

Divergent Mechanisms of Suicide Inactivation for Ethanolamine Ammonia-Lyase

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SUPPORTING INFORMATION

(Tables S1–S2 and relevant full references, Total 17 pages including this page)

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**TABLE S1: GAUSSIAN Archive Entries for the MPW1K/6-31+G(d,p)
Optimized Geometries**

1a

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1\1\GINC-LC22\FOpt\RmPWPW91\6-31+G(d,p)\C2H8N1O1(1+)\GMS501\20-Apr-200
4\0\0\#P MPWPW91/6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=32768000
GFINPUT IOP(3/76=0572004280)\2-aminoethanol mpw1k/6-31+G**\1,1\C,-0.
5956595632,0.7373357154,-0.2591283382\N,-1.3284925057,-0.5147399917,0.
1029796572\H,-0.7067224727,-1.2976508923,-0.1233386305\H,-1.5336174271
,-0.5643099228,1.0972762929\H,-1.1168629107,1.589396439,0.1636807607\H
,-0.6087678989,0.7984021831,-1.3427092179\C,0.8210655823,0.5953228547,
0.250545247\O,1.2109153821,-0.6900463122,-0.1531386007\H,0.8619169791,
0.7021141259,1.3368231871\H,2.1343668466,-0.8615450193,0.0240247187\H,
-2.2022025978,-0.6173868699,-0.4039969944\H,1.4315778499,1.3785789755,
-0.196010364\Version=x86-Linux-G03RevB.05\State=1-A\HF=-210.7158829\R
MSD=9.122e-09\RMSF=3.476e-06\Dipole=-1.3470027,-0.1341836,0.3933369\PG
=C01 [X(C2H8N1O1)]\@
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TS:1a→3a

```
1\1\ GINC-RADOM-BAROSSA082\FTS\UmPWPW91\6-31+G(d,p)\C4H13N1O2(1+,2)\SA
NDALG\27-Nov-2004\0\0\#MPWPW91/6-31+G(D,P) OPT=(TS,NOEIGEN,CALCFC) IOP(
3/76=0572004280)\Ado=ethanol H abstraction allgem aminoeth mpw1k/6-31
+G**\1,2\C,1.8545060794,-0.6522215344,-0.4478942134\N,3.2743705049,-0
.2542067346,-0.141812939\H,3.2763243012,0.7600340704,-0.0066838674\H,3
.6089189409,-0.6775187813,0.7192351148\H,1.7743990929,-1.7320101329,-0
.3885537681\H,1.6705145971,-0.3259747052,-1.4682122418\C,0.9481207849,
0.0556209262,0.508464774\O,1.3700933456,1.3757676893,0.5358043014\H,0.
8738234633,-0.4040917508,1.4938494628\H,0.8046838569,1.9270205161,1.07
478933358\H,3.9215554925,-0.4952948288,-0.8867645712\H,-0.2695143342,-0
.0220957073,-0.0316109288\C,-2.5289782098,-0.2864653038,0.3763984219\C
,-1.4782491107,0.0067263489,-0.6533597574\H,-2.4941226833,0.4601947513
,1.1751983423\H,-2.3527173008,-1.2676423056,0.8261689802\H,-1.39047164
31,-0.7519852227,-1.4253753588\H,-1.5154712675,1.0109379256,-1.0640132
121\O,-3.7610495599,-0.2518489046,-0.291425499\H,-4.4732635978,-0.4354
395858,0.3179775147\Version=x86-Linux-G03RevB.02\State=2-A\HF=-365.03
00449\S2=0.762441\S2-1=0.\S2A=0.750067\RMSD=6.122e-09\RMSF=5.712e-06\D
ipole=4.3549463,-0.6324153,0.7300891\PG=C01 [X(C4H13N1O2)]\@
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3a

```
1\1\GINC-LC72\FOpt\UmPWPW91\6-31+G(d,p)\C2H7N1O1(1+,2)\GMS501\20-Apr-2
004\0\0\#P MPWPW91/6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=3276800
0 GFINPUT IOP(3/76=0572004280)\2-aminoethanol radical mpw1k/6-31+G**\
1,2\C,0.5401231432,0.7406412499,0.2756496223\N,1.3739126003,-0.473634
8392,-0.0466494339\H,0.8534241923,-1.3076104334,0.2255218279\H,1.54967
12458,-0.5408652502,-1.0464208809\H,1.0388763787,1.6166294945,-0.12393
38912\H,0.5219860615,0.8005696319,1.3657407549\C,-0.7950241568,0.53884
21217,-0.3143738608\O,-1.3326924628,-0.6341778643,0.0676232776\H,-1.42
13640365,1.363276895,-0.6120744867\H,-2.2354586409,-0.7456291497,-0.23
07592423\H,2.2664223809,-0.4744046285,0.4398311654\Version=x86-Linux-
G03RevB.05\State=2-A\HF=-210.054179\S2=0.755084\S2-1=0.\S2A=0.750019\R
MSD=6.419e-09\RMSF=1.293e-06\Dipole=1.3502851,-0.2130494,-0.2272736\PG
=C01 [X(C2H7N1O1)]\@
```

4a

```
1\1\GINC-LC28\FOpt\UmPWPW91\6-31+G(d,p)\C2H7N1O1(1+,2)\GMS501\20-Apr-2
004\0\#P MPWPW91/6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=3276800
0 GFINPUT IOP(3/76=0572004280)\gem substituted aminoethanol radical m
pw1k/6-31+G**\1,2\C,-1.1738089072,-0.8990066625,-0.0988675041\H,-1.55
80440638,-1.6853703633,0.5299738522\H,-1.6011547045,-0.730182862,-1.07
58562717\C,-0.1082616672,0.0017511827,0.386593644\O,-0.186198156,1.299
941038,-0.0705876371\H,0.0133545421,-0.0595765077,1.4693502864\N,1.237
7895884,-0.4036913015,-0.1865772203\H,1.2019180389,-0.3370086129,-1.20
25652714\H,1.4994515268,-1.3512772497,0.0710476166\H,-0.9932670644,1.7
289794492,0.2162266515\H,1.9552233003,0.2442798318,0.1362079356\Ver
sion=x86-Linux-G03RevB.05\State=2-A\HF=-210.0413447\S2=0.755173\S2-1=0.\
S2A=0.750015\RMSD=7.349e-09\RMSF=2.055e-06\Dipole=1.0311337,-0.8529534
,0.1330682\PG=C01 [X(C2H7N1O1)]\@
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TS:4a→5a

```
1\1\ GINC-RADOM-BAROSSA135\FTS\UmPWPW91\6-31+G(d,p)\C4H13N1O2(1+,2)\SA
NDALG\26-Nov-2004\0\#MPWPW91/6-31+G(D,P) OPT=(TS,NOEIGEN,CALCFC) IOP(
3/76=0572004280)\H abstraction allgem aminoeth mpw1k/6-31+G**\1,2\C,
0.7555398078,-0.8522311554,-0.2317113386\C,1.8215283707,0.0436026132,0
.2793726892\O,1.9193200462,1.2007890762,-0.4445644652\H,0.7397633314,-
0.950091801,-1.3116041982\H,-0.4082541782,-0.1859603169,0.0347355259\H
,1.744984287,0.2069191559,1.3538865651\N,3.2006064038,-0.6356611746,0.
090593657\H,3.3627549745,-0.7455117651,-0.9082646011\H,3.2427963507,-1
.5531258882,0.5253627782\H,1.9259957784,1.9832820796,0.1045807532\H,3.
9536370227,-0.0601020571,0.4609542458\H,0.6385924879,-1.7888248825,0.3
01570727\C,-2.660270157,-0.3947758203,-0.164167212\C,-1.51776479,0.464
0484528,0.2953749975\H,-2.6330160677,-1.3620483405,0.3448142325\H,-2.5
842094001,-0.5752172156,-1.2393604565\H,-1.405941522,1.3895104848,-0.2
604083924\H,-1.4893558062,0.6173893578,1.3703434598\O,-3.8303278503,0.
3099571878,0.1517536541\H,-4.5981290409,-0.1764252428,-0.1414945663\Ver
sion=x86-Linux-G03RevB.02\State=2-A\HF=-365.0270744\S2=0.762197\S2-1
=0.\S2A=0.750067\RMSD=6.801e-09\RMSF=5.117e-06\Dipole=4.4484066,-1.250
8399,0.4729411\PG=C01 [X(C4H13N1O2)]\@
```

