Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Nature or number of species in transition state: The key role of catalytically active molecules in hydrogen transfer stages in atmospheric aldehyde reactions

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Table S1. ZPE corrected energies and Gibbs free energies of the structures and TSs in solution of the proposed mechanism of 2-methylimidazole formation and the stage barriers

Reagents, TSs	E (+ZPE), a.u.	E (+ZPE), kcal·mol^{-1}	G, a.u.	G, kcal·mol^{-1}
Glyoxal trans	-227.528273	-142776.2	-227.553966	-142792.3
Glyoxal cis	-227.524176	-142773.6	-227.550075	-142789.8
Water	-76.344532	-47906.9	-76.362183	-47918.0
Ammonia	-56.465527	-35432.7	-56.484601	-35444.6
CH_3CHO	-153.588522	-96378.3	-153.613441	-96393.9
1-aminoethanol ($CH_3CHOH(NH_2)$)	-210.059008	-131814.0	-210.086300	-131831.1
Bc ($OHCCHOH(NH_2)$)	-284.006604	-178216.8	-284.035583	-178235.0
Y	-494.084746	-310042.9	-494.119706	-310064.8
2	-417.740043	-262135.8	-417.773239	-262156.7
OH PreIm	-341.392646	-214227.1	-341.423458	-214246.5
PreIm	-265.053854	-166323.8	-265.082198	-166341.6
2MI	-265.085874	-166343.9	-265.115056	-166362.2
TS_{A1} ($CH_3CHO+NH_3$)	-210.008551	-131782.4	-210.035552	-131799.3
TS_{A2} ($OHCCHO+NH_3$)	-283.954008	-178183.8	-283.982711	-178201.8
TS_B (precyclization)	-494.038022	-310013.6	-494.073173	-310035.6
TS_C (cyclization)				
TS_D (-H_2O)	-417.669010	-262091.3	-417.702515	-262112.3
TS_E (-H_2O)	-341.324727	-214184.5	-341.356076	-214204.2
TS_F (H transfer)	-265.006073	-166293.8	-265.034410	-166311.6
Energy barriers (no catalyst)				
A1 ($CH_3CHO+NH_3$)	0.045498	28.6	0.062490	39.2
A2 ($OHCCHO+NH_3$)	0.039792	25.0	0.055856	35.1
B (precyclization)	0.027590	17.3	0.048710	30.6
C (cyclization)				
D (-H_2O)	0.071033	44.6	0.070724	44.4
E (-H_2O)	0.067919	42.6	0.067382	42.3
F (H transfer)	0.047781	30.0	0.047788	30.0

Table S2. ZPE corrected energies and Gibbs free energies of the structures and TSs with participation of one water molecule in solution of the proposed mechanism of 2-methylimidazole formation and the stage barriers

Reagents, TSs	E (+ZPE), a.u.	E (+ZPE), kcal·mol^{-1}	G, a.u.	G, kcal·mol^{-1}
Glyoxal trans	-227.528273	-142776.2	-227.553966	-142792.3
Glyoxal cis	-227.524176	-142773.6	-227.550075	-142789.8
Water	-76.344532	-47906.9	-76.362183	-47918.0
Ammonia	-56.465527	-35432.7	-56.484601	-35444.6
CH_3CHO	-153.588522	-96378.3	-153.613441	-96393.9
1-aminoethanol ($CH_3CHOH(NH_2)$)	-210.059008	-131814.0	-210.086300	-131831.1
Bc ($OHCCHOH(NH_2)$)	-284.006604	-178216.8	-284.035583	-178235.0
Y	-494.084746	-310042.9	-494.119706	-310064.8
2	-417.740043	-262135.8	-417.773239	-262156.7
OH_PreIm	-341.392646	-214227.1	-341.423458	-214246.5
PreIm	-265.053854	-166323.8	-265.082198	-166341.6
2MI	-265.085874	-166343.9	-265.115056	-166362.2
TS_{A1} ($CH_3CHO+NH_3$)	-286.386372	-179710.2	-286.415868	-179728.7
TS_{A2} ($OHCCHO+NH_3$)	-360.329744	-226110.3	-360.360610	-226129.7
TS_B (precyclization)	-570.415651	-357941.2	-570.454085	-357965.4
TS_C (cyclization)	-570.376579	-357916.7	-570.414596	-357940.6
TS_D (-H_2O)	-494.039760	-310014.6	-494.075657	-310037.2
TS_E (-H_2O)	-417.699739	-262110.6	-417.733257	-262131.6
TS_F (H transfer)	-341.331078	-214188.5	-341.361992	-214207.9
Energy barriers (1H_2O)				
A1 ($CH_3CHO+NH_3$)	0.012209	7.7	0.044357	27.8
A2 ($OHCCHO+NH_3$)	0.008588	5.4	0.040140	25.2
B (precyclization)	-0.005507	-3.5	0.029981	18.8
C (cyclization)	0.052699	33.1	0.067293	42.2
D (-H_2O)	0.044815	28.1	0.059765	37.5
E (-H_2O)	0.037439	23.5	0.052384	32.9
F (H transfer)	0.067308	42.2	0.082389	51.7

Table S3. ZPE corrected energies and Gibbs free energies of the structures and TSs with participation of two water molecules in solution of the proposed mechanism of 2-methylimidazole formation and the stage barriers

Reagents, TSs	E (+ZPE), a.u.	E (+ZPE), kcal·mol^{-1}	G, a.u.	G, kcal·mol^{-1}
Glyoxal trans	-227.528273	-142776.2	-227.553966	-142792.3
Glyoxal cis	-227.524176	-142773.6	-227.550075	-142789.8
Water	-76.344532	-47906.9	-76.362183	-47918.0
Ammonia	-56.465527	-35432.7	-56.484601	-35444.6
CH_3CHO	-153.588522	-96378.3	-153.613441	-96393.9
1-aminoethanol ($CH_3CHOH(NH_2)$)	-210.059008	-131814.0	-210.086300	-131831.1
Bc ($OHCCHOH(NH_2)$)	-284.006604	-178216.8	-284.035583	-178235.0
Y	-494.084746	-310042.9	-494.119706	-310064.8
2	-417.740043	-262135.8	-417.773239	-262156.7
OH PreIm	-341.392646	-214227.1	-341.423458	-214246.5
PreIm	-265.053854	-166323.8	-265.082198	-166341.6
2MI	-265.085874	-166343.9	-265.115056	-166362.2
TS_{A1} ($CH_3CHO+NH_3$)	-362.742370	-227624.3	-362.775515	-227645.1
TS_{A2} ($OHCCHO+NH_3$)	-436.685799	-274024.5	-436.719829	-274045.8
TS_B (precyclization)	-646.770871	-405854.9	-646.812247	-405880.8
TS_C (cyclization)	-646.686625	-405802.0	-646.724831	-405826.0
TS_D (-H_2O)	-570.399885	-357931.3	-570.439721	-357956.3
TS_E (-H_2O)	-494.060132	-310027.4	-494.097626	-310051.0
TS_F (H transfer)	-417.717906	-262122.0	-417.752157	-262143.4
Energy barriers ($2H_2O$)				
A1 ($CH_3CHO+NH_3$)	0.000743	0.5	0.046893	29.4
A2 ($OHCCHO+NH_3$)	-0.002935	-1.8	0.043104	27.0
B (precyclization)	-0.016195	-10.2	0.034002	21.3
C (cyclization)	0.087185	54.7	0.119241	74.8
D (-H_2O)	0.029222	18.3	0.057884	36.3
E (-H_2O)	0.021578	13.5	0.050198	31.5
F (H transfer)	0.025012	15.7	0.054407	34.1

Table S4. ZPE corrected energies and Gibbs free energies of the structures and TSs with participation of one methanol molecule in solution of the proposed mechanism of 2-methylimidazole formation and the stage barriers

Reagents, TSs	E (+ZPE), a.u.	E (+ZPE), kcal·mol^{-1}	G, a.u.	G, kcal·mol^{-1}
Glyoxal trans	-227.528273	-142776.2	-227.553966	-142792.3
Glyoxal cis	-227.524176	-142773.6	-227.550075	-142789.8
Water	-115.545412	-72505.8	-115.568169	-72520.1
Ammonia	-56.465527	-35432.7	-56.484601	-35444.6
CH_3CHO	-153.588522	-96378.3	-153.613441	-96393.9
1-aminoethanol ($CH_3CHOH(NH_2)$)	-210.059008	-131814.0	-210.086300	-131831.1
Bc ($OHCCHOH(NH_2)$)	-284.006604	-178216.8	-284.035583	-178235.0
Y	-494.084746	-310042.9	-494.119706	-310064.8
2	-417.740043	-262135.8	-417.773239	-262156.7
OH PreIm	-341.392646	-214227.1	-341.423458	-214246.5
PreIm	-265.053854	-166323.8	-265.082198	-166341.6
2MI	-265.085874	-166343.9	-265.115056	-166362.2
TS_{A1} ($CH_3CHO+NH_3$)	-325.590741	-204311.3	-325.623512	-204331.8
TS_{A2} ($OHCCHO+NH_3$)	-399.534861	-250711.9	-399.569739	-250733.8
TS_B (precyclization)	-609.620084	-382542.4	-609.661472	-382568.4
TS_C (cyclization)				
TS_D ($-H_2O$)	-533.244963	-334616.3	-533.284724	-334641.2
TS_E ($-H_2O$)	-456.905103	-286712.3	-456.942331	-286735.7
TS_F (H transfer)	-380.538038	-238791.2	-380.572741	-238813.0
Energy barriers ($1CH_3OH$)				
A1 ($CH_3CHO+NH_3$)	0.008720	5.5	0.042699	26.8
A2 ($OHCCHO+NH_3$)	0.004351	2.7	0.036997	23.2
B (precyclization)	-0.009060	-5.7	0.028580	17.9
C (cyclization)				
D ($-H_2O$)	0.040492	25.4	0.056684	35.6
E ($-H_2O$)	0.032955	20.7	0.049296	30.9
F (H transfer)	0.061228	38.4	0.077626	48.7

Table S5. ZPE corrected energies and Gibbs free energies of the structures and TSs with participation of two methanol molecules in solution of the proposed mechanism of 2-methylimidazole formation and the stage barriers

Reagents, TSs	E (+ZPE), a.u.	E (+ZPE), kcal·mol^{-1}	G, a.u.	G, kcal·mol^{-1}
Glyoxal trans	-227.528273	-142776.2	-227.553966	-142792.3
Glyoxal cis	-227.524176	-142773.6	-227.550075	-142789.8
Water	-115.545412	-72505.8	-115.568169	-72520.1
Ammonia	-56.465527	-35432.7	-56.484601	-35444.6
CH_3CHO	-153.588522	-96378.3	-153.613441	-96393.9
1-aminoethanol ($CH_3CHOH(NH_2)$)	-210.059008	-131814.0	-210.086300	-131831.1
Bc ($OHCCHOH(NH_2)$)	-284.006604	-178216.8	-284.035583	-178235.0
Y	-494.084746	-310042.9	-494.119706	-310064.8
2	-417.740043	-262135.8	-417.773239	-262156.7
OH PreIm	-341.392646	-214227.1	-341.423458	-214246.5
PreIm	-265.053854	-166323.8	-265.082198	-166341.6
2MI	-265.085874	-166343.9	-265.115056	-166362.2
TS_{A1} ($CH_3CHO+NH_3$)	-441.152558	-276827.4	-441.192876	-276852.7
TS_{A2} ($OHCCHO+NH_3$)	-515.100434	-323230.4	-515.142252	-323256.7
TS_B (precyclization)	-725.180562	-455057.7	-725.227045	-455086.9
TS_C (cyclization)				
TS_D ($-H_2O$)	-648.810417	-407134.7	-648.857323	-407164.1
TS_E ($-H_2O$)	-572.470604	-359230.7	-572.515406	-359258.9
TS_F (H transfer)				
Energy barriers ($2CH_3OH$)				
A1 ($CH_3CHO+NH_3$)	-0.007685	-4.8	0.041504	26.0
A2 ($OHCCHO+NH_3$)	-0.015810	-9.9	0.032653	20.5
B (precyclization)	-0.024126	-15.1	0.031176	19.6
C (cyclization)				
D ($-H_2O$)	0.020450	12.8	0.052254	32.8
E ($-H_2O$)	0.012866	8.1	0.044390	27.9
F (H transfer)				

