.385991

H(298.15 K)= -591.33688

C	1.79859500	3.56861600	-0.14600200
C	2.01405300	2.54513300	-1.26234200
C	2.93508000	1.40837800	-0.80643800
C	2.32923900	0.76730600	0.44884000
C	2.15050300	1.76061300	1.58634800
C	1.24197200	2.90385000	1.11386000
H	1.05305400	2.11889700	-1.57415800
H	2.46135100	3.02000800	-2.14092900
H	2.75528800	4.05135400	0.09129200
H	1.11757700	4.35503900	-0.48311300
H	1.71072300	1.26609100	2.46114800
H	3.13116200	2.15462400	1.87419200
H	0.24133800	2.50614000	0.91008200
H	1.14120200	3.62888100	1.92495600
H	3.89874100	1.83650200	-0.49804200
C	3.18312100	0.35878800	-1.89171300
H	3.59360200	0.85530100	-2.77517700
H	2.22841200	-0.09291400	-2.18355300
C	3.65952100	-1.39887300	-0.14470700
N	3.37850500	-0.31198800	0.85210500
C	4.15454500	-0.72194300	-1.41328600

H	4.27651200	-1.49941400	-2.17168200
H	5.14022800	-0.28581600	-1.22215100
N	3.64077900	-0.82259400	3.16116900
N	3.49002700	-0.61051100	2.07790700
O	1.17323000	0.10688700	0.09484600
H	2.72037100	-1.93538300	-0.30062700
H	0.61870800	-0.05912700	0.87096700
H	4.40433400	-2.06242300	0.29425800

1-a-TS

G(298.15 K)= -591.362738

H(298.15 K)= -591.312753

C	1.76943500	3.67861900	-0.29602100
C	2.02685900	2.62992900	-1.37534500
C	2.95614400	1.51154400	-0.89340900
C	2.28314700	0.85559500	0.38551400
C	2.04212900	1.90381600	1.46659700
C	1.15596300	3.03674500	0.94738900
H	1.08126200	2.18174700	-1.70123300
H	2.49696100	3.08605200	-2.25252200
H	2.71511100	4.16639500	-0.02774100
H	1.10458000	4.45544300	-0.68335900
H	1.57058600	1.41395600	2.32932100
H	3.01256800	2.29043700	1.79376600
H	0.16200200	2.64239700	0.70629700
H	1.02400100	3.77474400	1.74229300
H	3.90952200	1.94576600	-0.56986500
C	3.21006300	0.43240600	-1.94128200
H	3.69454300	0.88816200	-2.80961200
H	2.25436400	0.01485600	-2.27439000
C	3.48299500	-1.23908100	-0.06101500
N	3.35194800	-0.05495100	0.77271100
C	4.09836100	-0.66070600	-1.36580400
H	4.20436300	-1.51129800	-2.04343500

H	5.09675500	-0.27403000	-1.14466500
N	3.04801900	-1.06970700	3.34295400
N	2.91241900	-0.68465900	2.32320700
O	1.13147300	0.20489700	-0.03403400
H	2.52076800	-1.71176200	-0.26507100
H	0.49539800	0.15106600	0.69363300
H	4.18997600	-1.92320400	0.40630800

1-b

G(298.15 K)= -591.384267

H(298.15 K)= -591.335752

C	3.25209600	0.93366900	-1.67968700
C	2.28479300	-0.14350100	-2.17663400
C	1.96152200	-1.18397400	-1.09412400
C	1.31605800	-0.51815500	0.12759400
C	2.72271500	1.62347800	-0.43310300
H	2.71984700	-0.65749700	-3.03802400
H	1.35595200	0.32752000	-2.51239400
H	3.38449300	1.70452700	-2.44310700
H	4.23902900	0.51271400	-1.46964700
H	1.17831900	-1.85142900	-1.47509400
C	3.17299300	-2.03380200	-0.69198900
H	3.53836800	-2.54867400	-1.58590100
H	3.98773600	-1.38732300	-0.34352200
C	2.29357800	-2.31923100	1.64573000
C	2.83264900	-3.03731000	0.40931900
H	3.71913400	-3.62076000	0.67180200
H	2.07729500	-3.74371200	0.04253500
H	2.00714900	-3.03466600	2.42036600
O	0.19638500	0.16832900	-0.27808800
N	2.38307900	0.54855800	0.56358500
N	2.39455600	0.89754400	1.78264600
N	2.45640200	1.15187100	2.86538500

H	3.08295300	-1.69083200	2.07800000
C	1.06890500	-1.47659000	1.28306200
H	0.26270200	-2.13040500	0.93312900
H	0.66960900	-0.93408000	2.14923900
H	3.46353900	2.27473500	0.03083200
H	-0.38770400	0.34984300	0.47276600
H	1.80052400	2.17648900	-0.62775600

1-b-TS

G(298.15 K)= -591.359949

H(298.15 K)= -591.310257

C	3.25515800	0.92994600	-1.67507100
C	2.30066700	-0.14205000	-2.18270400
C	2.00999000	-1.17564400	-1.09404800
C	1.42496800	-0.43802900	0.18731400
C	2.69781700	1.58319400	-0.37556000
H	2.73448600	-0.64941600	-3.04956300
H	1.36406100	0.32092700	-2.50518600
H	3.36592900	1.75116900	-2.38731600
H	4.24961800	0.52612100	-1.47256600
H	1.15212800	-1.79280300	-1.38827600
C	3.18710700	-2.09232800	-0.75500000
H	3.44365800	-2.64931100	-1.66175200
H	4.06795000	-1.50187800	-0.48087400
C	2.38625200	-2.30539400	1.62837900
C	2.85169600	-3.05856000	0.38261100
H	3.72565400	-3.67179900	0.61769500
H	2.05669900	-3.74107800	0.05590000
H	2.11827500	-3.00541000	2.42382700
O	0.28945200	0.25091600	-0.21313700
N	2.54350200	0.43870000	0.50213800
N	2.19739500	1.13703300	2.05218700
N	2.39895800	1.54893300	3.05047900

H	3.20046800	-1.67957900	2.01272600
C	1.16868200	-1.44068400	1.30722100
H	0.33877600	-2.06850000	0.96611200
H	0.81092700	-0.89838600	2.19316300
H	3.44616200	2.25468700	0.04344200
H	-0.31264500	0.35286000	0.53785600
H	1.75042800	2.08682100	-0.57485700

1-c

G(298.15 K)= -591.385648

H(298.15 K)= -591.336664

C	-2.22162400	3.08486400	1.11336300
C	-1.43126500	2.86616800	-0.17942700
C	-1.64076300	1.46077000	-0.77261300
C	-1.30856200	0.43364400	0.31356000
C	-2.09400200	0.61434800	1.60536600
C	-1.86296400	2.02580700	2.15636800
H	-1.71202000	3.60256400	-0.93853000
H	-0.36440700	3.00888000	0.02660200
H	-2.00665800	4.08306200	1.50507800
H	-3.29895300	3.05373600	0.91097800
H	-3.15972300	0.45660400	1.41178100
H	-1.76587600	-0.14783900	2.31967800
H	-2.45768500	2.15509300	3.06416200
H	-0.80899300	2.12665800	2.43729600
H	-0.92048800	1.30453200	-1.58811100
C	-3.04622000	1.26243600	-1.35638200
H	-3.20582000	2.02782400	-2.12065000
H	-3.81166100	1.41975200	-0.58830500
C	-3.00314000	-1.22062900	-0.94607700
N	-1.67831700	-0.95742900	-0.30135400

C	-3.21367800	-0.12408600	-1.97659400
H	-4.21947600	-0.24632200	-2.38533800
H	-2.50086800	-0.26080700	-2.79581100
N	-0.50589600	-2.76252500	0.71216500
N	-1.09136600	-1.93385000	0.25411600
H	-2.95394500	-2.21199400	-1.39690200
O	0.02780000	0.36535500	0.63049600
H	0.56973000	0.52875700	-0.15661400
H	-3.76988000	-1.20972000	-0.16582500

1-c-TS

G(298.15 K)= -591.359837

H(298.15 K)= -591.310168

C	-2.27752700	3.15608600	1.11371200
C	-1.48491800	2.96699600	-0.18009600
C	-1.68120800	1.58202100	-0.81790800
C	-1.29033600	0.51046700	0.29104500
C	-2.10229300	0.68787500	1.57062100
C	-1.90334700	2.09092400	2.14509000
H	-1.77743600	3.71027400	-0.92892800
H	-0.41927400	3.11234200	0.02205900
H	-2.07528600	4.15258200	1.51618300
H	-3.35438700	3.11315100	0.91127900
H	-3.16293300	0.51730800	1.37024000
H	-1.76320500	-0.08099800	2.27567700
H	-2.51232100	2.19554200	3.04657500
H	-0.85555700	2.21040300	2.43859600
H	-0.95628700	1.45761700	-1.63157600
C	-3.07936100	1.33439300	-1.37885600
H	-3.26001300	2.05474500	-2.18206100
H	-3.84702200	1.50524800	-0.61762100

C	-2.83124700	-1.10962300	-0.81069500
N	-1.48472700	-0.72852300	-0.43663200
C	-3.18330600	-0.08208700	-1.92236000
H	-4.19556000	-0.33342900	-2.24701700
H	-2.50655700	-0.22678100	-2.76850500
N	-0.34473600	-2.81316200	1.01204500

1-d

G(298.15 K)= -591.385135

H(298.15 K)= -591.335946

C	-1.40896300	3.59574200	0.37707000
C	-1.41247200	2.89473000	-0.98432900
C	-2.06810000	1.50375100	-0.92793500
C	-1.36946800	0.69078900	0.16688800
C	-1.38097600	1.35051200	1.53790500
C	-0.72106600	2.73278400	1.43620600
H	-1.94208100	3.49613300	-1.72959400
H	-0.38072400	2.78006600	-1.33327700
H	-0.89513900	4.55722400	0.29060700
H	-2.43511600	3.81657400	0.69454600
H	-2.40973600	1.45995800	1.89378700
H	-0.85900100	0.70187800	2.24942700
H	-0.76057200	3.21294700	2.41698100
H	0.33758400	2.61142500	1.17934900
H	-1.86679500	0.97985600	-1.87234400
C	-3.58940600	1.57653300	-0.72886200
H	-4.01057700	2.14532000	-1.56247000
H	-3.83220500	2.13360200	0.18312900
C	-3.65064800	-0.63836100	0.45446400
N	-2.15728700	-0.66688100	0.31900300

N	-0.92013400	-1.93588400	0.68624900
H	-2.79914900	-2.11336900	-1.23339900
O	0.04869200	0.60178300	0.63480700
H	0.59745200	0.58639600	-0.16399500
H	-3.55001500	-1.04815900	0.00938700

C	-4.24258800	0.19587200	-0.67001900
H	-5.31777500	0.28435400	-0.49421700
H	-4.11032900	-0.33000900	-1.62238700
N	-1.22238900	-2.42467100	-0.99098900
N	-1.69155700	-1.59855200	-0.41219800
O	-0.11048300	0.35387400	-0.27016200
H	-3.82973300	-0.20158900	1.43819100
H	0.46874900	0.15602300	0.48150000
H	-3.99859700	-1.67121300	0.46775400

1-d-TS

G(298.15 K)= -591.359504

H(298.15 K)= -591.310085

C	-1.37760700	3.58221700	0.34337300
C	-1.38351100	2.84652900	-1.00040100
C	-2.06523000	1.47462700	-0.91689700
C	-1.42862000	0.64953000	0.20867600
C	-1.50829700	1.39011400	1.59366600
C	-0.76021300	2.71956100	1.44264800
H	-1.89440000	3.44297600	-1.76255100
H	-0.35184000	2.70326200	-1.33677100

H	-0.81443400	4.51433000	0.24512100
H	-2.39841100	3.86121700	0.63086400
H	-2.54927400	1.58173600	1.86110400
H	-1.06410700	0.75664100	2.36637700
H	-0.80664200	3.22873800	2.40970100
H	0.29384500	2.52336200	1.22468200
H	-1.84349000	0.91605500	-1.83857200
C	-3.58627000	1.55779800	-0.75106800
H	-4.00293000	2.04093000	-1.63914800
H	-3.84809500	2.19390100	0.10108700
C	-3.53954600	-0.61419300	0.53678500
N	-2.09045900	-0.61121700	0.50243500
C	-4.21225600	0.17614500	-0.57831800
H	-5.27935300	0.24797000	-0.35904500
H	-4.11089100	-0.40412200	-1.50466000
N	-1.33805600	-2.40032300	-1.56206200
N	-1.71706000	-1.54569800	-0.98581000
O	-0.11606200	0.37889500	-0.14097800
H	-3.71945500	-0.16966100	1.53122500
H	0.35051700	-0.03346000	0.60214300
H	-3.86841100	-1.65173700	0.61694000

2-a

G(298.15 K)= -748.453869

H(298.15 K)= -748.394291

C	2.02723300	3.52479700	-0.21665300
C	2.31370200	2.42371800	-1.25696200
C	3.04671200	1.19717800	-0.70881000
C	2.20308800	0.61985300	0.43215600
C	2.00014400	1.62103000	1.55511400
C	1.32849500	2.89368400	1.00604700
H	1.35249000	2.07808200	-1.65572100

H	2.87562100	2.81785800	-2.10727600
H	1.27546500	4.16891400	-0.69191500
H	1.36443100	1.18984700	2.33884600
H	2.97174300	1.84382500	2.00189400
H	0.30403500	2.63239300	0.71932600
H	1.24323500	3.61270300	1.82563800
H	4.00514200	1.49786000	-0.26839100
C	3.31588700	0.13847200	-1.78086600
H	3.89977500	0.59183500	-2.58658600
H	2.36344700	-0.19123300	-2.21099300
C	3.33709100	-1.68340200	-0.03285100
N	3.04712700	-0.58280400	0.94750000
C	4.07819000	-1.05530800	-1.20255900
H	4.21360700	-1.83393100	-1.95744300
H	5.07153500	-0.74122000	-0.86650300
N	2.84903400	-1.18602700	3.24178500
N	2.90945200	-0.92512800	2.16074900
O	1.03488800	0.10881500	-0.09004000
H	2.37448100	-2.10649900	-0.33082100
H	0.36171200	0.01285500	0.59921200
H	3.93460300	-2.43272400	0.48651800
C	3.19529400	4.50549700	0.13423500
C	2.56628700	5.81842000	0.63051600
H	3.34721200	6.52815700	0.92209700
H	1.96266200	6.28274000	-0.15634400
H	1.92274300	5.65837700	1.50162500
C	4.15102900	4.01034600	1.22924000
H	3.63834200	3.88085100	2.18776300
H	4.64753200	3.07129800	0.96776400
H	4.93648900	4.75759600	1.38330100
C	4.01888700	4.82533100	-1.11965200
H	4.61594400	3.96693300	-1.44416500
H	3.37441000	5.12953900	-1.95203400

H 4.70969800 5.64826000 -0.91040300

2-a-TS

G(298.15 K)= -748.430605

H(298.15 K)= -748.370393

C 1.99347800 3.60942000 -0.23464900

C 2.23886400 2.51535300 -1.28746600

C 3.04606400 1.30119100 -0.81807100

C 2.25549000 0.67019200 0.39997200

C 2.08455100 1.69940300 1.50812800

C 1.36342100 2.95969000 1.01312700

H 1.26425200 2.14234100 -1.62271700

H 2.73839500 2.92127700 -2.17136000

H 1.21097700 4.24233400 -0.67416200

H 1.50090300 1.24137100 2.31890800

H 3.07418300 1.92356300 1.91088700

H 0.32967100 2.68723000 0.77262600

H 1.30726400 3.67056900 1.84229200

H 4.02896900 1.61138800 -0.44909900

C 3.22539000 0.24446400 -1.90443400

H 3.79095700 0.67937400 -2.73357300

H 2.24492500 -0.05310200 -2.29010900

C 3.24740800 -1.51991600 -0.08738500

N 3.20757100 -0.36069200 0.78977700

C 3.96794900 -0.96085700 -1.34623200

H 4.00709400 -1.79120500 -2.05542100

H 4.99349900 -0.69478400 -1.07676800

N 2.70958600 -1.40849900 3.31126900

N 2.64642800 -0.99078500 2.29726600

O 1.06275200 0.15630400 -0.08799600

H 2.25008600 -1.88181500 -0.34293700

H 0.38799700 0.16476200 0.60555400

H 3.86177100 -2.29142200 0.37522600

C 3.16281200 4.60457300 0.05996200

C 2.54211800 5.90176300 0.60577900

H 3.32704800 6.62220400 0.85726500

H 1.88434200 6.36235600 -0.13867600

H 1.95517700 5.72256200 1.51233000

C 3.90737000 4.95003200 -1.23593700

H 4.50251900 4.10705000 -1.60234600

H 3.20975900 5.24820800 -2.02676100

H 4.59278900 5.78499600 -1.05967800

C 4.18480300 4.11136900 1.09378400

H 3.72723500 3.96312700 2.07706800

H 4.67789400 3.18212300 0.79373900

H 4.96816200 4.86705400 1.21387500

2-b

G(298.15 K)= -748.451834

H(298.15 K)= -748.392564

C 3.37251700 1.01058800 -1.65094800

C 2.26822600 0.08348800 -2.16523500

C 1.82184300 -0.94514300 -1.11327100

C 1.29186300 -0.24450300 0.13999800

C 2.95855600 1.71334400 -0.36814800

H 2.62099900 -0.45188200 -3.05090900

H 1.40356800 0.68161500 -2.46812600

H 3.58493700 1.78725900 -2.39013700

H 4.30320700 0.46324700 -1.48008600

H 0.95426800 -1.48285300 -1.51223400

C 2.92919700 -1.93921000 -0.74854200

H 3.27608400 -2.42212700 -1.66562600

H	3.78955500	-1.37697800	-0.36516500
C	2.01951700	-2.24618800	1.56546400
C	2.56637900	-2.98219800	0.32568600
H	3.52964800	-3.41197200	0.63058900
H	1.61776700	-2.95200300	2.29804100
O	0.27052600	0.60593700	-0.21128500
N	2.49993000	0.65154700	0.59322800
N	2.60704200	0.92261600	1.82530900
N	2.74499700	1.10196900	2.91641700
H	2.86020400	-1.74823400	2.06449800
C	0.93245500	-1.20841200	1.25646200
H	0.01589300	-1.69001300	0.90918800
H	0.65271200	-0.65243500	2.16053900
H	3.78448000	2.24557700	0.10322100
H	-0.27063000	0.82604700	0.56119000
H	2.11137800	2.38660500	-0.52035400
C	1.72929700	-4.22369500	-0.12836900
C	2.02248600	-5.36780400	0.85658300
H	1.77285800	-5.09350500	1.88651100
H	1.43235000	-6.25258400	0.59759900
H	3.08116300	-5.64587400	0.82699100
C	2.17394500	-4.67938100	-1.52386800
H	1.85904400	-3.97519300	-2.30085800
H	3.26294000	-4.78770200	-1.57900200
H	1.72634500	-5.65078800	-1.75653700
C	0.20843800	-4.01203300	-0.14961600
H	-0.18778700	-3.80915200	0.85068500
H	-0.09950200	-3.20384900	-0.81960000
H	-0.27524800	-4.92744600	-0.50651000

2-b-TS

G(298.15 K)= -748.426949

H(298.15 K)= -748.366561

C	3.37712800	1.02076700	-1.64062600
C	2.27658400	0.11195000	-2.17056200
C	1.85812300	-0.91782800	-1.11826100
C	1.40885600	-0.15840400	0.19824900
C	2.94290700	1.68653600	-0.29896400
H	2.62323400	-0.41228900	-3.06618300
H	1.40804300	0.71217000	-2.45419000
H	3.58254500	1.85214500	-2.31942300
H	4.31265200	0.48017300	-1.48271200
H	0.91881800	-1.39057300	-1.42570000
C	2.92115800	-1.98063700	-0.83295100
H	3.13899800	-2.49464200	-1.77238000
H	3.85061000	-1.48061400	-0.54008200
C	2.10871500	-2.22430500	1.53388400
C	2.58258300	-2.99232100	0.28260800
H	3.54912300	-3.43851600	0.55114300
H	1.73087400	-2.91378200	2.29422000
O	0.37754000	0.70457400	-0.14408000
N	2.64525600	0.53497700	0.52816700
N	2.42664000	1.18981300	2.12285200
N	2.70012200	1.49114000	3.14324700
H	2.97603500	-1.72492600	1.98140300
C	1.02854400	-1.17179300	1.26767900
H	0.09816400	-1.62516900	0.92140500
H	0.78468200	-0.63236300	2.19307700
H	3.78828400	2.22467900	0.12769600
H	-0.20110500	0.84425100	0.61917200
H	2.07373700	2.32810400	-0.45342000
C	1.70332500	-4.22531300	-0.10897800
C	1.97582900	-5.33999700	0.91554100
H	1.73437100	-5.02883200	1.93656000

H	1.36668300	-6.22020200	0.68655500
H	3.02826100	-5.64166600	0.89241500
C	2.11690700	-4.75384100	-1.48931700
H	1.79576700	-4.08735400	-2.29606200
H	3.20352600	-4.87895700	-1.55839000
H	1.65418900	-5.72995600	-1.66576100
C	0.19012000	-3.96752100	-0.12356300
H	-0.19049700	-3.72029300	0.87262800
H	-0.09602000	-3.17096100	-0.81709000
H	-0.32600300	-4.87717200	-0.44827200

2-c

G(298.15 K)= -748.462231

H(298.15 K)= -748.400869

C	-2.13151200	3.07194200	1.12868000
C	-1.31345800	2.79561200	-0.14296500
C	-1.58050500	1.40966400	-0.75719800
C	-1.30837100	0.35998700	0.32053400
C	-2.10977000	0.57531900	1.59390000
C	-1.83273800	1.97294700	2.16002900
H	-1.51567300	3.54219700	-0.91594400
H	-0.24648300	2.86480700	0.09831600
H	-3.20093300	2.99828900	0.87677100
H	-3.17712500	0.46462100	1.37761600
H	-1.83269200	-0.19973900	2.31605400
H	-2.44747400	2.09870000	3.05392500
H	-0.78344200	2.02471600	2.47315600
H	-0.85303000	1.23546400	-1.56288700
C	-2.98178300	1.27523900	-1.36875400
H	-3.09759700	2.05547600	-2.12599300
H	-3.75569000	1.45175200	-0.61375500
C	-3.04546900	-1.21137900	-0.98559900
N	-1.72510300	-1.00893700	-0.30983700
C	-3.19100900	-0.09693400	-2.00822600

H	-4.19266900	-0.17522200	-2.43749100
H	-2.46804000	-0.25336600	-2.81489800
N	-0.64158400	-2.86876100	0.70303000
N	-1.18694200	-2.01334900	0.24460600
H	-3.02639100	-2.19930700	-1.44607500
O	0.01820400	0.23258800	0.66079000
H	0.58011500	0.38049400	-0.11523900
H	-3.82718800	-1.17740800	-0.22099800
C	-1.93084300	4.51536600	1.67589300
C	-2.48761900	5.52899000	0.66521000
H	-2.41541300	6.54183000	1.07433400
H	-1.93474600	5.51895800	-0.27808800
H	-3.54211100	5.32683400	0.44745500
C	-2.71144400	4.68286000	2.98777600
H	-2.25838700	4.11855400	3.80774600
H	-2.72344400	5.73691400	3.28279600
H	-3.75009900	4.35107700	2.87509000
C	-0.45325600	4.83691000	1.93661200
H	-0.36788200	5.82352200	2.40371500
H	0.00808400	4.11041800	2.61322600
H	0.12769300	4.86044100	1.00999500

2-c-TS

G(298.15 K)= -748.43635

H(298.15 K)= -748.37451

C	-2.17935100	3.14755200	1.12571400
C	-1.35382600	2.89633300	-0.14399400
C	-1.60677400	1.53084400	-0.80170700
C	-1.28732200	0.43314300	0.30025200
C	-2.11618900	0.65310200	1.55933700
C	-1.86813600	2.04312900	2.14707500
H	-1.56111500	3.65110100	-0.90889700
H	-0.28855000	2.96496900	0.09786000

H	-3.24733500	3.06253300	0.87139500
H	-3.17921900	0.53338200	1.33506000
H	-1.83248900	-0.12952600	2.27383500
H	-2.49847900	2.14716900	3.03289400
H	-0.82470400	2.11147800	2.47427900
H	-0.87027400	1.38494900	-1.60148800
C	-3.00052800	1.35108600	-1.39817000
H	-3.13036900	2.08708600	-2.19710100
H	-3.77957100	1.54604200	-0.65461400
C	-2.88123500	-1.10504100	-0.84616100
N	-1.52791600	-0.79240800	-0.43573100
C	-3.15208700	-0.05423400	-1.95913400
H	-4.16455200	-0.25606600	-2.31616500
H	-2.45744700	-0.22326600	-2.78603100
N	-0.52711600	-2.93219100	1.03454400
N	-1.05260800	-2.02855700	0.69666900
H	-2.88839000	-2.10712700	-1.27413600
O	0.04696500	0.45514200	0.67205300
H	0.61027200	0.40717900	-0.11522400
H	-3.61744400	-1.01081300	-0.04491100
C	-1.99627700	4.58907700	1.68502100
C	-2.59567600	5.60117600	0.69767200
H	-2.51960300	6.61302100	1.10852100
H	-2.07467100	5.60037300	-0.26385000
H	-3.65475200	5.38979600	0.51400300
C	-2.75169800	4.72649300	3.01480500
H	-2.26824400	4.16440600	3.81880400
H	-2.78009700	5.77724300	3.32017400
H	-3.78503200	4.37297900	2.92122400
C	-0.52000100	4.93685700	1.91724900
H	-0.44426600	5.91528200	2.40272400
H	-0.02738200	4.20633700	2.56708900
H	0.03759800	4.99152800	0.97763400

2-d

G(298.15 K)= -748.461133

H(298.15 K)= -748.399859

C	-1.31703200	3.56117900	0.33902400
C	-1.27876300	2.78874300	-0.99071200
C	-1.99627900	1.42956500	-0.92768200
C	-1.37600200	0.61906700	0.21192000
C	-1.40790900	1.33028500	1.55377900
C	-0.69409000	2.68483200	1.43633000
H	-1.73385300	3.36762600	-1.79972100
H	-0.23455800	2.60821700	-1.26803600
H	-2.36933900	3.72553800	0.61819100
H	-2.44347200	1.49138200	1.86800700
H	-0.93661200	0.69150700	2.30816400
H	-0.75612700	3.17236000	2.41116800
H	0.36945500	2.51853500	1.22491300
H	-1.77462500	0.87743300	-1.85137900
C	-3.52139600	1.56399600	-0.80378600
H	-3.88047300	2.12330900	-1.67221800
H	-3.78841300	2.15393100	0.08001400
C	-3.72145800	-0.59980100	0.44777200
N	-2.22612600	-0.69779800	0.37762800
C	-4.22568100	0.20914600	-0.73603400
H	-5.30522300	0.33841400	-0.62439200
H	-4.05768000	-0.35698500	-1.65980100
N	-1.33841600	-2.51718700	-0.88247000
N	-1.78324700	-1.66144700	-0.32862000
O	-0.11828200	0.21314300	-0.16727800
H	-3.92068000	-0.11282400	1.40351500
H	0.42413700	0.01646400	0.61167700
H	-4.11431400	-1.61577000	0.49036300
C	-0.68935300	4.98155200	0.23393600

C	-0.64765600	5.63446500	1.62333500
H	0.09770900	5.16696100	2.27325600
H	-0.38514700	6.69305300	1.53088700
H	-1.62361200	5.57008400	2.11850800
C	-1.56883800	5.85934700	-0.66874500
H	-1.61685500	5.48211500	-1.69392300
H	-2.59044700	5.92039300	-0.27790300
H	-1.16343800	6.87532600	-0.71257500
C	0.73267300	4.94600500	-0.34060600
H	1.16635400	5.95111200	-0.31402700
H	1.38903100	4.28792200	0.23815700
H	0.73994300	4.61006000	-1.38158900

2-d-TS

G(298.15 K)= --748.436621

H(298.15 K)= --748.374267

C	-1.28899900	3.54599600	0.30789000
C	-1.32405200	2.76895600	-1.01979100
C	-2.04909800	1.42029800	-0.91924200
C	-1.43534600	0.58189600	0.20562700
C	-1.48535000	1.34722300	1.57419000
C	-0.69523200	2.64961700	1.40206200
H	-1.82488800	3.35290500	-1.79718400
H	-0.30021100	2.58250500	-1.36019500
H	-2.32642400	3.77256800	0.59979900
H	-2.51855900	1.57305300	1.84484000
H	-1.05472700	0.71605600	2.35647100
H	-0.71560100	3.15054400	2.37358500
H	0.34896600	2.41053200	1.17710700
H	-1.85035800	0.85197100	-1.84032000
C	-3.56647900	1.55386300	-0.75041000
H	-3.96918300	2.04371600	-1.64130400

H	-3.80656500	2.20391800	0.09742100
C	-3.58595000	-0.60683500	0.55475200
N	-2.13809500	-0.65261900	0.51556200
C	-4.23640400	0.19492900	-0.56519600
H	-5.29981900	0.30361800	-0.34316800
H	-4.15758800	-0.39655000	-1.48662400
N	-1.45275000	-2.48759500	-1.53249400
N	-1.80077000	-1.61545400	-0.96299000
O	-0.13446100	0.26264500	-0.14713300
H	-3.74609400	-0.14665500	1.54548300
H	0.32290000	-0.15297600	0.59989900
H	-3.94937600	-1.63172500	0.64626400
C	-0.58073500	4.92735200	0.19173300
C	-0.68925400	5.67098000	1.53178600
H	-0.10194300	5.18962800	2.31890300
H	-0.31264200	6.69296200	1.42358600
H	-1.73091300	5.72809200	1.86762100
C	-1.28569300	5.77608900	-0.87618900
H	-1.13297800	5.37831100	-1.88314400
H	-2.36397400	5.82944400	-0.68743800
H	-0.88963400	6.79639000	-0.86336400
C	0.90214600	4.79544700	-0.17880300
H	1.35111200	5.79163200	-0.24998500
H	1.46267000	4.23593400	0.57629100
H	1.03971500	4.30330400	-1.14606100

3-a

G(298.15 K)= -748.462319

H(298.15 K)= -748.40119

C	1.69134000	3.54149500	-0.21813400
C	1.90354900	2.45446600	-1.28329600
C	2.85620300	1.35516800	-0.80406300
C	2.27493400	0.74150300	0.47348300