5a

```
1\1\GINC-LC6\FOpt\RmPWPW91\6-31+G(d,p)\C2H8N1O1(1+)\GMS501\20-Apr-2004
\0\#P MPWPW91/6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=32768000 G
FINPUT IOP(3/76=0572004280)\gem substituted aminoethanol mpw1k/6-31+G
**\1,1\C,-1.2999820965,-0.6260152187,-0.0816950521\C,-0.0717720985,0.
1085335606,0.3744404685\O,0.0448330043,1.3266021557,-0.2332267085\H,-1
.3397037626,-0.6700242644,-1.1680893796\H,-2.1718492362,-0.0747803778,
0.257162342\H,0.0017645859,0.1551961441,1.4597980896\N,1.1616330207,-0
.6798562555,-0.0775475262\H,1.1782679972,-0.6959737622,-1.0958419346\H
,1.1602971264,-1.6391783952,0.2595611\H,0.2459375022,2.0344882008,0.37
76282644\H,2.0191973637,-0.2281948173,0.2298807157\H,-1.3534815862,-1.
6304662363,0.3320746557\Version=x86-Linux-G03RevB.05\State=1-A\HF=-21
0.7157796\RMSD=4.705e-09\RMSF=9.584e-07\Dipole=1.4958977,-0.9028305,0.
5963773\PG=C01 [X(C2H8N1O1)]\@
```

2a

```
1\1\GINC-LC118\FOpt\RmPWPW91\6-31+G(d,p)\C2H4O1\GMS501\02-Mar-2004\0\
#P MPWPW91/6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=32768000 IOP(3
/76=0572004280)\ethanaldehyde iop=1 MPW1K/6-31+G(d,p)//opt\0,1\C,0.9
246700951,-0.7138747453,0.\C,0.0023866972,0.4592052866,0.\O,-1.1954287
198,0.3823437254,0.\H,0.4907996257,1.4492193882,0.\H,1.5730160079,-0.6
685315027,0.8750890374\H,1.5730160079,-0.6685315027,-0.8750890374\H,0.
364257363,-1.6428894332,0.\Version=x86-Linux-G03RevB.03\State=1-A'\HF
=-153.7884354\RMSD=1.552e-09\RMSF=1.353e-06\Dipole=1.199514,-0.1148504
,0.\PG=CS [SG(C2H2O1),X(H2)]\@
```

Ammonium cation

```
1\1\GINC-SC6\FOpt\RmPWPW91\6-31+G(d,p)\H4N1(1+)\GMS501\15-Apr-2004\0\
#P MPWPW91/6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=13107200 GFINP
UT IOP(3/76=0572004280)\ammonium ion mpw1k/6-31+G**\1,1\N,0.,0.,0.\H
,0.5877407838,0.5877407838,0.5877407838\H,-0.5877407838,-0.5877407838,
0.5877407838\H,0.5877407838,-0.5877407838,-0.5877407838\H,-0.587740783
8,0.5877407838,-0.5877407838\Version=DEC-AXP-OSF/1-G03RevB.05\State=1
-A1\HF=-56.890131\RMSD=2.239e-09\RMSF=3.145e-08\Dipole=0.,0.,0.\PG=TD
[O(N1),4C3(H1)]\@
```

Ammonium radical cation

```
1\1\GINC-SC6\FOpt\UmPWPW91\6-31+G(d,p)\H3N1(1+,2+)\GMS501\15-Apr-2004\0
\#P MPWPW91/6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=19660800 GFI
NPUT IOP(3/76=0572004280)\ammonia radical cation mpw1k/6-31+G**\1,2\
N,0.,0.,0.\H,0.,0.,1.0186946639\H,0.8822154576,0.,-0.509347332\H,-0.88
22154576,0.,-0.509347332\Version=DEC-AXP-OSF/1-G03RevB.05\State=2-A2"
\HF=-56.1801316\S2=0.75466\S2-1=0.\S2A=0.750012\RMSD=3.599e-09\RMSF=1.
835e-08\Dipole=0.,0.,0.\PG=D03H [O(N1),3C2(H1)]\@
```