Table S6. ZPE corrected energies and Gibbs free energies of the structures and TSs with participation of one ethanol molecule in solution of the proposed mechanism of 2-methylimidazole formation and the stage barriers

Reagents, TSs	E (+ZPE), a.u.	E (+ZPE), kcal·mol^{-1}	G, a.u.	G, kcal·mol^{-1}
Glyoxal trans	-227.528273	-142776.2	-227.553966	-142792.3
Glyoxal cis	-227.524176	-142773.6	-227.550075	-142789.8
Water	-154.775561	-97123.1	-154.800999	-97139.1
Ammonia	-56.465527	-35432.7	-56.484601	-35444.6
CH_3CHO	-153.588522	-96378.3	-153.613441	-96393.9
1-aminoethanol ($CH_3CHOH(NH_2)$)	-210.059008	-131814.0	-210.086300	-131831.1
Bc ($OHCCHOH(NH_2)$)	-284.006604	-178216.8	-284.035583	-178235.0
Y	-494.084746	-310042.9	-494.119706	-310064.8
2	-417.740043	-262135.8	-417.773239	-262156.7
OH PreIm	-341.392646	-214227.1	-341.423458	-214246.5
PreIm	-265.053854	-166323.8	-265.082198	-166341.6
2MI	-265.085874	-166343.9	-265.115056	-166362.2
TS_{A1} ($CH_3CHO+NH_3$)	-364.820432	-228928.3	-364.855115	-228950.1
TS_{A2} ($OHCCHO+NH_3$)	-438.765151	-275329.3	-438.801925	-275352.4
TS_B (precyclization)	-648.850650	-407159.9	-648.893696	-407187.0
TS_C (cyclization)				
TS_D (-H_2O)	-572.475310	-359233.7	-572.516614	-359259.6
TS_E (-H_2O)	-496.135618	-311329.8	-496.174592	-311354.3
TS_F (H transfer)	-419.768837	-263408.9	-419.805145	-263431.7
Energy barriers ($1C_2H_5OH$)				
A1 ($CH_3CHO+NH_3$)	0.009178	5.8	0.043926	27.6
A2 ($OHCCHO+NH_3$)	0.004210	2.6	0.037641	23.6
B (precyclization)	-0.009477	-5.9	0.029186	18.3
C (cyclization)				
D (-H_2O)	0.040294	25.3	0.057624	36.2
E (-H_2O)	0.032589	20.4	0.049865	31.3
F (H transfer)	0.060578	38.0	0.078052	49.0

Table S7. ZPE corrected energies and Gibbs free energies of the structures and TSs with participation of two ethanol molecules in solution of the proposed mechanism of 2-methylimidazole formation and the stage barriers

Reagents, TSs	E (+ZPE), a.u.	E (+ZPE), kcal·mol^{-1}	G, a.u.	G, kcal·mol^{-1}
Glyoxal trans	-227.528273	-142776.2	-227.553966	-142792.3
Glyoxal cis	-227.524176	-142773.6	-227.550075	-142789.8
Water	-154.775561	-97123.1	-154.800999	-97139.1
Ammonia	-56.465527	-35432.7	-56.484601	-35444.6
CH_3CHO	-153.588522	-96378.3	-153.613441	-96393.9
1-aminoethanol ($CH_3CHOH(NH_2)$)	-210.059008	-131814.0	-210.086300	-131831.1
Bc ($OHCCHOH(NH_2)$)	-284.006604	-178216.8	-284.035583	-178235.0
Y	-494.084746	-310042.9	-494.119706	-310064.8
2	-417.740043	-262135.8	-417.773239	-262156.7
OH PreIm	-341.392646	-214227.1	-341.423458	-214246.5
PreIm	-265.053854	-166323.8	-265.082198	-166341.6
2MI	-265.085874	-166343.9	-265.115056	-166362.2
TS_{A1} ($CH_3CHO+NH_3$)	-519.613532	-326062.4	-519.657357	-326089.9
TS_{A2} ($OHCCHO+NH_3$)	-593.561431	-372465.4	-593.606554	-372493.8
TS_B (precyclization)	-803.637145	-504289.9	-803.688434	-504322.1
TS_C (cyclization)				
TS_D ($-H_2O$)	-727.271414	-456369.7	-727.322226	-456401.6
TS_E ($-H_2O$)	-650.931831	-408465.9	-650.980609	-408496.5
TS_F (H transfer)				
Energy barriers ($2C_2H_5OH$)				
A1 ($CH_3CHO+NH_3$)	-0.008361	-5.2	0.042683	26.8
A2 ($OHCCHO+NH_3$)	-0.016509	-10.4	0.034011	21.3
B (precyclization)	-0.020411	-12.8	0.035447	22.2
C (cyclization)				
D ($-H_2O$)	0.019751	12.4	0.053011	33.3
E ($-H_2O$)	0.011937	7.5	0.044847	28.1
F (H transfer)				

Table S8. ZPE corrected energies and Gibbs free energies of the structures and TSs with participation of one formic acid molecule in solution of the proposed mechanism of 2-methylimidazole formation and the stage barriers

Reagents, TSs	E (+ZPE), a.u.	E (+ZPE), kcal·mol^{-1}	G, a.u.	G, kcal·mol^{-1}
Glyoxal trans	-227.528273	-142776.2	-227.553966	-142792.3
Glyoxal cis	-227.524176	-142773.6	-227.550075	-142789.8
Water	-189.534636	-118934.8	-189.558717	-118949.9
Ammonia	-56.465527	-35432.7	-56.484601	-35444.6
CH_3CHO	-153.588522	-96378.3	-153.613441	-96393.9
1-aminoethanol ($CH_3CHOH(NH_2)$)	-210.059008	-131814.0	-210.086300	-131831.1
Bc ($OHCCHOH(NH_2)$)	-284.006604	-178216.8	-284.035583	-178235.0
Y	-494.084746	-310042.9	-494.119706	-310064.8
2	-417.740043	-262135.8	-417.773239	-262156.7
OH_PreIm	-341.392646	-214227.1	-341.423458	-214246.5
PreIm	-265.053854	-166323.8	-265.082198	-166341.6
2MI	-265.085874	-166343.9	-265.115056	-166362.2
TS_{A1} ($CH_3CHO+NH_3$)	-399.593013	-250748.4	-399.627772	-250770.2
TS_{A2} ($OHCCHO+NH_3$)	-473.538291	-297149.8	-473.574017	-297172.2
TS_B (precyclization)				
TS_C (cyclization)				
TS_D ($-H_2O$)	-607.267074	-381065.9	-607.306446	-381090.6
TS_E ($-H_2O$)	-530.922094	-333158.7	-530.959322	-333182.0
TS_F (H transfer)	-454.576182	-285250.9	-454.610313	-285272.3
Energy barriers (1HCOOH)				
A1 ($CH_3CHO+NH_3$)	-0.004328	-2.7	0.028987	18.2
A2 ($OHCCHO+NH_3$)	-0.009855	-6.2	0.023267	14.6
B (precyclization)				
C (cyclization)				
D ($-H_2O$)	0.007605	4.8	0.025510	16.0
E ($-H_2O$)	0.005188	3.3	0.022853	14.3
F (H transfer)	0.012308	7.7	0.030602	19.2

Table S9. ZPE corrected energies and Gibbs free energies of the structures and TSs with participation of one acetic acid molecule in solution of the proposed mechanism of 2-methylimidazole formation and the stage barriers

Reagents, TSs	E (+ZPE), a.u.	E (+ZPE), kcal·mol^{-1}	G, a.u.	G, kcal·mol^{-1}
Glyoxal trans	-227.528273	-142776.2	-227.553966	-142792.3
Glyoxal cis	-227.524176	-142773.6	-227.550075	-142789.8
Water	-228.772739	-143557.1	-228.800146	-143574.3
Ammonia	-56.465527	-35432.7	-56.484601	-35444.6
CH_3CHO	-153.588522	-96378.3	-153.613441	-96393.9
1-aminoethanol ($CH_3CHOH(NH_2)$)	-210.059008	-131814.0	-210.086300	-131831.1
Bc ($OHCCHOH(NH_2)$)	-284.006604	-178216.8	-284.035583	-178235.0
Y	-494.084746	-310042.9	-494.119706	-310064.8
2	-417.740043	-262135.8	-417.773239	-262156.7
OH_PreIm	-341.392646	-214227.1	-341.423458	-214246.5
PreIm	-265.053854	-166323.8	-265.082198	-166341.6
2MI	-265.085874	-166343.9	-265.115056	-166362.2
TS_{A1} ($CH_3CHO+NH_3$)	-438.830426	-275370.3	-438.867971	-275393.8
TS_{A2} ($OHCCHO+NH_3$)				
TS_B (precyclization)				
TS_C (cyclization)				
TS_D (-H_2O)	-646.501957	-405686.1	-646.544820	-405713.0
TS_E (-H_2O)	-570.157895	-357779.5	-570.198248	-357804.8
TS_F (H transfer)	-493.811620	-309871.5	-493.848808	-309894.8
Energy barriers (1CH_3COOH)				
A1 ($CH_3CHO+NH_3$)	-0.003638	-2.3	0.030217	19.0
A2 ($OHCCHO+NH_3$)				
B (precyclization)				
C (cyclization)				
D (-H_2O)	0.010825	6.8	0.028565	17.9
E (-H_2O)	0.007490	4.7	0.025356	15.9
F (H transfer)	0.014973	9.4	0.033536	21.0

Table S10. ZPE corrected energies and Gibbs free energies of the structures and TSs with participation of one ammonia molecule in solution of the proposed mechanism of 2-methylimidazole formation and the stage barriers

Reagents, TSs	E (+ZPE), a.u.	E (+ZPE), kcal·mol^{-1}	G, a.u.	G, kcal·mol^{-1}
Glyoxal trans	-227.528273	-142776.2	-227.553966	-142792.3
Glyoxal cis	-227.524176	-142773.6	-227.550075	-142789.8
Water	-76.344532	-47906.9	-76.362183	-47918.0
Ammonia	-56.465527	-35432.7	-56.484601	-35444.6
CH_3CHO	-153.588522	-96378.3	-153.613441	-96393.9
1-aminoethanol ($CH_3CHOH(NH_2)$)	-210.059008	-131814.0	-210.086300	-131831.1
Bc ($OHCCHOH(NH_2)$)	-284.006604	-178216.8	-284.035583	-178235.0
Y	-494.084746	-310042.9	-494.119706	-310064.8
2	-417.740043	-262135.8	-417.773239	-262156.7
OH_PreIm	-341.392646	-214227.1	-341.423458	-214246.5
PreIm	-265.053854	-166323.8	-265.082198	-166341.6
2MI	-265.085874	-166343.9	-265.115056	-166362.2
TS_{A1} ($CH_3CHO+NH_3$)	-266.496132	-167228.9	-266.526083	-167247.6
TS_{A2} ($OHCCHO+NH_3$)	-340.448777	-213634.8	-340.480642	-213654.8
TS_B (precyclization)	-550.530162	-345462.9	-550.568628	-345487.0
TS_C (cyclization)				
TS_D ($-H_2O$)	-474.156209	-297537.5	-474.192447	-297560.3
TS_E ($-H_2O$)	-397.818906	-249635.1	-397.852499	-249656.2
TS_F (H transfer)				
Energy barriers ($1NH_3$)				
A1 ($CH_3CHO+NH_3$)	0.023444	14.7	0.056560	35.5
A2 ($OHCCHO+NH_3$)	0.010550	6.6	0.042526	26.7
B (precyclization)	0.000977	0.6	0.037856	23.8
C (cyclization)				
D ($-H_2O$)	0.049361	31.0	0.065393	41.0
E ($-H_2O$)	0.039267	24.6	0.055560	34.9
F (H transfer)				

