Interconversion of (*S*)-Glutamate and (2*S*,3*S*)-3-Methylaspartate: A Distinctive B_{12}-Dependent Carbon-Skeleton Rearrangement

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Supporting Information

(Tables S1 and S2, 15 pages)

Table S1: G3(MP2)-RAD(p) Total Energies (Hartrees) at 0 K for Relevant Species

3	-173.53080
TS:3→4	-173.49379
aminomethyl	-95.703061
aminomethyl radical	-95.05572
ethene	-78.45179
3-H$^+$	-173.87587
protonated aminomethyl	-96.043786
protonated aminomethyl radical	-95.37245
5	-172.33142
TS:5→6	-172.28647
iminomethyl radical	-93.84525
TS:5→7	-172.31147
7	-172.31708
5-H$^+$	-172.67440
TS:5-H$^+$→5'-H$^+$	-172.66716
(*S*)-glutamate model (related to **8**)	-550.97824
8-H$^+$	-550.68885
protonated glycine	-284.43418
protonated 2-glycyl radical	-283.77218
8-H$^-$	-549.79824
deprotonated glycine	-283.55415
deprotonated 2-glycyl radical	-282.91388
8	-550.33059
TS:8→9	-550.30779
acrylic acid	-266.84716
glycine	-284.09868
2-glycyl radical	-283.47022
TS:9→10	-550.30524
10	-550.32287
3-methylaspartate model (related to **10**)	-550.98377
2-amino-5-methyltetrahydrofuran-3,4-diol (**III**)	-476.95493
model 5'-deoxyadenosyl radical (related to **III**)	-476.29401
11	-549.46028

TS:11→12	-549.45622
12	-549.45625
TS:12→13	-549.45501
13	-549.45924
2-aminoethyl cation	-134.09255
TS for hydride anion removal (Equation 3)	-307.61835
ethylamine	-134.94807

Table S2. GAUSSIAN 98 Archive Entries for the RMP2/6-31G(d)//B3-LYP/6-31G(d,p) Calculations for Relevant Species

3

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@16\GINC-PC\SP\ROMP2-FC\6-31G(d)\C3H8N1(2)\SDW501\22-Dec-1999\0\\#ROMP
2/6-31G(D) MAXDISK=5242880000\\aminopropyl radical with Cs symmetry //
B3-LYP/6-31G(d,p)\\0,2\C,0,0.,0.,0.\C,0,0.,0.,1.48864\C,0,1.427149,0.,
-0.630381\N,0,1.47481,0.,-2.091388\H,0,-0.532764,-0.882277,-0.382473\H
,0,-0.532764,0.882277,-0.382473\H,0,1.97594,0.877662,-0.270243\H,0,1.9
7594,-0.877662,-0.270243\H,0,0.981279,0.813185,-2.4541\H,0,0.981279,-0
.813185,-2.4541\H,0,0.090885,-0.926579,2.04642\H,0,0.090885,0.926579,2
.04642\\Version=SGI-G98RevA.6\State=2-A'\HF=-172.6447696\MP2=-173.1813
823\RMSD=6.987e-09\PG=CS [SG(C3N1),X(H8)]\\@
```

TS:3→4

```
@18\GINC-PC\SP\ROMP2-FC\6-31G(d)\C3H8N1(2)\SDW501\22-Dec-1999\0\\#ROMP
2/6-31G(D) MAXDISK=5242880000\\fragmentation-recombination TS for the
rearrangement of aminopropyl radical //B3-LYP/6-31G(d,p)\\0,2\C,0,0.,0
.,0.\C,0,0.,0.,1.36328\C,0,2.123159,0.,-0.878473\N,0,2.157718,0.,-2.27
9327\H,0,-0.198106,-0.91715,-0.548363\H,0,-0.198106,0.91715,-0.548363\
H,0,2.481439,0.915859,-0.417597\H,0,2.481439,-0.915859,-0.417597\H,0,1
.763923,0.830519,-2.706561\H,0,1.763923,-0.830519,-2.706561\H,0,0.0463
6,-0.923683,1.932463\H,0,0.04636,0.923683,1.932463\\Version=SGI-G98Rev
A.6\State=2-A'\HF=-172.5836874\MP2=-173.1320762\RMSD=9.087e-09\PG=CS [
SG(C3N1),X(H8)]\\@
```

aminomethyl