NH₃···1a···NH₃

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1\1\GINC-LC80\Freq\RmPWPW91\6-31+G(d,p)\C2H14N3O1(1+)\GMS501\02-Nov-20
04\0\#MPWPW91/6-31+G(D,P) FREQ=NORAMAN IOP(3/76=0572004280)\two nh3
aminoethanol mpw1k/6-31+G**\1,1\C,-0.6812160909,1.0584261091,-0.25909
12182\C,0.8156079091,1.0477241091,-0.0253632182\O,1.1827469091,-0.2943
578909,-0.0348922182\H,-1.1389380909,2.0195751091,-0.0484872182\H,-0.9
042980909,0.7698261091,-1.2819122182\H,2.1686849091,-0.4156488909,-0.0
369522182\N,-1.2810040909,0.0204891091,0.6139627818\H,-2.2569250909,-0
.2710788909,0.3051507818\H,-0.6375010909,-0.7752688909,0.5688307818\N,
-3.8210750909,-0.7529108909,-0.2323442182\H,-4.2851500909,-1.344812890
9,0.4425597818\H,-4.4421250909,0.0254871091,-0.4035732182\H,-3.7803540
909,-1.2810278909,-1.0929072182\H,-1.3156980909,0.3227461091,1.5808907
818\N,3.8592659091,-0.7082388909,-0.0788952182\H,4.2478579091,-0.55799
68909,-0.9980572182\H,4.0170019091,-1.6787228909,0.1495767818\H,4.4086
459091,-0.1622778909,0.5678537818\H,1.2964209091,1.6250311091,-0.81636
82182\H,1.0537449091,1.5267561091,0.9301957818\Version=IA32L-G03RevC.
02\State=1-A'\HF=-323.8715064\RMSD=5.438e-09\RMSF=1.574e-06\Dipole=-1.3
010462,-0.0439587,0.3872627\PG=C01[X(C2H14N3O1)]\@
```

TS:NH₃...1a...NH₃→NH₃...3a...NH₃

1\1\GINC-SC36\FTS\UmpPWPW91\6-31+G(d,p)\C4H19N3O2(1+,2)\GMS501\18-Nov-2004\0\#\MPWPW91\6-31+G(D,P) OPT=(TS,NOEIGEN,CALCFC,TIGHT) IOP(3/76=0572004280)\TS1 Ado=ethanol twp NH3 and 2-aminoethanol substrate mpwlk/6-31+G**\1,2\C,-1.5507722931,0.0998545714,0.3656296536\C,-0.1173891968,-0.292373296,0.5881434284\O,0.0887737294,-1.4724782181,-0.0798677706\H,-1.8862864434,0.8811854557,1.0393663968\H,-1.6958777185,0.4270119454,-0.6611197763\H,1.0266039047,-1.8011575925,-0.0040722025\N,-2.4096696592,-1.1053241827,0.5397465605\H,-3.367299801,-1.0034345672,0.0870876903\H,-1.8922405287,-1.8738054808,0.1066035547\N,-4.8980362498,-0.8230390758,-0.6894498972\H,-5.5449116766,-1.5532021335,-0.4257768964\H,-5.3532425929,0.0528770844,-0.4739527858\H,-4.8181474899,-0.8637446414,-1.6959838568\H,-2.526056369,-1.3385872408,1.5191219409\N,2.6097325731,-2.4232830215,0.0224579867\H,3.2815628731,-1.7784553029,-0.3668625181\H,2.629607796,-3.2494768467,-0.5573554832\H,2.9516715988,-2.695215925,0.9320077089\H,0.5892976276,0.6721385776,0.0507599097\H,0.1785624973,-0.3152566936,1.6398164752\C,2.3425888299,2.1747523184,0.3260206604\C,1.3429005316,1.6139456398,-0.6369206871\H,2.9118437267,1.3644572255,0.7929263943\H,1.8311609596,2.7212920537,1.1230820236\O,3.1951968026,3.0256230853,-0.3984178472\H,0.6167799398,2.332520627,-1.0036248533\H,1.7725562728,1.0190901932,-1.4363903227\H,3.8044972909,3.461052883,0.194130661\Version=Al64T-G03RevC.02\State=2-A\HF=-478.1850053\S2=0.762584\S2-1=0.\S2A=0.750069\RMSD=9.842e-09\RMSF=8.592e-07\Dipole=-3.1815202,-2.0310245,1.1020132\PG=C01 [X(C4H19N3O2)]\@

NH₃...4a...NH₃

1\1\GINC-LC101\Freq\UmpPWPW91\6-31+G(d,p)\C2H13N3O1(1+,2)\GMS501\02-Nov-2004\0\#\MPWPW91\6-31+G(D,P) FREQ=NORAMAN IOP(3/76=0572004280)\two nh3 gemaminoethanol radical mpwlk/6-31+G**\1,2\C,-0.025989963,1.3780201111,-0.5134861481\C,0.088351037,0.0210351111,0.0760268519\O,1.159269037,-0.7016288889,-0.3646961481\H,-0.463928963,2.1925081111,0.0405238519\H,0.380759037,1.5540921111,-1.4973301481\H,0.022210037,0.0686781111,1.1672558519\H,2.035425037,-0.3514288889,-0.0232981481\N,-1.084365963,-0.8230118889,-0.3470441481\H,-2.031301963,-0.4422028889,-0.0335231481\H,-1.067764963,-0.9025288889,-1.3595271481\N,-3.579821963,0.1212741111,0.4558108519\H,-4.308027963,-0.5464468889,0.2424738519\H,-3.836018963,0.9796591111,-0.0119231481\H,-3.645782963,0.3051491111,1.4472568519\H,-0.948320963,-1.7603948889,0.0207058519\N,3.577939037,0.0822831111,0.4539588519\H,4.208266037,-0.2902168889,-0.2417531481\H,3.847058037,-0.3245518889,1.3376578519\H,3.762852037,1.0725671111,0.5147268519\Version=IA32L-G03RevC.02\State=2-A\HF=-323.200977\S2=0.755317\S2-1=0.\S2A=0.750016\RMSD=4.961e-09\RMSF=9.400e-07\Dipole=-1.2856917,0.028458,0.4739618\PG=C01 [X(C2H13N3O1)]\@

TS:NH₃...4a...NH₃→NH₃...5a...NH₃

1\1\GINC-SC7\FTS\UmpWPW91\6-31+G(d,p)\C4H19N3O2(1+,2)\GMS501\18-Nov-2004\0\0\#MPWPW91/6-31+G(D,P) OPT=(TS,NOEIGEN,CALCFC,TIGHT) IOP(3/76=0572004280)\TS2 Ado=ethanol twp NH3 and gemaminoethanol mpw1k/6-31+G**\1,2\C,0.5872527491,-0.7023613011,-0.5954721241\C,1.0671630532,0.6555759512,-0.1964528159\O,0.441950905,1.6709745193,-0.8551131323\H,1.0424903426,0.775228868,0.8898364986\H,-0.1986866825,2.1754366762,-0.2781486308\N,2.5286899453,0.8021089858,-0.5697341622\H,3.1699228877,0.0905025228,-0.109462435\H,2.6008881647,0.7166640505,-1.5790556781\N,4.2744543818,-1.0379337434,0.6305465671\H,5.2261967113,-0.6982326783,0.6182649932\H,4.2846683176,-1.9265213853,0.1495446129\H,4.0576041707,-1.2388099016,1.5966843293\H,2.8349168982,1.7414468815,-0.3358020033\N,-1.3313928887,3.1078131589,0.5504958689\H,-1.7865571108,3.6579320116,-0.1641320363\H,-0.9632448729,3.7600642941,1.2268829032\H,-2.055947288,2.5786052122,1.0131099526\H,1.0596445799,-1.5356807741,-0.0860068582\H,-0.6964661475,-0.7443244402,-0.1748275564\H,0.5004742574,-0.8369603456,-1.668705777\C,-2.537361597,-2.0877893026,0.0132349242\C,-1.951004751,-0.7278088068,0.2455129681\H,-1.9561509508,-2.8447332042,0.5467227356\H,-2.5092830306,-2.3295664103,-1.0520669734\O,-3.8594001572,-2.0440782018,0.4869792934\H,-2.4029251014,0.0550405934,-0.3547981604\H,-1.8754077026,-0.4593666263,1.2954258995\H,-4.2911002201,-2.881513937,0.331509265\Vers ion=Al64T-G03RevC.02\State=2-A\HF=-478.1841503\S2=0.762606\S2-1=0.\S2A=0.750072\RMSD=4.039e-09\RMSF=6.061e-07\Dipole=3.6584495,0.5980865,0.4321584\PG=C01 [X(C4H19N3O2)]\@

6

1\1\GINC-LC140\FOpt\RmpWPW91\6-31+G(d,p)\C2H6O3\GMS501\02-Mar-2004\0\0\#P MPWPW91/6-31+G(D,P) OPT=TIGHT MAXDISK=39321600 IOP(3/76=0572004280)\conformer #4 triolethane MPW1K/6-31+G(d,p)//iop=1 opt\0,1\O,-1.5649348298,0.0271747225,-0.5546018268\C,-0.9068095909,-0.0635628795,0.6821205887\C,0.5877030238,0.0310173185,0.4676492022\H,-1.2430172483,0.7767449252,1.2825238374\H,-1.1485448573,-0.9909635429,1.2024987492\O,0.9264121776,1.1852197099,-0.218296093\O,0.9392036818,-1.1152140655,-0.2589521432\H,1.1248325431,0.0662621219,1.4160644373\H,-1.3209405844,-0.7408322245,-1.0703209979\H,0.2623205926,1.3134738285,-0.8999678208\H,1.8345407199,-1.0068546781,-0.5746164466\Version=x86-Linux-G03RevB.03\State=1-A\HF=-305.4091103\RMSD=4.274e-09\RMSF=3.550e-06\Dipole=0.2488835,-0.3882108,0.1343673\PG=C01 [X(C2H6O3)]\@

TS:6→7

1\1\GINC-RADOM-BAROSSA102\FTS\UmpWPW91\6-31+G(d,p)\C4H11O4(2)\SANDALG\29-Nov-2004\0\0\# MPWPW91/6-31+G(D,P) OPT=(TIGHT,TS,NOEIGEN,CALCFC) IOP(3/76=0572004280)\trioleth Ado=ethanol H abstract mpw1k/6-31+G**\0,2\O,-0.875535276,1.3857648452,-0.6698656755\C,-0.7549665849,0.0096647712,-0.6765900265\C,-1.8204010219,-0.6533857782,0.1532284228\H,-0.7374428127,-0.3468036251,-1.7011885399\H,0.4039754544,-0.3376540035,-0.1675993732\O,-3.0939942341,-0.4820040378,-0.3808869766\O,-1.7263359627,-0.0681757214,1.4223899169\H,-1.6632215597,-1.7303563174,0.2051867588\H,-0.9491618467,1.6614138376,0.245804549\H,-3.179456648,0.4318395011,-0.6568609767\H,-2.4779337175,-0.3482191262,1.9416443968\C,2.609491162,0.2594034795,-0.379442534\C,1.6518579558,-0.62014939,0.3557241615\H,2.5627081651,0.0473143418,-1.4512667957\O,3.9133645646,0.017590345,0.1113536704\H,2.3358695575,1.3077795354,-0.2372989718\H,1.5380425147,-0.3912272596,1.409720016\H,1.7806977458,-1.6818210944,0.1707090088\H,4.5300413472,0.5891322665,-0.340297696\Version=x86-Linux-G03RevB.02\State=2-A\HF=-459.721694\S2=0.762778\S2-1=0.\S2A=0.750071\RMSD=5.080e-09\RMSF=1.520e-06\Dipole=-0.3493312,0.2733422,-0.0622544\PG=C01 [X(C4H11O4)]\@

7

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1\1\GINC-LC140\FOpt\UmpPWPW91\6-31+G(d,p)\C2H5O3(2)\GMS501\02-Mar-2004\
0\#\#P MPWPW91/6-31+G(D,P) OPT=TIGHT MAXDISK=26214400 IOP(3/76=05720042
80)\trioleth_radical iop=1 MPW1K/6-31+G(d,p)/opt/\0,2\O,1.8925801087
,-0.079076114,-0.0570572365\C,0.732880019,-0.7551369253,-0.026925785\C
,-0.5031157197,-0.0179416648,0.357837059\H,0.830491199,-1.8014260345,0
.2126279011\O,-1.6457572458,-0.6340308167,-0.1267986053\O,-0.334740909
3,1.2831734716,-0.1386949282\H,-0.6496501075,0.0213391983,1.442398582\
H,1.6845869674,0.8481555118,-0.199283086\H,-1.505860347,-0.8316272672,
-1.053558475\H,-1.0348091359,1.8414978048,0.1927535934\Version=x86-Li
nux-G03RevB.03\State=2-A\HF=-304.7473918\S2=0.75491\S2-1=0.\S2A=0.7500
17\RMSD=9.067e-09\RMSF=3.045e-06\Dipole=-0.3826998,0.4322094,0.1264291
\PG=C01 [X(C2H5O3)]\@
```