Table S11. Cartesian coordinates of the all structures and TSs

Structures
Glyoxal trans C 0.32908000 0.68982200 0.00010800 O -0.32908000 1.69863800 -0.00011000 H 1.43561100 0.67280900 0.00023100 C -0.32908000 -0.68982200 0.00010800 O 0.32908000 -1.69863800 -0.00011000 H -1.43561100 -0.67280900 0.00023100
Water O 0.00000000 0.11943000 0.00000000 H 0.75536800 -0.47771900 0.00000000 H -0.75536800 -0.47771900 0.00000000
Ammonia N 0.00000000 0.00000500 -0.12038800 H -0.80679200 0.47179400 0.28088100 H 0.81200500 0.46276400 0.28088000 H -0.00521400 -0.93459400 0.28095800
Acetaldehyde C 0.23040800 0.39778000 -0.00008200 H 0.29945600 1.50603300 0.00030700 O 1.23497900 -0.27680500 -0.00025800 C -1.16734400 -0.14955000 0.00010100 H -1.70353900 0.22580000 -0.87800400 H -1.15683700 -1.23959900 -0.00038000 H -1.70292600 0.22498300 0.87893700
1-aminoethanol ($CH_3CHOH(NH_2)$) C 0.03576700 0.02250300 0.36381500 H 0.06447000 0.06977300 1.46073900 O 0.54474300 1.29113500 -0.04427300 H 0.65937900 1.23434300 -1.00209200 N 0.89185700 -1.01931100 -0.19274100 H 1.79515700 -1.00486700 0.27183800 H 0.48989300 -1.93815700 -0.03268200 C -1.40319500 -0.18031300 -0.09934900 H -1.82015400 -1.11050600 0.29718700 H -2.02192500 0.65154300 0.24130100 H -1.43701200 -0.22187700 -1.19227300
Bc ($OHCCHOH(NH_2)$) C 0.94692900 -0.51475800 0.26700100 O 1.85495000 0.03519900 -0.30538500 H 1.05834700 -1.53145900 0.70014900 O -0.49523800 1.35755000 -0.05749000 H -1.42657100 1.60255600 -0.11369000 N -1.41809100 -0.79850600 -0.31609600 H -1.06406900 -1.04608800 -1.23579300 H -1.64446600 -1.65148000 0.18367800 C -0.46958400 0.03248800 0.41630000 H -0.73836700 -0.03236000 1.48153000
Y C 1.49667000 -0.31329000 -0.25482100 C 0.56326700 -1.06690300 0.72898300 C 1.24655900 -3.38208100 -0.04926700 N 1.21781400 -0.70483500 -1.63273700 H 1.33612200 0.75891300 -0.07534600 H 0.67880200 -0.57534400 1.70187700 N 0.80927900 -2.47212100 0.97414300 C 0.87579100 -4.81680600 0.30173800 H 1.24616700 -5.50092300 -0.46359500 H 1.31551100 -5.10235500 1.26385200 H -0.20781500 -4.91828700 0.37993500 H 0.79345700 -3.07348200 -0.98808300 O 2.85287800 -0.54286900 0.05577700 H 3.00408600 -1.49094100 -0.12536300 H 0.22008900 -0.62518000 -1.80437400 O -0.76169600 -0.86497100 0.22653700 H 1.23891300 -2.64802200 1.87241700 H -1.33457600 -1.44979000 0.73580900 O 2.67961800 -3.30261600 -0.31806100 H 1.69227600 -0.06553800 -2.26273700 H 3.13707300 -3.74812300 0.40647500
2 C 0.95653100 -0.69428500 -0.29917500 C 0.92541700 0.70201800 0.36764500 C -1.22964300 0.18609100 -0.32366600 N -0.45436000 -1.03383600 -0.59272200 H 1.53398000 -0.62255500 -1.22591400

H 1.58834000 0.74620800 1.23535400 N -0.45867900 0.83981000 0.75468900 C -2.66303600 -0.10316200 0.08205300 H -3.17918400 -0.65587600 -0.70635600 H -2.68005400 -0.69345700 1.00287200 H -3.20507400 0.82875600 0.25958300 H -1.22321800 0.79929500 -1.23641200 O 1.54634600 -1.62913700 0.58394800 H 1.77094300 -2.41744000 0.07785400 H -0.71562800 -1.72149200 0.11200400 O 1.36615000 1.63531300 -0.63500900 H -0.72452900 1.80713500 0.91263100 H 1.42623300 2.50367200 -0.22212000
OH_PreIm C -1.20686900 0.00655000 0.37795700 C -0.63245500 1.29607800 -0.17294800 C 1.14476200 0.12225200 0.44653100 N -0.04018900 -0.51626200 1.05615600 H -2.04787900 0.14711300 1.06410000 H -1.25442200 2.07254600 -0.60923200 N 0.63627500 1.35195900 -0.17707800 C 1.87119600 -0.73563100 -0.59296900 H 2.26413500 -1.64105800 -0.12350000 H 1.17356900 -1.02223200 -1.38317600 H 2.70566200 -0.18424400 -1.03220800 H 1.84799700 0.41394200 1.23391900 O -1.65586200 -0.75240900 -0.76079300 H -2.31690800 -1.38271800 -0.45519200 H -0.00859700 -1.52877600 1.05114600
PreIm C -0.23726200 -1.31686600 0.73948700 C -0.23726200 -1.31686600 -0.73948700 C -0.24496300 0.73938600 0.00000000 N -0.24242400 -0.11599300 1.18981400 H -0.23317900 -2.19184600 1.38079600 H -0.23317900 -2.19184600 -1.38079600 N -0.24242400 -0.11599300 -1.18981400 C 0.93849400 1.71009600 0.00000000 H 0.90169800 2.34067400 0.88900900 H 1.87711800 1.15142800 0.00000000 H 0.90169800 2.34067400 -0.88900900 H -1.18477600 1.30682800 0.00000000
2MI C -1.48217600 0.63718500 0.00027800 C -1.43422200 -0.73066700 -0.00031400 C 0.62082000 -0.07565100 -0.00011100 N -0.16397400 1.04174100 -0.00011900 H -2.29817400 1.34008900 0.00042200 H -2.26171400 -1.42367900 -0.00052300 N -0.12278100 -1.16749500 0.00044300 C 2.11286800 -0.02296100 -0.00010300 H 2.49386100 0.49939600 -0.88255400 H 2.49386500 0.49761400 0.88340300 H 2.50559200 -1.03909500 -0.00109600 H 0.15998000 1.99723200 -0.00038800
Methanol C 0.66745900 -0.01911200 0.00000100 H 1.08944100 0.98743400 -0.00069900 H 1.03372200 -0.54507300 -0.89089700 H 1.03383200 -0.54388800 0.89156000 O -0.75354500 0.12227500 0.00000200 H -1.13339200 -0.76200300 0.00001000
Ethanol C -0.08232600 0.55142000 -0.00002000 H -0.13632200 1.19778000 0.88681700 H -0.13625900 1.19771800 -0.88690800 O -1.15467900 -0.39870600 -0.00004000 H -1.98372300 0.09046400 0.00029800 C 1.22262400 -0.22367000 0.00002100 H 2.07711800 0.45821500 -0.00023200 H 1.28749200 -0.86029400 0.88663100 H 1.28733500 -0.86073900 -0.88628700
Formic acid C -0.13249400 0.39841600 0.00000000 H -0.09866200 1.49590800 -0.00000100 O -1.13702700 -0.26342900 0.00000000 O 1.11548600 -0.08982200 0.00000000 H 1.06595400 -1.06039500 0.00000100

Acetic acid
C -0.09182000 0.12487100 0.00012700
C 1.39200200 -0.11803100 0.00003000
H 1.66874500 -0.70105200 0.88094900
H 1.66831900 -0.70158400 -0.88082700
H 1.92037600 0.83231700 -0.00064300
O -0.63362100 1.20508900 -0.00001800
O -0.78273700 -1.03663500 -0.00001300
H -1.72766400 -0.81834700 -0.00017700

TSs

no catalyst

TS_{A1}
C 1.44149100 0.29637900 -0.10891800
H 1.76069600 1.25680500 0.30614100
H 1.41482300 0.36056000 -1.20094200
H 2.17415700 -0.46532000 0.16693700
C 0.07422700 -0.13500800 0.40770700
H 0.05418400 -0.10431000 1.51115800
O -0.44089800 -1.27679300 -0.15688100
N -1.03939200 0.81712600 -0.09718200
H -1.30836900 -0.27985400 -0.53293700
H -0.74390600 1.55555800 -0.73303200
H -1.64295600 1.20280000 0.62526300

TS_{A2}
C -0.36436000 0.09191300 0.48163700
H -0.56585900 -0.04002600 1.56341600
H -1.51673700 0.44747600 -0.66745600
N -1.43109200 -0.71162100 -0.29521100
H -1.09957100 -1.41843400 -0.95063200
H -2.18512200 -1.09359900 0.27146700
O -0.63570100 1.30584400 -0.05691400
C 1.02346400 -0.51144300 0.22210400
H 1.15796600 -1.54920000 0.59924900
O 1.91974500 0.08819500 -0.31458700

TS_{B}
C -1.62293700 -0.31919200 -0.36955900
H -1.52976000 -0.23722500 -1.46044700
C -0.68038800 0.68423000 0.30253900
H -0.56267000 0.37239800 1.35862600
N 0.71699700 0.67495200 -0.31660700
H 0.67478700 0.40458000 -1.30085200
C 1.80748400 -0.08201100 0.34613100
H 1.70119400 0.12072200 1.41832200
C 3.16380200 0.37572100 -0.15143600
H 3.31507800 1.43426900 0.06531400
H 3.94339500 -0.20326800 0.34608500
H 3.24452600 0.21216300 -1.22885900
O -0.94415600 2.01271200 0.10170600
H 0.37848300 1.85651000 -0.22865400
N -2.95532900 -0.09589100 0.13559400
H -3.11367200 0.90613100 0.19954700
H -3.65219900 -0.48401600 -0.49150100
O -1.20172800 -1.66028500 -0.05765300
H -1.60724700 -1.86435800 0.79690600
O 1.66375600 -1.45564500 0.06275000
H 0.72566800 -1.69807000 0.17214200

TS_{D}
C -0.59618300 1.20926900 -0.41691300
H -0.65383500 1.90720400 -1.25944200
C -0.77203000 -0.22700200 -0.86516400
H -1.56397300 -0.61319600 -1.47944100
O -1.67783900 -1.91152500 0.41461900
O -1.61993600 1.47723000 0.52631000
H -1.52183000 2.40053800 0.78810700
H -2.50155600 -2.37742100 0.61242600
C 1.14449600 -0.16731200 0.39239800
C 2.61963200 -0.42075200 0.14914100
H 3.21624600 0.19542400 0.82467300
H 2.86000100 -1.46890900 0.33503100
H 2.88321800 -0.17747000 -0.88349700
N 0.26674600 -0.93766000 -0.53551300
H -0.04575000 -1.90824000 -0.30348000
H 0.86042300 -0.47953200 1.40235600
N 0.74446400 1.21760600 0.15740600
H 1.39530600 1.67111700 -0.47418900

TS_{E}
C -0.89257000 0.53504100 0.72831100
H -1.75607400 0.63467300 1.36006200

C -0.14465200 1.57796200 0.02780000
H -0.39668800 2.63119100 0.01948800
O -2.32866600 -0.78882600 -0.45211200
H -3.25551900 -0.98117100 -0.64955700
C 0.86830100 -0.34485600 -0.36875400
C 2.22047400 -0.83547400 0.14217300
H 2.18456100 -1.91277900 0.30913100
H 2.99228300 -0.61464000 -0.59577200
H 2.46849800 -0.33707500 1.08110700
N 0.86031300 1.09042200 -0.60593100
H 0.61120400 -0.83803600 -1.31254000
N -0.22898700 -0.59354700 0.58356300
H -0.94753500 -1.34571600 0.38437100