C	2.08882100	1.77432600	1.57007000
C	1.16149000	2.89059800	1.06886700
H	0.94509700	1.98949700	-1.54354300
H	2.31859400	2.88021900	-2.20166300
H	2.68100400	3.96371100	0.02297400
H	1.66135100	1.30930600	2.46712700
H	3.06605500	2.19110500	1.83715300
H	0.16051400	2.47615000	0.89723600
H	1.07219700	3.62687800	1.86989100
H	3.81483800	1.81036000	-0.52012500
C	3.11410700	0.27747600	-1.85943700
H	3.50617200	0.75312500	-2.76249400
H	2.16599400	-0.20234900	-2.12671300
C	3.64467000	-1.41323900	-0.06103200
N	3.34769100	-0.30120500	0.90329000
C	4.11221500	-0.76722100	-1.35596400
H	4.24244300	-1.56610300	-2.09035200
H	5.09052100	-0.30517000	-1.18985500
N	3.61719500	-0.75109100	3.22468500
N	3.46235200	-0.56690100	2.13705900
O	1.12844800	0.04751900	0.15399300
H	2.71743700	-1.97710900	-0.18995000
H	0.57903400	-0.09093700	0.93898200
H	4.40954800	-2.04360900	0.39232400
C	0.82449300	4.73224700	-0.71991300
C	-0.51529700	4.26310700	-1.30280900
H	-1.13361100	5.13142200	-1.55276500
H	-0.37789000	3.68247500	-2.21987500
H	-1.07734400	3.65092900	-0.58996500
C	0.54709100	5.70344400	0.43641500
H	1.47297100	5.97210300	0.95784700
H	0.09765400	6.62377700	0.05027000
H	-0.14763600	5.28010000	1.16762900

C	1.59522700	5.50100500	-1.80291000
H	1.00848900	6.36179300	-2.13965700
H	2.54830700	5.87437100	-1.41270900
H	1.80334600	4.88308200	-2.68075200

3-a-TS

G(298.15 K)= -748.438953

H(298.15 K)= --748.377342

C	1.68551200	3.62923300	-0.33608000
C	1.90834500	2.52395400	-1.37589200
C	2.89502300	1.44912800	-0.91199000
C	2.30572700	0.81331200	0.41471300
C	2.09032200	1.89539700	1.46333000
C	1.15312200	2.99106900	0.95408800
H	0.95808800	2.03367300	-1.61648200
H	2.31039000	2.93629200	-2.30677600
H	2.66991400	4.06386900	-0.09658000
H	1.67201500	1.43255100	2.36733900
H	3.06560300	2.31559900	1.72915900
H	0.15536800	2.56852500	0.78173100
H	1.05397800	3.73622200	1.74593700
H	3.85168500	1.91732100	-0.65164900
C	3.12600900	0.34624900	-1.94103700
H	3.55564900	0.78754800	-2.84493000
H	2.16681800	-0.10515700	-2.21476900
C	3.53832100	-1.26037600	-0.02796500
N	3.41722900	-0.05453700	0.77615400
C	4.07081300	-0.70643100	-1.37921200
H	4.16388900	-1.57462300	-2.03614200
H	5.06872800	-0.28872600	-1.22164600
N	3.27340300	-0.96826500	3.39542100
N	3.07489900	-0.64212800	2.36538900
O	1.15403900	0.11795700	0.07581900

H	2.57964300	-1.76231300	-0.16872400
H	0.55731900	0.07137000	0.83658800
H	4.28525600	-1.91214400	0.42308000
C	0.81093500	4.80100300	-0.86803500
C	-0.51175000	4.30475700	-1.46733000
H	-1.13946900	5.16037900	-1.73667200
H	-0.35021000	3.71654200	-2.37574100
H	-1.07552100	3.69107500	-0.75706400
C	0.50068300	5.78046500	0.27263200
H	1.41390100	6.06828000	0.80603600
H	0.04432500	6.68979600	-0.13086900
H	-0.19952800	5.35470100	0.99720400
C	1.58959200	5.56775800	-1.94659600
H	0.99648200	6.41557500	-2.30434000
H	2.52989700	5.95980800	-1.54411100
H	1.82266900	4.94277800	-2.81331600

3-b

G(298.15 K)= -748.461666

H(298.15 K)= -748.40046

C	3.22010300	1.01754200	-1.65997300
C	2.30516700	-0.09639900	-2.17538900
C	1.99216000	-1.14378300	-1.09608300
C	1.29400500	-0.49796500	0.10371100
C	2.63548200	1.69151500	-0.42926100
H	2.77893500	-0.59703200	-3.02402800
H	1.36788700	0.33903600	-2.53486500
H	3.34318900	1.78995500	-2.42338400
H	4.21621200	0.63318300	-1.42406200
H	1.24550500	-1.84159400	-1.49487400
C	3.22615200	-1.94053800	-0.65644700
H	3.64727200	-2.40899100	-1.55073200
H	3.98857800	-1.25282700	-0.27013900
C	2.30585900	-2.27224500	1.63709300

C	2.90856700	-2.98783900	0.42001400
H	2.12518700	-3.65143700	0.01853500
H	2.00560000	-2.98845200	2.40441900
O	0.15820400	0.14519400	-0.32737700
N	2.30918200	0.60781700	0.56146300
N	2.29272200	0.95084700	1.78123500
N	2.33197300	1.20280800	2.86571000
H	3.05933700	-1.61842400	2.09673200
C	1.06283100	-1.46859100	1.24873100
H	0.28581500	-2.14809300	0.88249900
H	0.63096800	-0.94673200	2.11215000
H	3.34098800	2.36977300	0.05070100
H	-0.44857800	0.30491200	0.41024600
H	1.69947700	2.21138800	-0.64804700
C	4.11398900	-3.90675100	0.76777900
C	5.34439800	-3.10545100	1.21308700
H	5.73953900	-2.48347100	0.40428300
H	5.12200600	-2.45834400	2.06766600
H	6.14029700	-3.79243800	1.51869500
C	3.71845200	-4.87403800	1.89354400
H	2.77819000	-5.38705800	1.66060800
H	4.49482900	-5.63461100	2.02266900
H	3.60058800	-4.36173900	2.85270800
C	4.48766900	-4.74688400	-0.46236800
H	5.28651500	-5.44978700	-0.20536200
H	3.62810400	-5.32705600	-0.81569200
H	4.84936100	-4.13042400	-1.28988700

3-b-TS

G(298.15 K)= -748.436561

H(298.15 K)= -748.374794

C	3.17606700	0.96264400	-1.74328000
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C	2.24483600	-0.15265900	-2.19779500
C	2.00106500	-1.15647900	-1.07020700
C	1.42008000	-0.39446900	0.19414600
C	2.62255700	1.64176400	-0.45543400
H	2.67768200	-0.67581300	-3.05565000
H	1.28973800	0.27301700	-2.51762800
H	3.25099400	1.76287400	-2.48361100
H	4.18533300	0.59445500	-1.54560200
H	1.15335000	-1.80256800	-1.32975600
C	3.20601200	-2.03773800	-0.73471500
H	3.43932500	-2.59825900	-1.64449200
H	4.08222700	-1.42088000	-0.50265000
C	2.47164100	-2.19319400	1.65146500
C	2.92747000	-3.00249100	0.42903100
H	2.08115300	-3.63770500	0.11999000
H	2.24781200	-2.84896500	2.49647500
O	0.25789400	0.25178600	-0.20092700
N	2.51878100	0.52186700	0.46057900
N	2.18489600	1.25250500	1.99692100
N	2.39218300	1.68560800	2.98501200
H	3.27651100	-1.52154300	1.97279700
C	1.21964900	-1.37606500	1.34049600
H	0.39916100	-2.03448900	1.03700600
H	0.87280400	-0.82277700	2.22391800
H	3.35805800	2.34811600	-0.07250500
H	-0.35092900	0.31906800	0.54832800
H	1.65697600	2.11090500	-0.65186500
C	4.10625200	-3.96931500	0.73753800
C	5.28276200	-3.24456700	1.40512000
H	6.12269800	-3.93672700	1.52430500
H	5.63284900	-2.39839700	0.80470500
H	5.01751500	-2.87291800	2.39942700
C	3.61525700	-5.08589500	1.67080800

H	2.78512000	-5.63676800	1.21540400
H	4.42554500	-5.79608800	1.86444000
H	3.28043900	-4.70052900	2.63786900
C	4.59988400	-4.62582200	-0.55943800
H	5.30445300	-5.43002100	-0.32524500
H	3.76670300	-5.06045900	-1.12382100
H	5.11799800	-3.91210700	-1.20648200

3-c

G(298.15 K)= --748.447849

H(298.15 K)= -748.388324

C	-2.44018300	2.95355800	0.99573500
C	-1.66023900	2.70569200	-0.32159400
C	-1.60018900	1.27126600	-0.88310700
C	-1.21197200	0.33109100	0.26002700
C	-2.10770600	0.45070700	1.48258800
C	-2.04254000	1.88359100	2.02822700
H	-2.00602400	3.36855200	-1.11916800
H	-0.62630200	3.00231200	-0.11257200
H	-2.00388900	3.89332400	1.35649600
H	-3.12828100	0.17184400	1.20873500
H	-1.75852700	-0.25766500	2.24134500
H	-2.66488900	1.95181200	2.92527000
H	-1.01158100	2.06622300	2.34776200
H	-0.77466800	1.23146100	-1.60902500
C	-2.86202700	0.83748400	-1.63616500
H	-3.02424700	1.54677800	-2.45271000
H	-3.73928900	0.89994900	-0.98741200
C	-2.52293200	-1.58792400	-1.08942300
N	-1.33433000	-1.11711000	-0.31345200
C	-2.74405800	-0.57663100	-2.20041800
H	-3.65891000	-0.85864900	-2.72707700
H	-1.91511000	-0.63753600	-2.91262000

N	-0.02801000	-2.70880800	0.87725900
N	-0.67451600	-1.98343200	0.33374800
H	-2.28892500	-2.58284000	-1.46875100
O	0.09522800	0.46053200	0.67132600
H	0.66888600	0.66180700	-0.08347300
H	-3.37559400	-1.64516200	-0.40636600
C	-3.97912900	3.27301800	0.95794100
C	-4.92099700	2.08055900	1.19238700
H	-4.72210500	1.58420000	2.14732000
H	-5.95181600	2.44763000	1.22937400
H	-4.88755900	1.32854300	0.40125800
C	-4.24170600	4.26502200	2.10665400
H	-3.69773500	5.20123900	1.94464600
H	-5.30849200	4.49909800	2.17819000
H	-3.92426800	3.85122600	3.07008600
C	-4.36682000	3.96003900	-0.35525800
H	-5.40093400	4.31494500	-0.29852900
H	-3.72574500	4.82578300	-0.55499200
H	-4.29535600	3.27897200	-1.20920900

3-c-TS

G(298.15 K)= -748.421878

H(298.15 K)= -748.36179

C	-2.48056700	3.02138400	0.98378500
C	-1.70310800	2.80004800	-0.33695800
C	-1.63655000	1.38625500	-0.94136300
C	-1.17913400	0.41385400	0.22752600
C	-2.09977600	0.52599500	1.43669100
C	-2.06441700	1.94710900	2.00541400
H	-2.06056300	3.46919200	-1.12503000
H	-0.66933500	3.09564200	-0.13300500
H	-2.05449200	3.96317000	1.35108700
H	-3.11555400	0.24029800	1.15777100

H	-1.74032400	-0.19191900	2.18455900
H	-2.69833400	1.99031600	2.89578200
H	-1.04172900	2.14779800	2.33746600
H	-0.81836200	1.37500600	-1.67237900
C	-2.89660200	0.90701800	-1.65320500
H	-3.07685600	1.56299500	-2.51052600
H	-3.76832500	0.98789500	-1.00148900
C	-2.38543900	-1.44246200	-0.91820500
N	-1.14336800	-0.86691100	-0.45044400
C	-2.73744100	-0.52897300	-2.12505600
H	-3.66038500	-0.93439200	-2.54572500
H	-1.95103500	-0.61404300	-2.87950000
N	0.14882900	-2.70449600	1.18952100
N	-0.52022800	-1.93872700	0.77372000
H	-2.18781400	-2.45563200	-1.26732100
O	0.10731600	0.70338300	0.65483900
H	0.71146900	0.71993200	-0.10275400
H	-3.18803800	-1.42624900	-0.17695100
C	-4.02417800	3.32018700	0.95369800
C	-4.42731700	4.00898400	-0.35406500
H	-5.46628700	4.34811300	-0.29105200
H	-3.80029200	4.88549000	-0.55141000
H	-4.35049300	3.33458700	-1.21305600
C	-4.29454300	4.30237500	2.10898900
H	-3.76384400	5.24656600	1.94958900
H	-5.36395400	4.52183800	2.18673300
H	-3.96706200	3.88751300	3.06858600
C	-4.94930800	2.11420100	1.18628700
H	-4.73869400	1.61272600	2.13597600
H	-5.98411400	2.46848300	1.23298400
H	-4.91421500	1.36802100	0.38973700

3-d

G(298.15 K)= -748.446491

H(298.15 K)= -748.387377

C	-1.65257500	3.49327400	0.37203300
C	-1.72100900	2.74086800	-0.98363600
C	-2.15217500	1.26095400	-0.97994600
C	-1.35470000	0.53927700	0.10731800
C	-1.47528300	1.17536100	1.48104200
C	-0.93511700	2.61317300	1.41262600
H	-2.34598500	3.27852500	-1.70162500
H	-0.70424100	2.76296000	-1.38951500
H	-0.96066800	4.31584800	0.15254500
H	-2.51904400	1.16680100	1.80379900
H	-0.90773900	0.57700000	2.20202400
H	-0.99071200	3.05810600	2.40998900
H	0.12925900	2.56549900	1.15820600
H	-1.82294800	0.81890700	-1.93051800
C	-3.66828300	1.05827600	-0.87263900
H	-4.13172700	1.54830800	-1.73390700
H	-4.05601100	1.56265000	0.01571300
C	-3.40843300	-1.12946900	0.32205000
N	-1.92631800	-0.92273000	0.23298100
C	-4.08176100	-0.41245900	-0.83631000
H	-5.16360500	-0.50409200	-0.71036900
H	-3.82019400	-0.91234500	-1.77583000
N	-0.69136200	-2.51368900	-1.04118600
N	-1.29850500	-1.76945300	-0.47984900
O	-0.05423000	0.39951100	-0.32037700
H	-3.68704700	-0.71133800	1.29104500
H	0.53952900	0.28070900	0.43678200
H	-3.58956900	-2.20435900	0.34542600
C	-2.91917100	4.24035100	0.93008400
C	-3.76418500	3.46334400	1.95272800

H	-3.17216100	3.14988000	2.81814600
H	-4.55641500	4.12051800	2.32567100
H	-4.26014900	2.58254800	1.53978500
C	-2.39622200	5.49066900	1.66222200
H	-1.88350600	6.16369800	0.96734400
H	-3.22283300	6.04134900	2.12226600
H	-1.69064700	5.22254300	2.45625900
C	-3.82721200	4.71042200	-0.21119000
H	-4.31640200	3.87257500	-0.71791600
H	-4.61138000	5.36469300	0.18319700
H	-3.26149700	5.27753300	-0.95862300

3-d-TS

G(298.15 K)= -748.421361

H(298.15 K)= -748.361727

C	-1.63310800	3.48587600	0.32083400
C	-1.70415500	2.69546800	-1.01384400
C	-2.16097300	1.22984900	-0.96196100
C	-1.40281300	0.49424700	0.14628800
C	-1.58792600	1.21133100	1.52959200
C	-0.97388100	2.61295000	1.40145300
H	-2.31655800	3.22245600	-1.75012900
H	-0.68568100	2.68793900	-1.41437900
H	-0.90390500	4.27328400	0.09450900
H	-2.64877600	1.27005700	1.77361200
H	-1.08720800	0.63450900	2.31225000
H	-1.03833700	3.08854400	2.38520600
H	0.09046500	2.50071200	1.17770300
H	-1.82932000	0.74700300	-1.89376400
C	-3.67462700	1.04025100	-0.84800900
H	-4.13815300	1.44391100	-1.75301200
H	-4.07142000	1.62182400	-0.01317900
C	-3.29593900	-1.08219700	0.45897500

N	-1.86508300	-0.85359900	0.43831900	C	1.83611000	3.59252200	-0.19806000
C	-4.06252900	-0.42541400	-0.68164300	C	2.13309900	2.55746900	-1.28444300
H	-5.13206800	-0.53262600	-0.49082500	C	3.03387100	1.41405100	-0.78855700
H	-3.83988300	-0.98711900	-1.59811000	C	2.32730100	0.80015400	0.44650100
N	-0.83585200	-2.51459300	-1.61302400	C	2.07303700	1.78636800	1.57696800
N	-1.34307800	-1.72329600	-1.04498300	C	1.21083400	2.93903500	1.03680200
O	-0.06737800	0.41985300	-0.21678700	H	1.19545000	2.10294300	-1.62461900
H	-3.55783200	-0.64894700	1.44022800	H	2.59323400	3.02111400	-2.16169500
H	0.46022400	0.06345300	0.51438900	H	2.75787000	4.11142900	0.08854500
H	-3.46059700	-2.15667300	0.55596300	H	1.15275600	4.34745300	-0.59630000
C	-2.88188800	4.29891600	0.82817400	H	1.55097200	1.27933300	2.39751400
C	-2.32512700	5.55258100	1.52889800	H	3.02174100	2.17000700	1.95967700
H	-1.77211700	6.18080900	0.82321300	H	0.21790400	2.55278300	0.78154600
H	-3.13865700	6.15031600	1.95182100	H	1.07400600	3.67292100	1.83427600
H	-1.64704700	5.28538100	2.34693000	C	3.20941400	0.32499500	-1.86124000
C	-3.78028100	3.59215400	1.85726000	H	3.70288300	0.76498500	-2.73292900
H	-3.22099000	3.27853800	2.74432800	H	2.21418800	0.00324400	-2.18474200
H	-4.54779600	4.29575100	2.19538100	C	3.47511300	-1.46737400	-0.07551000
H	-4.31091400	2.72371100	1.46041800	N	3.29018200	-0.33258000	0.89391100
C	-3.74933900	4.76243100	-0.34691900	C	4.01924600	-0.87954700	-1.37089500
H	-4.25962700	3.92536000	-0.83435600	H	3.99316600	-1.67560200	-2.11940400
H	-4.51602700	5.45800100	0.00907400	H	5.06275200	-0.59512300	-1.22085800
H	-3.14920700	5.28223000	-1.10176800	N	3.51980600	-0.78969600	3.21736400

4-a

G(298.15 K)= -1028.804303

H(298.15 K)= -1028.748556

G-CAM-B3LYP(298.15 K)= -1028.775462

H-CAM-B3LYP (298.15 K)= -1028.719314

O	1.17537500	0.18950700	-0.00178400
H	2.49484000	-1.93041300	-0.20411900
H	0.56024900	0.03699900	0.73080900
H	4.16969500	-2.17381200	0.37802300
S	4.68776700	2.03254600	-0.21781400
C	5.13229800	3.15892900	-1.56784700
H	4.52439600	4.06475400	-1.55563400
H	6.17431400	3.42805400	-1.39087600
H	5.05968200	2.66695900	-2.53922400

4-a-TS

G(298.15 K)= -1028.779974

H(298.15 K)= -1028.723776

G-CAM-B3LYP(298.15 K)= -1028.750194

H-CAM-B3LYP (298.15 K)= -1028.693642

C	1.88443400	3.67148400	-0.32979600
C	2.15677200	2.60484000	-1.38813600
C	3.08147500	1.47913300	-0.90074500
C	2.35390200	0.85067700	0.38905600
C	2.10963100	1.90036800	1.46829900
C	1.25981100	3.05102900	0.92061400
H	1.21458500	2.13690500	-1.69371000
H	2.59870500	3.04131900	-2.28893900
H	2.81506500	4.18451700	-0.06192200
H	1.20859300	4.42448100	-0.74384300
H	1.59018100	1.41319800	2.30415700
H	3.07165700	2.26341800	1.83661600
H	0.25716100	2.68013500	0.67933800
H	1.14006600	3.80131400	1.70568900
C	3.21909400	0.35777800	-1.93824600
H	3.73602300	0.75099600	-2.81928300
H	2.21674700	0.05516600	-2.25626600
C	3.37892000	-1.33081900	-0.03268700
N	3.35915800	-0.12818800	0.78320000
C	3.98256600	-0.83531900	-1.38192500
H	3.92637400	-1.69496400	-2.05383600
H	5.03272400	-0.58723800	-1.22274200

N	3.05133400	-1.05468000	3.37995000
N	2.90045400	-0.69044200	2.35446700
O	1.18376400	0.26280400	-0.06961100
H	2.37967000	-1.73860600	-0.18991800
H	0.50812400	0.27881600	0.62337300
H	4.05568400	-2.05349600	0.42114900
S	4.73932400	2.11074400	-0.37505800
C	5.12897500	3.24046700	-1.73973600
H	4.51229100	4.13986600	-1.71032800
H	6.17283000	3.52087900	-1.59333600
H	5.03389700	2.74671700	-2.70843500

4b

G(298.15 K)= -1028.80375

H(298.15 K)= -1028.748635

G-CAM-B3LYP(298.15 K)= -1028.774631

H-CAM-B3LYP (298.15 K)= -1028.718907

C	3.23180600	1.06902200	-1.65035000
C	2.19877900	0.07897700	-2.19267400
C	1.83742600	-1.04490700	-1.20154400
C	1.27284100	-0.44741600	0.11401100
C	2.75323300	1.68430800	-0.34837500
H	2.57668700	-0.38161100	-3.11004200
H	1.28343300	0.61840800	-2.45212200
H	3.36999600	1.88274600	-2.36667800
H	4.20686200	0.59909000	-1.50062200
C	3.04369400	-1.94214300	-0.88020700
H	3.40603900	-2.39245200	-1.80868300
H	3.85838100	-1.30413700	-0.51782100

C	2.28028800	-2.35336200	1.47871200
C	2.75550000	-3.00482100	0.17979000
H	3.66263300	-3.58576800	0.36542600
H	1.98912100	-3.70152400	-0.17920100
H	2.01259200	-3.11062200	2.21924400
O	0.16402200	0.30576000	-0.18282100
N	2.40046500	0.54627300	0.56822500
N	2.48803000	0.79304200	1.80956900
N	2.61712100	0.96443900	2.90225900
H	3.10178700	-1.77002100	1.91405600
C	1.05877000	-1.46644500	1.22597400
H	0.21627500	-2.08057600	0.89746600
H	0.72942400	-0.95460700	2.13823000
H	3.52348200	2.27419100	0.14821400
H	-0.39083300	0.42967300	0.60132100
H	1.84591200	2.27951800	-0.48004900
S	0.41489600	-2.00699700	-1.90614600
C	1.25994700	-3.14199200	-3.04045900
H	0.46244700	-3.62856000	-3.60384600
H	1.90282300	-2.60683300	-3.74159000
H	1.83100600	-3.90489400	-2.50916200

4b-TS

G(298.15 K)= -1028.777868

H(298.15 K)= -1028.721997

G-CAM-B3LYP(298.15 K)= -1028.691587

H-CAM-B3LYP (298.15 K)= -1028.748371

C	3.32649500	1.03240800	-1.59517900
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C	2.28842500	0.09594800	-2.19287500
C	1.88200600	-1.01985800	-1.21942700
C	1.37652700	-0.34308700	0.15068600
C	2.81129300	1.61851900	-0.24580700
H	2.67563100	-0.36337700	-3.10789600
H	1.39620600	0.66632300	-2.46359200
H	3.49188900	1.90057500	-2.23812600
H	4.28916800	0.54492500	-1.43234500
C	3.01588500	-2.01280200	-0.92587900
H	3.29430800	-2.51225300	-1.85780300
H	3.89979700	-1.44995600	-0.60775600
C	2.24950000	-2.34261600	1.45932700
C	2.66758700	-3.03299300	0.16049200
H	3.53489300	-3.67354000	0.34065900
H	1.85138000	-3.68094000	-0.18076000
H	1.95075800	-3.08315200	2.20548200
O	0.30204200	0.47573000	-0.15531600
N	2.57505600	0.41245100	0.51233900
N	2.31352900	0.97852400	2.14346000
N	2.58609300	1.26008800	3.16985600
H	3.10008100	-1.79241800	1.87840400
C	1.07613500	-1.39475000	1.21690700
H	0.20415000	-1.95335300	0.86832700
H	0.77556500	-0.87677400	2.13670000
H	3.60836200	2.19015900	0.22730000
H	-0.33435100	0.47665800	0.57384500
H	1.90563900	2.20806200	-0.40076900
S	0.35914800	-1.85116900	-1.87537100
C	1.07350500	-3.11281700	-2.96513500
H	1.57760600	-3.90360200	-2.40792300
H	0.22113600	-3.54334800	-3.49338300
H	1.75139500	-2.67249800	-3.69793700

4c

G(298.15 K)= -1028.807934

H(298.15 K)= -1028.751986

G-CAM-B3LYP(298.15 K)= -1028.723933

H-CAM-B3LYP (298.15 K)= -1028.779729

C	-2.23686200	3.07244800	1.06181100
C	-1.45454200	2.85797900	-0.23876700
C	-1.63990100	1.44882000	-0.83985300
C	-1.29249500	0.43011600	0.27428400
C	-2.09783100	0.61581200	1.55631000
C	-1.86708800	2.02408400	2.10796800
H	-1.76276900	3.59554700	-0.98500000
H	-0.38811400	3.01824600	-0.04013000
H	-2.01316000	4.07502300	1.43652200
H	-3.31537100	3.04518500	0.87009800
H	-3.16201400	0.45708300	1.36242700
H	-1.76856300	-0.14867300	2.26742500
H	-2.45956400	2.15442200	3.01673600
H	-0.81238600	2.12890300	2.38323700
C	-3.07536700	1.23701100	-1.35803400
H	-3.25831900	1.97076200	-2.14873900
H	-3.78844500	1.46005800	-0.55716200
C	-3.03598500	-1.24451600	-0.86613700
N	-1.66213600	-0.96702100	-0.33529900
C	-3.33575900	-0.16952600	-1.89811100
H	-4.38654500	-0.27034900	-2.17970600
H	-2.73118800	-0.35005100	-2.78970200
N	-0.41504600	-2.75435900	0.62112900
N	-1.03213900	-1.93389600	0.19212200
H	-3.01850600	-2.24209700	-1.30510700
O	0.03193200	0.37398300	0.60952200
H	0.56987100	0.58777600	-0.17664000
H	-3.73391700	-1.22729900	-0.02475500

S	-0.42085600	1.14152700	-2.21065800
C	-0.26462400	2.77507900	-2.98357900
H	0.20486400	3.49735600	-2.31730600
H	0.37660700	2.61752600	-3.85169800
H	-1.23426800	3.13909900	-3.32600900

4c-TS

G(298.15 K)= -1028.779804

H(298.15 K)= -1028.723646

G-CAM-B3LYP(298.15 K)= -1028.694512

H-CAM-B3LYP (298.15 K)= -1028.751112

C	-2.29511900	3.13648300	1.05643400
C	-1.52490100	2.95278700	-0.25379300
C	-1.69517600	1.56365000	-0.89698900
C	-1.28435300	0.49493200	0.24173300
C	-2.09224700	0.68695900	1.52496300
C	-1.88566300	2.08995100	2.08924900
H	-1.85783300	3.69507000	-0.98540500
H	-0.45872300	3.12392800	-0.06987300
H	-2.09004200	4.14159500	1.43483700
H	-3.37517600	3.08496700	0.87827300
H	-3.15554700	0.51608300	1.34542900
H	-1.74216600	-0.08004900	2.22674900
H	-2.47471800	2.19835300	3.00317300
H	-0.83205300	2.21922200	2.35512900
C	-3.12502000	1.29424400	-1.37786100
H	-3.34965300	1.98636500	-2.19576200
H	-3.83549200	1.51385600	-0.57489100
C	-2.86256900	-1.15193300	-0.75083800
N	-1.50414400	-0.75671600	-0.47036500
C	-3.30275300	-0.13839300	-1.85343100
H	-4.35046000	-0.37139900	-2.05505600

H	-2.72409100	-0.32956100	-2.75813200
N	-0.26233500	-2.81739000	0.96934700
N	-0.85921500	-1.94738000	0.66379100
H	-2.85368200	-2.15697100	-1.17149500
O	0.04827000	0.58263300	0.58019700
H	0.57964300	0.69530300	-0.22783200
H	-3.52848800	-1.08712500	0.11116400
S	-0.48420300	1.31573800	-2.28125400
C	-0.38860300	2.96629800	-3.02747000
H	0.07900000	3.68861200	-2.35985200
H	0.23688600	2.83869000	-3.91198900
H	-1.37411300	3.31206000	-3.34265700

4d

G(298.15 K)= **-1028.806166**

H(298.15 K)= **-1028.751487**

G-CAM-B3LYP(298.15 K)= **-1028.777144**

H-CAM-B3LYP (298.15 K)= **-1028.721862**

C	-1.29678400	3.61130700	0.51800600
C	-1.10314400	2.92522500	-0.83859800
C	-1.78341500	1.54718900	-0.91900300
C	-1.28382300	0.69573300	0.27371500
C	-1.49989900	1.35868700	1.63175300
C	-0.79784800	2.72107800	1.65576000
H	-1.49160300	3.54418800	-1.65385400
H	-0.02904700	2.79696000	-1.00572600
H	-0.74458800	4.55500400	0.51424200
H	-2.34986200	3.86699300	0.67841000
H	-2.56665700	1.49225400	1.82768900

H	-1.11324800	0.68727900	2.40584200
H	-0.97472300	3.19109000	2.62593200
H	0.28439600	2.57624800	1.56052000
C	-3.32253900	1.67738700	-0.87468900
H	-3.63021800	2.28497500	-1.72949300
H	-3.61547800	2.22840000	0.02459000
C	-3.61579000	-0.55910200	0.24856500
N	-2.11908000	-0.62278000	0.29400300
C	-4.05981200	0.33525000	-0.89944000
H	-5.13486800	0.50194800	-0.79478200
H	-3.90548100	-0.18074200	-1.85225100
N	-1.05348600	-2.46534100	-0.77488600
N	-1.57332300	-1.59182900	-0.32359000
O	0.02296200	0.32705000	0.06537200
H	-3.90651400	-0.16167500	1.22215700
H	0.45820300	0.13007100	0.90867000
H	-3.98567600	-1.58168300	0.17295600
S	-1.41875500	0.69697100	-2.52052200
C	0.31849100	1.07930600	-2.88466500
H	0.96860000	0.77133500	-2.06815800
H	0.55214000	0.49553000	-3.77657500
H	0.45195900	2.13650900	-3.11303700