8

```
1\1\GINC-LC54\FOpt\UmpPWPW91\6-31+G(d,p)\C2H3O2(2)\GMS501\02-Mar-2004\0
\#\#P MPWPW91/6-31+G(D,P) OPT=(MAXCYCLE=100,TIGHT) MAXDISK=26214400 IOP
(3/76=0572004280)\glycolrad iop=1 MPW1K/6-31+G(d,p)// opt/\0,2\H,1.35
17034796,-0.3670811153,0.\O,1.2927328858,0.6005095921,0.\C,0.009188400
6,0.889670784,0.\C,-0.9177774955,-0.1761607767,0.\O,-0.5023328009,-1.3
389987407,0.\H,-0.2381366432,1.9376305652,0.\H,-1.9852329461,0.0563036
949,0.\Version=x86-Linux-G03RevB.03\State=2-A\HF=-228.3448224\S2=0.7
70241\S2-1=0.\S2A=0.750119\RMSD=5.164e-09\RMSF=5.469e-06\Dipole=-0.262
2625,0.8707635,0.\PG=CS [SG(C2H3O2)]\@
```

TS:8→9

```
1\1\GINC-RADOM-BAROSSA126\FTS\UmpPWPW91\6-31+G(d,p)\C4H9O3(2)\SANDALG\
29-Nov-2004\0\#\# MPWPW91/6-31+G(D,P) OPT=(TIGHT,TS,NOEIGEN,CALCFC) IOP
(3/76=0572004280)\glycolrad Ado=ethanol H abstract mpw1k/6-31+G**\0,
2\H,1.3754372972,0.8724342936,-1.5863584808\O,1.1466204321,-0.04376099
78,-1.3974996018\C,-0.2191772696,-0.1081869293,-1.3513527809\H,-0.6020
523903,-1.0374152123,-1.7685094322\H,-0.5855141905,-0.1768994621,-0.15
47347749\C,-0.8829052475,1.1020285115,-1.859208721\O,-0.2525253667,2.1
055239791,-2.1008638063\H,-1.9764963002,1.0728911361,-1.9559164465\C,0
.4559405687,-1.0564291877,1.7555913243\C,-0.7845831068,-0.3608463357,1
.3052636719\H,1.3288221815,-0.4415828381,1.5296802552\H,0.5688382969,-
2.0025984574,1.2205153391\O,0.3465195179,-1.2840726882,3.1464381698\H,
-1.6969533025,-0.9455084922,1.3299097713\H,-0.9052997033,0.6638286774,
1.636835039\H,1.1526517766,-1.6860683428,3.4622196709\Version=x86-Lin
ux-G03RevB.02\State=2-A\HF=-383.2987937\S2=0.765404\S2-1=0.\S2A=0.7501
37\RMSD=5.221e-09\RMSF=1.137e-06\Dipole=-0.2413616,-0.71575,-0.0025525
\PG=C01 [X(C4H9O3)]\@
```