TS_F
C -1.45245900 -0.66594900 0.08774000
C -1.40156500 0.72869900 0.06386800
C 0.61430600 0.03531000 -0.12899500
H -2.31141000 -1.31969400 0.09918900
H -2.23321700 1.41890600 0.11380200
H 0.33822800 -0.75314100 -1.10791000
N -0.13838600 1.16009100 -0.08297000
N -0.19274600 -1.15840000 0.01208100
C 2.09438700 0.00663300 0.11616100
H 2.52502600 -0.94714500 -0.18957800
H 2.57906000 0.81350900 -0.43420500
H 2.29223000 0.14756400 1.18228100

1 H_2O

TS_{A1}
C 2.07401500 -0.13360100 -0.06288700
H 2.61958700 0.72242800 0.34247200
H 2.14938600 -0.13027200 -1.15365500
H 2.53520000 -1.05014300 0.30959300
C 0.61236400 -0.12259700 0.34903300
H 0.52484300 -0.05527100 1.44782000
O -0.10386000 -1.13630600 -0.20061800
O -2.25376500 -0.10269800 0.14182400
H -1.21577600 -0.80436700 -0.04988600
H -2.75266900 -0.10901100 -0.68200300
N -0.05444000 1.21262300 -0.11265400
H 0.14226500 1.38127800 -1.09872300
H 0.23581900 2.02503600 0.42878500
H -1.11484400 0.98117900 -0.00234500

TS_{A2}
C -0.21424300 0.07550400 0.42526800
H -0.04687300 0.24969900 1.50787300
H 0.31636800 1.37131400 -1.20237900
N 0.58389700 1.23845900 -0.22746700
H 0.51049500 2.12710600 0.26480600
H 1.62346700 0.79720200 -0.19262600
O 2.53590500 -0.34823200 -0.12247400
H 2.94260000 -0.39524900 0.74978000
H 1.42344300 -0.92134300 -0.05794300
O 0.25475700 -1.09062500 -0.05039900
C -1.70562400 0.31903500 0.17935600
H -2.06391800 1.32669700 0.48028100
O -2.44987000 -0.51012700 -0.27528500

TS_B
C -1.84793800 -0.22089800 -0.39190800
H -1.85749900 0.62939400 -1.08604300
C -0.61819600 -0.07507200 0.52936900
H -0.54782200 -0.97693500 1.15165500
N 0.60237000 -0.06203300 -0.39630900
H 0.47880900 -0.75508100 -1.13730800
C 1.90677700 -0.27493800 0.31267600
H 1.89212600 0.43237700 1.14506500
C 3.05274900 0.00708400 -0.63758800
H 2.98405300 1.02180300 -1.03361700
H 3.99609600 -0.10116000 -0.10203700
H 3.03748600 -0.70355000 -1.46771800
O -0.62005000 1.07041400 1.27201000
H -0.33133800 1.88187000 0.49608700
O 0.10468100 2.43871900 -0.57755100
H 0.84616100 3.01329200 -0.36029100
H 0.56785200 0.97091500 -0.76781900
N -3.01785800 -0.32392400 0.45107700
H -2.94234700 0.36072200 1.19853500
H -3.85642200 -0.10847900 -0.07838000
O -1.72669800 -1.37427400 -1.22187900

H -1.93535600 -2.13296200 -0.65959500
O 1.99556500 -1.60530900 0.75480100
H 1.58829200 -1.68397000 1.62373800

TS_C
C 0.19583000 1.42721100 0.00500400
C 0.68349200 0.53291100 1.20999700
C -1.69851100 0.08974000 -0.70338100
H -0.50131600 2.17193600 0.38708700
H 0.96502600 1.24519200 1.99974800
N -0.50519700 0.53343400 -0.91741900
H 0.13719900 -0.10506600 -1.43340600
N -0.27136300 -0.40158100 1.56322100
H -0.30025400 -1.78301300 0.81760300
C -2.79230900 0.74419600 0.05247000
H -2.47444000 1.58875800 0.65503000
O 1.97315300 -0.09940900 0.76652100
H 2.56081700 0.61948200 0.49354400
O 1.29603800 2.01902800 -0.63015400
H 0.99803700 2.77662500 -1.14573800
H -1.95828800 -0.80386300 -1.26382300
H -0.30422000 -0.49511400 2.57322100
O -0.32510400 -2.67710800 0.26483800
H -1.25805100 -2.85770800 0.11369000
O 1.26214800 -1.48594500 -1.55807100
H 0.66107700 -2.09387900 -1.06348100
H 1.74461300 -1.07393300 -0.81218600
H -3.26351900 0.00371400 0.69987800
H -3.55166000 1.06701900 -0.67140000

TS_D
C 0.98162200 -1.21656100 0.41366900
H 1.57204300 -1.47843200 1.30171800
C -0.28901700 -0.52955200 0.87242500
H -0.94540600 -0.94000100 1.62482600
O -1.74164600 -1.02936800 -0.58507400
O 0.68306300 -2.39340600 -0.30821300
H 1.50671100 -2.88704500 -0.38824700
H -2.22979300 -1.78500400 -0.24037300
C 0.79445300 1.02001700 -0.39176000
C 1.54744400 2.31479300 -0.14299500
H 2.31036700 2.45837600 -0.91127200
H 0.86152800 3.16337500 -0.17748300
H 2.02813100 2.29120800 0.83865000
N -0.22798500 0.75486300 0.64954800
H -1.21577900 1.21350900 0.55208500
H 0.26113000 1.07726300 -1.34833300
N 1.65379000 -0.16936700 -0.35459700
H 2.54838100 0.05737300 0.06185700
O -2.67069600 1.12167900 0.04334200
H -2.74502300 1.66779000 -0.74671200
H -2.30570000 -0.06030700 -0.33983700

TS_E
C -0.36672000 0.70589600 0.83029800
H -1.10735400 0.90185300 1.58779100
C 0.58109100 1.65751700 0.22852100
H 0.53783100 2.73347800 0.34230700
O -2.02001500 0.83362900 -0.60250400
H -2.73078600 1.31096000 -0.15852300
C 1.17268300 -0.37106600 -0.40817800
C 2.39795500 -1.18407500 -0.00143800
H 2.14077700 -2.24297600 0.05128800
H 3.19061200 -1.04761800 -0.73798300
H 2.75620600 -0.85550600 0.97609700
N 1.45577700 1.05667600 -0.48642800
H -2.73302600 -1.67663300 0.63618700
H 0.81480400 -0.69115600 -1.39489400
N 0.06624100 -0.50013800 0.55498000
H -0.74301800 -1.23202200 0.42785100
O -2.14141600 -1.53496300 -0.11115400
H -2.19878300 -0.33511400 -0.39593900

TS_F
C -1.91009300 -0.12776600 0.32027800
H -2.94579300 -0.18424900 0.62670800
C -1.22283800 -1.07362100 -0.51939300
H -1.56904900 -2.02017700 -0.90850400
O 2.05467700 -1.15549100 0.53467800
H 0.95196700 -1.17390400 -0.62282000
C 0.16258600 0.53364200 0.16546000
C 0.90238100 1.70879000 -0.46889400

H 1.02674600 2.49345900 0.27780000
H 1.88550900 1.37439900 -0.80033400
H 0.34525800 2.10725100 -1.31909200
N 0.00014300 -0.63775900 -0.66966200
H 1.01427300 -0.01533500 0.83641000
N -1.09390400 0.81258600 0.72195700
H 2.91778900 -0.80757400 0.28163100

2 H_2O

TS_{A1}
C -2.53221100 0.16957900 -0.19471100
H -2.86184900 0.04413900 0.84005400
H -2.99151800 -0.60342700 -0.81496800
H -2.86765900 1.14607400 -0.54678800
C -1.01621400 0.12312200 -0.26077600
H -0.66344700 0.21171600 -1.29706500
O -0.45266900 1.04903700 0.57340700
H 0.53771300 1.21845600 0.25395300
N -0.52687500 -1.27262100 0.17081900
H -0.77495700 -1.41924500 1.14948000
H -0.94455300 -2.02164800 -0.38157700
O 1.88409500 1.28641100 -0.27351600
H 2.43363500 1.68388900 0.40978500
H 0.56749000 -1.30900800 0.07321600
O 2.06424300 -1.13941800 -0.13020600
H 2.07652600 -0.01825700 -0.20835000
H 2.50194900 -1.34878400 0.70196200

TS_{A2}
C -1.32460200 -0.22361100 -0.82984300
H -1.63028400 0.36186200 -1.72140200
C -1.03221000 0.61144500 0.43123800
H -1.98050700 1.10072600 0.69683300
O -1.27912200 -1.42587100 -0.84922100
O -0.51750200 -0.05823000 1.48293800
N -0.08545300 1.74247400 -0.00240200
H -0.49211900 2.36115200 -0.70454300
H 0.86372000 1.27571700 -0.39514200
H 0.12650100 2.30110500 0.82290500
O 1.93341300 0.43157100 -0.86422500
H 1.75700300 -0.46618400 -0.19012900
H 2.79125600 0.80643700 -0.63892500
O 1.36874900 -1.38486600 0.64021000
H 0.95013600 -2.07322900 0.11263600
H 0.30903400 -0.69273900 1.14859500

TS_{B}
C 1.87858400 -0.27291700 0.34858400
H 1.82637100 0.80159000 0.55761000
C 0.59306100 -0.69177200 -0.38593500
H 0.60845300 -1.77499100 -0.53422900
N -0.57823400 -0.40220600 0.54661700
H -0.56288800 -1.08790100 1.30171800
C -1.91366000 -0.39470800 -0.16357400
H -1.90874100 0.54238400 -0.72383200
C -3.02731400 -0.41540200 0.86009200
H -2.91022100 0.41014200 1.56419300
H -3.98468200 -0.31262400 0.34866400
H -3.02239700 -1.36190900 1.40653300
O 0.41505000 -0.07380300 -1.60423200
H 0.34659800 0.96800800 -1.45376100
O 0.19957100 2.35771400 -1.06893200
H -0.52004700 2.77182800 -1.55569100
H -0.46211200 0.60606600 0.98500700
N 3.00858000 -0.67512000 -0.45853400
H 2.82198200 -0.46324800 -1.43445200
H 3.83878900 -0.15923500 -0.18600300
O 1.93304200 -0.89767400 1.62755300
H 2.24666200 -1.79872400 1.46958600
O -2.02736400 -1.49880700 -1.01558100
H -1.46702100 -1.31527300 -1.78322100
O -0.42234900 2.07475900 1.24627200
H 0.28448500 2.34911400 1.83888600
H -0.11526900 2.31732000 0.14676500

TS_{C}
C -0.64821700 -0.65729000 0.58209700
C -0.07560500 -1.69135500 1.51127200
H -0.81114400 -2.49850200 1.58060400
H 0.85837500 -2.07000900 1.09958300
H 0.06818400 -1.26996600 2.50942800
H 0.00296300 1.67734800 0.94408300

O -1.46831300 2.28646300 0.58551100
H -1.97498900 1.69010100 -0.18931500
H -2.10217500 2.40219200 1.33950500
H -1.32473900 0.07925800 0.97248400
O -2.52960100 -1.47531300 0.07009700
H -2.18857100 -2.08942200 -0.63797500
O -2.45772200 0.72364000 -1.07739100
H -2.70906800 -0.52019600 -0.46107900
H -3.03863900 1.02149800 -1.82163700
N 0.84274100 1.02240000 0.96674800
H 1.40167600 0.93674500 1.81281000
N -0.26863900 -0.56232000 -0.73802900
H -0.98029900 0.04472700 -1.24609000
C 1.58093600 0.92122000 -0.27609400
H 1.36400400 1.78071400 -0.92279500
C 1.12807000 -0.38967000 -1.05678300
H 1.21422600 -0.22237400 -2.13768000
O 1.95630800 -1.49541900 -0.63066200
H 2.78948100 -1.04613200 -0.29441100
O 3.01066200 0.73584800 -0.07380000
H 3.41022800 1.56426700 0.29845800