4d-TS

G(298.15 K)= **-1028.782299**

H(298.15 K)= **-1028.726797**

G-CAM-B3LYP(298.15 K)= **-1028.697882**

H-CAM-B3LYP (298.15 K)= **-1028.7534**

C	-1.65485700	3.65920400	0.32637200
C	-1.86704500	3.02998700	-1.05297600
C	-2.44081400	1.60637900	-0.98972900

C	-1.52618700	0.72052700	-0.07542300
C	-1.38469800	1.38035800	1.36815500
C	-0.77078900	2.76916300	1.19552200
H	-2.54301700	3.63988300	-1.66046000
H	-0.89923200	3.00067900	-1.56229300
H	-1.18484800	4.63749200	0.19568900
H	-2.61303800	3.83716400	0.82722800
H	-2.35724300	1.45498000	1.85504300
H	-0.74811800	0.72767600	1.97062700
H	-0.64884900	3.19487000	2.19580400
H	0.22544700	2.67704200	0.75302800
C	-3.87559300	1.57369000	-0.42548100
H	-4.53056100	2.11552800	-1.11215700
H	-3.90310300	2.11538000	0.52388600
C	-3.42249300	-0.68920800	0.61463800
N	-2.01746600	-0.57280700	0.26690400
C	-4.38915900	0.14834400	-0.21872700
H	-5.35429600	0.16416100	0.29147900
H	-4.54760600	-0.35143300	-1.18051600
N	-1.60066800	-2.41757800	-1.79078500
N	-1.89306200	-1.46117100	-1.32775000
O	-0.28048900	0.60085300	-0.66600500
H	-3.41436400	-0.37734000	1.67263900
H	0.31726700	0.10385000	-0.08657800
H	-3.66552300	-1.75323900	0.63316500
S	-2.56562800	0.87053700	-2.66910900
C	-1.04610700	1.35405900	-3.53022200
H	-0.16989500	1.04328500	-2.96342800
H	-1.07964200	0.82215200	-4.48211600
H	-1.02741000	2.42683100	-3.72211000

5a

G(298.15 K)= -705.833815

H(298.15 K)= -705.779563

C	1.82129800	3.64089800	-0.22464200
C	2.02950400	2.60078100	-1.32654500
C	2.94121800	1.46352800	-0.84933900
C	2.27939400	0.83142400	0.40167600
C	2.09940100	1.83415200	1.53081000
C	1.22937900	2.99625700	1.03009300
H	1.07048200	2.16309000	-1.62247900
H	2.46291600	3.05124200	-2.22491100
H	2.78069700	4.10958700	0.02368300
H	1.15725400	4.43176100	-0.58353500
H	1.62462200	1.34794500	2.39150900
H	3.08139000	2.20602900	1.83518600
H	0.22299500	2.62222400	0.81015700
H	1.13169600	3.72962800	1.83400600
C	3.15698900	0.38916400	-1.92315300
H	3.55819600	0.85596300	-2.82693900
H	2.18487200	-0.03587000	-2.19048700
C	3.57998200	-1.36582800	-0.16241500
N	3.26538900	-0.28104900	0.81916000
C	4.10513100	-0.70511800	-1.42926300
H	4.21495600	-1.48692100	-2.18467000
H	5.09540300	-0.28639500	-1.23013700
N	3.86136600	-0.54558500	3.09967900
N	3.56667000	-0.43845100	2.02836100
O	1.11748600	0.21028300	0.00495600
H	2.64412200	-1.90276600	-0.33397000
H	0.55327600	0.02687100	0.77033500
H	4.31033900	-2.02881000	0.30046900
C	4.99908600	2.65627200	-1.24714600
H	4.52112200	3.57749900	-1.59784000
H	5.90232100	2.91722800	-0.69545200
H	5.27912000	2.04613700	-2.11305900

O 4.17600600 1.94563800 -0.33963300

5a-TS

G(298.15 K)= -705.808124

H(298.15 K)= -705.753419

C 1.85840100 3.70809600 -0.37599200

C 2.05983100 2.63085700 -1.44076300

C 3.01871500 1.53392700 -0.97050800

C 2.37006400 0.89502800 0.35597500

C 2.18146900 1.96657200 1.42216400

C 1.29181100 3.10035700 0.90698100

H 1.10493200 2.16253700 -1.69675100

H 2.46340100 3.05596100 -2.36587400

H 2.81538600 4.19516500 -0.15626500

H 1.18201000 4.47788700 -0.75642400

H 1.72891600 1.50103300 2.30769800

H 3.16913000 2.34226600 1.70051800

H 0.28248500 2.71734800 0.71601500

H 1.20175200 3.85904600 1.68814100

C 3.19552800 0.40865200 -1.99139500

H 3.63836900 0.81590100 -2.90526800

H 2.21203700 0.01291400 -2.25843500

C 3.48111600 -1.24199200 -0.09030700

N 3.41179600 -0.05232700 0.73121100

C 4.08133200 -0.68425200 -1.41719700

H 4.15262900 -1.54668100 -2.08371100

H 5.08754500 -0.30833500 -1.22151700

N 3.10385200 -1.03770300 3.31908200

N 2.95914900 -0.64426100 2.30370000

O 1.19252900 0.27615300 -0.03949500

H 2.50166800 -1.68677700 -0.27519600

H 0.55268500 0.28582800 0.68676200

H 4.18106400 -1.94548800 0.35834100

C 4.97464900 2.84491800 -1.46610400

H 4.47975400 3.80541600 -1.64300100

H 5.95184100 3.02623000 -1.01904000

H 5.11360900 2.33068400 -2.42298700

O 4.26053800 2.04833500 -0.53295000

5b

G(298.15 K)= -705.774925

H(298.15 K)= -705.829047

C 3.21964200 1.02923800 -1.69467500

C 2.24914700 -0.02049400 -2.24222800

C 1.92299200 -1.12815400 -1.22738700

C 1.29661500 -0.50515200 0.05360700

C 2.71360900 1.64320500 -0.40080200

H 2.68672700 -0.47227900 -3.13622800

H 1.30623500 0.45194400 -2.53470500

H 3.33358400 1.84146400 -2.41671700

H 4.21179500 0.60041300 -1.53183100

C 3.15437000 -1.96449600 -0.84905100

H 3.56581700 -2.40728900 -1.76176100

H 3.93281800 -1.30603500 -0.45016300

C 2.26798600 -2.39638700 1.46220700

C 2.82163800 -3.03603000 0.18888400

H 3.71760900 -3.61744400 0.42068100

H 2.07754800 -3.72974500 -0.21870600

H 1.97655800 -3.16029300 2.18698200

O 0.19171300 0.22628700 -0.29927000

N 2.38718600 0.50616600 0.52818200

N 2.41314900 0.78276400 1.76788400

N 2.49126100 0.97886200 2.86086200

H 3.05345400 -1.79733200 1.94076900

C 1.04352400 -1.53482500 1.14411300

H	0.24463800	-2.16446600	0.74233900
H	0.64122900	-1.04394900	2.03895900
H	3.46601100	2.25960100	0.09099500
H	-0.41187200	0.31845600	0.45194200
H	1.79106300	2.21083300	-0.54423500
C	1.14719400	-2.80530700	-2.77995700
H	0.19167200	-3.22997800	-3.08900800
H	1.58400100	-2.27034300	-3.62957200
H	1.81758200	-3.62143600	-2.48803000
O	0.85838800	-1.94203800	-1.69397600

5b-TS

G(298.15 K)= -705.809038

H(298.15 K)= -705.754095

C	3.33294100	0.97162500	-1.59257400
C	2.35403400	-0.02606200	-2.19156200
C	1.97525800	-1.11891600	-1.18675700
C	1.44583900	-0.41251300	0.16868700
C	2.77094800	1.59507300	-0.28649400
H	2.80088800	-0.48925500	-3.07620000
H	1.43869300	0.48469000	-2.50480000
H	3.49491500	1.81593400	-2.26685900
H	4.30490600	0.51788200	-1.38832100
C	3.11180300	-2.09715100	-0.88947200
H	3.38552600	-2.59620500	-1.82488200
H	3.99310500	-1.53082700	-0.57115300
C	2.33516600	-2.40972600	1.48333000
C	2.74506000	-3.11494500	0.19121500
H	3.59732000	-3.77511000	0.37125200
H	1.91595800	-3.74257900	-0.15711500
H	2.04819200	-3.14033000	2.24423900
O	0.33665800	0.37345300	-0.11514300
N	2.55592500	0.41776200	0.53765600

N	2.11705900	1.07394100	2.07465100
N	2.26015300	1.50160000	3.07635000
H	3.18484100	-1.84471000	1.88543700
C	1.15688600	-1.47472300	1.22890100
H	0.29707300	-2.04214800	0.86246100
H	0.83092800	-0.95564700	2.13784000
H	3.53304800	2.21694600	0.18100400
H	-0.25941800	-0.16389200	-0.66226600
H	1.85033300	2.14489700	-0.48495800
C	0.85448000	-2.62369800	-2.70476600
H	1.44323400	-3.52102400	-2.49146500
H	-0.17146500	-2.91387300	-2.92815700
H	1.27720300	-2.10524600	-3.57080600
O	0.77934900	-1.77015800	-1.56876700

5c

G(298.15 K)= -705.838163

H(298.15 K)= -705.783637

C	-2.23527400	3.11675900	1.14747600
C	-1.45740000	2.94994100	-0.16183700
C	-1.62569100	1.55847200	-0.79454400
C	-1.28526600	0.50359200	0.28503300
C	-2.05641500	0.64720600	1.58699300
C	-1.83726500	2.04826400	2.16377500
H	-1.77492800	3.70360100	-0.88904400
H	-0.38799600	3.10359800	0.02718100
H	-2.03823500	4.11329900	1.55144600
H	-3.31391700	3.06497200	0.95751200
H	-3.12222900	0.47434500	1.40725800
H	-1.70311800	-0.12677700	2.27577000
H	-2.41776300	2.15081600	3.08378400
H	-0.78012200	2.16247600	2.42614300
C	-3.03307300	1.34919100	-1.37229300

H	-3.23298200	2.14310700	-2.09751600
H	-3.77786500	1.46880600	-0.57894400
C	-2.96161300	-1.13880700	-1.03544000
N	-1.65345700	-0.87098300	-0.36468600
C	-3.18266800	-0.01756000	-2.03652500
H	-4.18794000	-0.13393000	-2.44718900
H	-2.46664700	-0.11888300	-2.85611900
N	-0.36382800	-2.68397800	0.46769100
N	-1.00038400	-1.85146900	0.08922200
H	-2.88845500	-2.11599200	-1.51296600
O	0.05691800	0.45364800	0.54669600
H	0.51378800	0.68238900	-0.28449200
H	-3.73650400	-1.16670400	-0.26376800
C	-0.50981700	2.23991100	-2.83847800
H	-0.16006700	3.21149300	-2.47818500
H	0.22776500	1.82652500	-3.52558600
H	-1.45765100	2.36800200	-3.37150900
O	-0.63038700	1.30072800	-1.77965900

5c-TS

G(298.15 K)= -705.808846

H(298.15 K)= -705.75431

C	-2.31041800	3.15810400	1.13555900
C	-1.55354200	3.04267900	-0.18923500
C	-1.68985200	1.67526200	-0.86989500
C	-1.26118700	0.56586500	0.21211700
C	-2.03549100	0.69656200	1.52039000
C	-1.85269900	2.08697500	2.12315400
H	-1.91000300	3.80169300	-0.89327200
H	-0.48620400	3.22261200	-0.01836700
H	-2.13943700	4.15410500	1.55208900
H	-3.39021900	3.07095000	0.96658600
H	-3.09805600	0.50207700	1.35505800

H	-1.65088700	-0.08076800	2.19181500
H	-2.42314700	2.15066700	3.05300500
H	-0.79678400	2.23451800	2.37038100
C	-3.09144200	1.39214400	-1.40765600
H	-3.32019000	2.12569000	-2.18711300
H	-3.83572000	1.53501800	-0.61924700
C	-2.80833500	-1.05929800	-0.87250600
N	-1.46571200	-0.67144800	-0.53233200
C	-3.17154600	-0.01418300	-1.97384100
H	-4.18244600	-0.27443500	-2.29445000
H	-2.49178600	-0.13339200	-2.81931900
N	-0.23693800	-2.75504600	0.87238300
N	-0.84121300	-1.88402500	0.58422000
H	-2.78623900	-2.05640400	-1.31115400
O	0.08651200	0.67720600	0.48626300
H	0.53831700	0.82913600	-0.36191200
H	-3.52066200	-1.00068600	-0.04650500
C	-0.58290500	2.50910300	-2.85770900
H	-0.18011100	3.42934000	-2.42615600
H	0.11554700	2.12570400	-3.60046500
H	-1.53969600	2.72224900	-3.34581400
O	-0.71224800	1.48289100	-1.88054700

5d

G(298.15 K)= -705.831431

H(298.15 K)= -705.778769

C	-1.24479200	3.61484700	0.50933300
C	-0.98361400	2.90467900	-0.82505900
C	-1.67953900	1.53926300	-0.89614800
C	-1.23647400	0.71393100	0.33745500
C	-1.53177200	1.38102800	1.67140200
C	-0.82793700	2.74589000	1.69844700
H	-1.32666600	3.51373300	-1.66781700
H	0.09575300	2.75967600	-0.93596200

H	-0.68254800	4.55223300	0.52486700
H	-2.30244900	3.88550800	0.59926800
H	-2.60697200	1.51815000	1.80872800
H	-1.18143600	0.72868600	2.47835400
H	-1.06365200	3.24519100	2.64109400
H	0.25675600	2.59330600	1.67687600
C	-3.21212200	1.68305500	-0.93075000
H	-3.45500200	2.27496500	-1.81726300
H	-3.56734800	2.24323400	-0.06148900
C	-3.52978400	-0.55695000	0.16850000
N	-2.03271300	-0.62390900	0.27429900
C	-3.92374200	0.33071100	-1.00173300
H	-5.00732600	0.46839400	-0.97284900
H	-3.67707100	-0.17286300	-1.94072400
N	-0.97870000	-2.21995500	-1.15945800
N	-1.48995900	-1.45174400	-0.54179300
O	0.08958100	0.37505700	0.18694100
H	-3.85075700	-0.15743300	1.13125100
H	0.47033300	0.12054900	1.04101700
H	-3.89587700	-1.58062700	0.08590900
C	-0.12626800	0.94824500	-2.71374600
H	0.72305500	0.77817600	-2.04855600
H	-0.11333200	0.20474300	-3.51220600
H	-0.05446300	1.94469200	-3.15960800
O	-1.37206900	0.76635400	-2.04966800

5d-TS

G(298.15 K)= -705.810484

H(298.15 K)= -705.754725

C	-1.59867200	3.71967100	0.41223100
C	-1.84894700	3.16777800	-0.99346100
C	-2.42021600	1.74441700	-0.99134800
C	-1.52276200	0.82960200	-0.10995600
C	-1.34052800	1.39060200	1.34613800

C	-0.71094200	2.78129900	1.22472500
H	-2.53808400	3.82109800	-1.53766600
H	-0.90487600	3.14962200	-1.55098900
H	-1.12557900	4.70141700	0.32826000
H	-2.54919100	3.87427600	0.93623400
H	-2.30143600	1.45872400	1.85935900
H	-0.69448300	0.70023000	1.89204600
H	-0.56867200	3.16309100	2.23972400
H	0.27507700	2.69000500	0.76115400
C	-3.87663100	1.69049800	-0.51683200
H	-4.49329800	2.27931900	-1.20152100
H	-3.96401600	2.17432100	0.46085100
C	-3.48142700	-0.59815700	0.43640900
N	-2.06734100	-0.49345200	0.17415200
C	-4.38397000	0.25538300	-0.44369100
H	-5.39853900	0.21520800	-0.04385400
H	-4.40412600	-0.19243200	-1.44419000
N	-1.60937500	-2.12496400	-2.17936100
N	-1.90969100	-1.34870900	-1.46329800
O	-0.26500000	0.66869200	-0.65576500
H	-3.50518900	-0.26859100	1.49234300
H	-0.36591700	0.75406400	-1.61988100
H	-3.73859600	-1.65875000	0.46396400
C	-2.83641400	1.78483000	-3.39054900
H	-2.34751200	2.74561400	-3.57337300
H	-2.66461200	1.12638700	-4.24141200
H	-3.91337400	1.93783500	-3.27058900
O	-2.27557500	1.12169900	-2.26466000

6c

G(298.15 K)= -1185.884643

H(298.15 K)= -1185.816215

C	-2.17305800	3.04148600	1.07356900
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C	-1.41293800	2.76818500	-0.23680800
C	-1.66254100	1.37248200	-0.84283700
C	-1.32845800	0.33945400	0.25858600
C	-2.10525600	0.56107000	1.54866500
C	-1.81686600	1.95935600	2.10002300
H	-1.68269600	3.51263900	-0.98992400
H	-0.33725500	2.86761300	-0.04845700
H	-3.25294500	2.96255100	0.87810100
H	-3.17756300	0.44149700	1.37139100
H	-1.79600900	-0.21085500	2.26085900
H	-2.39697700	2.08542700	3.01636000
H	-0.75631100	2.02317500	2.36893600
C	-3.11062500	1.20873000	-1.34282300
H	-3.28103900	1.95211900	-2.12737100
H	-3.80693300	1.44862600	-0.53256500
C	-3.14376600	-1.27393400	-0.85985600
N	-1.75544200	-1.04266900	-0.34442100
C	-3.42182600	-0.18654900	-1.88509700
H	-4.47894700	-0.25266100	-2.15294600
H	-2.83551700	-0.38346200	-2.78526200
N	-0.55777200	-2.87536600	0.58904200
N	-1.15150800	-2.03189300	0.17183300
H	-3.16282900	-2.27041000	-1.30157400
O	-0.00109300	0.23733400	0.57200700
H	0.53077300	0.43369200	-0.22279100
H	-3.83058300	-1.23737300	-0.01005500
C	-1.94953500	4.49598600	1.58647000
C	-2.61073900	5.48914200	0.61965300
H	-2.50169100	6.50902000	1.00200100
H	-2.15789600	5.46537300	-0.37564900
H	-3.68096000	5.28040300	0.51460700
C	-2.61680500	4.66249500	2.95946500
H	-2.08215500	4.11664700	3.74180800

H	-2.62399500	5.71959900	3.24279600
H	-3.65429400	4.30991600	2.94047000
C	-0.46085000	4.84576500	1.71681500
H	-0.35458500	5.82626400	2.19198300
H	0.07647900	4.11902500	2.33484100
H	0.03302100	4.90026300	0.74190400
S	-0.47532400	1.03261100	-2.23582100
C	-0.27461800	2.66246900	-3.00640200
H	0.23194500	3.36583900	-2.34675100
H	0.34525400	2.48463900	-3.88607000
H	-1.23658000	3.06156300	-3.33136900

6c-TS

G(298.15 K)= -1185.856474

H(298.15 K)= -1185.788023

C	-2.21369600	3.10519900	1.06154400
C	-1.45934800	2.84519100	-0.25229300
C	-1.70118500	1.46594400	-0.89089000
C	-1.31995600	0.38740100	0.24296300
C	-2.10785200	0.63142200	1.52622200
C	-1.83570100	2.02651600	2.08331200
H	-1.74283500	3.59182000	-0.99909000
H	-0.38345500	2.94804300	-0.07372100
H	-3.29404200	3.01407500	0.87310200
H	-3.17914600	0.50795900	1.35518200
H	-1.79125100	-0.14246700	2.23654100
H	-2.41822800	2.14179000	2.99972300
H	-0.77653500	2.10621400	2.35025400
C	-3.14405100	1.25075300	-1.36077000
H	-3.34741500	1.94761700	-2.18008100
H	-3.84124900	1.49990900	-0.55518800
C	-2.97455200	-1.20064600	-0.72180600
N	-1.59878400	-0.86026700	-0.45542600

C	-3.37994100	-0.17637600	-1.82816000	C	-1.85486100	1.45130300	-0.96120000
H	-4.43716600	-0.36930200	-2.02250600	C	-1.32538900	0.63743800	0.24097100
H	-2.81467900	-0.39510400	-2.73505800	C	-1.47150500	1.37242800	1.56863100
N	-0.42251500	-2.95044900	0.99690600	C	-0.74995100	2.72378500	1.50606600
N	-0.99154100	-2.06432600	0.68457300	H	-1.53335800	3.38776100	-1.80660100
H	-3.01166200	-2.20797400	-1.13548600	H	-0.07828300	2.64548600	-1.13647500
O	0.01825600	0.42022200	0.56875100	H	-2.35224700	3.77456200	0.55856900
H	0.54590100	0.50810100	-0.24484100	H	-2.52732400	1.53325600	1.80074000
H	-3.63044900	-1.10168100	0.14485000	H	-1.06381600	0.73587000	2.36132000
C	-2.00223600	4.56183100	1.57451600	H	-0.88917800	3.21408200	2.47136700
C	-2.66952400	5.55071800	0.60744700	H	0.32707700	2.55829600	1.37970000
H	-2.57441900	6.57015600	0.99452500	C	-3.38948400	1.60862100	-0.87430800
H	-2.21008800	5.53721400	-0.38512300	H	-3.71454600	2.18954800	-1.74128000
H	-3.73658700	5.33026700	0.49473200	H	-3.64700400	2.19581300	0.01230100
C	-2.67307500	4.72139600	2.94647800	C	-3.68154200	-0.56900500	0.35229400
H	-2.13731400	4.17648100	3.72863700	N	-2.18495300	-0.65992800	0.35352300
H	-2.68592700	5.77779100	3.23217500	C	-4.14594000	0.27811700	-0.82280700
H	-3.70878800	4.36387000	2.92439600	H	-5.21538800	0.46492100	-0.69723500
C	-0.51648600	4.92302800	1.70720000	H	-4.02403900	-0.28147900	-1.75550700
H	-0.41917200	5.90668200	2.17767600	N	-1.19624200	-2.56524000	-0.67998300
H	0.02449100	4.20386300	2.33068400	N	-1.68035800	-1.66347000	-0.24520100
H	-0.02008300	4.97651700	0.73351200	O	-0.03662500	0.22845900	-0.00270900
S	-0.51404900	1.16728000	-2.28808500	H	-3.93129900	-0.11817800	1.31407800
C	-0.34871800	2.81141200	-3.03594400	H	0.43096500	0.06600800	0.83041300
H	0.16010500	3.51143800	-2.37438600	H	-4.07204000	-1.58663500	0.33889000
H	0.26057600	2.65319700	-3.92686700	C	-0.63714200	5.00874300	0.28787600
H	-1.31970400	3.20358300	-3.34193900	C	-0.71440900	5.67908300	1.66741700
6d				H	-0.03798200	5.21085200	2.38814500
G(298.15 K)= -1185.882789				H	-0.42950700	6.73265700	1.58644000
H(298.15 K)= -1185.815795				H	-1.73222000	5.63436400	2.07184300
				C	-1.42445700	5.87873700	-0.70281000
C	-1.28526500	3.59466000	0.36170700	H	-1.36136600	5.50048100	-1.72683700
C	-1.14469600	2.81559800	-0.95826200	H	-2.48186700	5.93311500	-0.42161500

H	-1.02307400	6.89710200	-0.70587600
C	0.83112900	4.95633800	-0.15537300
H	1.26638800	5.95965300	-0.10314600
H	1.42979300	4.30388800	0.48854500
H	0.93303500	4.60757100	-1.18757500
S	-1.55766200	0.54173600	-2.54521800
C	0.17468300	0.87687000	-2.97510500
H	0.84519300	0.56358000	-2.17726200
H	0.36257000	0.27752500	-3.86749400
H	0.32611100	1.92800000	-3.22118500

6d-TS

G(298.15 K)= **-1185.8584**

H(298.15 K)= **-1185.790891**

C	-1.24369700	3.57416100	0.32807200
C	-1.20990400	2.81577800	-1.00940300
C	-1.35359700	0.57873800	0.17769500
C	-1.46511700	1.36762100	1.55380700
C	-0.67138200	2.66527500	1.41978300
H	-1.68024900	3.40209600	-1.80381300
H	-0.16262100	2.65965200	-1.28683400
H	-2.29272600	3.78875700	0.57971000
H	-2.50634800	1.58134300	1.79519400
H	-1.05492700	0.72612400	2.33786700
H	-0.70205900	3.15051800	2.39969400
H	0.37432500	2.42546100	1.20495700
C	-3.45041300	1.60155000	-0.78705400
H	-3.86098200	2.12849600	-1.65197300
H	-3.64721700	2.23257100	0.08362400
C	-3.50837500	-0.56787300	0.50687900
N	-2.05671700	-0.62175500	0.49063600
C	-4.15007700	0.25412600	-0.60693100
H	-5.20264700	0.40476100	-0.35929100

H	-4.12211900	-0.32931800	-1.53369900
N	-1.42551400	-2.69379400	-1.27205300
N	-1.68821300	-1.67056900	-0.95829800
O	-0.02925200	0.27955000	-0.09182800
H	-3.70379500	-0.13279400	1.50133200
H	0.35696200	-0.21028600	0.65045400
H	-3.87229800	-1.59526100	0.56343900
C	-0.54253700	4.96293200	0.25763600
C	-0.86710900	5.75185800	1.53504000
H	-0.47663100	5.26491900	2.43305000
H	-0.41755900	6.74847800	1.48212500
H	-1.94901400	5.87517400	1.65471200
C	-1.08191300	5.76065000	-0.93792400
H	-0.73507200	5.35282000	-1.89169000
H	-2.17794000	5.77031400	-0.94532300
H	-0.73541600	6.79706000	-0.87916700
C	0.98132800	4.83945600	0.12674100
H	1.41944400	5.83469400	0.00016100
H	1.43122800	4.39345400	1.01872200
H	1.27188800	4.23957400	-0.74178300
S	-1.73530300	0.58355800	-2.59034200
C	-0.00942100	0.83446500	-3.08367100
H	0.66522000	0.47774900	-2.30693200
H	0.11516000	0.23749000	-3.98818900
H	0.18399500	1.88120500	-3.31856200
C	-1.92658700	1.45592500	-0.98271100

7a

G(298.15 K)= **-822.262656**

H(298.15 K)= **-822.203642**

C	1.72441100	3.49933100	-0.32137500
C	2.13455700	2.42040000	-1.32472000

C	3.09541700	1.38269900	-0.69173500
C	2.29414700	0.78735200	0.49919700
C	1.88488800	1.80605800	1.55682400
C	1.01992100	2.88706800	0.88993900
H	1.24759800	1.89011200	-1.68465400
H	2.61373500	2.86803300	-2.19778200
H	2.61438000	4.04929900	0.00844300
H	1.06138400	4.22165600	-0.80540900
H	1.31642100	1.30792800	2.35156200
H	2.76402000	2.26610100	2.01084300
H	0.06815800	2.44590100	0.57558400
H	0.79002100	3.65202800	1.63528500
C	3.38768400	0.23305000	-1.68573900
H	3.90836200	0.64404200	-2.55447600
H	2.43987800	-0.18400300	-2.03828300
C	3.57215900	-1.46036100	0.18200700
N	3.20836500	-0.31969900	1.09568500
C	4.24096500	-0.86359000	-1.04676700
H	4.40088600	-1.68196900	-1.75319400
H	5.22206300	-0.46833900	-0.76698800
N	2.96372000	-0.82890900	3.40948500
N	3.04237900	-0.61482400	2.31944400
O	1.19945900	0.12548200	-0.02701300
H	2.64293600	-1.97921500	-0.06401100
H	0.51838500	0.00216000	0.65043300
H	4.23861700	-2.11792000	0.73986900
C	4.43116300	2.05890200	-0.32186700
C	5.09352600	2.75137700	-1.34900200
C	5.07555000	2.00173300	0.91919000
C	6.32024200	3.37162900	-1.14339200
H	4.65162900	2.80779700	-2.33863500
C	6.30636200	2.62424000	1.13133400
H	4.64985500	1.46551700	1.75558300

C	6.93548800	3.31565200	0.10473900
H	6.79593600	3.89757900	-1.96479000
H	6.76856100	2.55578900	2.11068200
H	7.89295800	3.79817100	0.26995900

7a-TS

G(298.15 K)= -822.239386

H(298.15 K)= -822.179691

C	1.77966600	3.62275700	-0.49654100
C	2.26660100	2.51441000	-1.42798100
C	3.14998200	1.47015500	-0.70350400
C	2.16592000	0.87338600	0.43379200
C	1.67698300	1.95697300	1.39133000
C	0.92161900	3.04953800	0.63121100
H	1.41307000	1.99393800	-1.87174100
H	2.84752600	2.93589600	-2.25193900
H	2.64231800	4.15226000	-0.07332000
H	1.20193000	4.35363300	-1.06885300
H	1.02071800	1.48517900	2.13495400
H	2.52282200	2.38955800	1.92729000
H	-0.00575400	2.64121500	0.21403200
H	0.63441400	3.83177200	1.33793400
C	3.49456100	0.28899100	-1.63122800
H	4.15618400	0.64456500	-2.42567600
H	2.57993000	-0.08203900	-2.10165100
C	3.27060500	-1.31301900	0.31442700
N	3.03138500	-0.09824500	1.07946600
C	4.17662200	-0.82240000	-0.84816800
H	4.36185300	-1.70481100	-1.46527300
H	5.13175800	-0.48383200	-0.43855400
N	2.06037000	-1.00647600	3.50265500
N	2.18439000	-0.64553400	2.47233100
O	1.11458900	0.25429800	-0.23621700
H	2.34771300	-1.74109800	-0.07929000

H	0.30236800	0.32610400	0.28455100
H	3.81860100	-2.01601600	0.94026800
C	4.44958300	2.12946700	-0.20515300
C	4.95104900	2.10514100	1.10126700
C	5.22221400	2.78786300	-1.17590000
C	6.15455100	2.73288800	1.42542600
H	4.42722400	1.58361200	1.89086700
C	6.42328600	3.40936700	-0.85686000
H	4.89240800	2.81207900	-2.20972300
C	6.89575000	3.39170700	0.45336800
H	6.50794300	2.69558600	2.45073000
H	6.98957800	3.90659400	-1.63757500
H	7.83074900	3.87919700	0.70854000

7b

G(298.15 K)= -822.262511

H(298.15 K)= -822.204088

C	3.07532000	0.96000800	-1.72612800
C	2.04086000	-0.09433800	-2.12219000
C	1.79291300	-1.18228500	-1.04606200
C	1.32348400	-0.49935800	0.26868800
C	2.72009800	1.62304000	-0.40801900
H	2.36791400	-0.59258900	-3.03876700
H	1.08485500	0.39150700	-2.34363900
H	3.11141600	1.74480800	-2.48620600
H	4.07699200	0.52771700	-1.65977400
C	3.09206900	-1.96152100	-0.71765000
H	3.46037700	-2.44430200	-1.62483600
H	3.87375200	-1.25871900	-0.41173100
C	2.45685900	-2.29145900	1.69004200
C	2.89194100	-2.98512100	0.39953500
H	3.82324000	-3.53208700	0.56870900
H	2.13433500	-3.71882000	0.09922700

H	2.24461900	-3.02094400	2.47507700
O	0.21223000	0.27198600	0.03089800
N	2.48860500	0.52001900	0.58566700
N	2.67893100	0.82387200	1.80101900
N	2.89990000	1.04494400	2.87037500
H	3.28084700	-1.66870500	2.06056400
C	1.19876400	-1.45015400	1.45413400
H	0.36222900	-2.11192100	1.21717100
H	0.90199500	-0.89271200	2.35122000
H	3.52504500	2.24836900	-0.02191500
H	-0.24235100	0.48930900	0.85887800
H	1.79128200	2.19540600	-0.46769400
C	0.72995400	-2.14778600	-1.61430800
C	1.12062800	-2.97690400	-2.67754500
C	-0.60292500	-2.22942300	-1.19462800
C	0.23314100	-3.86384900	-3.27632600
H	2.13535800	-2.93319000	-3.05951600
C	-1.49328700	-3.12334600	-1.78955800
H	-0.97859000	-1.58608900	-0.41118000
C	-1.08277200	-3.94880800	-2.82891700
H	0.57480700	-4.48914000	-4.09485600
H	-2.51726000	-3.16377800	-1.43221300
H	-1.77782800	-4.64363700	-3.28856000