```
@42\GINC-PC\SP\ROMP2-FC\6-31G(d)\C1H5N1\SDW501\10-Apr-2001\0\\#ROMP2/6
-31G* SCF=TIGHT MAXDISK=5242880000\\RMP2/6-31G(d) single-point calcula
tion on methylamine closed shell\\0,1\H,0,-1.295715665,-0.7818682786,0
.\C,0,-0.196983825,-0.677035063,0.\N,0,0.3134084456,0.6949671702,0.\H,
0,0.1850429006,-1.2041610898,0.8803139187\H,0,0.1850429006,-1.20416108
98,-0.8803139187\H,0,-0.0431631527,1.1938153224,0.8115948314\H,0,-0.04
31631527,1.1938153224,-0.8115948314\\Version=SGI64-G98RevA.9\State=1-A
'\HF=-95.2089862\MP2=-95.5064891\RMSD=3.617e-09\PG=CS [SG(C1H1N1),X(H4
)]\\@
```

aminomethyl radical

```
@5\GINC-RSCQC9\SP\ROMP2-FC\6-31G(d)\C1H4N1(2)\STACEY\13-Oct-1999\0\\#R
OMP2/6-31G(D) MAXDISK=1048576000\\aminomethyl radical //B3-LYP/6-31G(d
,p)\\0,2\C,0,-0.733276,0.,-0.045978\N,0,0.66225,0.,0.063615\H,0,-1.229
064,0.928138,0.219407\H,0,-1.229064,-0.928138,0.219407\H,0,1.111017,0.
830723,-0.304125\H,0,1.111017,-0.830723,-0.304125\\Version=IBM-RS6000-
G98RevA.6\State=2-A'\HF=-94.5820627\MP2=-94.8609653\RMSD=3.934e-09\PG=
CS [SG(C1N1),X(H4)]\\@
```

ethene