TS_D
C -1.32168100 -1.11972400 -0.59413200
H -1.71197200 -1.23728500 -1.61319600
C 0.02263500 -0.43137000 -0.68277700
H 0.86301500 -0.76733500 -1.26850000
O 1.11058300 -1.41874000 1.01275600
O -1.19513200 -2.39715200 -0.00101600
H -1.99725800 -2.89025200 -0.20458200
H 0.95284500 -2.34525200 0.80331100
C -1.30638100 1.01253600 0.49702800
C -1.96173900 2.33659100 0.14096100
H -2.89045700 2.45067000 0.70359500
H -1.30207100 3.16759300 0.39787900
H -2.18377300 2.37637800 -0.92826500
N -0.05974700 0.78174100 -0.26396400
H 0.81429200 1.38777600 -0.21765700
H -1.02889800 1.00520700 1.55719600
N -2.12267700 -0.15969900 0.16176900
H -2.94611000 0.11603400 -0.35754700
O 2.36206600 1.86866900 -0.21338500
H 2.57986300 2.24551500 0.64589600
H 2.01551000 -1.12632500 0.56302700
O 3.15058600 -0.49467300 -0.09498800
H 3.32358500 -0.87269900 -0.96271300
H 2.76655900 0.88264900 -0.19649400

TS_E
C -0.03475000 -0.65999000 0.79538900
H 0.78502500 -0.77433300 1.48360100
C -1.18111600 -1.55584400 0.55562100
H -1.26256700 -2.56702400 0.93296500
O 1.28744000 -1.73874500 -0.63980700
H 1.58938200 -2.54839400 -0.21128400
C -1.59146200 0.33690600 -0.50556100
C -2.59852200 1.42431500 -0.14357300
H -2.19318500 2.40621900 -0.39232700
H -3.51838000 1.26785600 -0.70739300
H -2.82086000 1.38762300 0.92438900
N -2.06447100 -1.00103400 -0.18419100
H 1.95466100 2.51588700 0.91010300
H -1.36710600 0.36410300 -1.57880800
N -0.33041000 0.47295600 0.23836400
H 0.36199000 1.27757000 0.18152800
O 1.71701100 2.14030500 0.05549500
H 2.08807000 -0.99351900 -0.46510500
O 2.98176000 -0.02079500 -0.19899900
H 2.31371400 1.28304000 -0.05161800
H 3.37884200 -0.24093000 0.64997000

TS_F
C 1.15312600 1.42829000 0.36117400
H 1.14213200 2.48688100 0.58565800
C 2.05129700 0.71121000 -0.46038800
H 2.90448000 1.09400200 -1.00572500
O -2.45023000 0.93752000 0.44848300
H -3.00702100 0.40806100 1.03105400
C 0.51273400 -0.63033900 0.21423300
C 0.04879800 -1.92275400 0.84750600
H -0.99651800 -1.84490100 1.15502200

H 0.14327500 -2.74959200 0.14093800
H 0.64290900 -2.16311000 1.73514600
N 1.67497600 -0.56769300 -0.52999400
H -0.45711300 -0.48274000 -0.85212600
N 0.21506000 0.59445700 0.81490700
H -1.53647100 0.93023200 0.85163300
O -1.40404000 -0.25119900 -1.54098100
H -2.01250200 0.20759500 -0.85376000
H -1.81499000 -1.08278700 -1.81739800

1 CH_3OH

TS_{A1}
C -2.52856600 -0.19993600 0.32571100
H -3.16771400 0.65342000 0.08518300
H -2.38547400 -0.25576500 1.40817200
H -3.02776100 -1.11354600 -0.00203900
C -1.17840400 -0.11134300 -0.36331900
H -1.31107700 0.00666900 -1.45271800
O -0.33722100 -1.11894300 -0.01556300
O 1.70860600 0.00155400 -0.60256600
H 0.71674600 -0.73861300 -0.33513100
N -0.47712600 1.23051300 0.02679400
H -0.50745400 1.36863700 1.03646000
H -0.87830300 2.04770700 -0.43040100
H 0.55089000 1.04867800 -0.26926500
C 2.64293000 -0.08339800 0.44754500
H 2.18546900 0.05768700 1.44399900
H 3.15027800 -1.06176100 0.46952500
H 3.42743600 0.68046200 0.34407200

TS_{A2}
C -0.64901500 0.06678300 0.37399100
H -0.37233800 0.15391900 1.44376700
H -0.43870800 1.56962500 -1.14668400
N -0.02107600 1.34735200 -0.24328500
H -0.07434100 2.16775100 0.35769100
H 1.03771500 0.99065700 -0.41730000
O 2.01722700 -0.07272300 -0.61512000
H 0.96910200 -0.73529600 -0.45331000
O -0.15788800 -1.01321100 -0.26072300
C -2.17251700 0.21166300 0.31474100
H -2.56025100 1.15706900 0.75023200
O -2.90566400 -0.62801700 -0.13787100
C 2.90174000 -0.27959000 0.47000500
H 2.41760200 -0.12631100 1.44873200
H 3.30561900 -1.30152200 0.46351300
H 3.75248900 0.41111600 0.41364800

TS_{B}
C -2.01796400 0.05492600 -0.40098800
H -1.77803200 0.89907800 -1.06066300
C -0.81403300 -0.18006700 0.53583600
H -1.00806200 -1.08533100 1.12538400
N 0.37805100 -0.47830900 -0.37957100
H 0.07272900 -1.07941700 -1.14831900
C 1.55556300 -1.08941300 0.32448900
H 1.71849300 -0.45956700 1.20209500
C 2.75722400 -1.08419800 -0.59865200
H 2.98719700 -0.07101900 -0.93241100
H 3.61859100 -1.48420000 -0.06346100
H 2.56348100 -1.71349800 -1.47074900
O -0.50866300 0.89443100 1.32081100
H -0.01012900 1.62189800 0.58013300
O 0.59987900 2.07983100 -0.45983800
H 0.64160300 0.52558300 -0.71534000
N -3.18733600 0.24907000 0.42570600
H -2.94340000 0.85706800 1.20282500
H -3.92274700 0.70711300 -0.10276100
O -2.20315400 -1.05596900 -1.27569800
H -2.62628000 -1.74671600 -0.74729300
O 1.25520100 -2.41469900 0.67652300
H 0.83260600 -2.43274200 1.54149700
C 1.82350000 2.69739800 -0.14008200
H 2.42330700 2.88076400 -1.04367600
H 1.67519800 3.67281300 0.35028500
H 2.44859700 2.09222000 0.54151100

TS_{D}
C 1.87376200 -0.58108100 0.27862600
H 2.63280700 -0.53748300 1.07059200
C 0.50537700 -0.63880900 0.92896200
H 0.24706000 -1.33384100 1.71283700

O -0.70749200 -1.80099000 -0.38473200
O 2.09330100 -1.72596200 -0.51790700
H 3.03065000 -1.73370200 -0.74169100
H -0.68957700 -2.71027600 -0.06774400
C 0.49224800 1.26463000 -0.32590500
C 0.50160700 2.75876300 -0.05933100
H 0.98640300 3.28245300 -0.88588700
H -0.52027900 3.13166800 0.03174000
H 1.03955400 2.97616100 0.86717500
N -0.11784200 0.49745200 0.78997400
H -1.19084600 0.41397900 0.87243700
H -0.10372700 1.04825100 -1.22008300
N 1.83225300 0.68479100 -0.45257500
H 2.52760500 1.32560600 -0.09059200
O -2.49083100 -0.42649400 0.51046100
H -1.62972700 -1.26379700 0.02213700
C -3.22896500 0.15725300 -0.53388600
H -4.05224700 0.77748600 -0.14716000
H -2.61888800 0.81114500 -1.18524600
H -3.68367600 -0.60031300 -1.19369100

TS_E
C 0.16104900 0.80588400 0.81308000
H -0.57432900 1.13031100 1.53013900
C 1.38819100 1.50659500 0.40246600
H 1.62318900 2.53674400 0.63894300
O -1.23733300 1.52076800 -0.71947000
H -1.85317900 2.12696000 -0.29148900
C 1.48199100 -0.54046800 -0.41857000
C 2.39107600 -1.69381200 -0.00436600
H 1.85664700 -2.64033000 -0.09751800
H 3.27026500 -1.71778600 -0.64912300
H 2.70898700 -1.56429500 1.03189400
N 2.14189200 0.75331200 -0.30603300
H 1.16528700 -0.66176200 -1.46196700
N 0.28075500 -0.44165100 0.42868900
H -0.66131200 -0.91547500 0.15550900
O -2.04526500 -0.74967300 -0.52882800
H -1.73078400 0.43729700 -0.68476800
C -3.12156000 -0.83031100 0.38013600
H -2.87348800 -0.42251200 1.37596700
H -3.99955800 -0.27416600 0.01773800
H -3.43396000 -1.87269300 0.52598900

TS_F
C -2.24953900 -0.62192500 0.48718700
H -3.18469700 -0.97719100 0.89823300
C -1.46699700 -1.29190300 -0.52060900
H -1.61517700 -2.25864100 -0.97838500
O 1.85587600 -0.45661000 0.14193400
H 0.52720900 -0.80196900 -1.05299200
C -0.46104300 0.59782300 0.15368300
C -0.20704400 1.95913200 -0.49034700
H -0.20149100 2.72134100 0.28911800
H 0.76730900 1.93750200 -0.97711800
H -0.98380400 2.19641100 -1.21961800
N -0.43551200 -0.52999500 -0.76280700
H 0.51855200 0.33400000 0.72730300
N -1.66843700 0.47864600 0.87634900
C 3.22928400 -0.34657900 0.27621200
H 3.75997400 -0.37422900 -0.69751400
H 3.54165100 0.60633700 0.75013200
H 3.68314500 -1.15053100 0.89381200

2 CH_3OH

TS_{A1}
C -3.23738700 -0.03967400 -0.00836600
H -3.42059800 0.08920200 1.06138800
H -3.69796500 -0.97154700 -0.34399400
H -3.70324900 0.79082500 -0.54060200
C -1.74501600 -0.01513300 -0.28383400
H -1.54029100 -0.18754300 -1.34913600
O -1.18015300 1.13840800 0.19364100
H -0.21484600 1.25050300 -0.19727600
N -1.06672600 -1.20775600 0.41105300
H -1.08627900 -1.05583900 1.41950600
H -1.53104100 -2.09302900 0.20859400
O 1.18224300 1.28356000 -0.63491400
H -0.02365400 -1.26367500 0.06478600
O 1.33171100 -1.13830700 -0.57469700
H 1.35175300 -0.02083900 -0.64106200

C 2.41816800 -1.61770900 0.20255200
H 2.39160300 -2.71202100 0.23679500
H 3.37910100 -1.31923300 -0.23561100
H 2.39091200 -1.24524800 1.23675800
C 1.91535500 1.82952800 0.43700900
H 2.99090400 1.60684200 0.35421000
H 1.81846200 2.92561000 0.47145900
H 1.58513800 1.44892400 1.42041100