7b-TS

G(298.15 K)= -822.237442

H(298.15 K)= -822.178209

C	3.42759700	0.62519000	-1.76073700
C	2.40474800	-0.42119000	-2.17467900
C	1.92608800	-1.31165900	-1.00828400

C	1.42914100	-0.33868100	0.20568600
C	2.88489700	1.47853800	-0.58539700
H	2.82215100	-1.07527300	-2.94690100
H	1.54446600	0.08720200	-2.61722800
H	3.61287500	1.33164700	-2.57363500
H	4.38637600	0.18871200	-1.47584300
C	3.08043400	-2.18968100	-0.47239000
H	3.34336400	-2.91256400	-1.25117500
H	3.96317900	-1.55875300	-0.33752400
C	2.32096400	-1.95180900	1.94595700
C	2.81470500	-2.90616100	0.86035500
H	3.73953000	-3.39311000	1.18218700
H	2.06879100	-3.69655600	0.74024900
H	2.03766900	-2.51278200	2.84003800
O	0.38833300	0.50884900	-0.15853900
N	2.61095700	0.46356300	0.41737600
N	2.25705900	1.37791800	1.83424800
N	2.43694900	1.91046500	2.77795200
H	3.12020000	-1.26324500	2.24092000
C	1.11097600	-1.16755300	1.44725900
H	0.29949500	-1.85267300	1.17561700
H	0.71352500	-0.48688800	2.20972000
H	3.67141500	2.13476400	-0.21446000
H	-0.45700000	0.09091500	0.05610000
H	1.99206200	2.03275800	-0.87957300
C	0.71886900	-2.13163700	-1.49657900
C	0.74040500	-3.53204100	-1.51605600
C	-0.40837600	-1.49786500	-2.04688900
C	-0.32963200	-4.26723100	-2.02176500
H	1.60356900	-4.07799400	-1.15985400
C	-1.48224100	-2.23075100	-2.54172800
H	-0.45313600	-0.41737300	-2.10888500
C	-1.45341400	-3.62221900	-2.52480500

H	-0.27417100	-5.35084400	-2.02242100
H	-2.33866200	-1.70659300	-2.95325400
H	-2.28958000	-4.19468400	-2.91257200

7c

G(298.15 K)= -822.264883

H(298.15 K)= -822.205853

C	-2.18754500	3.07191400	1.06920600
C	-1.33599600	2.78602200	-0.16876100
C	-1.51745400	1.36552100	-0.77852400
C	-1.31972900	0.37331600	0.39440900
C	-2.19579700	0.63540400	1.61785600
C	-1.93499900	2.03876500	2.16190300
H	-1.56941700	3.52244300	-0.94029000
H	-0.27694500	2.91735400	0.08389800
H	-1.94748000	4.07549300	1.43141700
H	-3.25185300	3.08198700	0.80715700
H	-3.25197400	0.52226800	1.35838100
H	-1.95254400	-0.12809100	2.36438400
H	-2.57896200	2.21493900	3.02698800
H	-0.89661600	2.10165100	2.50429900
C	-2.94390100	1.20349600	-1.36170200
H	-3.06187500	1.93681600	-2.16436800
H	-3.69498200	1.44591800	-0.60302100
C	-3.07314600	-1.25693100	-0.82490200
N	-1.74860300	-1.03981700	-0.15862500
C	-3.20226600	-0.19972900	-1.90896000
H	-4.21633100	-0.26781500	-2.30961100
H	-2.50650600	-0.42728800	-2.72155300
N	-0.74080700	-2.83214700	1.03709900
N	-1.25579300	-2.00738700	0.49440500
H	-3.07039200	-2.26884700	-1.23051900

O	-0.02650000	0.24911200	0.83746500
H	0.60234500	0.47315300	0.13403600
H	-3.85460600	-1.16866100	-0.06486800
C	-0.50123800	1.16950700	-1.92391300
C	0.28829700	0.02626500	-2.11385000
C	-0.39465600	2.18527800	-2.88730400
C	1.16422200	-0.08152800	-3.19507100
H	0.23742800	-0.81759100	-1.43732900
C	0.47065900	2.07672000	-3.96903300
H	-1.00377500	3.07901400	-2.80810900
C	1.26366600	0.94229300	-4.12686600
H	1.76140800	-0.98116300	-3.30056200
H	0.52282800	2.88435000	-4.69191100
H	1.94296200	0.85772800	-4.96832400

7c-TS

G(298.15 K)= -822.237534

H(298.15 K)= -822.177982

C	-2.06078100	3.09370300	1.16169500
C	-1.25133000	2.83026900	-0.10622000
C	-1.54494700	1.48582600	-0.82634300
C	-1.35363700	0.36116500	0.31666500
C	-2.20131700	0.63774300	1.56305600
C	-1.85134300	1.98346000	2.18617100
H	-1.43665600	3.63206300	-0.82452500
H	-0.18248800	2.85871400	0.13166600
H	-1.74825800	4.05638300	1.57584700
H	-3.12685900	3.18725800	0.92462900
H	-3.26606900	0.61009100	1.32267400
H	-1.99338800	-0.18436000	2.25902000
H	-2.47567300	2.14443600	3.06863800
H	-0.80755200	1.96817100	2.51461500
C	-2.98925300	1.40296700	-1.35189200
H	-3.11380500	2.14719000	-2.14352300

H	-3.70542100	1.65457300	-0.56473900
C	-3.08267600	-1.05770000	-0.78950800
N	-1.70813000	-0.86420500	-0.38634900
C	-3.28385900	0.01634200	-1.89913100
H	-4.32386900	-0.08771700	-2.21614700
H	-2.63971000	-0.21921100	-2.74960600
N	-0.90594500	-3.04535000	1.14529600
N	-1.35912200	-2.10554800	0.80042200
H	-3.18028600	-2.05515200	-1.21716500
O	-0.04232500	0.26563600	0.74953700
H	0.57716400	0.36678700	0.01220500
H	-3.80379400	-0.89942100	0.01467200
C	-0.56944300	1.33673200	-2.01249200
C	0.24143200	0.22547200	-2.27979500
C	-0.52124600	2.40095300	-2.92740700
C	1.08565900	0.19657700	-3.39179300
H	0.21612900	-0.65548900	-1.64897000
C	0.30936800	2.36847800	-4.04016200
H	-1.15354000	3.27108000	-2.78600200
C	1.12811700	1.26598100	-4.27528900
H	1.70158700	-0.68020000	-3.56229200
H	0.31273200	3.20919100	-4.72595100
H	1.78053800	1.23997400	-5.14142100

7d

G(298.15 K)= -822.261471

H(298.15 K)= -822.202946

C	-1.45092200	3.57887000	0.29524200
C	-1.41947600	2.81518000	-1.03087700
C	-2.03275900	1.38826600	-0.97635100
C	-1.36790800	0.64684200	0.22366900
C	-1.47036100	1.39946400	1.55029800
C	-0.79153100	2.76622800	1.40803100

H	-1.95008800	3.36810500	-1.81318400
H	-0.37786300	2.72551800	-1.35635300
H	-0.92630900	4.52973700	0.16576200
H	-2.47907500	3.82936900	0.57914700
H	-2.50940000	1.54422300	1.85044400
H	-0.99426200	0.78793400	2.32474700
H	-0.85249700	3.28913400	2.36536500
H	0.27133400	2.62503200	1.18219300
C	-3.55299400	1.49065000	-0.68097200
H	-4.02946800	2.00761400	-1.51804000
H	-3.70392800	2.14322500	0.18185200
C	-3.60986400	-0.65428000	0.67965800
N	-2.13547600	-0.70216100	0.42444100
C	-4.27915300	0.16280300	-0.41407600
H	-5.30740400	0.36466200	-0.10254400
H	-4.33507800	-0.45499300	-1.31307800
N	-1.31101500	-2.43515100	-0.99498400
N	-1.73419900	-1.61879400	-0.36966600
O	-0.06951200	0.29610100	-0.05507900
H	-3.70124300	-0.20871200	1.66982900
H	0.41301500	0.12626500	0.76826000
H	-3.97182800	-1.68094300	0.73509700
C	-1.74946000	0.70382400	-2.33165100
C	-2.77794600	0.35958900	-3.21906100
C	-0.43043900	0.50027500	-2.77516600
C	-2.51027300	-0.21714300	-4.45987100
H	-3.81436400	0.55505100	-2.97300000
C	-0.16137600	-0.08045400	-4.00960300
H	0.40310200	0.79437700	-2.15242300
C	-1.20078400	-0.45524500	-4.85723700
H	-3.33731100	-0.47304600	-5.11401200
H	0.87022200	-0.23036600	-4.31162300
H	-0.99135000	-0.90916900	-5.82028400

7d-TS

G(298.15 K)= **-822.237536**

H(298.15 K)= **-822.178914**

C	-1.35566100	3.54047100	0.31376600
C	-1.32494300	2.76848200	-1.00643800
C	-2.01443100	1.38128200	-0.96905400
C	-1.45029900	0.58036400	0.25720300
C	-1.59098500	1.39715200	1.60563600
C	-0.79562700	2.69460100	1.45289500
H	-1.80386700	3.34650800	-1.80379900
H	-0.28064600	2.62668800	-1.30083500
H	-0.76328900	4.45286900	0.20144400
H	-2.37448200	3.86103000	0.55886400
H	-2.63424300	1.62750800	1.82093300
H	-1.20378100	0.77780200	2.42019400
H	-0.85684700	3.22819800	2.40571600
H	0.25782400	2.46137100	1.27216100
C	-3.53372300	1.54840100	-0.73487600
H	-3.97252900	2.02737400	-1.61401200
H	-3.69532100	2.25123800	0.08505200
C	-3.60556700	-0.57079000	0.66974800
N	-2.15989000	-0.63357200	0.59380900
C	-4.28112600	0.24638300	-0.42193000
H	-5.30346600	0.46614800	-0.10681500
H	-4.35445900	-0.39895300	-1.30162900
N	-1.52192800	-2.60540100	-1.31490900
N	-1.84310800	-1.67256600	-0.82972400
O	-0.12032400	0.25691500	0.05676900
H	-3.73384900	-0.13342200	1.67369900
H	0.24028500	-0.15490000	0.85658600
H	-3.97903300	-1.59280000	0.75410000

C	-1.70363400	0.66307100	-2.29782700
C	-2.71254900	0.29339500	-3.19835900
C	-0.37459300	0.41889700	-2.68975000
C	-2.41857200	-0.34691300	-4.40019600
H	-3.75272500	0.50584800	-2.98861400
C	-0.07952400	-0.22547400	-3.88493600
H	0.44302900	0.71613700	-2.04728300
C	-1.10114900	-0.62733900	-4.74288800
H	-3.22948900	-0.62367400	-5.06569000
H	0.95711700	-0.41106300	-4.14662300
H	-0.87083900	-1.13677600	-5.67270700

8c

G(298.15 K)= -979.334217

H(298.15 K)= -979.262685

C	-2.08142900	3.03303700	1.16616800
C	-1.28385700	2.75013900	-0.11642600
C	-1.54148800	1.37209300	-0.79689800
C	-1.36658600	0.30771800	0.30928900
C	-2.20345300	0.55376500	1.55968400
C	-1.83962400	1.90398500	2.17156400
H	-1.51717200	3.51784400	-0.85428900
H	-0.20992700	2.82856000	0.09468700
H	-3.15155400	3.03033300	0.90807400
H	-3.26904900	0.52016400	1.31689600
H	-1.99483700	-0.25998600	2.26241600
H	-2.42741400	2.04537600	3.08160700
H	-0.78378400	1.87894300	2.46162200
C	-2.98394200	1.30619500	-1.36147900
H	-3.08095000	2.08819400	-2.11969200
H	-3.71218400	1.53801000	-0.57804200
C	-3.22027100	-1.17146000	-0.96006400
N	-1.87846400	-1.05364400	-0.30415000

C	-3.31486600	-0.05060100	-1.98203800
H	-4.33687200	-0.04921700	-2.36840000
H	-2.64254100	-0.26396500	-2.81782900
N	-0.95823600	-2.94963900	0.79940500
N	-1.43297700	-2.07492200	0.29947200
H	-3.26872100	-2.15849200	-1.42111800
O	-0.07324900	0.09238400	0.71407600
H	0.55152300	0.32034600	0.00802900
H	-3.98726600	-1.09047700	-0.18425100
C	-1.79937200	4.44988400	1.75201700
C	-1.94019200	5.51476800	0.65392300
H	-1.93063000	6.51332900	1.10170600
H	-1.11881100	5.47275000	-0.06740700
H	-2.88411100	5.39884200	0.10866700
C	-2.83853800	4.75820900	2.83936900
H	-2.77513700	4.06275200	3.68078500
H	-2.67758100	5.76579500	3.23553900
H	-3.85490900	4.71394600	2.43309000
C	-0.39639600	4.55404900	2.36497800
H	-0.21157400	5.58409800	2.68661200
H	-0.28838300	3.91101300	3.24345400
H	0.38587000	4.28884300	1.64632800
C	-0.55787400	1.19908700	-1.97486700
C	0.16451700	0.02968800	-2.25372500
C	-0.41546300	2.26618000	-2.87558200
C	1.01210400	-0.05562900	-3.35943400
H	0.07945500	-0.85145300	-1.62974900
C	0.42080100	2.18055600	-3.98182400
H	-0.97213000	3.18478600	-2.72730400
C	1.14829400	1.01835000	-4.22779000
H	1.55714500	-0.97693800	-3.53580100
H	0.50109300	3.02791500	-4.65471300
H	1.80458400	0.95163400	-5.08876900

8c-TS

G(298.15 K)= -979.234859

H(298.15 K)= -979.306079

C	-0.00071500	-0.00208000	0.00131000
C	-0.00162800	-0.00205500	1.53501500
C	1.38456500	-0.00090700	2.23373800
C	2.14243800	-1.28804500	1.62633300
C	2.16286800	-1.27212200	0.09690400
C	0.75879900	-1.23640700	-0.49362400
H	-0.53597300	0.87669200	1.90065000
H	-0.54879200	-0.87933600	1.89740900
H	0.54702000	0.88536400	-0.35029300
H	2.73765300	-0.42043600	-0.27241800
H	2.68807100	-2.18604500	-0.20786600
H	0.85373700	-1.22733400	-1.58162400
H	0.22517900	-2.15118400	-0.21357500
C	2.21323000	1.25685800	1.91459600
H	1.71288100	2.12201500	2.35896400
H	2.25584600	1.43617700	0.83695300
C	4.33079700	-0.11366600	1.87092400
N	3.45862900	-1.20505300	2.24290100
C	3.61958400	1.13170700	2.47643200
H	4.24687600	1.98381000	2.20600200
H	3.60630800	1.04595800	3.56551800
N	4.81501000	-3.59977900	1.82682200
N	4.24334800	-2.67128600	1.69050600
H	5.29556500	-0.26383900	2.35426400
O	1.54694800	-2.48156100	1.99681700
H	1.23111000	-2.44804200	2.91171000
H	4.44467500	0.01205500	0.79241000
C	-1.43510700	0.13552600	-0.59039800
C	-2.00540700	1.51953700	-0.24675100

H	-2.98151700	1.65019300	-0.72462600
H	-2.15151300	1.65500500	0.82869900
H	-1.34444200	2.31592200	-0.60606900
C	-1.36684700	0.02382800	-2.12050800
H	-1.12464900	-0.99191100	-2.44532900
H	-2.33602500	0.28639600	-2.55609400
H	-0.61474200	0.70599600	-2.53321100
C	-2.38969200	-0.94216600	-0.05937700
H	-3.35203900	-0.86672500	-0.57588400
H	-2.00038700	-1.95096000	-0.23064000
H	-2.58255500	-0.82447000	1.01107900
C	1.16659800	-0.08059900	3.75981700
C	1.76892300	-1.00161000	4.62726900
C	0.31700000	0.87961500	4.33360700
C	1.50395200	-0.98638500	5.99789300
H	2.47988500	-1.73472100	4.26427600
C	0.06258500	0.90402000	5.69889000
H	-0.14822700	1.63835000	3.71301100
C	0.64784800	-0.03880200	6.54140500
H	1.98462700	-1.72111700	6.63518500
H	-0.59698400	1.66452200	6.10360500
H	0.44501300	-0.02613700	7.60687200

8d

G(298.15 K)= -979.329905

H(298.15 K)= -979.259653

CC	2.37473100	-0.14484600	0.24262800
C	1.10339700	0.71911000	0.27802600
C	-0.23919200	-0.05526600	0.41209100
C	-0.24937400	-1.16630300	-0.67721600
C	0.98203800	-2.06604500	-0.63578600
C	2.23128200	-1.20579100	-0.85505200
H	1.13349300	1.42202400	1.11606900

H	1.05712800	1.31878200	-0.63733500
H	2.46594100	-0.66958300	1.20528800
H	1.06687200	-2.59183800	0.31652000
H	0.87593300	-2.82783700	-1.41636100
H	3.09910100	-1.86834600	-0.88331000
H	2.16256600	-0.71883900	-1.83455000
C	-0.29430000	-0.75509600	1.79770600
H	-0.29757400	0.01887900	2.56990600
H	0.63272400	-1.31093800	1.95386500
C	-1.58746100	-2.76185600	0.92763600
N	-1.48452400	-2.08790100	-0.40537900
C	-1.47298200	-1.71520000	2.02463900
H	-1.34195500	-2.23523100	2.97724400
H	-2.42390400	-1.18085400	2.08279500
N	-3.49557200	-1.19097800	-1.33170500
N	-2.57271800	-1.58471600	-0.85287100
O	-0.45193500	-0.64709800	-1.93324700
H	-0.77156200	-3.48443200	0.92965800
H	-0.15160400	-1.27782700	-2.60508000
H	-2.52912700	-3.31107200	0.94979100
C	3.67884900	0.69815000	0.11192900
C	4.89280400	-0.21191600	0.35000700
H	4.98595900	-0.98862200	-0.41417500
H	5.81346700	0.37951000	0.32633200
H	4.83077100	-0.69940800	1.32911800
C	3.69842600	1.79633800	1.18450000
H	2.96377800	2.58082900	0.98228700
H	3.49375200	1.38154200	2.17840800
H	4.68442700	2.27036800	1.21429400
C	3.81680100	1.35146500	-1.26984600
H	4.70566700	1.99029700	-1.28517700
H	3.93570400	0.60644300	-2.06208500
H	2.95575500	1.98104000	-1.51553500

C	-1.38770100	0.96163500	0.23368900
C	-2.27392300	1.27286900	1.27370000
C	-1.52338700	1.69270300	-0.96007300
C	-3.28682400	2.21744900	1.11254100
H	-2.18383300	0.80219700	2.24403100
C	-2.53672600	2.63024800	-1.12520000
H	-0.83303200	1.52989500	-1.77640000
C	-3.43493500	2.89060600	-0.09330400
H	-3.95422600	2.42592000	1.94228700
H	-2.61521400	3.16672000	-2.06527500
H	-4.22496500	3.62282000	-0.22263800

8d-TS

G(298.15 K)= --979.306777

H(298.15 K)= -979.236063

C	0.00074400	-0.00136100	-0.00338000
C	0.00095100	0.01440700	1.53313100
C	1.39398800	0.00400600	2.21410300
C	2.24548100	-1.16199000	1.60475500
C	2.29906100	-1.06091300	0.02966300
C	0.86619600	-1.16641900	-0.49291700
H	-0.51117500	0.90572000	1.90837400
H	-0.56370000	-0.85048200	1.89554300
H	0.46142500	0.93120600	-0.36169200
H	2.74815600	-0.12114500	-0.29104200
H	2.92041300	-1.88017000	-0.34425700
H	0.92976200	-1.18511400	-1.58462000
H	0.43769200	-2.12053900	-0.17209100
C	2.14513600	1.32113500	1.90373200
H	1.62472700	2.14303900	2.40191900
H	2.06807400	1.53824400	0.83637200
C	4.37087100	0.09331800	1.80754700
N	3.65100900	-1.15750900	1.93900200

C	3.62742000	1.32735000	2.29823800
H	4.11960000	2.21327800	1.89093100
H	3.75761800	1.36565800	3.38310500
N	3.94348500	-1.99412300	4.61252600
N	3.62526100	-1.46208300	3.70432700
O	1.72599700	-2.39099400	1.97062300
H	4.55052600	0.10547600	0.71952600
H	2.20752400	-3.09845800	1.51538800
H	5.35562900	-0.04038600	2.25903900
C	-1.43453800	-0.01006500	-0.61016500
C	-1.34338200	0.26404200	-2.11856200
H	-0.79249300	-0.51823100	-2.64829900
H	-2.34740200	0.30677100	-2.55247700
H	-0.85135000	1.22324100	-2.31321300
C	-2.27418100	1.10903500	0.02197800
H	-2.52662100	0.89216800	1.06379800
H	-1.74392900	2.06784600	-0.01129900
H	-3.21412600	1.22422100	-0.52650600
C	-2.14976500	-1.35051500	-0.39487100
H	-3.17766500	-1.28044000	-0.76462900
H	-1.66031300	-2.16451200	-0.93806500
H	-2.19933100	-1.62496200	0.66376500
C	1.17782600	-0.19840600	3.72785400
C	1.57621500	0.75921900	4.67164600
C	0.50816900	-1.33669900	4.21342100
C	1.37842000	0.56400300	6.03667900
H	2.04069700	1.68661700	4.36266500
C	0.31611900	-1.53646900	5.57486700
H	0.14769100	-2.08836400	3.52424200
C	0.76491900	-0.59448800	6.49840400
H	1.70890500	1.32542000	6.73531400
H	-0.19124500	-2.43375300	5.91394200
H	0.62097300	-0.75496300	7.56173200

Coordinates with explicit water molecule

4a-TS

G(298.15 K)= -1105.171159

H(298.15 K)= -1105.108048

C	0.00021500	-0.10736900	-0.00197800
C	0.06919800	-0.14605000	1.52357900
C	1.49682800	-0.02280400	2.07693700
C	2.05878900	1.36711500	1.49838400
C	2.04647800	1.38409300	-0.03011600
C	0.62120900	1.17988000	-0.54852300
H	-0.50815000	0.68495700	1.94234200
H	-0.37058300	-1.06740400	1.91739900
H	0.52317500	-0.97423400	-0.42247200
H	-1.04485500	-0.17841300	-0.31604400
H	2.42991000	2.35761900	-0.35696100
H	2.71785400	0.60893600	-0.40689800
H	0.00754900	2.03715700	-0.25015900
H	0.64111400	1.16172200	-1.64111300
C	1.51429500	0.07648200	3.60750300
H	1.16293900	-0.87014000	4.03032900
H	0.80731600	0.85436800	3.91076700
C	3.51779000	1.64574400	3.44114200
N	3.42126700	1.32110200	2.02920400
C	2.90654500	0.39124400	4.13528600
H	2.88605600	0.63388700	5.20035300
H	3.58035600	-0.45340000	3.98561300
N	5.09575100	3.17448000	0.77454500
N	4.26736600	2.62724000	1.24374400
O	1.28846500	2.36481100	2.05638600
H	2.94419800	2.53624600	3.70016900

H	1.47411900	3.21218600	1.58120800
H	4.56839300	1.73402500	3.71489900
C	1.52037400	-2.83260400	1.73066600
H	0.71068300	-2.85798300	0.99986900
H	2.16178000	-3.70199500	1.57969000
H	1.11772700	-2.86908200	2.74463100
O	2.17222000	4.52652800	0.74901700
H	2.34182100	5.28564500	1.32136400
H	1.63218300	4.86882500	0.02538800
S	2.59697300	-1.39160800	1.49147300

4b-TS

G(298.15 K)= -1105.169567

H(298.15 K)= -1105.107313

C	3.33567400	0.84916800	-1.63765100
C	2.38276500	-0.21610700	-2.16334000
C	1.99221500	-1.22417900	-1.07648400
C	1.37640200	-0.41636900	0.18157000
C	2.73157200	1.56030000	-0.39820100
H	2.84039100	-0.76020400	-2.99520200
H	1.48590200	0.28084200	-2.54048900
H	3.48606000	1.63419100	-2.38275000
H	4.31508000	0.44145900	-1.38037900
C	3.17869100	-2.09155600	-0.61494000
H	3.51519800	-2.68036200	-1.47345800
H	4.00706600	-1.43774000	-0.32337100
C	2.31240600	-2.19333600	1.75528900
C	2.83962200	-3.00112600	0.56956200
H	3.73646100	-3.55483700	0.86024200
H	2.09230300	-3.74517700	0.26937500
H	2.02601400	-2.86037400	2.57273800
O	0.27643500	0.28458900	-0.25592200
N	2.51667100	0.44706100	0.50622100

N	2.12742400	1.20819600	2.01253400
N	2.28431000	1.62117100	3.01817400
H	3.10719000	-1.54246700	2.13899700
C	1.09797200	-1.35570700	1.35642600
H	0.27273800	-1.99973100	1.04210900
H	0.72908100	-0.75420700	2.19525000
H	3.46867900	2.23595300	0.03382100
H	-0.22107200	0.61798000	0.53031500
H	1.80333100	2.07175500	-0.65938500
C	-0.36640700	-1.41244200	-2.75947400
H	0.14161200	-1.11619300	-3.67725000
H	-1.19179900	-2.07993900	-3.01259500
H	-0.75093000	-0.54451100	-2.22658100
O	-0.72743700	1.22840600	2.05042800
H	-1.48414900	0.75573400	2.41958400
H	-0.99807800	2.15470800	2.01507700
S	0.71351100	-2.39574200	-1.68194900

4c-TS

G(298.15 K)= -1105.166233

H(298.15 K)= -1105.104496

C	2.64413900	-1.60158600	-0.40298700
C	2.31438700	-0.15376000	-0.77064700
C	1.10905600	0.43485500	-0.01827000
C	-0.13126100	-0.57651900	-0.29503400
C	0.22789600	-2.01394100	0.09435100
C	1.44624600	-2.50733500	-0.68048500
H	3.16515300	0.50813700	-0.57336700
H	2.10912600	-0.11884500	-1.84383800
H	3.50526000	-1.91923500	-0.99731800
H	2.94220900	-1.68290800	0.64845000
H	0.42625900	-2.08824400	1.16589400
H	-0.66010800	-2.61729400	-0.12984600

H	1.66327600	-3.53830000	-0.38996300
H	1.21823700	-2.50604500	-1.75139000
C	1.35294200	0.55830800	1.49172400
H	2.15695800	1.28136800	1.65503200
H	1.69856800	-0.40054800	1.88914700
C	-1.07252800	0.00902200	1.93738000
N	-1.17381600	0.04476300	0.49596700
C	0.09658900	0.99231900	2.23266700
H	0.23798500	0.96512900	3.31531900
H	-0.20756300	2.00511200	1.95753900
N	-3.62971500	-0.92152800	-0.30834000
N	-2.59199900	-0.85694600	0.04828500
H	-1.99642100	0.40471000	2.35805500
H	-0.84762100	-0.98037100	2.34077100
C	1.12835700	2.12318000	-2.39620900
H	0.59715500	1.32665200	-2.91624500
H	0.77913300	3.08792000	-2.76816600
H	2.20139400	2.04538100	-2.56736800
O	-2.23150700	1.42331400	-1.87036800
H	-1.81949000	2.09010500	-1.30032300
H	-2.36840900	1.85511000	-2.72305900
S	0.73158200	2.14253400	-0.62300700
O	-0.50655600	-0.57230300	-1.61676300
H	-1.07932100	0.21743800	-1.81114400

4d-TS

G(298.15 K)= -1105.172072

H(298.15 K)= -1105.109158

C	0.01544700	0.07770500	-0.01137300
C	0.03255800	0.11753900	1.51917800
C	1.44907600	0.08002600	2.11096600
C	2.20331000	-1.17117600	1.54934400
C	2.22733000	-1.13340000	-0.04708500

C	0.77854000	-1.13737700	-0.53178000
H	-0.46868700	1.01676200	1.89161700
H	-0.52344500	-0.74981300	1.88672600
H	-1.02408200	0.03879900	-0.34821900
H	0.44529800	0.99477300	-0.42954100
H	2.74587900	-0.24512900	-0.40883500
H	2.76650500	-2.02276200	-0.38004800
H	0.79998600	-1.14624100	-1.62569200
H	0.29163600	-2.06044000	-0.20291300
C	2.26150800	1.34820300	1.78125400
H	1.77699700	2.20511500	2.25601100
H	2.22911400	1.53046900	0.70348800
C	4.38610900	-0.02172600	1.71177600
N	3.60632700	-1.24531000	1.82197700
C	3.71714200	1.24364500	2.23989800
H	4.28819300	2.10552900	1.88846000
H	3.78283800	1.24548200	3.33341000
N	4.09664800	-2.24678800	4.36308300
N	3.62323300	-1.62226500	3.58788100
O	1.59196700	-2.32203300	1.98405800
H	4.56135000	0.03167100	0.62509800
H	2.06213200	-3.10067600	1.58422800
H	5.36469100	-0.21788200	2.15396900
C	0.06752700	-1.14948800	4.35904900
H	0.23406100	-2.10360700	3.86122900
H	0.12617900	-1.27783900	5.44083700
H	-0.90886300	-0.73883800	4.10160300
O	3.04449700	-4.17821500	0.76600200
H	2.66354100	-5.05329900	0.62142200
H	3.87279600	-4.33169200	1.23737100
S	1.39536600	0.01496300	3.94864900

5a-TS

G(298.15 K)= -782.198305

H(298.15 K)= -782.137079

C	-0.06511100	-0.09800800	0.00916700
C	-0.04335100	-0.09130900	1.53739100
C	1.38379600	-0.02264000	2.08875900
C	2.02415600	1.33399400	1.51685700
C	2.03409000	1.30220700	-0.00973400
C	0.61118600	1.15456300	-0.55036700
H	-0.59670900	0.76971700	1.92300100
H	-0.52265400	-0.98759800	1.94555600
H	0.45641600	-0.98828000	-0.36184300
H	-1.09857500	-0.15795100	-0.34274200
H	2.48469500	2.23319200	-0.37245700
H	2.66028600	0.46503700	-0.32773000
H	0.02722300	2.04103100	-0.27677100
H	0.64769200	1.11610700	-1.64214700
C	1.43615300	0.04092600	3.61576200
H	1.00858000	-0.87540000	4.03363700
H	0.81461000	0.87333700	3.95501300
C	3.50271400	1.49824900	3.46146600
N	3.38527200	1.23095900	2.04549700
C	2.87170000	0.21455900	4.08349500
H	2.93767800	0.35690000	5.16452600
H	3.47946400	-0.64991100	3.80833900
N	5.07473600	3.11786300	0.83470400
N	4.24846000	2.55561800	1.28939300
O	1.30320900	2.37643000	2.05927300
H	2.94185600	2.38102900	3.77319200
H	1.50387000	3.19923800	1.55028000
H	4.55640200	1.55403500	3.73214000
C	1.77283200	-2.37872200	1.78687100
H	0.86198100	-2.60126600	1.22101900
H	2.57679000	-3.02236100	1.42985900