```
@6\GINC-RSCQC9\SP\ROMP2-FC\6-31G(d)\C2H4\STACEY\13-Oct-1999\0\\#ROMP2/
6-31G(D) MAXDISK=1048576000\\ethene //B3-LYP/6-31G(d,p)\\0,1\C,0,-0.66
5078,0.,0.\C,0,0.665078,0.,0.\H,0,-1.237954,0.923227,0.\H,0,-1.237954,
-0.923227,0.\H,0,1.237954,0.923227,0.\H,0,1.237954,-0.923227,0.\\Versi
on=IBM-RS6000-G98RevA.6\State=1-AG\HF=-78.0311614\MP2=-78.2849786\RMSD
=1.225e-09\PG=D02H [C2"(C1.C1),SG(H4)]\\@
```

3-H$^+$

@44\GINC-PC\SP\ROMP2-FC\6-31G(d)\C3H9N1(1+,2)\SDW501\20-Mar-2001\0\\#R
OMP2/6-31G* SCF=TIGHT MAXDISK=5242880000\\romp2/dz single point on rea
ctant for small model GM rearrangemnet with protonated migrating group
\\1,2\C,0,0.3948556144,-0.7653918789,0.\C,0,1.8905997516,-0.7522194232
,0.\C,0,-0.1527430113,0.670246284,0.\N,0,-1.6894294836,0.6711276221,0.
\H,0,0.018609208,-1.2930795243,-0.886898051\H,0,0.018609208,-1.2930795
243,0.886898051\H,0,0.1475973278,1.2267216426,0.8895841791\H,0,0.14759
73278,1.2267216426,-0.8895841791\H,0,-2.057156471,0.1865288723,0.82631
0693\H,0,-2.057156471,0.1865288723,-0.826310693\H,0,2.4418850358,-0.73
84762928,-0.9323394351\H,0,2.4418850358,-0.7384762928,0.9323394351\H,0
,-2.072137944,1.6229073582,0.\\Version=SGI64-G98RevA.9\State=2-A'\HF=-
173.0142291\MP2=-173.5472815\RMSD=5.315e-09\PG=CS [SG(C3H1N1),X(H8)]\\
@

protonated aminomethyl

@45\GINC-PC\SP\ROMP2-FC\6-31G(d)\C1H6N1(1+)\SDW501\10-Apr-2001\0\\#ROM
P2/6-31G* SCF=TIGHT MAXDISK=5242880000\\RMP2/6-31G(d) single-point cal
culation on methylamine protonated closed shell\\1,1\H,0,-1.3488075312
,-0.7480343425,0.\C,0,-0.2597778782,-0.7602674736,0.\N,0,0.2303449685,
0.6741206933,0.\H,0,0.119637092,-1.2496934044,0.8959077974\H,0,0.11963
7092,-1.2496934044,-0.8959077974\H,0,-0.0999718363,1.184472561,0.82709
78178\H,0,-0.0999718363,1.184472561,-0.8270978178\H,0,1.2557295096,0.7
212360181,0.\\Version=SGI64-G98RevA.9\State=1-A'\HF=-95.5726133\MP2=-9
5.8681733\RMSD=1.269e-09\PG=CS [SG(C1H2N1),X(H4)]\\@

protonated aminomethyl radical

@46\GINC-RSCQC9\SP\ROMP2-FC\6-31G(d)\C1H5N1(1+,2)\STACEY\19-Mar-2001\0
\\#ROMP2/6-31G* SCF=TIGHT MAXDISK=1048576000\\RMP2/6-31G(d) single-poi
nt calculation on protonated aminomethyl radical\\1,2\C,0,-0.826118320
3,0.0442203425,0.\N,0,0.6413420722,-0.0547654175,0.\H,0,1.0997041157,0
.8718344651,0.\H,0,-1.3015568847,0.1807977539,-0.9606829665\H,0,-1.301
5568847,0.1807977539,0.9606829665\H,0,0.9853625348,-0.5576970526,-0.82
87708165\H,0,0.9853625348,-0.5576970526,0.8287708165\\Version=IBM-RS60
00-G98RevA.6\State=2-A'\HF=-94.9251411\MP2=-95.1974896\RMSD=7.478e-09\
PG=CS [SG(C1H1N1),X(H4)]\\@

5

@15\GINC-RSCQC9\SP\ROMP2-FC\6-31G(d)\C3H6N1(2)\STACEY\02-Nov-1999\0\\#