9

```
1\1\GINC-LC54\FOpt\RmPWPW91\6-31+G(d,p)\C2H4O2\GMS501\02-Mar-2004\0\#\#
P MPWPW91/6-31+G(D,P) OPT=TIGHT MAXDISK=32768000 IOP(3/76=0572004280)\
\Glycolaldehyde iop=1 MPW1K/6-31+G(d,p)// opt/\0,1\H,1.3535158324,-0.4
142317368,0.\O,1.3303866561,0.5467586502,0.\C,0.0006193041,0.926142632
8,0.\H,-0.2362810259,1.5374495658,0.8776076985\H,-0.2362810259,1.53744
95658,-0.8776076985\C,-0.9202256253,-0.2526791417,0.\O,-0.5008363799,-
1.3790970169,0.\H,-1.9997180634,-0.0427414082,0.\Version=x86-Linux-G0
3RevB.03\State=1-A\HF=-228.9772435\RMSD=2.464e-09\RMSF=3.337e-06\Dipo
le=-0.8732797,0.6177588,0.\PG=CS [SG(C2H2O2),X(H2)]\@
```

10

```
1\1\GINC-LC54\FOpt\UmpPWPW91\6-31+G(d,p)\C2H3O2(2)\GMS501\02-Mar-2004\0
\\#P MPWPW91/6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=26214400 GF
INPUT IOP(3/76=0572004280)\Semidione ethane c2v MPW1K/6-31+G(d,p)// io
p=1\\0,2\H,0.,0.,1.0237672834\O,0.,1.1480866315,0.5795396785\O,0.,-1.1
480866315,0.5795396785\C,0.,0.7083308496,-0.6134019275\C,0.,-0.7083308
496,-0.6134019275\H,0.,1.3678952885,-1.4677895048\H,0.,-1.3678952885,-
1.4677895048\\Version=x86-Linux-G03RevB.03\State=2-B1\HF=-228.3275025\
S2=0.756604\S2-1=0.\S2A=0.750025\RMSE=5.308e-09\RMSE=2.282e-06\Dipole=
0.,0.,-1.1440872\PG=C02V [C2(H1),SGV(C2H2O2)]\\@
```

11

```
1\1\GINC-LC107\Freq\RmpPWPW91\6-31+G(d,p)\C2H9N2O1(1+)\GMS501\15-Apr-20
04\0\\#P MPWPW91/6-31+G(D,P) FREQ=NORAMAN MAXDISK=39321600 GFINPUT IOP
(3/76=0572004280)\freq HEH cation overall cis (cc) intra OH bonding C
1 symm mpw1k/6-31+G** terminal amino off center\\1,1\C,-0.0715840233,1
.0338999767,-0.1541320698\N,0.9256449767,0.0075189767,-0.5784670698\H,
-0.4329820233,1.5008259767,-1.0665390698\H,0.4231979767,1.7721599767,0
.4684789302\N,1.6800859767,-0.4732730233,0.5183299302\H,0.3372479767,-
0.7677640233,-0.9128680698\C,-1.1888710233,0.3041139767,0.5556209302\O
,-1.4920050233,-0.7669870233,-0.3032260698\H,-0.8625700233,-0.04830502
33,1.5326649302\H,-2.0292560233,0.9854579767,0.6778849302\H,-2.1809680
233,-1.3270320233,0.0503609302\H,1.4902279767,0.3474609767,-1.35559506
98\H,2.1590979767,-1.3211660233,0.2533129302\H,2.3546579767,0.22645297
67,0.7901349302\\Version=x86-Linux-G03RevB.05\State=1-A\HF=-266.017593
6\RMSE=2.236e-09\RMSE=6.834e-06\Dipole=1.2337126,0.2394021,-0.4291623\
\PG=C01 [X(C2H9N2O1)]\\@
```

TS:11→12

```
1\1\GINC-RADOM-BAROSSA012\FTS\UmpPWPW91\6-31+G(d,p)\C4H14N2O2(1+,2)\SA
NDALG\27-Nov-2004\0\\# MPWPW91/6-31+G(D,P) OPT=(TS,NOEIGEN,CALCFC) IOP
(3/76=0572004280)\TS1 HEH cation mpw1k/6-31+G** Ado=ethanol\\1,2\C,1.
3711537853,-0.6741818436,-0.5258814369\N,2.7924423182,-0.1917346605,-0
.4486006404\H,1.1081351049,-0.635647084,-1.5812778781\H,1.3327130272,-
1.7000853295,-0.1748377855\N,3.3675412875,-0.4591840067,0.8160418077\H
,2.7029348184,0.8271483524,-0.5369036874\C,0.5154145063,0.2565066184,0
.272022318\O,0.8878736258,1.5354766229,-0.1182125116\H,0.5512476538,0
.0969178415,1.3466339693\H,-0.7370896135,0.0110605117,-0.1181265686\H,0
.4238365943,2.2119780491,0.3722011551\H,3.3385900209,-0.5381321711,-1.
2366511572\H,4.2299376948,0.0564991494,0.9108250373\H,3.5550970611,-1.
4479264344,0.8913430643\C,-1.9902273649,-0.1595559742,-0.6150159748\H,
-1.9532757766,-1.1350652635,-1.0908918704\C,-2.9520820157,-0.076192497
3,0.5326182965\H,-2.076226053,0.6483114311,-1.3349518259\O,-4.23511150
37,-0.2544483172,-0.0052217255\H,-2.8661205586,0.8957931442,1.02719858
71\H,-2.7252863053,-0.8498503252,1.2715836009\H,-4.8920293519,-0.21225
5466,0.6867818678\\Version=x86-Linux-G03RevB.02\State=2-A\HF=-420.3311
381\S2=0.762467\S2-1=0.\S2A=0.750066\RMSE=8.147e-09\RMSE=6.584e-06\Dip
ole=4.1950775,-0.3977321,0.2332406\PG=C01 [X(C4H14N2O2)]\\@
```

12

1\1\GINC-LC118\Freq\UmpWPW91\6-31+G(d,p)\C2H8N2O1(1+,2)\GMS501\06-May-2004\0\#\#P MPWPW91/6-31+G(D,P) FREQ=NORAMAN MAXDISK=43253760 GFINPUT IOP(3/76=0572004280)\freq HEH C1 radical cation C1 symm mpw1k/6-31+G**\1,2\O,1.7911259286,-0.7264199286,-0.1902120714\C,1.4220339286,0.5033490714,0.2137119286\C,0.0432479286,0.8208680714,-0.1973210714\N,-0.8513610714,-0.2758659286,0.3134699286\H,-0.8114730714,-0.2908109286,1.3342129286\H,-0.4309800714,-1.1483599286,-0.0083120714\N,-2.1551740714,-0.1911899286,-0.2275730714\H,-2.6900870714,-1.0010549286,0.0502069286\H,-2.6031470714,0.6450070714,0.1173499286\H,-0.1108670714,0.8162270714,-1.2776590714\H,-0.3006130714,1.7636200714,0.2160179286\H,2.1580019286,1.2647910714,0.4100419286\H,2.7142129286,-0.9139719286,-0.0197850714\Version=x86-Linux-G03RevB.05\State=2-A\HF=-265.3555843\S2=0.755146\S2-1=0.\S2A=0.750019\RMSD=2.924e-09\RMSF=3.140e-06\Dipole=-0.6435951,-0.0038255,1.0039538\PG=C01 [X(C2H8N2O1)]\@