H	1.59672400	-2.58938400	2.84729000
O	2.21435700	-1.04726500	1.57592700
O	2.19012200	4.47027500	0.63359500
H	2.36060400	5.25986100	1.16279300
H	1.63125400	4.76911300	-0.09491600

5b-TS

G(298.15 K)= -782.195163

H(298.15 K)= -782.133984

C	3.35887300	0.92112300	-1.59231500
C	2.40197000	-0.12676600	-2.14679200
C	2.02394500	-1.16023600	-1.08265600
C	1.40412100	-0.35492800	0.19374700
C	2.77986000	1.60716400	-0.33030200
H	2.85758700	-0.64731000	-2.99524700
H	1.49883700	0.37477200	-2.50342900
H	3.51024900	1.72204300	-2.31970200
H	4.33750300	0.49822300	-1.35720700
C	3.20334500	-2.02620100	-0.62934800
H	3.53616900	-2.58861300	-1.50764400
H	4.03323400	-1.39155100	-0.30468600
C	2.26943300	-2.21141700	1.70877900
C	2.82003500	-2.97728400	0.50638700
H	3.69671800	-3.56114900	0.79989800
H	2.06437200	-3.68136000	0.14357300
H	1.95297500	-2.90708500	2.49080800
O	0.31714700	0.36155400	-0.25891500
N	2.53508500	0.48113000	0.56229800
N	2.15311700	1.19419300	2.05677600
N	2.27581000	1.51966100	3.09886100
H	3.05782600	-1.58353000	2.14183000
C	1.07505900	-1.34791600	1.30534700
H	0.26799300	-1.97254900	0.91276400

H	0.66942300	-0.78922300	2.15755400
H	3.53044100	2.25750100	0.11701700
H	-0.20247100	0.66795300	0.52237200
H	1.86201500	2.14633700	-0.57055500
O	-0.69905300	1.26138600	2.06790100
H	-1.46653100	0.80360400	2.43327500
H	-0.94316300	2.19553500	2.05353200
O	1.03150500	-2.06366100	-1.48021100
C	0.05356600	-1.67725000	-2.43979200
H	-0.63836400	-2.51796000	-2.49898100
H	-0.48852300	-0.78185000	-2.13284400
H	0.50537000	-1.52248900	-3.42463100

5c-TS

G(298.15 K)= -782.195215

H(298.15 K)= -782.134188

C	2.59220200	-1.52711000	-0.43396300
C	2.23267000	-0.05986300	-0.67919700
C	1.02363200	0.43047500	0.12634600
C	-0.18718000	-0.58612900	-0.21300000
C	0.19521000	-2.03293800	0.09460000
C	1.41026400	-2.44772400	-0.73241700
H	3.08575100	0.57782300	-0.42552500
H	2.00136800	0.09315000	-1.73892500
H	3.44384800	-1.78885900	-1.06745000
H	2.92052800	-1.66863800	0.60258100
H	0.41140100	-2.16327900	1.15756200
H	-0.68305000	-2.64184300	-0.15140900
H	1.66481700	-3.48552000	-0.50305700
H	1.15488500	-2.39573000	-1.79531100
C	1.26609000	0.49031200	1.63536700
H	2.05570800	1.22222800	1.83276600
H	1.63645700	-0.47093900	2.00129100

C	-1.15572200	-0.10862300	2.03363100
N	-1.24755000	-0.01107200	0.59655600
C	-0.00603700	0.88888600	2.36380200
H	0.11277400	0.85383200	3.44870500
H	-0.31659800	1.89528000	2.07712700
N	-3.67479300	-0.95414300	-0.30874200
N	-2.64839400	-0.89711000	0.08056700
H	-2.08738300	0.25349700	2.46736700
O	-0.54879400	-0.51362600	-1.53415500
H	-0.94917600	0.37318900	-1.72211000
H	-0.91172900	-1.10908000	2.39795300
C	1.50226000	2.71809800	-0.51412400
H	2.18741300	2.50150200	-1.33785300
H	0.93206400	3.61620500	-0.75028800
H	2.07520700	2.89339400	0.40250500
O	0.54302500	1.68024300	-0.34534500
O	-1.95858700	1.75792300	-1.64555100
H	-1.40207400	2.14748500	-0.95399900
H	-1.86253600	2.34394300	-2.40645400

5d-TS

G(298.15 K)= -782.197047

H(298.15 K)= -782.135431

C	-1.59238600	3.67526900	0.29214700
C	-1.75488000	3.01878300	-1.08280100
C	-2.34221400	1.60879000	-0.99601000
C	-1.45622900	0.75193500	-0.03066600
C	-1.37629000	1.41144600	1.40559500
C	-0.75863200	2.80040300	1.22786500
H	-2.40242900	3.62082800	-1.72913900
H	-0.77008800	2.96158700	-1.55605700
H	-1.10863800	4.64744900	0.16571600
H	-2.57166800	3.87082400	0.74361400

H	-2.36633300	1.49329400	1.85663900	C	0.04722200	-0.23409900	1.62643900
H	-0.75158500	0.77019600	2.03126400	C	1.50160000	-0.03985400	2.08092000
H	-0.68403300	3.25725600	2.21906200	C	1.94474300	1.39578400	1.50643800
H	0.25754800	2.69341100	0.83669300	C	1.80424200	1.46692200	-0.01055000
C	-3.79501900	1.59962900	-0.50052100	C	0.36032000	1.18279500	-0.43175400
H	-4.39156900	2.14025900	-1.24013400	H	-0.54700600	0.54910900	2.10964700
H	-3.88616800	2.13799300	0.44596800	H	-0.30982500	-1.18939200	2.02249000
C	-3.40432400	-0.66549200	0.53989700	H	0.41349900	-0.97603800	-0.37263700
N	-1.98448800	-0.55599500	0.26291300	H	-1.19137300	-0.28986500	-0.13178800
C	-4.31541100	0.17191600	-0.35056800	H	2.09950400	2.47520800	-0.33059700
H	-5.31950100	0.16443700	0.07813800	H	2.49475200	0.75340700	-0.46588800
H	-4.37066200	-0.30889800	-1.33274300	H	-0.29200200	1.98478100	-0.06514600
N	-1.46501000	-2.15118100	-2.03541700	H	0.30346900	1.20341300	-1.52264600
N	-1.80264700	-1.35675300	-1.35512500	C	1.62087300	0.02783800	3.60892700
O	-0.20116300	0.61346300	-0.57457200	H	1.35131600	-0.94565200	4.03056000
H	-3.43601600	-0.33340300	1.59164900	H	0.89404400	0.75681600	3.98000100
H	0.37609900	0.12263700	0.06819900	C	3.52529800	1.70667800	3.34571500
H	-3.65518800	-1.72756500	0.56040900	N	3.33719300	1.41045300	1.93527200
C	-1.40991200	1.18618000	-3.23520600	C	3.02680400	0.40844800	4.05072100
H	-0.39947100	1.03873000	-2.84914200	H	3.06258500	0.63059700	5.11983500
H	-1.60623600	0.46241400	-4.02795000	H	3.73368100	-0.39501200	3.83945700
H	-1.51046700	2.19533300	-3.64576700	N	4.91615800	3.23229100	0.58976300
O	-2.39850000	0.93508300	-2.24191700	N	4.09446500	2.72477800	1.11441800
O	1.11738800	-0.68087300	1.33027100	O	1.17348200	2.33965700	2.16693200
H	2.04244500	-0.43654000	1.45731300	H	2.93384600	2.56566500	3.66632100
H	1.11885800	-1.63762400	1.20287000	H	0.97375100	3.08193900	1.57534700

With explicit CH₂Cl₂ molecule

4a-TS

G(298.15 K)= -1988.378856

H(298.15 K)= -1988.307232

C -0.13362500 -0.15939700 0.11172400

C 1.67413500 -2.83164000 1.66577600
H 0.81174400 -2.89672700 1.00076800
H 2.35461000 -3.65518600 1.44596000
H 1.35693400 -2.91112300 2.70717300
C 1.86421800 5.99444200 0.59959100
H 2.62519800 5.86419000 -0.16381800

H	1.52885200	7.02408100	0.67475000
Cl	0.45595100	4.99124400	0.15083600
Cl	2.54506600	5.50731000	2.16745100
S	2.63597600	-1.32095100	1.37743100

4d-TS

G(298.15 K)= -1988.380405

H(298.15 K)= -1988.310849

C	-1.51580900	3.52789500	0.40140200
C	-1.68102100	2.94576300	-1.00480200
C	-2.30926200	1.54386300	-1.01100700
C	-1.48124900	0.59823500	-0.07456100
C	-1.37913400	1.21601800	1.39191200
C	-0.70396900	2.58153600	1.28101000
H	-2.30343400	3.59639000	-1.62706900
H	-0.69035700	2.89480700	-1.46624200
H	-1.00801400	4.49286600	0.32330400
H	-2.49027400	3.72259500	0.86305300
H	-2.36686900	1.31694000	1.84230600
H	-0.79115100	0.52188800	1.99875300
H	-0.60201300	2.97577900	2.29651900
H	0.30341400	2.45885300	0.87166700
C	-3.77335700	1.55597800	-0.52654000
H	-4.36669700	2.14372600	-1.23123500
H	-3.83115000	2.07202500	0.43592000
C	-3.47318000	-0.74146700	0.48224600
N	-2.04754400	-0.67905200	0.21226700
C	-4.35513800	0.14906100	-0.38827200
H	-5.34823900	0.19297600	0.06323600
H	-4.47304100	-0.32285400	-1.36963400
N	-1.57400500	-2.49878200	-1.84894400
N	-1.86800600	-1.54238400	-1.38678700

O	-0.21346400	0.43335000	-0.60199700
H	-3.51055200	-0.44232200	1.54308100
H	0.31826200	-0.12367200	-0.00865100
H	-3.76042600	-1.79438800	0.47010900
C	-0.78086600	1.29346000	-3.47172700
H	0.04617900	0.93320900	-2.86166800
H	-0.77797200	0.78652600	-4.43769600
H	-0.70720200	2.36890700	-3.63363600
C	2.28488600	-1.31511700	2.18026200
H	2.34181000	-1.48697900	3.25061600
H	3.11502500	-1.76702600	1.64640300
Cl	0.77243900	-2.04279000	1.57874800
Cl	2.31432800	0.43932800	1.88762500
S	-2.36733100	0.85328900	-2.71395400

5a-TS

G(298.15 K)= -1665.40728

H(298.15 K)= -1665.336469

C	-0.23428600	-0.16452100	0.14538500
C	-0.09667700	-0.16176800	1.66738300
C	1.36079200	-0.00380800	2.10944600
C	1.87591000	1.39014800	1.49519100
C	1.75696300	1.37454400	-0.02364400
C	0.30853700	1.13414400	-0.45235200
H	-0.67485200	0.65829600	2.10300200
H	-0.48285500	-1.08950400	2.10246900
H	0.31879400	-1.01355500	-0.27283500
H	-1.28453300	-0.29410700	-0.12852800
H	2.11548200	2.33719700	-0.41108800
H	2.41135100	0.58656500	-0.40427300
H	-0.31639500	1.97616400	-0.12986500
H	0.26451400	1.10515300	-1.54376900
C	1.52338300	0.06893700	3.62881500

H	1.18350600	-0.87043800	4.07518000	C	-0.71995700	2.60112500	1.39251000
H	0.87824400	0.86207900	4.01581400	H	-2.29187300	3.65769300	-1.52486400
C	3.48367200	1.64631000	3.32310100	H	-0.67569000	2.95834800	-1.36653700
N	3.26928600	1.36926000	1.91960000	H	-1.02259100	4.52518900	0.46315300
C	2.97617200	0.33015400	3.98951000	H	-2.50845100	3.73303900	0.95901100
H	3.11191500	0.48131500	5.06273900	H	-2.36688500	1.29414500	1.90891400
H	3.61234200	-0.49754100	3.66963600	H	-0.77894800	0.52349800	2.06589900
N	4.85666100	3.20889200	0.57958700	H	-0.64580400	2.98331100	2.41472400
N	4.03510600	2.69021300	1.09307200	H	0.29763400	2.49977600	1.00328400
O	1.13826000	2.39057700	2.11009400	C	-3.75005600	1.58935500	-0.47409700
H	2.90368100	2.50046900	3.67865700	H	-4.31556800	2.19170800	-1.18985400
H	1.02591100	3.13956700	1.50389700	H	-3.85355200	2.06615000	0.50380700
H	4.55126100	1.76035500	3.50609500	C	-3.43733100	-0.74534600	0.42597300
C	1.86938300	-2.32968900	1.76071600	N	-2.01217800	-0.65453700	0.18337100
H	0.94418800	-2.60816200	1.24565300	C	-4.30618200	0.16853400	-0.43073100
H	2.69155300	-2.91950800	1.35582400	H	-5.32063500	0.15800400	-0.02796200
H	1.76736700	-2.55108200	2.82850900	H	-4.34596900	-0.24885600	-1.44224600
O	2.21316100	-0.97166900	1.53105000	N	-1.48273200	-2.10856700	-2.21494400
C	1.99095900	6.10328300	0.64708800	N	-1.81980400	-1.35212200	-1.49244000
H	2.84577900	6.09703000	-0.02197400	O	-0.18139500	0.52171600	-0.54319000
H	1.57542500	7.09789200	0.77422800	H	-3.48174200	-0.47326000	1.49496900
Cl	0.72394700	5.06561700	-0.06353200	H	0.35961700	-0.04887100	0.02840000
Cl	2.51364700	5.50406400	2.23728200	H	-3.71361500	-1.80006800	0.38050700

5d-TS

G(298.15 K)= -1665.405454

H(298.15 K)= -1665.337565

C	-1.52437800	3.55535200	0.51118600	H	2.29650000	-1.46441500	3.32396100
C	-1.66874600	3.00059800	-0.90921200	H	3.11417500	-1.75275500	1.74348200
C	-2.28561500	1.60052700	-0.93640800	Cl	0.77337200	-2.01554000	1.60802200
C	-1.45003500	0.65445500	-0.00573800	Cl	2.31891600	0.45850600	1.95616700
C	-1.37261500	1.21970800	1.46643700				

XH analogs with explicit water molecule

4a-TS

G(298.15 K)= -1065.903931

H(298.15 K)= -1065.844277

C	0.01095700	-0.11724300	-0.00507400
C	0.08582700	-0.17543000	1.52013100
C	1.50782900	-0.02216300	2.08264600
C	2.06061800	1.36924700	1.49867500
C	2.04856900	1.38188200	-0.02943500
C	0.62211500	1.17735300	-0.54372300
H	-0.51706800	0.63037000	1.95237800
H	-0.31730100	-1.12232100	1.89663000
H	0.53254500	-0.97817300	-0.43636600
H	-1.03611600	-0.19029000	-0.31178600
H	2.43233600	2.35495700	-0.35720800
H	2.72004500	0.60657500	-0.40606600
H	0.00715000	2.03081100	-0.23761200
H	0.63760800	1.16579300	-1.63642800
C	1.51863500	0.08553700	3.61203600
H	1.16765100	-0.86107100	4.03337600
H	0.81376600	0.86816800	3.90740700
C	3.51728600	1.66004500	3.44115700
N	3.42038900	1.32686100	2.03230600
C	2.91088700	0.40325000	4.13732800
H	2.89351200	0.64563000	5.20241300
H	3.58670100	-0.44020000	3.98662200
N	5.10566100	3.17057100	0.76452000
N	4.27621300	2.62601800	1.23472100
O	1.28124400	2.36023000	2.05447100
H	2.94094600	2.54945300	3.69783600

H	1.46694200	3.21049200	1.58355000
H	4.56770400	1.75095200	3.71460500
O	2.17599200	4.52079000	0.76192700
H	2.34795700	5.27674500	1.33778900
H	1.64532900	4.86984000	0.03456400
S	2.60294100	-1.40081800	1.51456700
H	1.65166400	-2.34288900	1.60896300

4d-TS

G(298.15 K)= -1065.905956

H(298.15 K)= -1065.84576

C	0.02621000	0.02935500	-0.00942900
C	0.04296800	0.11045400	1.51871800
C	1.45798200	0.09603800	2.12395200
C	2.23239800	-1.14010200	1.58156200
C	2.26101800	-1.12295300	-0.01743300
C	0.81179700	-1.18340900	-0.49888700
H	-0.46034600	1.01754100	1.86634000
H	-0.50926200	-0.74518500	1.92190800
H	-1.01217600	-0.03310100	-0.34631000
H	0.44399900	0.94178700	-0.45044900
H	2.73882800	-0.21490300	-0.38661300
H	2.83386400	-1.99222600	-0.34601300
H	0.83499900	-1.22118500	-1.59207700
H	0.34876100	-2.10949200	-0.14519300
C	2.24346500	1.38379200	1.82225200
H	1.74595100	2.22101000	2.31996800
H	2.19526000	1.59084300	0.74890100
C	4.39635500	0.06226700	1.71268600
N	3.64941400	-1.18111200	1.82293900
C	3.70405000	1.30100500	2.26780900
H	4.25463600	2.18196000	1.93152300
H	3.77617200	1.27719000	3.36039300

N	4.19202800	-2.20178900	4.37665900
N	3.74495800	-1.59014300	3.57879000
O	1.64991500	-2.29153300	2.04214200
H	4.55105300	0.12470100	0.62316800
H	2.06797400	-3.07582400	1.59426900
H	5.38854400	-0.11553100	2.13188300
O	2.89648600	-4.19999800	0.70718900
H	2.37170400	-4.96581700	0.44253500
H	3.65740100	-4.55940000	1.18015800
S	1.32282700	-0.01055400	3.95821300
H	0.64057200	-1.16558300	3.98398800

5a-TS

G(298.15 K)= -742.945366

H(298.15 K)= -742.887401

C	-0.05516500	-0.10330000	0.00814300
C	-0.02919300	-0.10558500	1.53663700
C	1.39509900	-0.01755600	2.09073500
C	2.02825400	1.33743400	1.51561900
C	2.03814500	1.30226700	-0.01060200
C	0.61456300	1.15320800	-0.54915000
H	-0.61192000	0.73056600	1.93367600
H	-0.47086900	-1.02889200	1.93235000
H	0.46768000	-0.99112100	-0.36491200
H	-1.08960800	-0.16727100	-0.33998800
H	2.48844800	2.23273100	-0.37512000
H	2.66476600	0.46475600	-0.32746300
H	0.02960100	2.03770700	-0.27159700
H	0.64853000	1.11767800	-1.64110000
C	1.44470000	0.04013600	3.61715300
H	1.04230600	-0.89956200	4.00946700
H	0.80813800	0.85459500	3.97242300
C	3.50173700	1.51479200	3.46199100

N	3.38733900	1.24102100	2.04594300
C	2.87857400	0.22903900	4.08581400
H	2.94407500	0.37147200	5.16688700
H	3.48999700	-0.63156300	3.80877700
N	5.08208900	3.11316300	0.82845300
N	4.25408000	2.55517800	1.28524400
O	1.29872100	2.37498800	2.05657600
H	2.93708100	2.39688600	3.76842700
H	1.50244500	3.20065400	1.55368400
H	4.55490800	1.57674100	3.73330900
O	2.20596400	-1.06285000	1.59533200
O	2.19837800	4.47063200	0.64109500
H	2.36918300	5.25948300	1.17128000
H	1.64456900	4.77174600	-0.09034300
H	1.71711900	-1.89163500	1.69100100

5d-TS

G(298.15 K)= -742.948068

H(298.15 K)= -742.889377

C	-1.58182500	3.67998100	0.31162000
C	-1.77950000	3.03122400	-1.06019000
C	-2.35938800	1.61567900	-0.98938600
C	-1.48307200	0.75705500	-0.02915800
C	-1.37756900	1.41243700	1.40630700
C	-0.73807400	2.79136400	1.22446700
H	-2.44135900	3.63257700	-1.69117100
H	-0.80932400	2.96732500	-1.56743300
H	-1.09703000	4.65158400	0.18443700
H	-2.55174200	3.87437100	0.78481700
H	-2.36664300	1.51626200	1.85634800
H	-0.76452100	0.76122400	2.03294400
H	-0.63769800	3.23913100	2.21748100
H	0.26869400	2.67143500	0.81299500

C	-3.82415200	1.58745100	-0.55248900	H	0.53312700	0.88117100	-0.33978700
H	-4.40332000	2.10447700	-1.32257400	H	2.73703300	-0.40055400	-0.29214000
H	-3.95291800	2.14617300	0.37867600	H	2.70846800	-2.16811300	-0.28859900
C	-3.43843600	-0.64665800	0.55124700	H	0.86975300	-1.18515300	-1.63791000
N	-2.01567300	-0.54642300	0.28964200	H	0.24486800	-2.16146500	-0.30516800
C	-4.32988100	0.15696100	-0.38819600	C	2.18252300	1.19304700	1.94989500
H	-5.34847800	0.14357200	0.00413100	H	1.66822900	2.03577300	2.42101400
H	-4.34358100	-0.34856600	-1.36000700	H	2.22949700	1.40976200	0.87915300
N	-1.53754900	-2.23991500	-1.95725500	C	4.31676100	-0.14864200	1.87078200
N	-1.83736100	-1.40549600	-1.30854500	N	3.45629400	-1.26346600	2.19898600
O	-0.24589700	0.60837600	-0.60986300	C	3.58724400	1.06603700	2.51504500
H	-3.48839000	-0.27330900	1.58893200	H	4.20542800	1.93436300	2.27697600
H	0.35835100	0.12853100	0.01869900	H	3.56853400	0.94228500	3.60030200
H	-3.68947900	-1.70733900	0.60893200	N	4.83729600	-3.62670200	1.70654200
O	-2.32063700	0.99688000	-2.26058600	N	4.25966800	-2.69798200	1.59983900
O	1.13630600	-0.64153400	1.25804100	H	5.28120700	-0.30383200	2.35311700
H	2.05440100	-0.36685300	1.37368000	O	1.56134400	-2.55216800	1.90172000
H	1.16644700	-1.59896700	1.13862800	H	1.22216800	-2.54129300	2.80879800
H	-1.40134100	1.01795100	-2.56630200	H	4.43397100	0.01593500	0.79792600

**(M06-2X/6-31G(d,p)-
water(CPCM;UFF)**

8c-TS-OMe

G(298.15 K)= -1093.76551

H(298.15 K)= -1093.688425

C	-0.00633000	-0.02324100	-0.01982000	H	-1.43948000	0.11745800	-0.61392300
C	-0.01436300	-0.07479200	1.51315200	C	-2.02125900	1.48877800	-0.24031700
C	1.36711900	-0.08481300	2.22065300	H	-2.99970100	1.62073900	-0.71310600
C	2.14334400	-1.33968700	1.57288300	H	-2.16565200	1.60044600	0.83810000
C	2.17113400	-1.27143400	0.04497400	H	-1.36825600	2.29824800	-0.58455000
C	0.76961300	-1.23184300	-0.55129400	C	-1.36550000	0.04213900	-2.14598400
H	-0.55965900	0.78596300	1.90503500	H	-1.11657000	-0.96435400	-2.49378900
H	-0.55533500	-0.96875100	1.84256200	H	-2.33459600	0.30970800	-2.57872700
				H	-0.61561100	0.73765800	-2.54003000
				C	-2.38797500	-0.97912400	-0.11141200
				H	-3.34670100	-0.90350400	-0.63457400
				H	-1.98730900	-1.98085800	-0.29764300
				H	-2.59064100	-0.88322200	0.95942400
				C	1.14420100	-0.22705500	3.73963000

C	1.76171300	-1.15500300	4.58251900	H	2.06477200	1.54120900	0.78696800
C	0.27025900	0.69247600	4.35152000	C	4.36323500	0.07383100	1.81150500
C	1.50487300	-1.20292300	5.95567800	N	3.62039800	-1.15798000	1.98269100
H	2.48779200	-1.86394300	4.20112300	C	3.63554400	1.34217200	2.23938700
C	0.01389100	0.66856200	5.70888900	H	4.13632700	2.19813900	1.78186900
H	-0.21333800	1.46433600	3.76194500	H	3.77574800	1.43866300	3.31891500
C	0.62255700	-0.29129100	6.52753400	N	3.86832800	-1.86971400	4.68606200
H	2.01011500	-1.95100700	6.55348400	N	3.53460700	-1.37261600	3.76213600
H	-0.65792200	1.39012500	6.16113500	O	1.67919600	-2.36367200	1.99725400
O	0.30104900	-0.24514600	7.84123600	H	4.56200600	0.04000200	0.72739800
C	0.92303700	-1.18820400	8.69966300	H	2.17189400	-3.08817800	1.58262200
H	0.54486700	-0.98232400	9.69972400	H	5.33709400	-0.05547200	2.28686000
H	0.66290900	-2.21316500	8.41492300	C	-1.43476600	-0.02505500	-0.63807900
H	2.01192100	-1.07267200	8.68879800	C	-1.34107000	0.22658700	-2.15015000

8d-TS-OMe

G(298.15 K)= -1093.766776

H(298.15 K)= -1093.69089

C	-0.00098800	-0.00446600	-0.02797200	H	-0.78283400	-0.55981800	-2.66581000
C	-0.00641400	0.04563400	1.50812600	H	-2.34412900	0.25623300	-2.58785900
C	1.38243000	0.04051300	2.19482200	H	-0.85421900	1.18580800	-2.35725900
C	2.22782900	-1.15060600	1.61438200	C	-2.27935700	1.10108500	-0.02525600
C	2.29331600	-1.07588300	0.04043500	H	-2.53291300	0.89933600	1.01935600
C	0.86485600	-1.18013100	-0.49261700	H	-1.75169600	2.06074600	-0.07199000
H	-0.51268100	0.94986200	1.85980900	H	-3.21854400	1.20459200	-0.57766300
H	-0.58049700	-0.80580000	1.88775400	C	-2.14796200	-1.36365900	-0.40440500
H	0.46113400	0.92044900	-0.40366300	H	-3.17653200	-1.30007700	-0.77390000
H	2.75440100	-0.14571100	-0.29112700	H	-1.65723900	-2.18374200	-0.93705100
H	2.91087100	-1.90627900	-0.31446100	H	-2.19513400	-1.62412200	0.65792800
H	0.93508000	-1.21568200	-1.58355100	C	1.17667400	-0.13616400	3.70662700
H	0.42952300	-2.12720800	-0.16068300	C	1.60783000	0.81306100	4.64156000
C	2.14894700	1.34212600	1.85700900	C	0.48924600	-1.25766300	4.22133100
H	1.64245700	2.17884000	2.34546400	C	1.44757200	0.64092300	6.01424900
				H	2.08280600	1.73132100	4.32134900
				C	0.32755800	-1.45037400	5.57849800
				H	0.09771800	-2.00860300	3.54841000
				C	0.82303300	-0.51059300	6.49450200

H	1.81081400	1.40743200	6.68708500
H	-0.18657700	-2.32569800	5.96066700
O	0.63152100	-0.79503200	7.79926400
C	1.09863100	0.14561700	8.75543600
H	0.85558700	-0.27090900	9.73141100
H	2.18178300	0.28219500	8.67415700
H	0.59838600	1.11158400	8.63321300

8c-TS

G(298.15 K)= -979.313215

H(298.15 K)= -979.241851

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	1.53370500
C	1.38660900	0.00000000	2.23160300
C	2.14306500	-1.28774900	1.62372600
C	2.16259800	-1.27181700	0.09428500
C	0.75820700	-1.23494100	-0.49540600
H	-0.53340700	0.87917900	1.89967300
H	-0.54766700	-0.87683800	1.89641100
H	0.54825300	0.88700100	-0.35191500
H	2.73786100	-0.42059600	-0.27536500
H	2.68687000	-2.18616500	-0.21081200
H	0.85250500	-1.22592700	-1.58346200
H	0.22400400	-2.14928500	-0.21505400
C	2.21611500	1.25709100	1.91198800
H	1.71674000	2.12265000	2.35666800
H	2.25823600	1.43639300	0.83432300
C	4.33253100	-0.11516800	1.86703300
N	3.45969000	-1.20584600	2.23951200
C	3.62270000	1.13077700	2.47298500
H	4.25052900	1.98237100	2.20219500
H	3.61000200	1.04502100	3.56207700
N	4.81386000	-3.60167600	1.82258600

N	4.24287800	-2.67271200	1.68662600
H	5.29746300	-0.26614000	2.34979600
O	1.54681800	-2.48078200	1.99454500
H	1.23155200	-2.44702000	2.90962600
H	4.44587000	0.01047800	0.78845400
C	-1.43463100	0.13879200	-0.59085200
C	-2.00359100	1.52326400	-0.24684300
H	-2.97987800	1.65472800	-0.72413500
H	-2.14894600	1.65883400	0.82869600
H	-1.34218800	2.31911300	-0.60654100
C	-1.36737300	0.02706300	-2.12100400
H	-1.12620100	-0.98886800	-2.44598600
H	-2.33659500	0.29043300	-2.55600900
H	-0.61495500	0.70862200	-2.53414300
C	-2.38978300	-0.93812600	-0.05928000
H	-3.35237500	-0.86188800	-0.57521300
H	-2.00140700	-1.94723600	-0.23079100
H	-2.58191200	-0.82029000	1.01129200
C	1.16948500	-0.07953900	3.75781000
C	1.77157100	-1.00105800	4.62488800
C	0.32101600	0.88136200	4.33212100
C	1.50742900	-0.98563900	5.99567000
H	2.48171600	-1.73474500	4.26146000
C	0.06743400	0.90595200	5.69755600
H	-0.14395800	1.64048800	3.71181500
C	0.65242600	-0.03736300	6.53970700
H	1.98788100	-1.72077500	6.63266400
H	-0.59127000	1.66698800	6.10267600
H	0.45023500	-0.02455000	7.60529500