ROMP2/6-31G(D) MAXDISK=1048576000\\iminopropyl radical Cs symmetry wit
h twisted radical center //B3-LYP/6-31G(d,p)\\0,2\C,0,-0.1955050196,-0
.9265419125,0.\C,0,1.2913964184,-0.9253850963,0.\C,0,-0.8475384488,0.4
348430027,0.\N,0,-0.1741482333,1.5132872048,0.\H,0,-1.9483073675,0.407
4194722,0.\H,0,1.8358016609,0.0092695678,0.\H,0,1.8343660995,-1.863589
2356,0.\H,0,-0.5975613122,-1.4842531055,-0.8662039371\H,0,-0.597561312
2,-1.4842531055,0.8662039371\H,0,-0.7978178355,2.3249000097,0.\\Versio
n=IBM-RS6000-G98RevA.6\State=2-A"\HF=-171.4700726\MP2=-171.9962741\RMS
D=6.778e-09\PG=CS [SG(C3H4N1),X(H2)]\\@

TS:5→6

@13\GINC-PC\SP\ROMP2-FC\6-31G(d)\C3H6N1(2)\SDW501\22-Oct-1999\0\\#ROMP
2/6-31G(D) MAXDISK=5242880000\\fragmentation-recombination TS for rear
rangement of the iminopropyl radical //B3-LYP/6-31G(d,p)\\0,2\C,0,0.64
60327855,0.,-1.1410841435\C,0,-0.612518074,0.,-1.6479954453\C,0,0.5407
046249,0.,1.1863472989\N,0,-0.5362076264,0.,1.7991395182\H,0,1.5322204
039,0.,1.6593500238\H,0,-1.1487890352,0.9245117185,-1.8403117392\H,0,-
1.1487890352,-0.9245117185,-1.8403117392\H,0,1.2199280695,-0.919786275
2,-1.0747250796\H,0,1.2199280695,0.9197862752,-1.0747250796\H,0,-1.366
3611057,0.,1.1931407258\\Version=SGI-G98RevA.6\State=2-A'\HF=-171.4005
523\MP2=-171.9411416\RMSD=5.865e-09\PG=CS [SG(C3H2N1),X(H4)]\\@

iminomethyl radical

@12\GINC-PC\SP\ROMP2-FC\6-31G(d)\C1H2N1(2)\SDW501\22-Oct-1999\0\\#ROMP
2/6-31G(D) MAXDISK=5242880000\\iminomethyl radical //B3-LYP/6-31G(d,p)
\\0,2\C,0,0.5931249136,0.,-0.2684542332\N,0,-0.5350085131,0.,0.2413810
428\H,0,1.5303307213,0.,0.3073051398\H,0,-1.344020611,0.,-0.3862470405
\\Version=SGI-G98RevA.6\State=2-A'\HF=-93.39254\MP2=-93.6665183\RMSD=8
.169e-09\PG=CS [SG(C1H2N1)]\\

TS:5→7

@11\GINC-VPP11\SP\ROMP2-FC\6-31G(d)\C3H6N1(2)\SDW501\14-Oct-1999\0\\#R
OMP2/6-31G(D) MAXDISK=65536000\\addition-elimination TS for the rearra
ngement of the iminopropyl radical //B3-LYP/6-31G(d,p)\\0,2\N,0,-1.430
1152258,-0.4253769032,-0.3962568387\C,0,-0.5004952258,0.0355930968,0.4
276591613\H,0,-2.1063652258,-0.9825229032,0.1363311613\H,0,-0.53744422
58,-0.0863779032,1.5147131613\C,0,0.6159377742,0.8949110968,-0.0956828
387\H,0,0.4190897742,1.2915330968,-1.0904598387\H,0,0.9964947742,1.644
8710968,0.5983871613\C,0,1.2500697742,-0.4385189032,-0.0462308387\H,0,
1.8156767742,-0.7638519032,0.8194741613\H,0,1.2302807742,-1.0779249032
,-0.9191208387\\Version=Fujitsu-VP-Unix-G98RevA.6\HF=-171.424508\MP2=-
171.9792338\RMSD=1.169e-09\PG=C01 [X(C3H6N1)]\\@

7

@4\GINC-VPP08\SP\ROMP2-FC\6-31G(d)\C3H6N1(2)\SDW501\14-Oct-1999\0\\#RO
MP2/6-31G(D) MAXDISK=1572864000\\cyclopropylamino radical //B3-LYP/6-3
1G(d,p)\\0,2\C,0,-0.332896,0.,0.465267\C,0,0.887586,0.741073,-0.124118