13

1\1\GINC-LC58\FOpt\UmpWPW91\6-31+G(d,p)\C2H8N2O1(1+,2)\GMS501\06-May-2004\0\#\#P MPWPW91/6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=43253760 GFINPUT IOP(3/76=0572004280)\C2 rad gem substituted radical cation heh mpw1k/6-31G**\1,2\C,-0.5403700206,0.0498997774,0.35453\O,-1.4542296242,-0.9124805989,-0.01892\H,-0.3316900177,0.0429698634,1.42695\N,0.7165602191,-0.5319997049,-0.28283\H,0.7210706318,-1.534099703,-0.07509\H,0.5973401826,-0.443389754,-1.29043\N,1.8765199285,0.1736007728,0.09978\H,2.1089200248,-0.0602091314,1.05378\H,2.6436600326,-0.0792689112,-0.50505\H,-2.3459097222,-0.6745409662,0.23622\C,-0.8104905804,1.4092696662,-0.14391\H,-0.4137409346,2.2692398296,0.36751\H,-1.3922606313,1.5329394266,-1.04494\Version=x86-Linux-G03RevB.05\State=2-A\HF=-265.3423659\S2=0.755158\S2-1=0.\S2A=0.750016\RMSD=6.675e-09\RMSF=3.659e-06\Dipole=-0.8825282,-0.4830702,-0.0125716\PG=C01 [X(C2H8N2O1)]\@

TS:13→14

1\1\GINC-RADOM-BAROSSA093\FTS\UmpWPW91\6-31+G(d,p)\C4H14N2O2(1+,2)\SANDALG\26-Nov-2004\0\#\#P MPWPW91/6-31+G(D,P) OPT=(TS,NOEIGEN,CALCF) IOP(3/76=0572004280)\TS1 HEH rad allgem mpw1k/6-31+G** Ado=ethanol\1,2\C,1.3523952865,0.4426831994,0.1518632162\O,1.3477743453,1.806574785,0.0119230636\H,1.2739782042,0.1689359452,1.2046138708\N,2.8111727525,0.0832582387,-0.1990515837\H,3.4007617526,0.8117168684,0.2107732687\H,2.9011773812,0.1631270394,-1.2090357587\N,3.1373824282,-1.2376108784,0.1748691939\H,3.1833374944,-1.2926294426,1.181773466\H,4.0337778636,-1.4908316735,-0.2134240943\H,0.65341261,2.10139902,-0.5763302175\C,0.3923799627,-0.3046450251,-0.6924566235\H,0.4033626679,-1.3769279025,-0.5456502811\H,0.3913416731,-0.0166852326,-1.7405624669\H,-0.8480342655,0.066639787,-0.2435801334\C,-2.0383398362,0.4248970442,0.1871512977\C,-2.9564316198,-0.7460277365,-0.0146857502\H,-1.87459599,0.6868427105,1.2283047608\H,-2.2903445054,1.2902247437,-0.4188141198\O,-4.2140289518,-0.3401746988,0.4515848699\H,-2.5892166278,-1.6125091264,0.5419850439\H,-2.9937130976,-1.0151503496,-1.0734431684\H,-4.8551173318,-1.0363536816,0.3233702487\Version=x86-Linux-G03RevB.02\State=2-A\HF=-420.3291626\S2=0.762359\S2-1=0.\S2A=0.750069\RMSD=7.285e-09\RMSF=9.120e-07\Dipole=3.9065721,-0.6252193,-0.6197384\PG=C01 [X(C4H14N2O2)]\@

14

```
1\1\GINC-LC131\FOpt\RmPWPW91\6-31+G(d,p)\C2H9N2O1(1+)\GMS501\06-May-20
04\0\0\#P MPWPW91/6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=32768000
GFINPUT IOP(3/76=0572004280)\gem substituted heh mpw1k/6-31+G**\1,1
\C,-0.5199099583,-0.0319406785,0.35386\O,-1.4230586737,-1.0163618571,0
.06314\H,-0.2863899276,-0.0554703737,1.41767\N,0.7700906698,-0.5132389
95,-0.31499\H,0.8111219899,-1.5248589415,-0.17051\H,0.6701104767,-0.36
53291255,-1.31695\N,1.9026497317,0.2055924829,0.12666\H,2.0995600588,-
0.0450772601,1.08469\H,2.6991800323,-0.0247664776,-0.44893\H,-2.144559
0865,-0.6999927986,-0.48029\C,-0.8630117609,1.3493988738,-0.11833\H,-0
.0431326588,2.0374599437,0.06407\H,-1.1021917684,1.3551385617,-1.18206
\H,-1.7308522219,1.7026377413,0.43221\Version=x86-Linux-G03RevB.05\St
ate=1-A\HF=-266.0179159\RMSD=3.695e-09\RMSF=3.805e-06\Dipole=-1.034779
4,-0.359647,0.5480124\PG=C01 [X(C2H9N2O1)]\@
```

N₂H₅⁺

```
1\1\GINC-LC41\FOpt\RmPWPW91\6-31+G(d,p)\H5N2(1+)\GMS501\13-Apr-2004\0\
\#P MPWPW91/6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=40632320 GFIN
PUT IOP(3/76=0572004280)\protonated hydrazine cation mpw1k/6-31+G** C
s symm\1,1\N,0.034189774,0.7699782034,0.\N,0.050731394,-0.6485430226,
0.\H,-0.4424607461,1.0978780639,0.8273587011\H,-0.4424607461,1.0978780
639,-0.8273587011\H,-0.8596787366,-1.1139018548,0.\H,0.5750760265,-0.9
659502694,0.8141021182\H,0.5750760265,-0.9659502694,-0.8141021182\Ver
sion=x86-Linux-G03RevB.05\State=1-A'\HF=-112.1871869\RMSD=8.344e-09\RM
SF=1.342e-06\Dipole=-0.5190288,-1.087481,0.\PG=CS [SG(H1N2),X(H4)]\@
```

N₂H₄⁺

```
1\1\GINC-SC2\FOpt\UmPWPW91\6-31+G(d,p)\H4N2(1+,2)\GMS501\11-Aug-2004\0\
\#P MPWPW91/6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=32768000 GF
INPUT IOP(3/76=0572004280)\hydrazine radical cation mpw1k/6-31+G** C2h
symm\1,2\N,-0.0623904647,0.644893043,0.\N,0.0623904647,-0.644893043,
0.\H,-0.1102679152,1.1396594071,0.8763828402\H,-0.1102679152,1.1396594
071,-0.8763828402\H,0.1102679152,-1.1396594071,0.8763828402\H,0.110267
9152,-1.1396594071,-0.8763828402\Version=DEC-AXP-OSF/1-G03RevB.05\Sta
te=2-AG\HF=-111.5547992\S2=0.756267\S2-1=0.\S2A=0.750025\RMSD=6.419e-0
9\RMSF=3.553e-08\Dipole=0.,0.,0.\PG=C02H [SGH(N2),X(H4)]\@
```