8d-TS

G(298.15 K)= -979.313901

H(298.15 K)= -979.243181

C	0.00046200	-0.00153900	0.00115700	C	-0.00581900	-0.02869600	-0.00700600
C	0.00191000	-0.00220500	1.53771300	C	-0.02361200	-0.06496800	1.52643700
C	1.39597000	-0.00188700	2.21732500	C	1.35714400	-0.06937700	2.23726000
C	2.26268900	-1.14875500	1.59441800	C	2.13166500	-1.33650500	1.60842200
C	2.31133300	-1.03099500	0.02065900	C	2.17032100	-1.27763800	0.08004100
C	0.87923400	-1.15129000	-0.50048400	C	0.77242600	-1.24153500	-0.52478000
H	-0.52089400	0.87853300	1.92325200	H	-0.56946100	0.80139200	1.90432500
H	-0.55108600	-0.87835600	1.89100000	H	-0.56728600	-0.95478300	1.86220900
H	0.45049900	0.93964800	-0.34760100	H	0.53450900	0.87346700	-0.33130400
H	2.74616600	-0.08172900	-0.29126600	H	2.73940300	-0.40993900	-0.25937900
H	2.94311100	-1.83734000	-0.36305000	H	2.70912100	-2.17715100	-0.24260900
H	0.94154900	-1.15924800	-1.59232300	H	0.87969600	-1.20118400	-1.61082900
H	0.46426900	-2.11395000	-0.18734400	H	0.24581800	-2.16930200	-0.27639700
C	2.12766900	1.32940200	1.92178400	C	2.18196200	1.20151500	1.96117300
H	1.59486800	2.13854200	2.42769900	H	1.67298400	2.05515600	2.41774700
H	2.04925800	1.55625500	0.85660900	H	2.23405000	1.40361100	0.88841700
C	4.36985800	0.13621500	1.80861300	C	4.30876900	-0.15916100	1.91064100
N	3.66984500	-1.12664100	1.92355600	N	3.43668600	-1.25909400	2.24783300
C	3.60907100	1.35195700	2.31735500	C	3.58283600	1.07034700	2.53549900
H	4.08818800	2.25045500	1.92254800	H	4.20859700	1.93020700	2.28732600
H	3.73897700	1.37638900	3.40273000	H	3.56231800	0.96443000	3.62276100
N	3.97966700	-1.99997200	4.58474300	N	4.81825300	-3.64570100	1.78307200
N	3.65472100	-1.45955000	3.68413000	N	4.23776900	-2.71990900	1.66902700
O	1.76239600	-2.38871300	1.94972800	H	5.26722700	-0.31343400	2.40488900
H	4.54691100	0.16536800	0.72026900	O	1.53944500	-2.54385100	1.93477200
H	2.25723700	-3.08486800	1.49099500	H	1.21641700	-2.55576500	2.84691100
H	5.35772000	0.01114700	2.25556200	H	4.43522700	-0.00832100	0.83698400
C	-1.43495400	-0.01955200	-0.60453700	C	-1.43697400	0.10692600	-0.60749300
C	-1.34756500	0.26416600	-2.11142100	C	-2.02135000	1.48032600	-0.24566500
8c-TS-N02				H	-2.99660000	1.60869600	-0.72577900
G(298.15 K)= -1183.741613				H	-2.17380900	1.59873300	0.83095800
H(298.15 K)= -1183.663589				H	-1.36652700	2.28804600	-0.59039900
				C	-1.35524900	0.02133300	-2.13864100

H	-1.10405800	-0.98725900	-2.47854200
H	-2.32267500	0.28505000	-2.57725800
H	-0.60442800	0.71510000	-2.53387400
C	-2.38650100	-0.98741900	-0.10202800
H	-3.34312600	-0.91487700	-0.62929300
H	-1.98507000	-1.99005100	-0.28138000
H	-2.59396100	-0.88565200	0.96738000
C	1.12282400	-0.18062600	3.75825100
C	1.72386700	-1.11881900	4.60935100
C	0.26111300	0.76697300	4.33835500
C	1.45169400	-1.14034700	5.97456400
H	2.44303300	-1.83873300	4.23890700
C	-0.01470200	0.76917700	5.69615000
H	-0.20053400	1.53559500	3.72958500
C	0.58190600	-0.19821400	6.49291300
H	1.91539900	-1.87199800	6.62374100
H	-0.67813200	1.50395000	6.13410300
N	0.29285100	-0.21349900	7.93101900
O	-0.48296300	0.62018500	8.36396700
O	0.84369700	-1.05934400	8.61335600

8d-TS-NO2

G(298.15 K)= -1183.742797

H(298.15 K)= -1183.665663

C	0.00571000	-0.00874900	0.01464300
C	0.02135100	-0.00287800	1.55045600
C	1.42611700	-0.01357800	2.21293500
C	2.27578500	-1.16854800	1.58887300
C	2.30101900	-1.06938900	0.01290900
C	0.85955500	-1.17687700	-0.48584000
H	-0.48855300	0.88401900	1.93866500
H	-0.53587600	-0.87334400	1.91116800
H	0.46799800	0.92293600	-0.34303000

H	2.74215900	-0.12969100	-0.31835900
H	2.91726100	-1.88809000	-0.36943900
H	0.90731600	-1.19866800	-1.57809400
H	0.43516700	-2.12968900	-0.15548700
C	2.16469500	1.31113300	1.90927400
H	1.63401700	2.12987800	2.40124100
H	2.09301300	1.52661500	0.84135300
C	4.39447900	0.11320700	1.77235000
N	3.69451400	-1.14957600	1.88092300
C	3.64341300	1.32051600	2.31132800
H	4.12798400	2.22580300	1.93988500
H	3.77117900	1.31716500	3.39802900
N	4.06404100	-2.08189100	4.51864900
N	3.73220700	-1.52316300	3.63247000
O	1.77843100	-2.40021600	1.97026800
H	4.55126100	0.15786300	0.68099300
H	2.24287900	-3.10747600	1.49648400
H	5.39118900	-0.02055500	2.19667500
C	-1.43629100	-0.00629900	-0.57621900
C	-1.35821600	0.27427700	-2.08416000
H	-0.81647900	-0.50858900	-2.62228600
H	-2.36635900	0.32451400	-2.50769000
H	-0.86249200	1.23151000	-2.27883600
C	-2.26261900	1.11508000	0.06947700
H	-2.50739000	0.89443000	1.11237600
H	-1.72601200	2.07031100	0.03657300
H	-3.20667900	1.23928100	-0.47002600
C	-2.15668300	-1.34365500	-0.35956800
H	-3.18715700	-1.26673800	-0.72095400
H	-1.67533900	-2.15817900	-0.90912900
H	-2.19927900	-1.62134800	0.69852900
C	1.20258800	-0.21808600	3.72760900
C	1.55565300	0.76471500	4.66333300

C	0.54306100	-1.36561600	4.20731800
C	1.31516300	0.60124400	6.02308600
H	2.01785100	1.69225900	4.35495100
C	0.29954300	-1.55122300	5.55985700
H	0.22068200	-2.13537400	3.52056800
C	0.70194800	-0.56445300	6.44887100
H	1.59698900	1.36413400	6.73754100
H	-0.19822500	-2.44128600	5.92320300
N	0.45155600	-0.75284700	7.88214400
O	0.81427400	0.12592100	8.64453600
O	-0.10557700	-1.77835800	8.23306200

**(M06-2X/6-31G(d,p)-
DCM(CPCM;UFF)**

8c-TS-OMe

G(298.15 K)= -1093.758481

H(298.15 K)= -1093.681389

C	-0.00607200	-0.02351500	-0.01989400
C	-0.01344800	-0.07391600	1.51309000
C	1.36806300	-0.08433100	2.22080700
C	2.14396100	-1.33883100	1.57322400
C	2.17173200	-1.27133600	0.04512400
C	0.76994400	-1.23241100	-0.55067700
H	-0.55803100	0.78745000	1.90470900
H	-0.55557200	-0.96687100	1.84333100
H	0.53300000	0.88092700	-0.34084500
H	2.73737000	-0.40033200	-0.29257400
H	2.70883600	-2.16844600	-0.28811800
H	0.86914700	-1.18682200	-1.63741700
H	0.24581900	-2.16197000	-0.30327600
C	2.18326900	1.19369700	1.94953200
H	1.66879700	2.03620300	2.42081300
H	2.22964200	1.41043100	0.87868000

C	4.31808300	-0.14633500	1.87043400
N	3.45856100	-1.26300300	2.19821900
C	3.58822400	1.06752900	2.51467100
H	4.20556800	1.93695100	2.27791600
H	3.56867500	0.94318600	3.59990500
N	4.82721100	-3.62892900	1.70612400
N	4.25973200	-2.69385700	1.59904500
H	5.28324800	-0.30131900	2.35178000
O	1.56402200	-2.55170400	1.90328800
H	1.21027900	-2.53442900	2.80473700
H	4.43483900	0.01807500	0.79733600
C	-1.43947700	0.11626300	-0.61381700
C	-2.02215100	1.48695200	-0.23935700
H	-3.00029500	1.61876200	-0.71248100
H	-2.16787300	1.59771700	0.83901000
H	-1.36990400	2.29742600	-0.58271500
C	-1.36525900	0.04174200	-2.14590300
H	-1.11615900	-0.96442000	-2.49453700
H	-2.33434400	0.30889400	-2.57859000
H	-0.61614600	0.73809200	-2.54001300
C	-2.38692200	-0.98137800	-0.11167900
H	-3.34577500	-0.90599400	-0.63437700
H	-1.98626500	-1.98291200	-0.29897100
H	-2.58986700	-0.88648100	0.95919900
C	1.14578200	-0.22694200	3.73973200
C	1.76133600	-1.15677300	4.58204800
C	0.27357500	0.69396200	4.35225700
C	1.50480300	-1.20458200	5.95524600
H	2.48469500	-1.86798200	4.19963400
C	0.01765000	0.67021100	5.70941600
H	-0.20931300	1.46650100	3.76291300
C	0.62461900	-0.29116300	6.52792200
H	2.00800900	-1.95406000	6.55305300

H	-0.65277700	1.39238200	6.16260000
O	0.30354700	-0.24431500	7.84052400
C	0.92109200	-1.18909600	8.69993000
H	0.54211400	-0.98158600	9.69924900
H	0.65763200	-2.21318000	8.41499700
H	2.01038100	-1.07684800	8.69065000

8d-TS-OMe

G(298.15 K)= -1093.759722

H(298.15 K)= -1093.683914

C	-0.00875400	0.04716100	1.50660300
C	1.37891000	0.04318900	2.19520300
C	2.22524100	-1.15001200	1.61658300
C	2.29366400	-1.07446300	0.04272100
C	0.86636700	-1.17786800	-0.49371000
H	-0.51644200	0.95099200	1.85713800
H	-0.58281800	-0.80431600	1.88593500
H	0.45965000	0.92222800	-0.40506900
H	2.75620100	-0.14438900	-0.28737000
H	2.91187200	-1.90511800	-0.31108800
H	0.93865100	-1.21156600	-1.58460500
H	0.43030000	-2.12552800	-0.16445800
C	2.14717900	1.34350000	1.85609000
H	1.64180300	2.18130200	2.34390100
H	2.06253400	1.54179400	0.78593400
C	4.36066000	0.07093600	1.81755300
N	3.61461700	-1.15928700	1.99238800
C	3.63407900	1.34286600	2.23842300
H	4.13635900	2.19611800	1.77723200
H	3.77362600	1.44485300	3.31745400
N	3.85549300	-1.85812800	4.69609200
N	3.51735200	-1.36102400	3.77327500
O	1.67254100	-2.36225700	1.99702400

H	4.56327000	0.03350500	0.73447500
H	2.16509700	-3.08754000	1.58403500
H	5.33238000	-0.05777200	2.29769600
C	-1.43461900	-0.02601800	-0.64121100
C	-1.33947000	0.22324800	-2.15357500
H	-0.78206300	-0.56447600	-2.66816700
H	-2.34205900	0.25303300	-2.59201000
H	-0.85207700	1.18186600	-2.36225400
C	-2.28021800	1.10065500	-0.03076200
H	-2.53553400	0.90018600	1.01366600
H	-1.75322100	2.06067000	-0.07818700
H	-3.21860300	1.20328200	-0.58441700
C	-2.14714500	-1.36472700	-0.40602500
H	-3.17564800	-1.30188600	-0.77545200
H	-1.65679000	-2.18535700	-0.93820400
H	-2.19476000	-1.62440500	0.65647700
C	1.17494400	-0.13364100	3.70627300
C	1.60921800	0.81452100	4.64180400
C	0.48652000	-1.25501500	4.22148000
C	1.45339200	0.64038300	6.01416300
H	2.08242500	1.73357400	4.32111100
C	0.32964900	-1.44998500	5.57829400
H	0.09157000	-2.00412800	3.54857800
C	0.82967200	-0.51219800	6.49473700
H	1.81776300	1.40587700	6.68752400
H	-0.18477900	-2.32458200	5.96149800
O	0.64281400	-0.79916100	7.79769400
C	1.10934500	0.13915500	8.75656200
H	0.86645200	-0.28065200	9.73104200
H	2.19247100	0.27621500	8.67552100
H	0.60797900	1.10481100	8.63692100

8c-TS

G(298.15 K)= -979.306335

H(298.15 K)= -979.234937

C	0.00025700	0.00015700	-0.00023300
C	0.00071900	0.00087600	1.53343500
C	1.38726800	0.00054700	2.23170100
C	2.14346400	-1.28676600	1.62393700
C	2.16347200	-1.27109200	0.09434600
C	0.75896400	-1.23468900	-0.49525500
H	-0.53224100	0.88038800	1.89936600
H	-0.54790300	-0.87518500	1.89659000
H	0.54783500	0.88745600	-0.35283100
H	2.73859800	-0.41967100	-0.27548200
H	2.68756700	-2.18577500	-0.21054200
H	0.85264900	-1.22616300	-1.58335800
H	0.22543000	-2.14916700	-0.21431800
C	2.21679900	1.25769000	1.91186900
H	1.71726300	2.12316300	2.35650600
H	2.25867500	1.43696300	0.83411400
C	4.33372200	-0.11330000	1.86751000
N	3.46140400	-1.20555900	2.23928100
C	3.62344600	1.13196900	2.47326200
H	4.25071200	1.98458400	2.20394400
H	3.60960300	1.04561800	3.56235300
N	4.80260700	-3.60481300	1.82464500
N	4.24226900	-2.66947400	1.68704500
H	5.29911200	-0.26417800	2.34975200
O	1.54901600	-2.48023900	1.99531400
H	1.21859800	-2.44041700	2.90481600
H	4.44706700	0.01220200	0.78875900
C	-1.43466500	0.13765900	-0.59094900
C	-2.00480400	1.52145400	-0.24625000
H	-2.98085900	1.65248300	-0.72382100

H	-2.15144400	1.65624500	0.82925200
H	-1.34435000	2.31842900	-0.60526100
C	-1.36710900	0.02650900	-2.12111900
H	-1.12544700	-0.98909800	-2.44674200
H	-2.33640000	0.28909000	-2.55610600
H	-0.61566300	0.70906000	-2.53444100
C	-2.38855300	-0.94047400	-0.05960200
H	-3.35109800	-0.86509900	-0.57548100
H	-1.99971400	-1.94932300	-0.23155400
H	-2.58145800	-0.82322900	1.01090600
C	1.17045000	-0.07944200	3.75787300
C	1.76998100	-1.00338500	4.62422600
C	0.32424800	0.88299100	4.33274700
C	1.50615900	-0.98801100	5.99503800
H	2.47696900	-1.73965500	4.25985400
C	0.07100500	0.90741600	5.69817100
H	-0.13963800	1.64314800	3.71280900
C	0.65387100	-0.03773900	6.53961100
H	1.98429800	-1.72480500	6.63184500
H	-0.58593700	1.66955800	6.10396300
H	0.45179800	-0.02504500	7.60515900

8d-TS

G(298.15 K)= -979.306777

H(298.15 K)= -979.236063

C	0.00074400	-0.00136100	-0.00338000
C	0.00095100	0.01440700	1.53313100
C	1.39398800	0.00400600	2.21410300
C	2.24548100	-1.16199000	1.60475500
C	2.29906100	-1.06091300	0.02966300
C	0.86619600	-1.16641900	-0.49291700
H	-0.51117500	0.90572000	1.90837400
H	-0.56370000	-0.85048200	1.89554300

H	0.46142500	0.93120600	-0.36169200
H	2.74815600	-0.12114500	-0.29104200
H	2.92041300	-1.88017000	-0.34425700
H	0.92976200	-1.18511400	-1.58462000
H	0.43769200	-2.12053900	-0.17209100
C	2.14513600	1.32113500	1.90373200
H	1.62472700	2.14303900	2.40191900
H	2.06807400	1.53824400	0.83637200
C	4.37087100	0.09331800	1.80754700
N	3.65100900	-1.15750900	1.93900200
C	3.62742000	1.32735000	2.29823800
H	4.11960000	2.21327800	1.89093100
H	3.75761800	1.36565800	3.38310500
N	3.94348500	-1.99412300	4.61252600
N	3.62526100	-1.46208300	3.70432700
O	1.72599700	-2.39099400	1.97062300
H	4.55052600	0.10547600	0.71952600
H	2.20752400	-3.09845800	1.51538800
H	5.35562900	-0.04038600	2.25903900
C	-1.43453800	-0.01006500	-0.61016500
C	-1.34338200	0.26404200	-2.11856200
H	-0.79249300	-0.51823100	-2.64829900
H	-2.34740200	0.30677100	-2.55247700
H	-0.85135000	1.22324100	-2.31321300
C	-2.27418100	1.10903500	0.02197800
H	-2.52662100	0.89216800	1.06379800
H	-1.74392900	2.06784600	-0.01129900
H	-3.21412600	1.22422100	-0.52650600
C	-2.14976500	-1.35051500	-0.39487100
H	-3.17766500	-1.28044000	-0.76462900
H	-1.66031300	-2.16451200	-0.93806500
H	-2.19933100	-1.62496200	0.66376500
C	1.17782600	-0.19840600	3.72785400

C	1.57621500	0.75921900	4.67164600
C	0.50816900	-1.33669900	4.21342100
C	1.37842000	0.56400300	6.03667900
H	2.04069700	1.68661700	4.36266500
C	0.31611900	-1.53646900	5.57486700
H	0.14769100	-2.08836400	3.52424200
C	0.76491900	-0.59448800	6.49840400
H	1.70890500	1.32542000	6.73531400
H	-0.19124500	-2.43375300	5.91394200
H	0.62097300	-0.75496300	7.56173200

8c-TS-NO2

G(298.15 K)= -1183.733138

H(298.15 K)= -1183.655164

C	-0.00540900	-0.02891100	-0.00731200
C	-0.02289000	-0.06413400	1.52611900
C	1.35769000	-0.06873500	2.23750600
C	2.13229100	-1.33522000	1.60902400
C	2.17146700	-1.27733100	0.08045200
C	0.77342200	-1.24178500	-0.52429100
H	-0.56828200	0.80262900	1.90397300
H	-0.56780100	-0.95307400	1.86235100
H	0.53433600	0.87347400	-0.33239400
H	2.74057900	-0.40973100	-0.25962700
H	2.70990600	-2.17745300	-0.24158300
H	0.88007000	-1.20224800	-1.61041900
H	0.24743900	-2.16962700	-0.27512700
C	2.18220300	1.20231400	1.96083100
H	1.67282100	2.05585900	2.41712900
H	2.23401500	1.40416800	0.88793300
C	4.30985600	-0.15642500	1.91090100
N	3.43861200	-1.25789900	2.24811100

C	3.58324800	1.07231900	2.53544600
H	4.20819200	1.93331200	2.28862500
H	3.56174900	0.96590300	3.62271000
N	4.81019300	-3.64719100	1.78379600
N	4.23846700	-2.71585300	1.66952400
H	5.26901400	-0.31017500	2.40433200
O	1.54237200	-2.54316900	1.93693900
H	1.19519800	-2.54420200	2.84019900
H	4.43595100	-0.00591200	0.83699200
C	-1.43676000	0.10542100	-0.60789200
C	-2.02234900	1.47811300	-0.24540800
H	-2.99726500	1.60610700	-0.72595300
H	-2.17636300	1.59569700	0.83114000
H	-1.36846000	2.28697100	-0.58930900
C	-1.35450100	0.02050100	-2.13904200
H	-1.10288400	-0.98774200	-2.47964600
H	-2.32189300	0.28353600	-2.57777800
H	-0.60456900	0.71523500	-2.53431300
C	-2.38509000	-0.99014200	-0.10284300
H	-3.34162100	-0.91834400	-0.63009100
H	-1.98331500	-1.99253100	-0.28274900
H	-2.59346000	-0.88909000	0.96647700
C	1.12350500	-0.18072300	3.75857700
C	1.72042400	-1.12262900	4.60857600
C	0.26513000	0.76912100	4.33966700
C	1.44849300	-1.14410300	5.97401700
H	2.43491400	-1.84640700	4.23657600
C	-0.01016400	0.77116300	5.69776300
H	-0.19468100	1.53933500	3.73132500
C	0.58314400	-0.19883800	6.49336100
H	1.90833100	-1.87782100	6.62376200
H	-0.67085600	1.50731700	6.13777100
N	0.29489600	-0.21398400	7.93288000

O	-0.47629700	0.62349200	8.36490200
O	0.84317300	-1.06349700	8.61178200

8d-TS-NO2

G(298.15 K)= -1183.734227

H(298.15 K)= -1183.657095

C	0.00557000	-0.00802500	0.01351500
C	0.02044500	-0.00147900	1.54937100
C	1.42427400	-0.01232600	2.21343400
C	2.27400400	-1.16804300	1.59020400
C	2.30142100	-1.06877200	0.01388800
C	0.86026900	-1.17577800	-0.48647200
H	-0.48996000	0.88549100	1.93669600
H	-0.53740200	-0.87141600	1.91024300
H	0.46738500	0.92385800	-0.34461600
H	2.74294500	-0.12883200	-0.31646800
H	2.91843800	-1.88737300	-0.36805800
H	0.90904000	-1.19697100	-1.57874100
H	0.43514200	-2.12868500	-0.15736700
C	2.16406400	1.31177500	1.90939300
H	1.63412700	2.13082200	2.40168900
H	2.09190800	1.52758300	0.84147100
C	4.39357700	0.11219900	1.77427800
N	3.69200300	-1.15046500	1.88480600
C	3.64298000	1.32084200	2.31145100
H	4.12840700	2.22563600	1.93955400
H	3.77002200	1.31861300	3.39821700
N	4.05488900	-2.07834000	4.52411300
N	3.72702500	-1.51865200	3.63691300
O	1.77559600	-2.39975100	1.97026200
H	4.55111400	0.15576800	0.68318700
H	2.23493900	-3.10669100	1.49139000
H	5.38971200	-0.02188900	2.20014600

C	-1.43620200	-0.00688000	-0.57824500
C	-1.35737800	0.27247200	-2.08636000
H	-0.81604300	-0.51090300	-2.62422500
H	-2.36520200	0.32241300	-2.51029100
H	-0.86197000	1.22966700	-2.28205700
C	-2.26304800	1.11471200	0.06637900
H	-2.50868300	0.89487500	1.10924200
H	-1.72728100	2.07041300	0.03270800
H	-3.20681500	1.23821700	-0.47348900
C	-2.15594900	-1.34443900	-0.36066400
H	-3.18625000	-1.26817100	-0.72223100
H	-1.67490400	-2.15940500	-0.90988300
H	-2.19933200	-1.62159100	0.69755800
C	1.20157600	-0.21696300	3.72820600
C	1.55699000	0.76465500	4.66438300
C	0.54140700	-1.36405900	4.20788400
C	1.31875100	0.59992800	6.02449100
H	2.01824200	1.69278100	4.35602500
C	0.30041700	-1.55082100	5.56087700
H	0.21622000	-2.13252500	3.52095400
C	0.70591100	-0.56580000	6.45004200
H	1.60132000	1.36137300	6.74032200
H	-0.19802800	-2.44012500	5.92538600
N	0.45907300	-0.75623300	7.88492800
O	0.82551900	0.12179400	8.64547800
O	-0.09745200	-1.78210200	8.23357000

**(M06-2X/6-311+G(d,p)-
water(CPCM;UFF)**

8c-TS-OMe

G(298.15 K)= -1094.033251

H(298.15 K)= -1093.956107

C	-0.00520800	-0.02317400	-0.01901200
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C	-0.01434800	-0.07464600	1.51343400
C	1.36692000	-0.09086800	2.22054300
C	2.14308900	-1.34306500	1.57353700
C	2.16751300	-1.27517600	0.04662700
C	0.76708200	-1.23285300	-0.55105700
H	-0.55278800	0.78915700	1.90142500
H	-0.56115500	-0.96297700	1.84271500
H	0.53344300	0.87859300	-0.33944800
H	2.73221900	-0.40532200	-0.28903500
H	2.70260700	-2.16994400	-0.29049300
H	0.87151600	-1.18193000	-1.63534000
H	0.23907800	-2.16013800	-0.31171900
C	2.18186600	1.18725900	1.95127900
H	1.66581800	2.02813900	2.41996500
H	2.23145600	1.40206600	0.88249900
C	4.31682300	-0.14742700	1.87348900
N	3.46055800	-1.26893700	2.19489900
C	3.58524600	1.06239900	2.51806100
H	4.19923700	1.93202500	2.28015600
H	3.56755800	0.94067700	3.60196600
N	4.85487200	-3.59885100	1.66236500
N	4.26749200	-2.68249000	1.58424900
H	5.27971900	-0.30252100	2.35554300
O	1.56349400	-2.56004700	1.90472300
H	1.24591400	-2.56249100	2.81673000
H	4.43523700	0.01728600	0.80255100
C	-1.43853600	0.11986900	-0.61165700
C	-2.00991900	1.49910700	-0.25166100
H	-2.98835200	1.63105900	-0.72158700
H	-2.14832000	1.62396100	0.82447400
H	-1.35346400	2.29821500	-0.60898400
C	-1.36812600	0.02799900	-2.14281300
H	-1.13061400	-0.98355600	-2.47894800

H	-2.33427800	0.30128700	-2.57496200
H	-0.61238600	0.71092400	-2.54393700
C	-2.39463100	-0.96423300	-0.09680200
H	-3.34786600	-0.89221800	-0.62769200
H	-1.99767800	-1.96918000	-0.26399100
H	-2.60356900	-0.84878900	0.96930800
C	1.14215700	-0.23079600	3.73973300
C	1.76743000	-1.14761200	4.58453300
C	0.26213500	0.68238600	4.34969300
C	1.51028000	-1.19563100	5.95740000
H	2.50557900	-1.84507800	4.21017700
C	0.00544900	0.65916600	5.70602300
H	-0.22595400	1.45012100	3.76232700
C	0.61958300	-0.29322200	6.52596600
H	2.02378100	-1.93578200	6.55521400
H	-0.67209500	1.37665400	6.15328500
O	0.29624900	-0.25145700	7.83981000
C	0.91804500	-1.19404200	8.70241300
H	0.52922900	-0.99252600	9.69726300
H	0.66454300	-2.21652300	8.41069800
H	2.00367900	-1.06756300	8.69997300

8d-TS-OMe

G(298.15 K)= -1094.03494

H(298.15 K)= -1093.958604

C	0.00296900	-0.01186700	-0.01647900
C	0.00825900	0.02941800	1.51889000
C	1.40298700	0.02255100	2.19468300
C	2.24765200	-1.15878300	1.60267800
C	2.29069300	-1.08946100	0.03165500
C	0.85777900	-1.19086300	-0.49025600
H	-0.49320100	0.93062300	1.87944000
H	-0.56082800	-0.82342300	1.89658300

H	0.46577500	0.90995900	-0.39138700
H	2.74655100	-0.16232100	-0.30882000
H	2.90192600	-1.92034300	-0.32880400
H	0.92154800	-1.22228900	-1.57982900
H	0.41963700	-2.13553600	-0.16042900
C	2.15857700	1.33074700	1.85867100
H	1.64626000	2.16112200	2.34763300
H	2.07386800	1.52965600	0.79069200
C	4.37804500	0.09055600	1.77485400
N	3.65223400	-1.15111400	1.94945800
C	3.64496300	1.34112000	2.23670100
H	4.13353300	2.21010100	1.79420300
H	3.79121900	1.41505500	3.31567400
N	3.95678700	-1.87347400	4.62185500
N	3.61342400	-1.38424000	3.70706600
O	1.72441600	-2.38125100	1.99958600
H	4.54962700	0.07232000	0.68713400
H	2.18720600	-3.09895000	1.54681200
H	5.36311000	-0.03369100	2.22421100
C	-1.43479600	-0.02010300	-0.61680100
C	-1.34818200	0.23482100	-2.12873200
H	-0.80574600	-0.55722000	-2.64935000
H	-2.35289500	0.28054600	-2.55764400
H	-0.84970000	1.18673700	-2.33491800
C	-2.26553800	1.11184200	0.00404000
H	-2.51743100	0.90724200	1.04700400
H	-1.72777600	2.06440100	-0.04002000
H	-3.20376400	1.22709100	-0.54483500
C	-2.15880700	-1.35254100	-0.38299000
H	-3.18780400	-1.27646600	-0.74505300
H	-1.68032700	-2.17352100	-0.92239800
H	-2.20104100	-1.61572100	0.67728000
C	1.19711100	-0.15485900	3.70814700

C	1.61152900	0.79951400	4.64026300	H	2.25869400	1.42842700	0.84107000
C	0.51072300	-1.27489300	4.22140600	C	4.33067600	-0.11287000	1.87429700
C	1.42727300	0.63879800	6.01219100	N	3.46269700	-1.21241100	2.23678700
H	2.08830400	1.71606400	4.32446500	C	3.61677000	1.12677500	2.48127100
C	0.32541800	-1.45652300	5.57647900	H	4.24015800	1.98059800	2.21287000
H	0.12872000	-2.03075500	3.55115700	H	3.60315900	1.04164700	3.56883800
C	0.79768900	-0.50717600	6.49132100	N	4.83336500	-3.57363200	1.76689200
H	1.77659500	1.41269400	6.68164900	N	4.25185700	-2.65584600	1.66598200
H	-0.19223500	-2.33036600	5.95369300	H	5.29363100	-0.26362900	2.35767600
O	0.58012600	-0.77602700	7.79676100	O	1.54860600	-2.49011900	1.99646300
C	1.02623100	0.17525300	8.75483000	H	1.25503600	-2.47094900	2.91626800
H	0.75834600	-0.23077300	9.72675700	H	4.44652100	0.01488300	0.79796500
H	2.10966800	0.30615300	8.69683800	C	-1.43311500	0.14198500	-0.59025700
H	0.52889500	1.13721900	8.60899900	C	-1.98929300	1.53598200	-0.26445500

8c-TS

G(298.15 K)= -979.547403

H(298.15 K)= -979.476185

C	0.00110800	0.00027600	0.00047900	H	-2.96638500	1.66672000	-0.73743200
C	-0.00174500	-0.00221100	1.53367100	H	-2.12600800	1.68944800	0.80816800
C	1.38394100	-0.00806100	2.23264300	H	-1.32429600	2.31870000	-0.64179200
C	2.14199000	-1.29185900	1.62474300	C	-1.36901200	0.00931000	-2.11867300
C	2.15933100	-1.27451700	0.09633500	H	-1.14159700	-1.01288700	-2.42861100
C	0.75675500	-1.23459800	-0.49649400	H	-2.33424100	0.27972500	-2.55463100
H	-0.53010500	0.87835900	1.89661100	H	-0.60878300	0.67488400	-2.53994500
H	-0.55434900	-0.87486200	1.89377500	C	-2.39767800	-0.91891000	-0.04390000
H	0.54856300	0.88535900	-0.34991700	H	-3.35375900	-0.84790500	-0.56980100
H	2.73365400	-0.42383600	-0.27035500	H	-2.01346300	-1.93183600	-0.19112400
H	2.68176700	-2.18655800	-0.21298500	H	-2.59793400	-0.77682600	1.02062200
H	0.85701100	-1.21924400	-1.58218500	C	1.16450900	-0.08622200	3.75875800
H	0.21920100	-2.14756400	-0.22550900	C	1.77574600	-0.99674000	4.62788600
C	2.21237500	1.25033400	1.91650800	C	0.30940200	0.86798400	4.33148100
H	1.70979700	2.11326600	2.35844100	C	1.51342600	-0.98068100	5.99806800
				H	2.49776000	-1.71920400	4.27065600
				C	0.05721900	0.89433400	5.69621800
				H	-0.16108700	1.62261800	3.71369700
				C	0.65050400	-0.04034700	6.54010500