\C,0,0.887586,-0.741073,-0.124118\H,0,0.701082,-1.254704,-1.060457\H,0
,1.513554,-1.272784,0.585921\H,0,0.701082,1.254704,-1.060457\H,0,1.513
554,1.272784,0.585921\H,0,-0.391827,0.,1.554854\N,0,-1.484962,0.,-0.31
7105\H,0,-2.296366,0.,0.311772\\Version=Fujitsu-VP-Unix-G98RevA.6\Stat
e=2-A"\HF=-171.4576224\MP2=-171.9855154\RMSD=6.096e-09\PG=CS [SG(C1H2N
1),X(C2H4)]\\@

5-H$^+$

@10\GINC-VPP10\SP\ROMP2-FC\6-31G(d)\C3H7N1(1+,2)\SDW501\14-Oct-1999\0\
\#ROMP2/6-31G(D) MAXDISK=65536000\\protonated iminopropyl radical cati
on //B3-LYP/6-31G(d,p)\\1,2\N,0,-1.451033,0.695857,-0.137717\C,0,-0.18
2694,0.573522,-0.400031\H,0,-1.88724,1.607391,-0.032142\H,0,-2.055918,
-0.114103,-0.029033\H,0,0.377847,1.495787,-0.536944\C,0,0.542376,-0.72
3788,-0.418025\H,0,-0.138459,-1.579126,-0.459391\H,0,1.242595,-0.76105
5,-1.257798\C,0,1.247577,-0.597477,0.901463\H,0,2.229568,-0.142391,0.9
62631\H,0,0.745285,-0.89104,1.816252\\Version=Fujitsu-VP-Unix-G98RevA.
6\HF=-171.8386454\MP2=-172.3560791\RMSD=5.018e-09\PG=C01 [X(C3H7N1)]\\
@

TS:5-H$^+$→5'-H$^+$

@17\GINC-PC\SP\ROMP2-FC\6-31G(d)\C3H7N1(1+,2)\SDW501\22-Dec-1999\0\\#R
OMP2/6-31G(D) MAXDISK=5242880000\\TS for addition-elimination rearrang
ement of protonated iminopropyl radical //B3-LYP/6-31G(d,p)\\1,2\C,0,0
.1322769673,-0.49892875,-0.2656921187\C,0,-1.0863311546,0.13678125,0.5
539993735\C,0,0.2127189967,0.13678125,1.2007419838\H,0,0.7890857737,1.
05536125,1.2563887233\H,0,0.4563218913,-0.62262875,1.9391847592\H,0,-1
.478133348,1.05536125,0.1276353712\H,0,-1.8223915065,-0.62262875,0.804
7088888\H,0,0.1683992495,-1.57914875,-0.3382474991\N,0,0.6576389045,0.
17235125,-1.3209364975\H,0,1.0517038112,-0.32763875,-2.1124570629\H,0,
0.6795529405,1.18706125,-1.3649531299\\Version=SGI-G98RevA.6\State=2-A
"\HF=-171.8121133\MP2=-172.3559034\RMSD=7.102e-09\PG=CS [SG(C1H3N1),X(
C2H4)]\\@

(*S*)-glutamate model (related to **8**)

@27\GINC-VPP07\SP\ROMP2-FC\6-31G(d)\C5H9N1O4\SDW501\08-Nov-1999\0\\#RO
MP2/6-31G(D) MAXDISK=144179200\\(S)-glutamate //B3-LYP/6-31G(d,p)\\0,1
\C,0,-0.1030352714,-0.7913442965,-0.401770734\C,0,1.4281314079,-0.9071
053835,-0.4048479354\C,0,-0.6556836545,0.6671157562,-0.3961591019\H,0,
-0.4577372042,-1.2891655141,-1.3104623213\H,0,-0.521685302,-1.33307094
,0.453248772\H,0,-0.0808530088,1.2278205754,-1.1491690634\N,0,-0.63787
64789,1.3766216813,0.8744829528\H,0,0.0983436914,1.0085248076,1.470123
1664\H,0,-1.5246182885,1.2087187814,1.3445605781\H,0,1.7319915467,-1.8
998675931,-0.7577687378\C,0,2.1175804234,-0.7021032828,0.9267554688\O,
0,1.5970485449,-0.3820031862,1.9761921738\O,0,3.4454916314,-0.93673214
09,0.8277672123\H,0,3.8172996878,-0.7815473018,1.712821688\C,0,-2.0922