TS_{A2}
C 2.72542900 -0.40529300 -0.42240600
H 3.00576800 -1.26262500 -1.06108100
C 1.21678200 -0.20042200 -0.31355600
H 0.88724200 0.34271700 -1.21528600
O 3.53578900 0.29305800 0.13380900
O 0.60185600 -1.40501600 -0.13897300
N 0.91790700 0.73256600 0.84033500
H 1.03586100 0.21975000 1.71456700
H -0.15065600 1.06137300 0.73228500
H 1.55946700 1.52688000 0.85167100
O -1.54981900 1.23641900 0.41095100
H -1.74742000 0.21683800 -0.04318100
O -1.79771300 -0.98394900 -0.50837100
H -0.44314900 -1.28888400 -0.35210100
C -2.55651800 -1.78276500 0.37609600
H -3.44393700 -1.24355500 0.73907300
H -2.91018800 -2.69833200 -0.11856700
H -1.97951100 -2.09214600 1.26366700
C -1.84750600 2.26929400 -0.51824800
H -1.44866900 2.05420800 -1.51954500
H -2.93098500 2.41446200 -0.60890500
H -1.40919500 3.21238000 -0.17558500

TS_{B}
C 1.83856500 1.05425800 0.34792100
H 1.03533100 1.65934200 0.78340900
C 1.22277200 -0.15070200 -0.39205700
H 2.04363900 -0.78480300 -0.73755200
N 0.43449100 -0.94420400 0.63058000
H 1.07210500 -1.18216000 1.39274400
C -0.25060400 -2.18254300 0.09875800
H -0.64547500 -2.68854900 0.98052800
C 0.69981100 -3.09850600 -0.65860600
H 1.57020900 -3.36199700 -0.05322000
H 0.16243200 -4.01289600 -0.91236800
H 1.03644300 -2.63272000 -1.58672300
O 0.42734500 0.19259900 -1.46851100
H -0.28367800 0.92914500 -1.16854300
O -1.27878900 1.80440900 -0.66832600
H -0.35922200 -0.26043600 1.06224400
N 2.68956800 1.76322400 -0.58020300
H 2.24694800 1.80300100 -1.49351700
H 2.84009900 2.71693500 -0.26879900
O 2.59677500 0.59049200 1.46362400
H 3.44988900 0.30929800 1.10488300
O -1.35976200 -1.79215900 -0.66675500
H -1.01588700 -1.24073100 -1.38812300
O -1.30129100 0.73027000 1.48398600
H -1.37542500 1.30416500 0.46759500
C -2.48033700 1.63109600 -1.39495900
H -3.29808800 2.22307500 -0.96102800
H -2.35373400 1.95858000 -2.43520700
H -2.81062800 0.58043700 -1.41654900
C -2.55651800 0.18474000 1.86472600
H -2.87869700 -0.60951800 1.17822900
H -2.48902000 -0.23900400 2.87310900
H -3.33202300 0.96076200 1.87940800

TS_{D}
C -1.97493500 -1.12103800 -0.43036400
H -2.38965100 -1.35374300 -1.41986800
C -0.55527700 -0.63434500 -0.62433200
H 0.21175900 -1.17605900 -1.15436600
O 0.38012700 -1.41328200 1.24051000
O -2.00453000 -2.28844600 0.36547200
H -2.86629600 -2.70047400 0.24056400
H 0.18858900 -2.35585400 1.20186400
C -1.67627200 1.14823600 0.27506100
C -2.16709200 2.46203500 -0.30994900
H -3.06448700 2.78824500 0.21946100
H -1.40420000 3.23486700 -0.19783100

H -2.40025600 2.34379000 -1.37097900
N -0.48079000 0.63524500 -0.43031600
H 0.45599200 1.13809800 -0.48469500
H -1.38198500 1.29116300 1.32080700
N -2.63650300 0.04660300 0.14784100
H -3.43073800 0.32828800 -0.41213100
O 2.02760900 1.49302300 -0.43509500
H 1.34308100 -1.24757900 0.86429200
O 2.58030800 -0.82688700 0.21737000
H 2.32595900 0.50215300 -0.19200100
C 2.34594200 2.31791300 0.67796100
H 3.39287700 2.18818400 0.97939700
H 2.19695200 3.36700000 0.40605600
H 1.71511600 2.09946000 1.55243300
C 2.98485200 -1.68732600 -0.80868600
H 3.11161700 -1.16406600 -1.77397300
H 3.94882200 -2.18318800 -0.59484700
H 2.25647300 -2.50132700 -0.99104700

TS_E
C -0.61805100 -0.69895700 0.76668800
H 0.24143200 -0.84982900 1.39755200
C -1.90364100 -1.42208400 0.77092800
H -2.08501800 -2.35184300 1.29448300
O 0.34283000 -2.13267200 -0.61967800
H 0.62089000 -2.91066500 -0.12206300
C -2.16013800 0.36455900 -0.50173400
C -2.94698400 1.63517900 -0.19429300
H -2.43551300 2.50160700 -0.61623300
H -3.94107200 1.56113200 -0.63571600
H -3.04171200 1.76476400 0.88532600
N -2.77876900 -0.83041400 0.05053400
H -2.06653800 0.22484100 -1.58542900
N -0.81222900 0.38904700 0.08662200
H -0.03039400 1.06424300 -0.15061600
O 1.41576500 1.69286200 -0.51332400
H 1.24934900 -1.49070000 -0.70987700
O 2.28738000 -0.66102800 -0.72637600
H 1.85037500 0.75658800 -0.63029300
C 3.15173700 -1.02435400 0.31890800
H 3.52294600 -2.05695000 0.20644500
H 4.03668300 -0.37112600 0.35869600
H 2.67832000 -0.97032100 1.31821500
C 2.05796400 2.36831500 0.56371600
H 3.11996600 2.53773700 0.34899100
H 1.57942200 3.34088500 0.70368200
H 1.98473800 1.80996500 1.50649800

1 C_2H_5OH

TS_{A1}
C -2.81685200 -0.27222500 -0.48000600
H -3.48619400 -0.67753700 0.28309300
H -2.52969800 -1.06728200 -1.17325100
H -3.35136600 0.49601100 -1.04150300
C -1.57344800 0.34990500 0.12918100
H -1.85213200 1.11067400 0.87795000
O -0.68800600 0.79225600 -0.80050700
O 1.23282700 0.82037200 0.65345000
H 0.30188100 0.93123400 -0.20816400
N -0.83295000 -0.71422300 1.00557900
H -0.72538900 -1.58843900 0.49155200
H -1.30125700 -0.90724600 1.88936500
H 0.14311000 -0.27494700 1.14271100
C 2.42230700 0.35696000 0.05813200
H 2.80547800 1.09666500 -0.66647200
H 3.20503200 0.24926300 0.82548900
C 2.24693600 -0.98432200 -0.66511400
H 3.17055000 -1.29661900 -1.16325400
H 1.96265900 -1.77035800 0.04268400
H 1.45575600 -0.90478400 -1.41595800

TS_{A2}
C -1.15272300 0.08028800 0.35960900
H -0.82734600 0.19488000 1.41265500
H -0.88679900 1.48385100 -1.24449900
N -0.45951900 1.28226000 -0.34078400
H -0.43838500 2.13581200 0.21486700
H 0.56102300 0.85329400 -0.52095000
O 1.46896900 -0.30883600 -0.69225300
H 0.37000900 -0.87882900 -0.47258100
O -0.76420700 -1.05856100 -0.24202200

C -2.66468900 0.32609900 0.34891700
H -2.97508700 1.31333400 0.75156800
O -3.46662100 -0.48524300 -0.03317400
C 2.37189700 -0.53517500 0.37490100
H 1.90618400 -0.30441500 1.34914000
H 2.64927000 -1.59974100 0.40948100
C 3.63077700 0.30830500 0.20764400
H 3.38205400 1.37379800 0.22127000
H 4.35111000 0.11232500 1.00831400
H 4.10790300 0.08388200 -0.75062100

TS_B
C 2.02000300 -0.89749900 -0.45131700
H 1.33941800 -1.59327900 -0.95927700
C 1.18657300 -0.03258200 0.51807800
H 1.84431100 0.73231000 0.95052300
N 0.15523600 0.69653300 -0.35341700
H 0.60346000 1.01006100 -1.21743800
C -0.51863000 1.85070500 0.33362300
H -0.84293500 1.45377200 1.29832600
C -1.69152000 2.32618100 -0.49980500
H -2.40088500 1.51541000 -0.67388600
H -2.19994700 3.13216000 0.02959800
H -1.34029200 2.70626600 -1.46232800
O 0.52813300 -0.75059800 1.47263800
H -0.33391600 -1.23670700 0.88267700
O -1.21360600 -1.47009100 -0.03116900
H -0.57041800 -0.09081300 -0.52808100
N 3.06872200 -1.53088900 0.31536200
H 2.67835100 -1.86942800 1.19062900
H 3.43920200 -2.33213600 -0.18530700
O 2.57554800 -0.09735300 -1.49270900
H 3.33251000 0.36220000 -1.10378900
O 0.39557400 2.90536500 0.47907600
H 0.89099100 2.79379400 1.29730700
C -2.53277900 -1.39642000 0.45616200
H -2.71774500 -2.19453300 1.19469100
H -2.71917700 -0.44397700 0.98806500
C -3.54329200 -1.53294000 -0.67989700
H -3.38485300 -2.47764000 -1.20814600
H -4.57310100 -1.51035700 -0.30838600
H -3.41999400 -0.71986700 -1.40254100

TS_D
C 2.18596600 -0.79757600 0.17062100
H 3.03150700 -0.85102500 0.86826300
C 0.90968700 -0.63380100 0.97309900
H 0.64921600 -1.25843900 1.81343900
O -0.60184000 -1.64258700 -0.13715800
O 2.13745000 -1.97961400 -0.59963400
H 3.03023100 -2.13359600 -0.92838500
H -0.67864500 -2.54103100 0.20135300
C 1.02123500 1.21052100 -0.36413400
C 1.26452600 2.69666000 -0.17640000
H 1.71952700 3.11687900 -1.07572900
H 0.32044400 3.21391700 0.00496600
H 1.92913900 2.86742700 0.67455900
N 0.44246800 0.57650000 0.84911100
H -0.60799200 0.66046500 1.06078400
H 0.30496600 1.04712500 -1.17744900
N 2.24627100 0.44299400 -0.60181800
H 3.05697500 0.98715700 -0.33313400
O -2.06956300 -0.00579700 0.89142500
H -1.38664500 -0.97603700 0.35106300
C -2.82358100 0.63160700 -0.11080000
H -3.32049000 1.52524100 0.30120300
H -2.18304700 0.99461800 -0.93826200
C -3.88588900 -0.29849500 -0.70156400
H -4.48827400 0.20650800 -1.46457400
H -3.40482500 -1.16815200 -1.15913500
H -4.55330300 -0.65702800 0.08798300

TS_E
C 0.70084100 0.83188200 0.82637700
H 0.00969600 1.20069800 1.56556100
C 1.93704900 1.47132300 0.34904900
H 2.22522000 2.49452200 0.55464400
O -0.73041600 1.57696500 -0.66444200
H -1.30697800 2.21440500 -0.22726000
C 1.90960200 -0.59246900 -0.43468300
C 2.78650600 -1.77634600 -0.03758900

H 2.20984400 -2.70088900 -0.09125800
H 3.63548300 -1.84771200 -0.71828000
H 3.15354600 -1.64329200 0.98183800
N 2.62666100 0.67373200 -0.37598200
H 1.54125300 -0.71878200 -1.46034900
N 0.75237400 -0.42569300 0.46198300
H -0.21234600 -0.87045200 0.25317800
O -1.63397700 -0.65146600 -0.40020000
H -1.26612500 0.51937900 -0.59688400
C -2.70766400 -0.64625600 0.51645800
H -2.81945400 -1.64581700 0.96107800
H -2.51681400 0.04828400 1.35509600
C -4.01891200 -0.24726600 -0.16087800
H -4.23880300 -0.93120500 -0.98569400
H -4.85764100 -0.26840300 0.54305600
H -3.93951400 0.76378800 -0.57200300