H	2.00242800	-1.70714200	6.63587300
H	-0.60640900	1.65009900	6.09922700
H	0.44961400	-0.02638600	7.60437600

8d-TS

G(298.15 K)= -979.548063

H(298.15 K)= -979.477582

C	0.00424700	-0.00800700	0.00571200
C	0.00736000	-0.01197900	1.54142200
C	1.40312300	-0.01203100	2.21826100
C	2.27133400	-1.15449300	1.59340300
C	2.30864000	-1.04448600	0.02311800
C	0.87598800	-1.16169600	-0.49706100
H	-0.51160900	0.86784700	1.92903900
H	-0.54432600	-0.88716100	1.89245900
H	0.45561300	0.92967600	-0.34273700
H	2.74249300	-0.09943200	-0.29584100
H	2.93599100	-1.85261800	-0.36028100
H	0.93876600	-1.16749400	-1.58701700
H	0.45569000	-2.12120000	-0.18719700
C	2.12857400	1.32251200	1.92283500
H	1.59132000	2.12814900	2.42566600
H	2.05187900	1.54593500	0.85901300
C	4.37392100	0.14780100	1.79678000
N	3.68444700	-1.12036100	1.91815400
C	3.60922600	1.35419200	2.31722500
H	4.07956100	2.25667700	1.92500600
H	3.74356200	1.37413600	3.40049200
N	4.02971900	-1.97038600	4.55898400
N	3.69091300	-1.45010200	3.66107700
O	1.78688100	-2.40055100	1.95987500
H	4.53730900	0.18072000	0.70772600
H	2.25818700	-3.09284900	1.47714100

H	5.36638900	0.02988700	2.23163900
C	-1.43204700	-0.01790600	-0.59757600
C	-1.34450900	0.26992300	-2.10365500
H	-0.79797500	-0.50841800	-2.64035500
H	-2.34893600	0.32002000	-2.53265900
H	-0.85030600	1.22838600	-2.28891400
C	-2.27420300	1.09308500	0.04527200
H	-2.52602000	0.86483400	1.08331200
H	-1.74482400	2.05105700	0.02190000
H	-3.21253800	1.21144000	-0.50271500
C	-2.14333400	-1.36186300	-0.39388600
H	-3.16990700	-1.29021400	-0.76361600
H	-1.65138700	-2.16805000	-0.94347300
H	-2.19221500	-1.64419900	0.66108300
C	1.18259800	-0.23087000	3.72975400
C	1.55309800	0.72610100	4.68220100
C	0.52469300	-1.37989000	4.20102700
C	1.33541300	0.52373300	6.04293800
H	2.00956400	1.65961500	4.38738400
C	0.31297100	-1.58771500	5.55750100
H	0.18242400	-2.13232200	3.50619400
C	0.73044500	-0.64288600	6.49093400
H	1.64315800	1.28679900	6.74788700
H	-0.18623200	-2.49229300	5.88438800
H	0.56977400	-0.80801700	7.54965200

8c-TS-N02

G(298.15 K)= -1184.041426

H(298.15 K)= -1183.963203

C	-0.00482100	-0.02842900	-0.00604400
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C	-0.02401800	-0.06508100	1.52678700	H	-2.32164400	0.27830400	-2.57385500
C	1.35641200	-0.07621500	2.23743000	H	-0.60058800	0.69047400	-2.53700200
C	2.13083400	-1.34058800	1.60907400	C	-2.39309500	-0.97244700	-0.08869200
C	2.16660000	-1.28074100	0.08172800	H	-3.34397800	-0.90364200	-0.62404600
C	0.76999100	-1.24200400	-0.52479800	H	-1.99508800	-1.97801000	-0.24927700
H	-0.56301400	0.80431900	1.90065200	H	-2.60733200	-0.85174100	0.97581100
H	-0.57362300	-0.94930500	1.86220400	C	1.11988900	-0.18506600	3.75795000
H	0.53481600	0.87125000	-0.33028200	C	1.72863600	-1.11244200	4.61181000
H	2.73418300	-0.41351100	-0.25538100	C	0.25187800	0.75614700	4.33525700
H	2.70376600	-2.17782100	-0.24505800	C	1.45601900	-1.13402700	5.97551000
H	0.88174000	-1.19695100	-1.60846500	H	2.45957700	-1.82148200	4.24845900
H	0.24043300	-2.16772100	-0.28363100	C	-0.02476300	0.75913100	5.69139100
C	2.18119500	1.19507800	1.96397800	H	-0.21320500	1.52140100	3.72865100
H	1.67031200	2.04665600	2.41823500	C	0.57732800	-0.20075900	6.49051700
H	2.23678800	1.39575800	0.89337500	H	1.92883300	-1.85966300	6.62268400
C	4.30821300	-0.15912300	1.91537800	H	-0.69380300	1.49102800	6.12242400
N	3.44019400	-1.26652500	2.24417600	N	0.28623400	-0.21484600	7.93353400
C	3.58011400	1.06501000	2.54102400	O	-0.50212100	0.60251400	8.36129700
H	4.20222800	1.92639000	2.29506300	O	0.84899600	-1.04342600	8.61872700
H	3.55888900	0.95946400	3.62673800	8d-TS-NO2			
N	4.83451800	-3.61892600	1.73671200	G(298.15 K)= -1184.042669			
N	4.24518200	-2.70469500	1.65187800	H(298.15 K)= -1183.965321			
H	5.26493100	-0.31398200	2.40943500				
O	1.53991300	-2.55230500	1.93630800				
H	1.24693400	-2.58136500	2.85535400	C	0.00830700	-0.01505100	0.01754200
H	4.43644500	-0.00734900	0.84381600	C	0.02300500	-0.00928100	1.55249000
C	-1.43596400	0.10984800	-0.60539500	C	1.42834300	-0.01974100	2.21416200
C	-2.01019400	1.49075100	-0.25637900	C	2.28057700	-1.17271400	1.59195200
H	-2.98510600	1.61947000	-0.73422100	C	2.29687000	-1.08317800	0.01990200
H	-2.15747200	1.62146000	0.81790300	C	0.85586100	-1.18805600	-0.48022100
H	-1.35165200	2.28839900	-0.61298900	H	-0.48313200	0.87786200	1.93999900
C	-1.35726800	0.00883300	-2.13558200	H	-0.53444100	-0.87752700	1.91156200
H	-1.11708600	-1.00443700	-2.46448300	H	0.47246200	0.91234300	-0.34098300

$$G(298.15\text{ K}) = -1184.042669$$

C	0.00830700	-0.01505100	0.01754200
C	0.02300500	-0.00928100	1.55249000
C	1.42834300	-0.01974100	2.21416200
C	2.28057700	-1.17271400	1.59195200
C	2.29687000	-1.08317800	0.01990200
C	0.85586100	-1.18805600	-0.48022100
H	-0.48313200	0.87786200	1.93999900
H	-0.53444100	-0.87752700	1.91156200
H	0.47246200	0.91234300	-0.34098300
H	2.73785400	-0.14809300	-0.31832000

H	2.90903200	-1.90429600	-0.36002100	C	1.31337100	0.59316200	6.02162600
H	0.90561200	-1.20983300	-1.57051600	H	2.02021600	1.68256600	4.35915100
H	0.42545200	-2.13696100	-0.15185500	C	0.28799300	-1.55058900	5.55503300
C	2.16159700	1.30744000	1.90923200	H	0.20736800	-2.13121800	3.51940700
H	1.62784400	2.12304700	2.39921500	C	0.69512600	-0.56869400	6.44523800
H	2.08935000	1.51923900	0.84277900	H	1.59828500	1.35569600	6.73318600
C	4.39474400	0.12468900	1.76422100	H	-0.21546600	-2.43843700	5.91185000
N	3.70377600	-1.14198700	1.88469200	N	0.44291600	-0.75939900	7.88341700
C	3.64072700	1.32677700	2.30685400	O	0.83882700	0.09536000	8.64885300
H	4.11620300	2.23311900	1.93052400	O	-0.14776300	-1.76204900	8.22852800
H	3.77557800	1.32712500	3.39095700	C	1.20157600	-0.21696300	3.72820600
N	4.09818000	-2.02663800	4.51326200	C	1.55699000	0.76465500	4.66438300
N	3.75474000	-1.49790200	3.62261400	C	0.54140700	-1.36405900	4.20788400
O	1.79676100	-2.40883800	1.98570300	C	1.31875100	0.59992800	6.02449100
H	4.54018100	0.16681400	0.67252900	H	2.01824200	1.69278100	4.35602500
H	2.24122300	-3.11399900	1.49569800	C	0.30041700	-1.55082100	5.56087700
H	5.39469400	-0.00040200	2.17948600	H	0.21622000	-2.13252500	3.52095400
C	-1.43340200	-0.00553600	-0.57322800	C	0.70591100	-0.56580000	6.45004200
C	-1.35280900	0.27735200	-2.08056800	H	1.60132000	1.36137300	6.74032200
H	-0.81731200	-0.50765800	-2.61869700	H	-0.19802800	-2.44012500	5.92538600
H	-2.35954000	0.33592100	-2.50286400	N	0.45907300	-0.75623300	7.88492800
H	-0.85075500	1.23049000	-2.27166200	O	0.82551900	0.12179400	8.64547800
C	-2.25429800	1.11909600	0.07346000	O	-0.09745200	-1.78210200	8.23357000
H	-2.50374200	0.89604100	1.11326200	(B3LYP/6-31G(d,p)- water(CPCM;UFF) 8c-TS-OMe G(298.15 K)= -1094.242064 H(298.15 K)= -1094.163389			
H	-1.71099200	2.06908000	0.04545600				
H	-3.19400700	1.25080700	-0.46893400				
C	-2.16168000	-1.33886600	-0.36025400	C	-0.01111700	-0.03857500	-0.05162400
H	-3.19090100	-1.25262900	-0.71916500	C	-0.02106500	0.00442300	1.48885100
H	-1.68737400	-2.15252500	-0.91426200	C	1.34671500	-0.09070700	2.23811000
H	-2.20380200	-1.61970300	0.69546300				
C	1.20064400	-0.22210400	3.72767900				
C	1.55562900	0.75712900	4.66332900				
C	0.53489100	-1.36486700	4.20472300				

C	2.10466500	-1.39698600	1.61232200
C	2.08504000	-1.41292400	0.07618700
C	0.67821900	-1.33448300	-0.50613900
H	-0.46560100	0.94934700	1.80367300
H	-0.66327600	-0.79480300	1.86995300
H	0.59928300	0.80047500	-0.41590600
H	2.69015600	-0.59292300	-0.31658300
H	2.57646300	-2.35041400	-0.21497800
H	0.76054600	-1.37727100	-1.59508700
H	0.10439600	-2.21088000	-0.18852400
C	2.21051500	1.17036900	1.97329900
H	1.73271600	2.01737300	2.47499900
H	2.21830500	1.40387500	0.90431800
C	4.32812700	-0.20951500	1.81169400
N	3.46325000	-1.33038200	2.16234300
C	3.64293500	1.02203500	2.46982500
H	4.25391500	1.88456400	2.18846400
H	3.68442400	0.92219900	3.55649000
N	4.82105100	-3.63357600	1.92088300
N	4.21107500	-2.74055600	1.66899500
H	5.30846900	-0.38223900	2.25611300
O	1.52017400	-2.58614900	2.03324900
H	1.33809400	-2.54242100	2.98694400
H	4.41988900	-0.05423900	0.73435600
C	-1.43259000	0.19081500	-0.68117100
C	-1.99173700	1.55940700	-0.23324500
H	-2.91480000	1.78480000	-0.77779000
H	-2.23465100	1.58408400	0.83329700
H	-1.27944700	2.36717700	-0.43789100
C	-1.30420000	0.22324300	-2.22008700
H	-1.01448000	-0.74690100	-2.63392400
H	-2.26428900	0.49472500	-2.67159100
H	-0.56290000	0.96391500	-2.54180300

C	-2.43898700	-0.91130200	-0.29162300
H	-3.40607300	-0.71656600	-0.76790600
H	-2.10827800	-1.90232500	-0.61784100
H	-2.61122200	-0.95025300	0.78857800
C	1.08770300	-0.25330100	3.75738500
C	1.93440900	-0.94542200	4.63967900
C	-0.03137900	0.37871800	4.34468600
C	1.69127600	-1.02617900	6.01490600
H	2.82257300	-1.44541900	4.27190800
C	-0.28131600	0.32044300	5.70691900
H	-0.72783900	0.94406000	3.73924400
C	0.57553500	-0.38919900	6.56233600
H	2.38104700	-1.58586300	6.63427400
H	-1.14517300	0.82244800	6.13022800
O	0.23736100	-0.39712500	7.87803000
C	1.08475900	-1.09794500	8.78987600
H	0.63475000	-0.96933300	9.77415000
H	1.13295200	-2.16551500	8.54840000
H	2.09724200	-0.67952000	8.79465500

8d-TS-OMe

G(298.15 K)= -1094.243788

H(298.15 K)= -1094.166888

C	-0.00961200	-0.00882400	-0.01750600
C	0.00753200	0.00858400	1.52744300
C	1.41615700	0.01787300	2.19922300
C	2.28913200	-1.16012400	1.57690200
C	2.31105200	-1.06605500	0.01422500
C	0.87908600	-1.15854700	-0.52883800
H	-0.51795600	0.89099000	1.90276500
H	-0.54219900	-0.85992200	1.89725300
H	0.43814800	0.92866500	-0.37568700
H	2.78015600	-0.14146400	-0.32236600

H	2.92100500	-1.89409600	-0.36081500
H	0.95122300	-1.14181900	-1.61971900
H	0.45495300	-2.12720000	-0.24877000
C	2.15689700	1.34722800	1.85988000
H	1.64343400	2.17257300	2.36045900
H	2.04075200	1.54721900	0.79404900
C	4.40706700	0.11347500	1.80340300
N	3.67017400	-1.13311700	2.02242600
C	3.65905500	1.39055500	2.20160700
H	4.12531400	2.23874600	1.69267900
H	3.82332500	1.54923500	3.26992800
N	4.06701200	-1.78852600	4.55691000
N	3.52670800	-1.30106900	3.70772800
O	1.75375800	-2.39717700	1.95820600
H	4.61249200	0.07532100	0.72453400
H	2.28445200	-3.10329300	1.55717700
H	5.37548300	0.02012000	2.29875800
C	-1.46293500	-0.01208200	-0.61592100
C	-1.38054400	0.08102900	-2.15562300
H	-0.94570300	-0.81686300	-2.60432800
H	-2.38332300	0.20158800	-2.57922500
H	-0.78040000	0.94241500	-2.47101200
C	-2.23419200	1.22841600	-0.11472200
H	-2.43798200	1.18709100	0.95917500
H	-1.67883800	2.15124400	-0.31903700
H	-3.20040800	1.30179400	-0.62511800
C	-2.25901300	-1.27906800	-0.24061700
H	-3.25405500	-1.24144700	-0.69729000
H	-1.77107400	-2.19130700	-0.59800500
H	-2.40240300	-1.37276400	0.84044600
C	1.24787200	-0.19698700	3.71080800
C	1.65025700	0.76608100	4.66716200
C	0.54503000	-1.32729400	4.22074900

C	1.44228100	0.60483600	6.02922900
H	2.13349100	1.68060300	4.35368300
C	0.33659900	-1.50826900	5.57062600
H	0.18561800	-2.08552500	3.54069000
C	0.79419500	-0.55010900	6.50014200
H	1.77813400	1.37538000	6.71116700
H	-0.18543600	-2.38329100	5.94230200
O	0.55242000	-0.82327200	7.79271800
C	0.97907500	0.10923300	8.79641500
H	0.68183800	-0.32908700	9.74793300
H	2.06515600	0.23860600	8.77284100
H	0.48534200	1.07675600	8.66597000

8c-TS

G(298.15 K)= -979.744119

H(298.15 K)= -979.670756

C	-0.01644100	-0.05584600	-0.02649700
C	-0.01963700	-0.00762200	1.51382100
C	1.35903000	-0.06108700	2.24853000
C	2.11880600	-1.37144000	1.64142800
C	2.10645700	-1.39545400	0.10467300
C	0.69945700	-1.33744200	-0.48175800
H	-0.49262800	0.92193100	1.83053800
H	-0.63211800	-0.82525400	1.90488900
H	0.57297100	0.79587400	-0.39547900
H	2.70384900	-0.57134000	-0.29076700
H	2.60850300	-2.32912600	-0.17999900
H	0.78663400	-1.37486900	-1.57049000
H	0.14012300	-2.22495400	-0.16942400
C	2.21351100	1.19817800	1.95385600
H	1.73009300	2.05584900	2.43120200
H	2.22871400	1.40639100	0.88018800
C	4.33656100	-0.18033200	1.84309100

N	3.47049400	-1.29610700	2.20469900
C	3.64086300	1.06278500	2.46990400
H	4.25535200	1.92011500	2.18068000
H	3.66844000	0.98226300	3.55879900
N	4.84089600	-3.60500800	1.98353100
N	4.22602600	-2.71699000	1.72801100
H	5.31161900	-0.34163900	2.30296500
O	1.53160100	-2.56060500	2.05962800
H	1.34431200	-2.52676800	3.01207200
H	4.44038200	-0.04478900	0.76429700
C	-1.44554000	0.13990400	-0.64973400
C	-2.02512100	1.50470600	-0.21619800
H	-2.95826700	1.70463400	-0.75349300
H	-2.25658800	1.54168600	0.85256500
H	-1.33019000	2.32201800	-0.44136800
C	-1.32785600	0.15386200	-2.18976800
H	-1.03031300	-0.81836100	-2.59295000
H	-2.29392600	0.40893400	-2.63806100
H	-0.59712800	0.89850000	-2.52620800
C	-2.42981100	-0.97407700	-0.23818400
H	-3.40138400	-0.80652000	-0.71555800
H	-2.08090600	-1.96439500	-0.54719200
H	-2.59899800	-0.99656700	0.84293200
C	1.11259700	-0.17130400	3.77733800
C	1.87313300	-0.96487800	4.65581300
C	0.09455300	0.61411800	4.35396900
C	1.61129400	-0.99756900	6.02945200
H	2.70262900	-1.55779000	4.28982800
C	-0.16023900	0.59161900	5.72349100
H	-0.50895300	1.27014200	3.73925400
C	0.59049300	-0.22354100	6.57225400
H	2.21991100	-1.63084600	6.66734900
H	-0.95153400	1.21706300	6.12536200

H	0.38616900	-0.24691200	7.63799300
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8d-TS

G(298.15 K)= -979.741674

H(298.15 K)= -979.670423

C	-1.30407400	3.52106700	0.29547600
C	-1.32504300	2.70514900	-1.01571100
C	-2.01868000	1.30841000	-0.94872400
C	-1.42004800	0.50101100	0.27673500
C	-1.50436100	1.34491500	1.60617000
C	-0.72043200	2.65157600	1.42355600
H	-1.83703500	3.26315100	-1.80437800
H	-0.29781500	2.55829000	-1.35726000
H	-2.34092100	3.75767100	0.57225900
H	-2.53831200	1.56429500	1.87162400
H	-1.07894400	0.74203900	2.41447600
H	-0.76050700	3.17259600	2.38416700
H	0.32986000	2.41660600	1.22768600
C	-3.54014400	1.48766200	-0.66596400
H	-4.00439200	1.96110800	-1.53485600
H	-3.66599700	2.20419900	0.14713200
C	-3.58549000	-0.64369600	0.74336700
N	-2.13536200	-0.72614900	0.59147800
C	-4.30625500	0.20243900	-0.30623200
H	-5.29814900	0.45711200	0.07703100
H	-4.46626400	-0.43070600	-1.18244700
N	-1.62231000	-2.75199900	-1.11658900
N	-1.85716800	-1.72110100	-0.77261700
O	-0.09022000	0.16002000	0.03217900
H	-3.66866300	-0.21335100	1.75313100
H	0.28395100	-0.26321500	0.82117600
H	-3.97323500	-1.66079900	0.82538600

C	-0.60220700	4.91883000	0.14281300
C	-0.73656700	5.70305300	1.46706600
H	-0.16679500	5.24601600	2.28152200
H	-0.35775100	6.72282500	1.34033000
H	-1.78367400	5.77358700	1.78384700
C	-1.31088700	5.73789900	-0.95797900
H	-1.16330500	5.31204300	-1.95460200
H	-2.38946000	5.80276200	-0.77316400
H	-0.91505900	6.75878700	-0.98011800
C	0.89468600	4.79937400	-0.21012800
H	1.33571100	5.79830800	-0.29776500
H	1.45690700	4.26215600	0.56017300
H	1.05491800	4.28909600	-1.16494100
C	-1.74825200	0.57618900	-2.28550400
C	-2.78733800	0.21353800	-3.16762800
C	-0.42547700	0.34526200	-2.73173000
C	-2.52744400	-0.37734100	-4.40335100
H	-3.82129100	0.40362500	-2.91518300
C	-0.16519300	-0.25061200	-3.96164600
H	0.40954100	0.61975300	-2.10327200
C	-1.21492700	-0.62508700	-4.80402000
H	-3.35728900	-0.64072000	-5.05153900
H	0.86362300	-0.41940500	-4.26427500
H	-1.01147100	-1.09324400	-5.76207700

8c-TS-N02

G(298.15 K)= -1184.246548

H(298.15 K)= -1184.16696

C	-0.02163300	-0.05151500	-0.01896700
C	-0.02511400	-0.03721600	1.52222200

C	1.36253600	-0.07013800	2.24293900
C	2.12626200	-1.37064600	1.62682500
C	2.13030300	-1.35954800	0.08943200
C	0.72563100	-1.30407200	-0.50590300
H	-0.52539800	0.86856400	1.86444700
H	-0.60960500	-0.88257600	1.89701100
H	0.54400800	0.82422000	-0.36760300
H	2.72306500	-0.52231300	-0.28370800
H	2.64233300	-2.28231600	-0.21149000
H	0.82260800	-1.30398100	-1.59429600
H	0.17987000	-2.21112200	-0.22840000
C	2.21231400	1.19301500	1.94913100
H	1.72525900	2.05486900	2.41456900
H	2.23628300	1.39413000	0.87518100
C	4.33953000	-0.18896200	1.87537500
N	3.46386000	-1.30133500	2.22079400
C	3.63358500	1.05958500	2.48355300
H	4.25250900	1.91378500	2.19508200
H	3.64897100	0.98919700	3.57344200
N	4.85151700	-3.61581700	1.97555000
N	4.22862200	-2.72947700	1.73743600
H	5.30318400	-0.34924300	2.35876100
O	1.53171500	-2.57059500	2.00176800
H	1.32797900	-2.58339700	2.94978800
H	4.46731000	-0.05646700	0.79903200
C	-1.45666400	0.12087500	-0.63603700
C	-2.06936800	1.46119500	-0.17286600
H	-3.00770600	1.64902300	-0.70533300
H	-2.30117900	1.46954400	0.89650200
H	-1.39534700	2.30024800	-0.38066300
C	-1.34082500	0.16959300	-2.17543600
H	-1.02201700	-0.78732800	-2.59840000
H	-2.31298600	0.41174900	-2.61751100

H	-0.62764900	0.93742500	-2.49689000
C	-2.41175400	-1.02622200	-0.24715200
H	-3.38872000	-0.87097800	-0.71745300
H	-2.04072100	-2.00039300	-0.58080300
H	-2.57679300	-1.07809700	0.83360400
C	1.12210000	-0.16310200	3.77236600
C	1.79651800	-1.03739200	4.64446800
C	0.18939900	0.72527700	4.34711300
C	1.52960500	-1.06080000	6.01270800
H	2.57248200	-1.69969900	4.28291000
C	-0.08218500	0.72531000	5.70877400
H	-0.33471900	1.44660800	3.73355500
C	0.58623800	-0.18185000	6.52805500
H	2.05286000	-1.74505300	6.66762500
H	-0.79960500	1.41498700	6.13392400
N	0.29869200	-0.19893900	7.96503700
O	-0.53584300	0.59810500	8.39763700
O	0.90487200	-1.00965300	8.66798700

8d-TS-NO2

G(298.15 K)= -1184.245561

H(298.15 K)= -1184.166825

C	-0.00097000	-0.01665400	0.02068900
C	0.02854500	-0.03155500	1.56387000
C	1.44403800	-0.02725100	2.22938500
C	2.32292800	-1.16594900	1.57832300
C	2.31612200	-1.06337800	-0.00012500
C	0.87060400	-1.16880700	-0.50605100
H	-0.49969200	0.83713300	1.96562600
H	-0.51027200	-0.91336200	1.91784800
H	0.45658000	0.92010900	-0.32612700
H	2.75878700	-0.12606600	-0.33567200
H	2.93126100	-1.87841900	-0.39252600

H	0.93061600	-1.15520300	-1.59793700
H	0.45450900	-2.13812700	-0.21680500
C	2.15851800	1.32447800	1.93411900
H	1.61730300	2.12663500	2.44146900
H	2.06340700	1.54961300	0.87056100
C	4.42596500	0.18168500	1.76699900
N	3.75123200	-1.10626800	1.88131200
C	3.64767500	1.37648400	2.31084100
H	4.09923000	2.29176000	1.91898800
H	3.79247300	1.39730700	3.39477500
N	4.33617000	-2.15765300	4.33106400
N	3.85303400	-1.55218800	3.53715500
O	1.86382100	-2.42046000	1.96482900
H	4.57479400	0.24015000	0.67684500
H	2.33995900	-3.11123200	1.47627600
H	5.42811800	0.07567000	2.18692900
C	-1.45812700	0.00630900	-0.56809700
C	-1.38148600	0.11502600	-2.10704500
H	-0.96537000	-0.78565100	-2.56791100
H	-2.38417200	0.25760300	-2.52358900
H	-0.76795500	0.96907900	-2.41620800
C	-2.20629400	1.25312200	-0.04822700
H	-2.40230600	1.20447900	1.02686000
H	-1.63897100	2.16945900	-0.24838600
H	-3.17535800	1.34545200	-0.54984800
C	-2.26925000	-1.25316800	-0.20105100
H	-3.26417900	-1.19883100	-0.65600500
H	-1.79402800	-2.16889100	-0.56660800
H	-2.41271800	-1.35298400	0.87936700
C	1.22180700	-0.25742000	3.74861500
C	1.54167100	0.72669500	4.70306900
C	0.57114500	-1.42074900	4.21740500
C	1.26132100	0.55940400	6.05645800

H	2.00237300	1.65927100	4.41098200
C	0.28820200	-1.60871800	5.56417900
H	0.28650500	-2.19900000	3.52494900
C	0.64344000	-0.61427900	6.47263400
H	1.51434400	1.32680900	6.77616000
H	-0.20588700	-2.50751700	5.90937900
N	0.34886200	-0.80371400	7.89573400
O	0.67214800	0.09110400	8.67964400
O	-0.20764800	-1.84896100	8.23836900

**(CAM-B3LYP/6-31G(d,p)-
water(CPCM;UFF)**

8c-TS

G(298.15 K)= -979.20042

H(298.15 K)= -979.12837

C	-0.01290400	-0.05396000	-0.00952700
C	-0.01824200	-0.04293800	1.52475800
C	1.36216500	-0.06690700	2.23938100
C	2.12364600	-1.35208500	1.62848000
C	2.13586200	-1.34423200	0.09907500
C	0.73513000	-1.29870800	-0.49315600
H	-0.52900200	0.85287500	1.87354800
H	-0.59357700	-0.89586000	1.89445700
H	0.54998700	0.82265600	-0.35779400
H	2.72080500	-0.50340100	-0.27534700
H	2.65195700	-2.26242400	-0.20336700
H	0.82878100	-1.30451800	-1.58054200
H	0.19520500	-2.20562400	-0.20745600
C	2.19716200	1.19397800	1.94132200
H	1.70282600	2.05190500	2.40282900
H	2.22859300	1.39369700	0.86812800
C	4.31776300	-0.17333500	1.87454800
N	3.44667300	-1.27108700	2.22977100

C	3.61022800	1.06617200	2.48343300
H	4.22895000	1.92264400	2.20745700
H	3.61318700	0.98633800	3.57182300
N	4.82025700	-3.63910100	1.85450900
N	4.22745100	-2.72460000	1.69750000
H	5.28250500	-0.32864200	2.35543800
O	1.53443400	-2.54715400	2.00635800
H	1.28248800	-2.52899700	2.94146800
H	4.43855000	-0.04160400	0.79843900
C	-1.43865200	0.11070800	-0.62314700
C	-2.04983200	1.44709100	-0.17177100
H	-2.98814300	1.62894500	-0.70389200
H	-2.27898600	1.46267200	0.89672400
H	-1.37698100	2.28367300	-0.38722700
C	-1.32711200	0.14606600	-2.15570000
H	-1.01552800	-0.81546500	-2.57045200
H	-2.29776300	0.39054000	-2.59684500
H	-0.61020200	0.90603600	-2.48374000
C	-2.38769700	-1.02852700	-0.22492200
H	-3.36204800	-0.88173100	-0.70063400
H	-2.01253300	-2.00456700	-0.54442600
H	-2.55588200	-1.06599900	0.85470400
C	1.12408600	-0.16295200	3.76415800
C	1.76648600	-1.05445200	4.63082800
C	0.21956100	0.74161000	4.33974500
C	1.48949400	-1.06856100	5.99679800
H	2.52381500	-1.73823700	4.26927900
C	-0.04822800	0.73771500	5.70065100
H	-0.28238400	1.47961800	3.72596500
C	0.57803900	-0.17776000	6.53981800
H	2.00516400	-1.78132900	6.63132900
H	-0.75183800	1.45744400	6.10544600
H	0.36417700	-0.18648700	7.60305000

8d-TS

G(298.15 K)= -979.19908

H(298.15 K)= -979.128076

C	-1.30628400	3.51149900	0.29404900
C	-1.33257300	2.69861000	-1.00983800
C	-2.01981700	1.30806000	-0.94036700
C	-1.42536200	0.51262100	0.27318600
C	-1.50369100	1.35197100	1.60101000
C	-0.71384900	2.64620100	1.41092300
H	-1.84735300	3.25369700	-1.79731100
H	-0.30696200	2.55204800	-1.35384200
H	-2.34045400	3.74654600	0.57830300
H	-2.53428000	1.58243100	1.86516400
H	-1.08248600	0.74906000	2.41002700
H	-0.73671900	3.16766000	2.37019600
H	0.33061000	2.40384400	1.19924800
C	-3.53388200	1.48330100	-0.66403000
H	-3.99576400	1.96009100	-1.53055500
H	-3.66863000	2.19211200	0.15344800
C	-3.58139000	-0.61999800	0.75540200
N	-2.14149800	-0.69090800	0.64232100
C	-4.28409100	0.19304800	-0.31966600
H	-5.29238800	0.42745200	0.02812500
H	-4.39880200	-0.45209000	-1.19346400
N	-1.56554000	-2.74679000	-1.14318900
N	-1.84165900	-1.76437000	-0.72829400
O	-0.10738300	0.16198800	0.03120200
H	-3.67942100	-0.17093100	1.75625300
H	0.28144800	-0.22719900	0.82886100
H	-3.96215200	-1.63647700	0.86450700
C	-0.60828600	4.89911600	0.13778300
C	-0.74610900	5.68638500	1.45094700
H	-0.18070900	5.23265400	2.26863800