08359,0.628192797,-0.9045584861\O,0,-3.082260613,0.7340602498,-0.21474
52008\O,0,-2.1530585215,0.4199778524,-2.2413978423\H,0,-3.0979894125,0
.3731736617,-2.4653297485\H,0,1.8739080298,-0.2018939892,-1.1184510149
\\Version=Fujitsu-VP-Unix-G98RevA.6\HF=-548.5078401\MP2=-550.02254\RMS
D=9.737e-09\PG=C01 [X(C5H9N1O4)]\\@

8-H$^+$

@47\GINC-PC\SP\ROMP2-FC\6-31G(d)\C5H9N1O4(1+,2)\SDW501\15-Mar-2001\0\\
#ROMP2/6-31G* SCF=TIGHT MAXDISK=5242880000\\RMP2/6-31G(d) single-point
calculation on protonated (S)-glutmatme (8-H+)\\1,2\C,0,-0.017279,-0.
869303,-0.540252\C,0,1.477225,-0.943189,-0.449752\C,0,-0.645115,0.5528
18,-0.490007\H,0,-0.337463,-1.315857,-1.483829\H,0,-0.469741,-1.467903
,0.264719\H,0,-0.147568,1.213028,-1.203821\N,0,-0.533374,1.153207,0.88
515\H,0,0.331139,0.749178,1.380242\H,0,-1.408254,0.931305,1.386933\H,0
,2.049961,-1.359609,-1.271321\C,0,2.198216,-0.57584,0.757451\O,0,1.688
352,0.035326,1.712154\O,0,3.471946,-0.948589,0.752442\H,0,3.890914,-0.
667234,1.585837\C,0,-2.148629,0.488818,-0.797368\O,0,-2.982133,0.65868
8,0.064504\O,0,-2.373435,0.205117,-2.074075\H,0,-3.334827,0.147034,-2.
227053\H,0,-0.464879,2.173439,0.85161\\Version=SGI64-G98RevA.9\HF=-548
.2611726\MP2=-549.7563015\RMSD=5.351e-09\PG=C01 [X(C5H9N1O4)]\\@

protonated glycine

@49\GINC-PC\SP\ROMP2-FC\6-31G(d)\C2H6N1O2(1+)\SDW501\10-Apr-2001\0\\#R
OMP2/6-31G* SCF=TIGHT MAXDISK=5242880000\\RMP2/6-31G(d) single-point c
alculation on glycine with protonated NH2 group\\1,1\H,0,-1.9660944489
,-1.5391845145,0.000179341\O,0,-0.9902440893,-1.5418084506,-0.00001191
3\C,0,-0.5335552741,-0.307478062,-0.0001236071\O,0,-1.1748589942,0.723
6975985,0.0001691665\C,0,0.9985713648,-0.268051853,-0.0001177186\N,0,1
.355024537,1.1987734165,0.0000254757\H,0,1.8858962395,1.4823731772,-0.
8284879458\H,0,0.4278337257,1.6895132672,0.0000360436\H,0,1.8858394933
,1.4822269719,0.8286254216\H,0,1.4060307046,-0.7540483677,-0.888173634
6\H,0,1.4060506512,-0.7542281424,0.8878323704\\Version=SGI64-G98RevA.9
\HF=-283.1820966\MP2=-283.9560271\RMSD=2.711e-09\PG=C01 [X(C2H6N1O2)]\
\@

protonated 2-glycyl radical

@48\GINC-PC\SP\ROMP2-FC\6-31G(d)\C2H5N1O2(1+,2)\SDW501\15-Mar-2001\0\\
#ROMP2/6-31G* SCF=TIGHT MAXDISK=5242880000\\RMP2/6-31G(d) single-point
calculation on protonated 2-glycyl\\1,2\C,0,0.714542222,-0.6859541336,
0.\H,0,1.7804357406,-0.8731114123,0.\N,0,-0.2154966462,-1.8120294173,0
.\H,0,-0.1202013801,-2.4137973008,0.83049\H,0,-1.1622823555,-1.3631471
749,0.\C,0,0.,0.5943310711,0.\O,0,-1.2261567744,0.5835114192,0.\O,0,0.
7979600308,1.6455909546,0.\H,0,0.2690465155,2.4649784946,0.\H,0,-0.120
2013801,-2.4137973008,-0.83049\\Version=SGI64-G98RevA.9\State=2-A"\HF=