TS_F
C 2.77134500 -0.40538400 -0.37584000
H 3.76995100 -0.64293300 -0.71649100
C 2.02640600 -1.13699700 0.61782700
H 2.27577300 -2.05602200 1.12723200
O -1.31784300 -0.86736500 -0.31109600
H -0.04824300 -0.91400200 1.00143400
C 0.81499400 0.56517300 -0.20120700
C 0.35062700 1.90683600 0.36291100
H 0.28660300 2.62622400 -0.45379800
H -0.63584800 1.78531800 0.80854200
H 1.05355600 2.27589300 1.11209000
N 0.88715100 -0.51806000 0.76484200
H -0.08410200 0.14611900 -0.81280400
N 2.06939500 0.58551200 -0.85065100
C -2.69644200 -0.80964100 -0.40810200
H -3.03715500 -0.86747200 -1.46335400
H -3.16362000 -1.68663200 0.08814100
C -3.30439300 0.45680100 0.21603900
H -2.91963900 1.34896800 -0.28910200
H -4.39864000 0.46601300 0.14451500
H -3.02693200 0.52454900 1.27325900

2 C_2H_5OH

TS_{A1}
C -3.64733800 0.78877900 0.05932500
H -3.92417400 0.28884300 0.99114500
H -4.26925900 0.40534400 -0.75244100
H -3.83694200 1.85700400 0.17194400
C -2.17006200 0.58197600 -0.21726600
H -1.86851100 1.06606800 -1.15404700
O -1.40168600 0.98904000 0.84722500
H -0.46404900 1.21019700 0.47615900
N -1.89223100 -0.90721000 -0.46528300
H -2.17842200 -1.44553700 0.35290100
H -2.40066400 -1.26571400 -1.27367100
O 0.81952600 1.35366300 -0.29316200
H -0.80574900 -1.04334000 -0.61655700
O 0.69692600 -1.02944100 -0.69611300
H 0.84485600 0.08854700 -0.54569200
C 1.20680800 -1.69008400 0.45721600
H 2.24193600 -1.37010300 0.63898800
H 0.62838400 -1.40788100 1.35176500
C 1.94320300 1.79079700 0.43294100
H 1.82437900 2.85340800 0.69912500
H 2.04873000 1.24496200 1.38862200
C 1.16200100 -3.19929500 0.26562900
H 1.74494200 -3.48424100 -0.61439600
H 1.57167600 -3.71886400 1.13700800
H 0.13327500 -3.54077500 0.11650300
C 3.23400100 1.62344500 -0.37038200
H 3.16115000 2.17127600 -1.31471700
H 4.10413300 1.99388100 0.18208100
H 3.40011900 0.56759700 -0.60611100

TS_{A2}
C 2.81452500 -1.43978900 -0.41262900
H 2.78416500 -2.38068000 -0.99160700
C 1.45400600 -0.75812100 -0.29462500
H 1.27697200 -0.19974400 -1.22904700
O 3.82484100 -1.00160600 0.07813900
O 0.49574400 -1.69004200 -0.02082100
N 1.51022900 0.29512000 0.79020600
H 1.51095000 -0.16770600 1.69946600

H 0.58974800 0.93112000 0.68660000
H 2.36174300 0.85454400 0.72100000
O -0.69629700 1.51803400 0.37262400
H -1.21558400 0.58826000 -0.02645200
O -1.65802700 -0.54918600 -0.43359400
H -0.45925400 -1.26712300 -0.24379900
C -2.63018500 -1.03726300 0.47050500
H -3.39442300 -0.26576500 0.65224900
H -2.18058300 -1.26750300 1.45251800
C -0.66289600 2.54290200 -0.61635400
H 0.01434400 2.26882300 -1.44035400
H -1.66393000 2.65784300 -1.05222900
C -0.21181400 3.85715300 0.00417000
H 0.79609300 3.76081500 0.41843400
H -0.20111300 4.65902200 -0.73999400
H -0.88763400 4.14354300 0.81440100
C -3.30178900 -2.29303300 -0.07745200
H -2.56459600 -3.08877200 -0.22199200
H -4.07651500 -2.66199200 0.60272800
H -3.76316400 -2.07921500 -1.04584100

TS_B
C -1.03527900 0.10591800 1.44010700
C -1.82571100 0.57242600 0.19955000
N -1.09979500 0.30457700 -1.10056200
H -0.13471100 0.86955400 -1.05234000
H -1.64022800 0.75132800 -1.84267700
C -2.01112300 -1.96551800 -1.78373900
H -2.74059100 -1.46479800 -2.42328800
H -2.47085400 -2.17578300 -0.81975600
H -1.71292900 -2.90285300 -2.25598900
C -0.76389100 -1.12102400 -1.59294900
H -0.28933900 -0.91274100 -2.56008900
O 0.11371400 -1.74695200 -0.73180700
O 2.32124500 -0.63992100 -0.63503200
H 1.08912900 -1.31352800 -0.75255500
H -0.00714000 0.46864900 1.32105000
H -1.86873800 1.66386500 0.24936700
O -3.10179200 0.00590100 0.22472100
H -3.71839600 0.58077000 -0.24198200
O -1.04604000 -1.30113800 1.61477400
H -0.56687000 -1.68417600 0.84942000
N -1.62149000 0.76709200 2.58013200
H -2.56801300 0.41302000 2.69872400
H -1.10398600 0.50167200 3.41248600
O 1.20359200 1.44959100 -1.02155900
H 1.83883400 0.49438000 -0.81294800
C 1.51355600 2.54007300 -0.16680700
H 1.28958100 2.29673300 0.88412100
H 2.59066400 2.75011100 -0.21862400
C 2.76737700 -0.79871500 0.70117300
H 3.44448300 0.02465300 0.97109800
H 1.92217600 -0.75511100 1.40934300
C 0.72920200 3.77867100 -0.57949800
H 0.98602300 4.63460800 0.05154100
H 0.94717000 4.03375700 -1.62005700
H -0.34725900 3.60304200 -0.49134400
C 3.48858200 -2.13068300 0.87318900
H 3.85672600 -2.25479600 1.89655600
H 2.81244500 -2.96095600 0.64818200
H 4.33879100 -2.18983300 0.18784300

TS_D
C -2.48668000 -1.22113500 -0.46223800
H -2.84597800 -1.47842000 -1.46727700
C -1.03458300 -0.81119300 -0.58046300
H -0.26314100 -1.41265700 -1.03428400
O -0.26930700 -1.54397200 1.36695300
O -2.62892500 -2.34817500 0.37812600
H -3.49934200 -2.72492200 0.20938300
H -0.49420800 -2.48010300 1.35264400
C -2.12188500 1.06248800 0.16180300
C -2.51239400 2.36847900 -0.50963000
H -3.42606900 2.75717600 -0.05541200
H -1.72421400 3.11254300 -0.38035400
H -2.68217200 2.21173800 -1.57763500
N -0.91115100 0.46250400 -0.44200300
H 0.04838900 0.92038900 -0.46424200
H -1.88749300 1.23928900 1.21746400
N -3.12523500 0.00186100 0.01945900

H -3.86681000 0.29404500 -0.60367400
O 1.63531700 1.21406800 -0.34006600
H 0.72555100 -1.43145300 1.05956600
O 2.03500500 -1.07654600 0.51623700
H 1.87296200 0.23409700 0.00065200
C 1.92121900 2.12953400 0.71334400
H 2.92050300 1.92381300 1.12004000
H 1.20699600 2.00420500 1.54248200
C 2.52458600 -1.98919800 -0.42533200
H 2.37739800 -3.02638300 -0.07405300
H 1.98135600 -1.92456200 -1.39134000
C 4.01350900 -1.77007700 -0.70392000
H 4.40642600 -2.49620600 -1.42438900
H 4.17595700 -0.76428200 -1.10408400
H 4.58270800 -1.85813800 0.22650900
C 1.85544200 3.55495700 0.18726700
H 0.85579200 3.77739200 -0.19725800
H 2.08718600 4.27601200 0.97649200
H 2.57089500 3.68973700 -0.62840800

TS_E
C -0.85410800 -0.91276500 0.83684200
H -0.03547400 -0.75607300 1.51906400
C -1.93507400 -1.91633200 0.91354700
H -1.91763800 -2.78837900 1.55475700
O 0.43044500 -2.17102200 -0.27727800
H 0.86540000 -2.76673700 0.34508100
C -2.54826200 -0.41758800 -0.59124000
C -3.63885300 0.64251700 -0.47367000
H -3.32990000 1.55391800 -0.98820200
H -4.55804700 0.27355600 -0.92980400
H -3.82578200 0.87071300 0.57736400
N -2.88720500 -1.65246400 0.10287000
H -2.36705800 -0.66305400 -1.64483000
N -1.28477200 0.01397100 0.02438000
H -0.68848700 0.82240000 -0.27306500
O 0.62973800 1.75082200 -0.67235000
H 1.23185000 -1.32320100 -0.54601600
O 2.00773700 -0.40036300 -0.75423100
H 1.24892100 0.94031400 -0.73595800
C 3.04537000 -0.46451700 0.19925800
H 2.64367900 -0.55723400 1.22516600
H 3.62048100 0.47287000 0.18094300
C 1.08354400 2.59901700 0.38618200
H 2.12667200 2.88956000 0.20994500
H 1.05611400 2.06077600 1.34396100
C 3.99085100 -1.63627000 -0.06726400
H 4.40536100 -1.55980900 -1.07665700
H 4.81825400 -1.65669600 0.64987500
H 3.45213100 -2.58621600 0.00395500
C 0.19188600 3.83346900 0.45351700
H -0.71132300 3.64720500 1.04027600
H 0.72240400 4.67827200 0.89961800
H -0.10920300 4.11658300 -0.55837100

1 NH_3

TS_{A1}
C 2.13269500 -0.02629100 -0.02400800
H 2.59344600 0.87659700 0.39187600
H 2.24218100 -0.01696400 -1.11374200
H 2.66304000 -0.90133700 0.36165500
C 0.64124700 -0.14976000 0.32644200
H 0.54360000 -0.07120500 1.43849500
O 0.04829600 -1.21052800 -0.22087400
H -1.59467300 -0.85320300 -0.03058700
H -2.94324100 -0.04804800 -0.73673000
N -0.08280600 1.16707800 -0.12815800
H 0.13430800 1.33516800 -1.10977000
H 0.22247100 1.98152700 0.40154700
H -1.38585400 0.77557500 -0.01256100
N -2.30042700 -0.05972200 0.04866000
H -2.82266200 -0.08908000 0.91868800

TS_{A2}
C 1.74417800 0.31076000 0.23093800
C 0.26136800 -0.04762900 0.45251600
H 0.08019200 0.17207100 1.54024700
O -0.15153300 -1.19584800 -0.01026900
H -1.99824900 -0.97680100 0.01168500
H -3.24791800 -0.28225200 -0.89785400
N -0.52014700 1.16968300 -0.21810200

H -0.24279700 1.24915600 -1.19537700
H -0.36248300 2.06838900 0.23508800
H -1.77276500 0.67841300 -0.15548800
N -2.67287600 -0.18616900 -0.06641800
H -3.26916200 -0.12288500 0.75325500
O 2.53582500 -0.37025800 -0.37613500
H 2.05673100 1.27937300 0.69059100

TS_B
C -1.84428500 -0.19760900 -0.40604600
H -1.83071900 0.66836400 -1.08296800
C -0.62832300 -0.10553200 0.55623200
H -0.56666600 -1.11290900 1.04077800
N 0.60990500 -0.01105900 -0.37141600
H 0.48384600 -0.63559600 -1.16826300
C 1.86405300 -0.34958700 0.31719500
H 1.84836500 0.22499300 1.24976500
C 3.06772400 0.01636600 -0.53210900
H 3.06837800 1.08191700 -0.76813200
H 3.98655600 -0.22645000 0.00395800
H 3.04979000 -0.55062100 -1.46698200
O -0.68059800 0.91072600 1.41644700
H -0.25234800 2.31559800 0.38229600
H 1.09838000 3.12114000 -0.27077200
H 0.57895800 1.32169800 -0.65609300
N -3.03276100 -0.28410100 0.41394300
H -2.88866400 0.34110800 1.20440100
H -3.85126500 0.03235500 -0.09521800
O -1.75034800 -1.32490600 -1.28284300
H -1.90844900 -2.10178200 -0.73015800
O 1.95914500 -1.74425500 0.58784700
H 1.30257300 -1.96776300 1.25664000
N 0.30349100 2.52550800 -0.48241500
H -0.26378700 2.96116300 -1.20328100