H	-0.36551400	6.70362600	1.32031100
H	-1.79355000	5.75927700	1.76178800
C	-1.30815800	5.70812000	-0.96556500
H	-1.14794800	5.28122200	-1.95845400
H	-2.38763500	5.76586800	-0.79065900
H	-0.91846300	6.73004800	-0.98525700
C	0.88291800	4.77742000	-0.20699100
H	1.32156400	5.77505900	-0.30486700
H	1.44220200	4.25124400	0.57131300
H	1.04640600	4.25659400	-1.15417800
C	-1.75120100	0.59295900	-2.28446700
C	-2.78450100	0.25599300	-3.16760000
C	-0.43805600	0.34826400	-2.72092200
C	-2.52840700	-0.33213600	-4.40177300
H	-3.81690900	0.45813800	-2.91969200
C	-0.18004100	-0.24388900	-3.94874300
H	0.39726400	0.60923600	-2.08776000
C	-1.22482800	-0.59706600	-4.79584200
H	-3.35925000	-0.57945200	-5.05397800
H	0.84769600	-0.42528200	-4.24552400
H	-1.02312400	-1.06188100	-5.75509800

8c-TS-OMe

G(298.15 K)= -1093.653525

H(298.15 K)= -1093.57526

C	-0.01153500	-0.04536800	-0.02415700
C	-0.01151000	-0.04442800	1.51021900
C	1.36828400	-0.08679200	2.22513100
C	2.12999300	-1.36251200	1.59360900
C	2.13072600	-1.34281200	0.06452800
C	0.72667100	-1.29155600	-0.51795700
H	-0.51067900	0.85672400	1.86235600
H	-0.59694500	-0.89207400	1.87606100

H	0.55622700	0.82960400	-0.36891400
H	2.71328700	-0.49882500	-0.30688300
H	2.64474800	-2.25857600	-0.24879000
H	0.81236500	-1.29428900	-1.60602800
H	0.18540300	-2.19735900	-0.23104300
C	2.20030800	1.18074000	1.94608600
H	1.70629000	2.02745200	2.42880200
H	2.22305400	1.40159400	0.87644000
C	4.32338700	-0.17744500	1.83416800
N	3.46039100	-1.28425100	2.18095000
C	3.61826100	1.04787100	2.47308000
H	4.23153000	1.91151300	2.20730300
H	3.63131000	0.94749800	3.55962200
N	4.83415400	-3.64091400	1.76850600
N	4.23984300	-2.72520800	1.62394300
H	5.29465400	-0.33756700	2.30014300
O	1.54899500	-2.56180300	1.97031300
H	1.29915700	-2.54124600	2.90633500
H	4.43042900	-0.02617400	0.75915000
C	-1.43813700	0.13282500	-0.63211600
C	-2.04203200	1.46706600	-0.16492100
H	-2.97944500	1.66038100	-0.69458700
H	-2.27088700	1.47103500	0.90374100
H	-1.36475400	2.30260400	-0.37048500
C	-1.33028600	0.18395600	-2.16449600
H	-1.02246700	-0.77409200	-2.59001200
H	-2.30125700	0.43578800	-2.60078000
H	-0.61188600	0.94518000	-2.48629000
C	-2.39159700	-1.00619300	-0.24392900
H	-3.36710100	-0.84848100	-0.71379100
H	-2.02276800	-1.98013600	-0.57694200
H	-2.55559500	-1.05606600	0.83583300
C	1.13382100	-0.21952700	3.74632000

C	1.82601500	-1.07555900	4.60489100
C	0.18002400	0.62236300	4.34652800
C	1.57002800	-1.13117300	5.97556900
H	2.61398800	-1.71824300	4.23348300
C	-0.07742400	0.59066900	5.70171300
H	-0.37314200	1.33791400	3.75114300
C	0.60914300	-0.29847400	6.53404600
H	2.13692000	-1.82368900	6.58365900
H	-0.81420100	1.25370100	6.14127400
O	0.27731600	-0.26571000	7.84605900
C	0.95353300	-1.14787100	8.72898600
H	0.53726300	-0.96341800	9.71819100
H	0.78416600	-2.19382100	8.45403000
H	2.02957300	-0.94754400	8.74581500

8d-TS-OMe

G(298.15 K)= -1093.653656

H(298.15 K)= -1093.57638

C	-0.00264200	-0.01048400	-0.00699900
C	0.01990900	0.00979700	1.52984400
C	1.42039400	0.01611300	2.19798600
C	2.27999100	-1.14752200	1.57980000
C	2.30262000	-1.06016900	0.01211600
C	0.87094100	-1.16498100	-0.50949000
H	-0.50141600	0.89237600	1.90745300
H	-0.52979800	-0.85693100	1.90152800
H	0.44977800	0.92095000	-0.37212500
H	2.75561800	-0.12955700	-0.32516700
H	2.91708700	-1.88200000	-0.36472200
H	0.93461000	-1.16593000	-1.59980800
H	0.44936700	-2.12740600	-0.20937600
C	2.15432000	1.34036100	1.86758700

H	1.63817900	2.16011700	2.37129400
H	2.04673500	1.54969600	0.80325000
C	4.39155500	0.12693300	1.77016300
N	3.67806200	-1.12116900	1.93146000
C	3.64535700	1.37473600	2.22185600
H	4.11656200	2.24492100	1.75999100
H	3.80193700	1.47494300	3.29757500
N	4.06279800	-1.92286100	4.55000000
N	3.63307100	-1.40002600	3.67826400
O	1.77126400	-2.38020100	1.96341600
H	4.57745700	0.11692500	0.68508600
H	2.26758300	-3.08745700	1.52486300
H	5.37497900	0.01470000	2.22874300
C	-1.44765600	-0.01276100	-0.59808600
C	-1.36921000	0.09226400	-2.12965400
H	-0.93141600	-0.79931400	-2.58519000
H	-2.37233900	0.21079700	-2.54961000
H	-0.77415100	0.95820000	-2.43792300
C	-2.21728800	1.21479600	-0.08593700
H	-2.42711200	1.15629200	0.98474400
H	-1.65969200	2.13860000	-0.27277000
H	-3.17896900	1.29593700	-0.60093000
C	-2.23532900	-1.27924700	-0.23313000
H	-3.23407600	-1.23411500	-0.67781700
H	-1.75228400	-2.18503200	-0.60940700
H	-2.36602000	-1.38760500	0.84693400
C	1.23159100	-0.18643000	3.71115200
C	1.62404200	0.76999100	4.65433700
C	0.55276100	-1.31607500	4.21639000
C	1.41401300	0.60987500	6.01895500
H	2.10080000	1.68913800	4.34454800
C	0.34222700	-1.49646700	5.56604100
H	0.20183300	-2.08095400	3.53921000

C	0.78098800	-0.53878500	6.48822700
H	1.74446000	1.38589400	6.69662300
H	-0.17040500	-2.37734800	5.93589800
O	0.53674800	-0.80838500	7.78728200
C	0.95213400	0.13764900	8.76314000
H	0.66395800	-0.27830400	9.72714600
H	2.03652700	0.28179600	8.73890200
H	0.45314600	1.10077000	8.61935100

8c-TS-N02

G(298.15 K)= -1183.639513

H(298.15 K)= -1183.560793

C	-0.01381100	-0.05143900	-0.00517700
C	-0.02011100	-0.04656400	1.52932700
C	1.36262900	-0.07058400	2.24076900
C	2.12466800	-1.35451100	1.62673500
C	2.14001000	-1.33442300	0.09730900
C	0.73964900	-1.28994700	-0.49596300
H	-0.53276400	0.84770400	1.87907000
H	-0.59355700	-0.90200700	1.89602700
H	0.54428500	0.82993400	-0.34872600
H	2.72244600	-0.48891300	-0.26999300
H	2.65974000	-2.24851200	-0.21053300
H	0.83501200	-1.28657500	-1.58308200
H	0.20289500	-2.20109100	-0.21835300
C	2.19933500	1.19132900	1.94939800
H	1.70776700	2.05048000	2.41152500
H	2.22870300	1.39210500	0.87680500
C	4.31900000	-0.18303600	1.88284600
N	3.44342800	-1.27578100	2.23613400
C	3.61266700	1.05965200	2.49045800
H	4.23281300	1.91375900	2.21079200
H	3.62002300	0.98428400	3.57920000
N	4.82092400	-3.65352300	1.84811500

N	4.22422300	-2.74035700	1.70015000
H	5.28097600	-0.33936000	2.36870100
O	1.53261300	-2.55225600	1.98949800
H	1.29180800	-2.56442800	2.92674700
H	4.44362200	-0.05145000	0.80732500
C	-1.44119400	0.10967400	-0.61634400
C	-2.05825300	1.44082500	-0.15752500
H	-2.99685700	1.62147800	-0.68938600
H	-2.28900700	1.44929300	0.91076200
H	-1.38902600	2.28164200	-0.36756400
C	-1.33002200	0.15341100	-2.14869300
H	-1.01453600	-0.80467300	-2.56839000
H	-2.30196400	0.39579200	-2.58798000
H	-0.61670400	0.91824900	-2.47310400
C	-2.38437500	-1.03632100	-0.22363700
H	-3.35947700	-0.89131300	-0.69821300
H	-2.00502400	-2.00886200	-0.54871800
H	-2.55252100	-1.08049200	0.85576600
C	1.12405400	-0.16255400	3.76496100
C	1.76428400	-1.05838100	4.62966900
C	0.22280200	0.75028000	4.33562400
C	1.49227200	-1.07759300	5.99224200
H	2.51958700	-1.74351100	4.26943600
C	-0.05316200	0.75421700	5.69090300
H	-0.27380700	1.49035200	3.72214100
C	0.58093400	-0.17391500	6.50258500
H	1.98923400	-1.77978100	6.64780100
H	-0.74856900	1.46403500	6.11809500
N	0.28952200	-0.18640900	7.93506800
O	-0.51718400	0.62694100	8.36342900
O	0.86618900	-1.00980900	8.63165800

8d-TS-NO2

G(298.15 K)= -1183.639674

H(298.15 K)= -1183.561419

C	0.00439200	-0.01480300	0.02713000
C	0.03460700	-0.02983300	1.56282300
C	1.44297700	-0.02807900	2.22232700
C	2.31030700	-1.15989700	1.57536400
C	2.30781600	-1.05672100	0.00556000
C	0.86847800	-1.16549600	-0.49623600
H	-0.49171800	0.83805600	1.96617700
H	-0.50435200	-0.91129700	1.91509300
H	0.46165800	0.92037700	-0.32140500
H	2.74498600	-0.11825000	-0.33063900
H	2.92446000	-1.86859500	-0.38835800
H	0.92077600	-1.15896400	-1.58695500
H	0.45204100	-2.13075100	-0.19755800
C	2.15667100	1.31468000	1.92953300
H	1.61616200	2.11870800	2.43190100
H	2.06950200	1.53967000	0.86635400
C	4.40756200	0.16817900	1.76269500
N	3.73531800	-1.10809200	1.85484700
C	3.63719000	1.35473100	2.31597800
H	4.09733000	2.27166000	1.94222800
H	3.77342400	1.35780700	3.40028200
N	4.24666900	-2.13341400	4.39853300
N	3.82752400	-1.55594400	3.56007600
O	1.85115100	-2.40760000	1.95800100
H	4.55820000	0.23148400	0.67300200
H	2.31277800	-3.10016600	1.46109900
H	5.41091600	0.05320700	2.17535300
C	-1.44369100	0.00434900	-0.55594700
C	-1.37006300	0.13365400	-2.08588900
H	-0.94436100	-0.75517400	-2.55795100
H	-2.37360100	0.27002600	-2.49914900

H	-0.76680400	0.99792600	-2.38248400
C	-2.19930200	1.23057000	-0.02018900
H	-2.40467100	1.15725000	1.05049600
H	-1.63444900	2.15216100	-0.19551200
H	-3.16280200	1.32828300	-0.52869500
C	-2.23984600	-1.26122300	-0.20739500
H	-3.23827700	-1.20280000	-0.65104400
H	-1.76352500	-2.16532600	-0.59607900
H	-2.37147900	-1.38284300	0.87113200
C	1.21746500	-0.25103300	3.73669400
C	1.52929300	0.73468100	4.68091100
C	0.57839300	-1.41212400	4.20496500
C	1.25617300	0.56844600	6.03136500
H	1.98231000	1.66918300	4.38504000
C	0.30253100	-1.59929100	5.54831300
H	0.29831500	-2.19223300	3.51365000
C	0.65303900	-0.60417900	6.44723000
H	1.50447700	1.33779300	6.74983300
H	-0.18349200	-2.49989000	5.89857600
N	0.36550500	-0.79258200	7.86803000
O	0.68079800	0.10042500	8.64251500
O	-0.17593900	-1.83432600	8.21186900

**(wB97Z-D/6-31G(d,p)-
water(CPCM;UFF)**

8c-TS

G(298.15 K)= -979.460162

H(298.15 K)= -979.388083

C	-0.01340600	-0.05852100	-0.01317100
C	-0.02221900	-0.04809800	1.52058200
C	1.35677500	-0.07177200	2.23501100
C	2.11541100	-1.36546200	1.62654200
C	2.13213900	-1.35308700	0.09539100

C	0.73255500	-1.30372400	-0.49928600
H	-0.52844200	0.85342300	1.86341700
H	-0.60191100	-0.89835100	1.89295200
H	0.55161000	0.81947200	-0.35797600
H	2.71664300	-0.50886600	-0.27446800
H	2.64968300	-2.27029400	-0.20954500
H	0.83032200	-1.30543000	-1.58702600
H	0.18983500	-2.21074600	-0.21661200
C	2.19596400	1.18515100	1.93212300
H	1.69989200	2.04799400	2.38387500
H	2.23921300	1.37604800	0.85692200
C	4.30824100	-0.19210900	1.88233700
N	3.43394800	-1.28699200	2.23174200
C	3.60281800	1.05222100	2.48917600
H	4.22914200	1.90440100	2.21728000
H	3.59443900	0.96971400	3.57813600
N	4.78798500	-3.66464200	1.89705900
N	4.21322100	-2.74320700	1.70892300
H	5.26937800	-0.35004700	2.36980000
O	1.51788900	-2.55395600	2.00369000
H	1.26201700	-2.53095300	2.93486800
H	4.43540100	-0.05620500	0.80660300
C	-1.43920700	0.10998400	-0.62607300
C	-2.06719600	1.42332700	-0.12718700
H	-2.99367000	1.62828200	-0.67290200
H	-2.32295900	1.38359400	0.93569700
H	-1.38928800	2.26991700	-0.28405900
C	-1.32027500	0.19813100	-2.15720700
H	-0.98612000	-0.74451300	-2.59955400
H	-2.29386400	0.43545200	-2.59763000
H	-0.61556000	0.98279000	-2.45417900
C	-2.37372700	-1.05630100	-0.26961100
H	-3.35655200	-0.89413000	-0.72421200

H	-1.99355600	-2.01136300	-0.64464800	N	-2.12348700	-0.69522900	0.61901500
H	-2.52414900	-1.14839100	0.81025600	C	-4.28027400	0.19287200	-0.31234000
C	1.12325500	-0.15921800	3.76079700	H	-5.28429400	0.42114200	0.05096700
C	1.78816000	-1.02870600	4.63487000	H	-4.40239700	-0.44829700	-1.18895400
C	0.20906500	0.74134200	4.33028900	N	-1.55467200	-2.70936600	-1.22402000
C	1.52418400	-1.02527500	6.00462000	N	-1.83614000	-1.74093900	-0.77867900
H	2.55209000	-1.70814600	4.27658200	O	-0.09893200	0.18210400	0.01468500
C	-0.04691200	0.75426900	5.69488500	H	-3.65217700	-0.19170700	1.75375300
H	-0.30865000	1.46456900	3.71080100	H	0.29229300	-0.21043900	0.80530700
C	0.60282300	-0.13875000	6.54282900	H	-3.93899100	-1.64790300	0.84784900
H	2.05873300	-1.71830000	6.64553800	C	-0.60544000	4.90127800	0.14484000
H	-0.75795300	1.46978100	6.09448300	C	-0.76413900	5.69868100	1.45108700
H	0.40067800	-0.13317000	7.60854000	H	-0.23073800	5.23683300	2.28680300

8d-TS

G(298.15 K)= -979.460025

H(298.15 K)= -979.389008

C	-1.31172800	3.51723300	0.29826200	H	-0.35773900	6.70751500	1.32595000
C	-1.34260800	2.71187500	-1.01038800	H	-1.81955700	5.79341600	1.72969200
C	-2.02451800	1.32001300	-0.94248500	C	-1.28135100	5.70361400	-0.97994000
C	-1.41753800	0.51658000	0.26241800	H	-1.09545400	5.26899700	-1.96600300
C	-1.50343400	1.34978500	1.59757300	H	-2.36537900	5.75902400	-0.82915400
C	-0.71800400	2.64696100	1.41145800	H	-0.89145300	6.72638900	-0.99674500
H	-1.86813200	3.26774400	-1.79143900	C	0.89248200	4.76673300	-0.17061600
H	-0.31725000	2.57264000	-1.36193400	H	1.33690500	5.76121500	-0.28215300
H	-2.34605000	3.75461500	0.58422700	H	1.43424000	4.25489000	0.63049700
H	-2.53665900	1.57831500	1.85666600	H	1.06948700	4.22474700	-1.10444800
H	-1.08340200	0.74623200	2.40701000	C	-1.76035800	0.60704800	-2.28745500
H	-0.74517700	3.16373400	2.37379200	C	-2.79717400	0.25204600	-3.16121100
H	0.32840500	2.41009300	1.19932600	C	-0.44629900	0.36588400	-2.72708000
C	-3.53814500	1.48858700	-0.65654600	C	-2.54342300	-0.36040100	-4.38532400
H	-4.00678100	1.96753900	-1.51923100	H	-3.83064300	0.45568600	-2.91527000
H	-3.67278300	2.19492700	0.16428000	C	-0.19014500	-0.25070400	-3.94457000
C	-3.56088200	-0.62954200	0.74657700	H	0.39105100	0.64467600	-2.10294900
				C	-1.23854800	-0.62987100	-4.77856100
				H	-3.37546600	-0.62466600	-5.02952100
				H	0.83753000	-0.43190100	-4.24191700

H -1.03964600 -1.11570700 -5.72802100

8c-TS-OMe

G(298.15 K)= -1093.923466

H(298.15 K)= -1093.8461

C 0.00412500 -0.03148500 -0.04309100

C -0.01624200 -0.00886800 1.49012200

C 1.34245100 -0.08740300 2.23665900

C 2.10589200 -1.37725400 1.60858400

C 2.09828600 -1.38038600 0.07836300

C 0.69789000 -1.31253900 -0.50782500

H -0.48429500 0.92138500 1.81369900

H -0.64136000 -0.82917000 1.85469400

H 0.61254600 0.81276100 -0.39870900

H 2.68962500 -0.54589100 -0.30409800

H 2.60228200 -2.30643600 -0.22277100

H 0.78967100 -1.34023400 -1.59553600

H 0.12838800 -2.19634600 -0.20246400

C 2.18393800 1.17939000 1.98541700

H 1.69111900 2.01677600 2.48702900

H 2.20313600 1.41716700 0.91780600

C 4.29793500 -0.18145400 1.82591700

N 3.44235200 -1.29073100 2.17440800

C 3.60555100 1.03613100 2.49725400

H 4.21678800 1.90228600 2.23479500

H 3.63364000 0.91848300 3.58237500

N 4.80668900 -3.64621600 1.79988700

N 4.21953500 -2.73001900 1.62329900

H 5.27640000 -0.34704300 2.27503100

O 1.52690900 -2.56311100 2.01728800

H 1.32724100 -2.52445800 2.96299600

H 4.38665600 -0.01161700 0.75107800

C -1.41161200 0.19556700 -0.66078000

C -1.90002000 1.61517500 -0.32348200

H -2.85161100 1.81440600 -0.82665300

H -2.06792200 1.75573100 0.74828300

H -1.17833700 2.36900200 -0.65691200

C -1.32135700 0.08323100 -2.19213100

H -1.13476400 -0.94388000 -2.51801900

H -2.26368100 0.40337200 -2.64785400

H -0.52253000 0.71955400 -2.58955600

C -2.44340200 -0.82195600 -0.15001700

H -3.39443000 -0.68054300 -0.67371300

H -2.12005700 -1.85275500 -0.32584200

H -2.63985000 -0.70295400 0.91962400

C 1.08287700 -0.26101800 3.75020700

C 1.93744900 -0.93783600 4.62718200

C -0.04599800 0.34546500 4.33261800

C 1.68969300 -1.03447500 5.99666000

H 2.83768600 -1.41592100 4.25980900

C -0.30228500 0.27057500 5.68869400

H -0.74912300 0.90451800 3.72909200

C 0.56050200 -0.42861800 6.53991100

H 2.38925300 -1.58444700 6.61368200

H -1.17840500 0.75078500 6.11067800

O 0.21693000 -0.45612800 7.84657000

C 1.07634500 -1.13594600 8.74745700

H 0.62114200 -1.03291800 9.73147000

H 1.15925200 -2.19888100 8.49601800

H 2.07472000 -0.68554100 8.76069900

8d-TS-OMe

G(298.15 K)= -1093.9253

H(298.15 K)= -1093.848703

C	-0.00380500	-0.01072800	-0.02338900	H	-2.47603200	1.08423700	0.95516500
C	-0.00593400	0.03267400	1.51327300	H	-1.67997200	2.11776100	-0.24611100
C	1.38425200	0.03899800	2.19909300	H	-3.18402300	1.27364400	-0.64694200
C	2.24770800	-1.14361000	1.61233100	C	-2.21336600	-1.30848600	-0.30490900
C	2.29894700	-1.06734100	0.04084100	H	-3.21538200	-1.25742500	-0.74335500
C	0.87376900	-1.17521300	-0.49747000	H	-1.72288800	-2.19668500	-0.71421600
H	-0.52115100	0.92835000	1.87026900	H	-2.33555800	-1.45177000	0.77303800
H	-0.57092400	-0.82383300	1.88944300	C	1.18425200	-0.14851200	3.71030600
H	0.45575100	0.91592300	-0.39485800	C	1.60280600	0.79872100	4.65326300
H	2.75570600	-0.13766600	-0.29726200	C	0.50085000	-1.27559800	4.21767900
H	2.91884300	-1.89239600	-0.32051700	C	1.43214800	0.62055600	6.02169900
H	0.95361800	-1.19133000	-1.58728000	H	2.07510900	1.72057800	4.34222800
H	0.44364200	-2.13178800	-0.18837000	C	0.32850200	-1.47474800	5.57109400
C	2.13234300	1.35321200	1.85811000	H	0.12523300	-2.02865300	3.53930300
H	1.61835700	2.18456400	2.34679700	C	0.81125400	-0.53640400	6.49462700
H	2.03453700	1.55007500	0.78962800	H	1.78634400	1.38726700	6.69904900
C	4.36299700	0.11259100	1.81968800	H	-0.18074500	-2.35743200	5.94179900
N	3.63614300	-1.12385300	1.99330800	O	0.61556500	-0.82932100	7.79455400
C	3.62171700	1.38135300	2.22406000	C	1.09044200	0.08909600	8.76848400
H	4.10474600	2.23271100	1.74015300	H	0.85378300	-0.35117400	9.73572600
H	3.77141500	1.51109500	3.29813100	H	2.17350400	0.22721100	8.68611700
N	3.94019500	-1.86507700	4.65223600	H	0.58997600	1.05851700	8.67597600
N	3.54645800	-1.35841400	3.75309500	8c-TS-N02			
O	1.71918800	-2.36526100	1.99543700	G(298.15 K)= -1183.898761			
H	4.57432800	0.07411800	0.73910900	H(298.15 K)= -1183.820319			
H	2.21882300	-3.07801200	1.57781000	C	-0.00875100	-0.04160100	-0.01181300
H	5.33471500	0.00212900	2.30330600	C	-0.02478300	-0.06168400	1.52198500
C	-1.44014300	-0.02212500	-0.63493800	C	1.35297900	-0.07537700	2.23910300
C	-1.33881800	0.11387400	-2.16425500	C	2.12658800	-1.35423400	1.61516700
H	-0.87455500	-0.76111700	-2.62802100	C	2.14812900	-1.31580900	0.08469000
H	-2.33745200	0.21963800	-2.60030500	C	0.75158400	-1.26974300	-0.51820400
H	-0.75561700	0.99841400	-2.44388000	H	-0.55672200	0.81881500	1.88106400
C	-2.23600100	1.18371800	-0.10713400	H	-0.58432500	-0.93473200	1.87080400

H	0.54899800	0.84621900	-0.34226900
H	2.72493900	-0.45925800	-0.26844100
H	2.67695900	-2.22195400	-0.23285600
H	0.86061700	-1.24166300	-1.60414400
H	0.21410900	-2.18892300	-0.26495000
C	2.18134500	1.19482100	1.96234000
H	1.67744700	2.04808700	2.42353800
H	2.22439100	1.40041100	0.89024800
C	4.30627500	-0.16551300	1.89826100
N	3.43978700	-1.27016300	2.23041300
C	3.58806400	1.06512100	2.52097000
H	4.20742600	1.92559900	2.25987300
H	3.58213600	0.97097600	3.60906800
N	4.82888900	-3.63466700	1.85215900
N	4.23668500	-2.72034900	1.68652300
H	5.26637900	-0.32046300	2.38844300
O	1.53834300	-2.55488500	1.96533800
H	1.29751000	-2.57387900	2.89984300
H	4.43557100	-0.01316300	0.82519300
C	-1.43772200	0.12326400	-0.61846000
C	-1.99732200	1.50860800	-0.25086500
H	-2.96262200	1.66612100	-0.74252000
H	-2.16289600	1.62191500	0.82451400
H	-1.31949300	2.30511000	-0.57683100
C	-1.35030400	0.04586900	-2.15201100
H	-1.10646800	-0.96217500	-2.49910600
H	-2.31237000	0.31947900	-2.59649200
H	-0.59219600	0.73537200	-2.54046600
C	-2.41111600	-0.95681300	-0.12149400
H	-3.37053600	-0.85767700	-0.63923300
H	-2.03343300	-1.96573900	-0.31523600
H	-2.60841800	-0.86584700	0.95081200
C	1.11445300	-0.18207300	3.76207400

C	1.78479800	-1.05999500	4.62393600
C	0.19011300	0.70642700	4.33616500
C	1.51976300	-1.08650100	5.98881200
H	2.55792600	-1.72481600	4.26111800
C	-0.08035700	0.70293400	5.69402600
H	-0.32873200	1.43495300	3.72614700
C	0.58433200	-0.20751500	6.50410800
H	2.04310600	-1.77440400	6.63956800
H	-0.79401900	1.39571500	6.12007600
N	0.30073900	-0.22720800	7.93984800
O	-0.52278300	0.56620400	8.37232000
O	0.90117900	-1.03613400	8.63253500

8d-TS-NO2

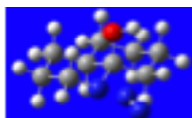
G(298.15 K)= -1183.899881

H(298.15 K)= -1183.821944

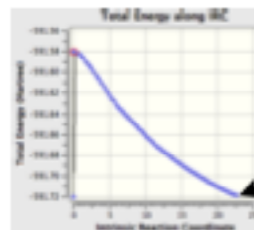
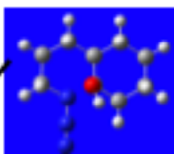
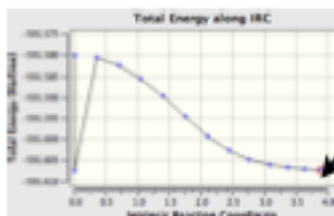
C	0.00358100	-0.01188500	0.01776300
C	0.02280900	-0.00941700	1.55390300
C	1.42713400	-0.01350900	2.21883800
C	2.29170300	-1.16014600	1.58878200
C	2.30565800	-1.06124100	0.01594700
C	0.86812600	-1.16998200	-0.49062400
H	-0.49303100	0.87143900	1.94478100
H	-0.52956400	-0.88143000	1.91254600
H	0.46329600	0.92066900	-0.33785400
H	2.74465700	-0.12238600	-0.32007700
H	2.92411200	-1.87486100	-0.37220700
H	0.92611700	-1.17306800	-1.58173700
H	0.44634300	-2.13106400	-0.18351200
C	2.15191200	1.32217900	1.91788600
H	1.61555100	2.13556800	2.41153400
H	2.06919700	1.53905400	0.85177600
C	4.39552200	0.14852500	1.78337700

N	3.71067900	-1.11811900	1.88969800	C	1.29878000	0.56467100	6.03542500
C	3.63284000	1.35531100	2.30679200	H	2.00088000	1.67770200	4.38572900
H	4.10157200	2.25910300	1.91290600	C	0.30003200	-1.58537800	5.54751200
H	3.76940300	1.37911000	3.39153300	H	0.24273500	-2.15354100	3.50539800
N	4.15025200	-2.08940900	4.47168600	C	0.69011400	-0.60720800	6.45145600
N	3.76152000	-1.52567800	3.60848500	H	1.57563400	1.32280000	6.75601200
O	1.81528800	-2.39875500	1.97181300	H	-0.19219500	-2.48381100	5.89593600
H	4.56041400	0.19277800	0.69413800	N	0.43715500	-0.81178100	7.87827500
H	2.27955000	-3.09580700	1.49072500	O	0.79962000	0.05882900	8.65683200
H	5.39230500	0.03057400	2.21130900	O	-0.12328200	-1.84353300	8.21999300
C	-1.44177700	-0.00179600	-0.57255100	C	0.65303900	-0.60417900	6.44723000
C	-1.35961800	0.16643900	-2.09969200	H	1.50447700	1.33779300	6.74983300
H	-0.90770000	-0.70161400	-2.58796200	H	-0.18349200	-2.49989000	5.89857600
H	-2.36326200	0.28751000	-2.51971700	N	0.36550500	-0.79258200	7.86803000
H	-0.77437200	1.05293400	-2.36836600	O	0.68079800	0.10042500	8.64251500
C	-2.22138500	1.19728100	-0.00673400	O	-0.17593900	-1.83432600	8.21186900
H	-2.44419200	1.07764700	1.05727200				
H	-1.66246900	2.13088700	-0.13647500				
H	-3.17776000	1.30326800	-0.52844800				
C	-2.21728000	-1.29085300	-0.25915400				
H	-3.22174200	-1.22833500	-0.69028400				
H	-1.73292800	-2.17382200	-0.68664400				
H	-2.33405100	-1.45172300	0.81688100				
C	1.20190000	-0.23018300	3.73268700				
C	1.54325400	0.74403400	4.67998500				
C	0.54978600	-1.38559900	4.19991500				

Selected IRCs for **1a** (leads to fused lactam) and **1d** (lead to bridged lactam).



Ia-TS



Id-TS