15

```
1\1\GINC-SC160\FOpt\RmPWPW91\6-31+G(d,p)\C2H4O1\GMS501\16-Apr-2004\0\
\#P MPWPW91/6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=13107200 GFIN
PUT IOP(3/76=0572004280)\enol of acetaldehyde OH in Cs symm mpw1k/6-31
+G**\0,1\C,-1.1352337766,-0.4203024667,0.\C,0.1906927382,-0.394720369
6,0.\O,0.9778290708,0.6975712383,0.\H,0.4414116739,1.4886629129,0.\H,0
.7866986948,-1.2946745508,0.\H,-1.7320871396,0.480840722,0.\H,-1.65140
95651,-1.3652619726,0.\Version=DEC-AXP-OSF/1-G03RevB.05\State=1-A'\HF
=-153.7716808\RMSD=2.937e-09\RMSF=3.771e-06\Dipole=-0.3759839,0.198200
1,0.\PG=CS [SG(C2H4O1)]\@
```

16

```
1\1\GINC-LC12\FOpt\RmPWPW91\6-31+G(d,p)\C2H6N1O1(1+)\GMS501\30-Apr-200
4\0\#P MPWPW91\6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=26214400
GFINPUT IOP(3/76=0572004280)\aminoacetaldehyde Cs symm mpw1k/6-31+G**
cis\1,1\N,1.3193725987,0.2629514383,0.\C,0.0052888419,0.9559313309,0
.\H,-0.0908900122,1.5855887253,0.8808115046\H,-0.0908900122,1.58558872
53,-0.8808115046\H,1.8801597679,0.4690892386,0.8211101637\H,1.88015976
79,0.4690892386,-0.8211101637\H,1.0898036467,-0.7499384829,0.\C,-1.046
360361,-0.1386911834,0.\O,-0.6952161929,-1.2837250056,0.\H,-2.09579269
09,0.1662816474,0.\Version=x86-Linux-G03RevB.05\State=1-A'\HF=-209.47
68385\RMSD=7.453e-09\RMSF=2.880e-06\Dipole=1.5059806,1.5717478,0.\PG=C
S [SG(C2H2N1O1),X(H4)]\@
```

17

```
1\1\GINC-LC5\FOpt\RmPWPW91\6-31+G(d,p)\C2H8N1O2(1+)\GMS501\04-May-2004
\0\#P MPWPW91\6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=39321600 G
FINPUT IOP(3/76=0572004280)\Cs gem diol hydrate of aminoacetaldehyde
mpw1k/6-31+G**\1,1\N,-0.3651958902,-1.5521818717,0.\C,0.8724254871,-0
.7226946701,0.\H,1.4413003025,-0.9522453104,0.8935020264\H,1.441300302
5,-0.9522453104,-0.8935020264\C,0.3890057012,0.7120496529,0.\O,-0.3720
867716,0.8219251834,-1.1565793843\O,-0.3720867716,0.8219251834,1.15657
93843\H,1.2324945767,1.4024822926,0.\H,-0.5760594493,1.727763188,-1.38
51221541\H,-0.5760594493,1.727763188,1.3851221541\H,-0.9229183997,-1.3
129243743,0.8204561248\H,-0.9229183997,-1.3129243743,-0.8204561248\H,-
0.1759670378,-2.5493290293,0.\Version=x86-Linux-G03RevB.05\State=1-A'
\HF=-285.9239926\RMSD=2.867e-09\RMSF=1.842e-06\Dipole=-0.0273616,-1.02
69564,0.\PG=CS [SG(C2H2N1),X(H6O2)]\@
```

TS:17→18

```
1\1\GINC-RADOM-BAROSSA059\FTS\UmPWPW91\6-31+G(d,p)\C4H13N1O3(1+,2)\SA
NDALG\27-Nov-2004\0\# MPWPW91\6-31+G(D,P) OPT=(TS,NOEIGEN,CALCFC) IOP
(3/76=0572004280)\Ado=ethanol initial H abstraction gemdiolaminoacet
mpw1k/6-31+G**\1,2\N,-2.3116699215,1.9880564488,0.4694357666\C,-1.638
0940124,0.6485542887,0.5031751735\H,-1.4328786474,0.4016915103,1.53862
66704\H,-2.3087670567,-0.0766089905,0.05717434\C,-0.3773062669,0.80444
29797,-0.296608982\O,-0.7335385236,1.2277910242,-1.5609013391\O,0.3916
444364,1.7197954721,0.3845731604\H,0.2550655078,-0.3743560238,-0.39927
37768\H,-0.2070105911,0.8226364756,-2.2497724262\H,1.1992105001,1.9275
4659,-0.0858153192\H,-1.6779230618,2.6838488441,0.8619995524\H,-2.4809
736292,2.2478518313,-0.5023377183\H,-3.1898005611,2.0109639962,0.97856
86267\C,0.9333823266,-1.5231494726,-0.6258351523\H,0.1672843394,-2.206
8987248,-0.9791314924\H,1.6412785811,-1.2647803102,-1.4088021315\C,1.5
798672087,-1.9331556606,0.6652195383\O,2.2686464515,-3.1245853621,0.40
08839889\H,2.2605229349,-1.1510465044,1.0117625323\H,0.8197267515,-2.0
826332302,1.4378831296\H,2.7348399329,-3.4187724891,1.1809176995\Vers
ion=x86-Linux-G03RevB.02\State=2-A'\HF=-440.238138\S2=0.76241\S2-1=0.\S
2A=0.750061\RMSD=5.249e-09\RMSF=3.223e-06\Dipole=-2.6699984,2.54946,0.
723589\PG=C01 [X(C4H13N1O3)]\@
```

18

```
1\1\GINC-LC9\FOpt\UmpPWPW91\6-31+G(d,p)\C2H7N1O2(1+,2)\GMS501\05-May-20
04\0\#\#P MPWPW91/6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=36044800
GFINPUT IOP(3/76=0572004280)\Clrad of hydrate of aminoacetaldehyde m
pw1k/6-31+G** C1 symm\1,2\N,-1.6241596366,-0.006301818,-0.4733744007\
C,-0.7744074504,-0.2619444596,0.7559361875\H,-1.1107415346,0.430182314
9,1.5203404812\H,-0.9497064752,-1.2844189871,1.0696334406\C,0.64621537
21,-0.0166547158,0.392655994\O,1.2409608564,-0.9256060432,-0.417629455
4\O,0.7932128108,1.2505919132,-0.0267608885\H,1.6810451167,-1.61926596
07,0.0754897225\H,1.6782160254,1.4019284109,-0.3665236613\H,-1.4443561
038,0.9397407932,-0.8079982068\H,-1.3698508432,-0.6485559968,-1.221146
8618\H,-2.6197255975,-0.1037897551,-0.2926044473\Version=x86-Linux-G0
3RevB.05\State=2-A\HF=-285.257954\S2=0.753862\S2-1=0.\S2A=0.75001\RMSD
=8.634e-09\RMSF=2.674e-06\Dipole=-1.7892678,-0.4895701,-0.2571304\PG=C
01 [X(C2H7N1O2)]\@
```