TS_D
C 1.06879000 -1.05910800 0.40342500
H 1.66246200 -1.15817900 1.32426600
C -0.29934000 -0.49308900 0.77608800
H -0.81364000 -0.92701000 1.62938300
O -1.43400800 -1.26505200 -0.49600400
O 0.97900000 -2.35147700 -0.19551400
H 1.86730700 -2.72257600 -0.19681500
H -1.34252600 -2.21624900 -0.37652100
C 0.69125300 1.15079700 -0.38748400
C 1.43753200 2.43541400 -0.04166000
H 2.20940000 2.65824200 -0.78478900
H 0.74096500 3.27709000 -0.00954300
H 1.90707500 2.33817900 0.94235500
N -0.32358700 0.82274500 0.61760800
H -1.94145800 1.11614700 0.27232200
H 0.20937600 1.28616300 -1.37013400
N 1.60756200 -0.02246000 -0.46724600
H 2.53907200 0.24275500 -0.17179700
H -3.20331800 1.27887400 -0.92018600
H -2.60869000 -0.24349800 -0.32464400
N -2.90505000 0.76856900 -0.09367100
H -3.62784900 0.81623800 0.61920400

TS_E
C 0.41500700 0.75866200 -0.73637300
H 0.93255200 1.06004800 -1.64346800
C -0.58290600 1.64387500 -0.06757300
H -0.54980200 2.72964700 -0.07785400
C -1.13414100 -0.44201800 0.35476800
C -2.36781200 -1.21105300 -0.11434500
H -2.11671600 -2.26318900 -0.26771600
H -3.17226000 -1.14618500 0.62250900
H -2.72001000 -0.79730300 -1.06325300
N -1.45645400 0.98357000 0.58700700
H -0.81804300 -0.84383100 1.33222100
N -0.04569200 -0.49991200 -0.62332500
O 1.82947200 1.06830700 0.38027400
H 2.38620000 1.68954100 -0.10558800
H 1.15967800 -1.35910600 -0.26536700
H 2.84431900 -1.94806000 -0.50608100
H 2.42233300 -0.54889600 0.39179500
N 2.19396100 -1.55300500 0.16752500
H 2.17237200 -2.13048700 1.00330000

1HCOOH

TS_{A1}

C 2.81053900 -0.38331400 0.18137100
H 3.26812100 0.40362500 0.78190100
H 3.11228500 -0.28380500 -0.86271300
H 3.16369200 -1.35264900 0.54952500
C 1.30652400 -0.37170700 0.29006600
H 0.91596500 -0.21820400 1.30717900
O 0.61859200 -1.02054500 -0.53982000
N 0.94685300 1.58403300 -0.13722000
H 1.30953400 1.79391800 -1.06273500
H 1.28249600 2.28629000 0.51583700
H -0.07550600 1.59142300 -0.16328800
C -2.44605400 -0.05141700 0.13635400
H -3.51436400 -0.20001200 0.35877900
O -1.97188700 1.06406100 0.00093900
O -1.81169000 -1.19217600 0.04966800
H -0.79637100 -1.08090800 -0.19698000

TS_{A2}
C 0.92119600 -0.15536400 -0.43178200
H 0.48953300 0.06988400 -1.42172900
H 0.88926800 1.72273400 1.17325900
N 0.53785200 1.62662100 0.22396500
H 0.83171500 2.42581900 -0.33212200
H -0.48707500 1.56339400 0.24108700
O 0.37666700 -0.98381400 0.33720700
C 2.43978400 0.02182200 -0.40463100
H 2.82896200 0.77842800 -1.11607000
O 3.16125700 -0.60857400 0.32519700
C -2.76701200 -0.13061600 -0.05845000
H -3.84782300 -0.29051600 -0.18519300
O -2.11230500 -1.26414100 -0.03906100
H -1.09453200 -1.12931000 0.10940300
O -2.29297200 0.98879900 0.04325600

TS_{D}
C 1.70078900 -0.97213400 0.55847700
H 2.14163100 -1.05741100 1.55814700
C 0.24860600 -0.53117600 0.70679100
H -0.39917300 -0.95805500 1.46029300
O -0.57855600 -1.37676200 -0.72984700
O 1.75597200 -2.23168300 -0.08592800
H 2.66109600 -2.55488700 -0.02411300
H -0.38047300 -2.32168700 -0.67984800
C 1.28305100 1.13989900 -0.47300700
C 1.75635300 2.56275800 -0.23880900
H 2.59803000 2.79094200 -0.89617500
H 0.95168500 3.26809700 -0.45609400
H 2.06695100 2.69309300 0.80124700
N 0.17733000 0.75970300 0.43389700
H -0.76904000 1.17590800 0.36915700
H 0.92916200 1.02841200 -1.50434100
N 2.30984000 0.12792800 -0.18379100
H 3.06289000 0.53970000 0.35358500
C -3.28263900 0.33060400 0.06701500
H -4.37798300 0.50420100 0.14121800
O -2.53768600 1.31177600 0.25429400
O -2.95653400 -0.86717600 -0.19879900
H -1.59750100 -1.19066900 -0.51437100

TS_{E}
C -0.39619800 -0.86133400 0.76430200
H 0.15812900 -1.13957000 1.65048100
C -1.69752600 -1.46625700 0.35341800
H -1.99902400 -2.47982000 0.59049700
O 0.73197800 -1.67385900 -0.42326300
H 0.94451200 -2.56040300 -0.09897400
C -1.66072900 0.58362200 -0.48371800
C -2.51784200 1.78786800 -0.11236800
H -1.93002700 2.70395400 -0.19650400
H -3.37316300 1.85646200 -0.78615100
H -2.87547700 1.68861600 0.91452200
N -2.39370100 -0.67520400 -0.36303600
H -1.32516300 0.66601400 -1.52561600
N -0.50980700 0.42008900 0.41271000
H 0.32535800 1.02510300 0.40872400
C 2.93100000 0.76243100 -0.03773100
H 3.96404600 1.15804100 -0.09359000
O 2.02825600 1.52896900 0.32591500
O 2.83710500 -0.46898400 -0.36904100
H 1.70441400 -1.05958500 -0.38340300

TS_{F}

C 2.36670600 -0.52008200 -0.55327000
H 3.29268500 -0.79689600 -1.03736000
C 1.58590800 -1.35733500 0.31522400
H 1.72943600 -2.38882600 0.60003800
C 0.58474500 0.61736100 -0.00003300
C 0.23389500 1.84149200 0.83999000
H -0.73804000 1.68606300 1.30893300
N 0.55445200 -0.64632500 0.68177400
H -0.37803400 0.48738400 -0.72736800
N 1.78756200 0.64069800 -0.71796900
H 0.18106200 2.71345100 0.18855400
H 0.98779200 2.01068300 1.61090400
C -2.48374400 -0.33284500 -0.35432500
H -3.53751400 -0.51125200 -0.65819800
O -2.13358600 -0.72870300 0.77653200
H -0.34630600 -0.95069400 1.09116800
O -1.78019500 0.26594400 -1.22763400

1 CH_3COOH

TS_{A1}
C 3.29026600 -0.43892800 0.26691100
H 3.74352000 0.32528900 0.89978200
H 3.64560200 -0.33520800 -0.75994100
H 3.59491300 -1.42358900 0.63707800
C 1.78158100 -0.38022700 0.30125800
H 1.35208500 -0.24063600 1.30578800
O 1.11817400 -1.00962900 -0.56610700
N 1.49349100 1.55329300 -0.11558400
H 1.90371300 1.75832400 -1.02220300
H 1.81732100 2.24131200 0.55847600
H 0.47231700 1.58225800 -0.18735300
C -1.96540500 0.03988900 -0.00289600
O -1.41338100 1.12672100 -0.12073600
O -1.34959500 -1.12325700 -0.07111200
H -0.33330300 -1.03021900 -0.27845400
C -3.44941300 -0.09760300 0.23950800
H -3.90346500 -0.64991600 -0.58662200
H -3.62073100 -0.67427100 1.15110800
H -3.91015400 0.88414600 0.32638800

TS_D
C 2.16854200 -0.88421400 0.57056300
H 2.60366100 -0.93347800 1.57552000
C 0.69104000 -0.53944900 0.70193700
H 0.05623300 -1.01578400 1.43621600
O -0.06985400 -1.44556100 -0.76551800
O 2.31639700 -2.14141900 -0.06358400
H 3.23442700 -2.41481600 0.03638100
H 0.17666600 -2.37763800 -0.70121700
C 1.62186400 1.19647300 -0.46698500
C 1.99994700 2.64507500 -0.21602400
H 2.83507200 2.93102300 -0.85909500
H 1.15571500 3.30013400 -0.44058100
H 2.28684900 2.78671600 0.82932600
N 0.53086000 0.73870200 0.42141800
H -0.44692300 1.08298100 0.33592400
H 1.28675800 1.07166800 -1.50312400
N 2.70887900 0.25064900 -0.17290900
H 3.43505800 0.70964500 0.36283400
C -2.88170900 0.10941100 0.02148500
O -2.17652300 1.13270100 0.17047100
O -2.45650400 -1.07272200 -0.20321500
H -1.09973100 -1.31102400 -0.54048700
C -4.39852900 0.24941700 0.10316000
H -4.79983900 -0.48580700 0.80442000
H -4.68537300 1.25421400 0.41149000
H -4.83179500 0.03243700 -0.87720500

TS_E
C -0.96785800 -0.87549500 0.77946800
H -0.46368300 -1.24446000 1.66163400
C -2.32649700 -1.29244200 0.33013500
H -2.77292400 -2.25474000 0.55113900
O 0.07416700 -1.84728700 -0.41840200
H 0.18223800 -2.74733700 -0.08101100
C -1.97928700 0.73482400 -0.48782900
C -2.66521800 2.04696500 -0.12595000
H -1.95081800 2.86999600 -0.18803000
H -3.48521500 2.24006800 -0.81906400
H -3.05852800 1.99416600 0.89129000
N -2.88590100 -0.40758100 -0.39742800

H -1.60763900 0.77510200 -1.51985900 N -0.88404000 0.40516000 0.43225200 H 0.03823200 0.87643500 0.44428500 C 2.57437200 0.29930600 0.00270800 O 1.75084200 1.14715400 0.39325100 O 2.30614800 -0.90328600 -0.36204600 H 1.11421200 -1.34645000 -0.37423400 C 4.04858700 0.66479000 -0.06983700 H 4.62703500 -0.02687300 0.54733000 H 4.39992400 0.55340500 -1.09862300 H 4.21288400 1.68730600 0.26678900
TS_F C 2.70328400 -0.72034700 -0.64538100 H 3.56371800 -1.11312300 -1.16894000 C 1.90586300 -1.42927100 0.31932400 H 1.96840000 -2.45511500 0.65056400 C 1.08062800 0.61382000 -0.04705600 C 0.91140800 1.90992400 0.73990200 H -0.03334400 1.87792400 1.28325700 N 0.97685300 -0.60196900 0.71202500 H 0.05832000 0.53166400 -0.68635300 N 2.22799300 0.48091000 -0.84305700 H 0.89351300 2.74722200 0.04261500 H 1.73270100 2.04490900 1.44608900 C -2.09128200 -0.12020900 -0.08348600 O -1.63965800 -0.51233700 1.02239700 H 0.04905200 -0.78939500 1.16057100 O -1.40902800 0.38845600 -1.03338900 C -3.58370900 -0.26679600 -0.35251700 H -3.73390000 -1.06742300 -1.08252700 H -4.12065600 -0.51360700 0.56298700 H -3.97939500 0.65268200 -0.78781000