19

```
1\1\GINC-LC145\Freq\UmpPWPW91\6-31+G(d,p)\C2H7N1O2(1+,2)\GMS501\05-May-
2004\0\#\#P MPWPW91/6-31+G(D,P) FREQ=NORAMAN MAXDISK=32768000 GFINPUT I
OP(3/76=0572004280)\freq all gem C2radical hydrate of aminoacetaldehy
de mpw1k/6-31+G**\1,2\C,1.2137580238,0.9497649524,-0.1192589762\H,1.9
048070238,0.8694099524,-0.9409069762\C,0.1297890238,-0.0496760476,0.00
26530238\H,1.3231420238,1.7157409524,0.6323370238\O,-0.0484569762,-0.5
857460476,1.2501840238\O,0.2146730238,-0.9696450476,-0.9897659762\N,-1
.2367079762,0.6593989524,-0.1932559762\H,-0.1003509762,-1.8255180476,-
0.6895179762\H,0.7914890238,-0.7605860476,1.6799860238\H,-1.3467599762
,1.4397479524,0.4490850238\H,-1.9879999762,-0.0040020476,-0.0114229762
\H,-1.3183819762,0.9920099524,-1.1504769762\Version=x86-Linux-G03RevB
.05\State=2-A\HF=-285.2498658\S2=0.75508\S2-1=0.\S2A=0.750014\RMSD=3.8
91e-09\RMSF=3.439e-06\Dipole=-1.0625654,0.8014752,0.1437984\PG=C
01 [X(C2H7N1O2)]\@
```

TS:19→20

```
1\1\ GINC-RADOM-BAROSSA103\FTS\UmpPWPW91\6-31+G(d,p)\C4H13N1O3(1+,2)\SA
NDALG\26-Nov-2004\0\#\# MPWPW91/6-31+G(D,P) OPT=(TS,NOEIGEN,CALCFC) IOP
(3/76=0572004280)\Ado=ethanol H abstraction allgemaminoacet mpw1k/6-3
1+G**\1,2\H,-0.353862052,-1.7770986505,0.0930076034\H,-0.5518238372,-
1.078445653,-1.5767789329\C,-0.5233191771,-0.8936461931,-0.5092956183\
H,0.626353819,-0.1705075026,-0.32078017\C,-1.607104073,-0.0149299315,0
.0008170304\O,-1.5533284967,0.0829239513,1.3556447776\O,-1.7444598661,
1.1904616282,-0.6307190793\N,-2.9935900658,-0.6539844709,-0.3064566595
\H,-1.8466727,0.9512135004,1.6404263989\H,-0.891612087,1.5415222322,-0
.8927426226\H,-3.1025527257,-1.5131858391,0.2243987728\H,-3.0945120816
,-0.8503960657,-1.2980859113\H,-3.7327019179,-0.0077196477,-0.03636121
89\C,1.7261721103,0.5295457416,-0.1524969091\C,2.8393579761,-0.4542186
485,0.0720587207\H,1.5135405864,1.1553779178,0.7092326229\H,1.83133869
96,1.10053227,-1.0712162797\O,4.0023095997,0.3102321601,0.2315860846\H
,2.6334207807,-1.0552918455,0.961199805\H,2.9220268633,-1.1288960849,-
0.783920973\H,4.7553762004,-0.2586610623,0.3782239161\Version=x86-Lin
ux-G03RevB.02\State=2-A\HF=-440.2378665\S2=0.762344\S2-1=0.\S2A=0.7500
68\RMSD=6.760e-09\RMSF=2.006e-06\Dipole=-3.5504257,-1.1829085,-0.60046
32\PG=C01 [X(C4H13N1O3)]\@
```

20

```
1\1\GINC-LC91\FOpt\RmPWPW91\6-31+G(d,p)\C2H8N1O2(1+)\GMS501\04-May-200
4\0\#P MPWPW91/6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100,CALCFC) MAXDISK=36
044800 GFINPUT IOP(3/76=0572004280)\allgem hydrate of aminoacetaldehy
de mpwlk/6-31+G**\1,1\H,-1.3707347653,1.3765675076,0.8978915717\H,-1.
3576345891,1.4010004734,-0.8827491194\C,-1.3174188912,0.7679754003,-0.
0004043676\H,-2.183231304,0.1110717324,0.006677514\C,-0.079776878,-0.0
858663359,0.0100072539\O,-0.0006216705,-0.7920578538,1.1672577223\O,0.
1366402967,-0.8405184159,-1.1080948559\N,1.1590451828,0.8293589602,-0.
0078438778\H,0.42241359,-1.6411075567,1.0192748598\H,-0.6824045688,-1.
1660583304,-1.4848454784\H,1.2237141649,1.3499678856,0.8628106365\H,1.
1351593119,1.4757162137,-0.7921761306\H,1.9944274863,0.2552851251,-0.1
028969584\\Version=x86-Linux-G03RevB.05\State=1-A\HF=-285.9258565\RMSD
=3.838e-09\RMSF=2.190e-06\Dipole=0.9487056,0.9141296,-0.3750879\PG=C01
[X(C2H8N1O2)]\\@
```

21

```
1\1\GINC-LC12\FOpt\RmPWPW91\6-31+G(d,p)\C2H4O2\GMS501\30-Apr-2004\0\#
P MPWPW91/6-31+G(D,P) OPT=(TIGHT,MAXCYCLE=100) MAXDISK=39321600 GFINPU
T IOP(3/76=0572004280)\acetic acid mpwlk/6-31+G**\0,1\C,-0.001408788
4,0.150223427,0.\O,0.1940856123,1.3341474193,0.\O,-1.2344425072,-0.368
7918735,0.\H,-1.8540283132,0.3648793556,0.\C,1.0488426675,-0.909414405
1,0.\H,2.0284505983,-0.4485174952,0.\H,0.9319148,-1.5420301791,0.87647
27318\H,0.9319148,-1.5420301791,-0.8764727318\\Version=x86-Linux-G03Re
vB.05\State=1-A'\HF=-229.0236015\RMSD=4.932e-09\RMSF=1.454e-06\Dipole=
-0.1393642,-0.7145112,0.\PG=CS [SG(C2H2O2),X(H2)]\\@
```

TABLE S2: G3(MP2)-RAD//MPW1K/6-31+G(d,p) Total Energies (Hartrees) at 0 K

Species	
1a	– 210.41381
TS:1a→3a	– 364.52321
3a	– 209.76173
4a	– 209.75202
TS:4a→5a	– 364.52405
5a	– 210.41687
2a	– 153.59921
Ethanol	– 154.79020
Ethanol radical	– 154.12847
Ammonium cation	– 56.79285
Ammonium radical cation	– 56.09629
NH₃•••1a•••NH₃	– 323.40468
TS:NH₃•••1a•••NH₃→NH₃•••3a•••NH₃	– 477.51409
NH₃•••4a•••NH₃	– 322.74670
TS:NH₃•••4a•••NH₃→NH₃•••5a•••NH₃	– 477.51667
6	– 305.09265
TS:6→7	– 459.20076
7	– 304.43931
8	– 228.11124
9	– 228.73902
TS:8→9	– 382.85381
10	– 228.09675
H₂O	– 76.34219

11	– 265.65508
TS:11→12	– 419.76392
12	– 265.00226
13	– 264.99258
TS:13→14	– 419.76522
14	– 265.65800
15	– 153.58317
N_2H_5^+	– 112.02613
$\text{N}_2\text{H}_4\bullet^+$	– 111.40302
16	– 209.20592
17	– 285.57468
TS:17→18	– 439.68478
18	– 284.91566
19	– 284.91358
TS:19→20	– 439.68796
20	– 285.57959
21	– 228.78205

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