-282.5427001\MP2=-283.2953486\RMSD=8.774e-09\PG=CS [SG(C2H3N1O2),X(H2)
]\\@

8-H$^-$

@50\GINC-PC\SP\ROMP2-FC\6-31G(d)\C5H7N1O4(1-,2)\SDW501\30-Mar-2001\0\\
#ROMP2/6-31G* SCF=TIGHT MAXDISK=5242880000\\RMP2/6-31G(d) single-point
calculation on 4-glutamyl radical with depronated COOH in migrating g
roup\\-1,2\C,0,0.0710385567,-0.7146364897,-0.5684339972\C,0,-1.2801465
279,-1.0040086359,-0.0650667996\C,0,0.9539164103,0.0102985812,0.542302
8798\H,0,0.6107241712,-1.6362785122,-0.8077500225\H,0,0.0516268679,-0.
0562170037,-1.4423712219\H,0,0.8763855267,-0.598840731,1.4517459639\N,
0,0.5982663646,1.3905407604,0.7968986254\H,0,-0.3760562988,1.578561275
8,0.5697625083\H,0,1.1970540496,1.9244444161,0.1618667063\H,0,-1.45564
26546,-1.9072294311,0.5123717891\C,0,-2.3580980808,-0.0756731445,-0.15
00575911\O,0,-2.3299911837,1.064581248,-0.6292667798\O,0,-3.5461081141
,-0.5556482855,0.3776948078\H,0,-4.1600720461,0.18548028,0.2570174098\
C,0,2.4621440797,-0.0927357568,0.0104341037\O,0,2.9035118921,0.9734451
262,-0.4800954538\O,0,2.9694610563,-1.2277747066,0.1196667903\\Version
=SGI64-G98RevA.9\HF=-547.3118594\MP2=-548.8203494\RMSD=5.618e-09\PG=C0
1 [X(C5H7N1O4)]\\@

deprotonated glycine

@51\GINC-PC\SP\ROMP2-FC\6-31G(d)\C2H4N1O2(1-)\SDW501\10-Apr-2001\0\\#R
OMP2/6-31G* SCF=TIGHT MAXDISK=5242880000\\RMP2/6-31G(d) single-point c
alculation on Glycine with COO- group\\-1,1\H,0,-0.4835754085,0.940349
4433,1.4861340768\N,0,0.460808689,1.3019395357,1.2882656254\H,0,0.2443
490578,2.1439456557,0.7502991289\C,0,0.9239835779,0.2989687406,0.30153
80354\C,0,-0.2396882775,-0.4556056876,-0.4401614934\O,0,-1.3817971069,
-0.2983101019,0.077017905\O,0,0.1052241125,-1.1461940418,-1.4272992899
\H,0,1.5895301054,0.7585448055,-0.4398983632\H,0,1.5308475754,-0.46056
18234,0.8195976071\\Version=SGI64-G98RevA.9\HF=-282.2502569\MP2=-283.0
321933\RMSD=7.693e-09\PG=C01 [X(C2H4N1O2)]\\@

deprotonated 2-glycyl radical

@52\GINC-PC\SP\ROMP2-FC\6-31G(d)\C2H3N1O2(1-,2)\SDW501\30-Mar-2001\0\\
#ROMP2/6-31G* SCF=TIGHT MAXDISK=5242880000\\RMP2/6-31G* single point c
alculation on 2-glycyl radical with COO- group\\-1,2\C,0,-0.6330301428
,-0.7415019154,-0.0361386107\H,0,-0.6670174032,-1.8280715848,-0.072736
7695\N,0,-1.8260611017,-0.0186759133,-0.1856614774\H,0,-2.5732163387,-
0.2878599187,0.4553869416\H,0,-1.523229736,0.9528139982,-0.0300139295\
C,0,0.6401561392,0.039104386,0.0278393223\O,0,0.4713042757,1.305038545
3,0.0648198797\O,0,1.7165876257,-0.6165092859,0.0597788489\\Version=SG
I64-G98RevA.9\HF=-281.6281607\MP2=-282.3923649\RMSD=6.285e-09\PG=C01 [
X(C2H3N1O2)]\\@

8

```
@20\GINC-PC\SP\ROMP2-FC\6-31G(d)\C5H8N1O4(2)\SDW501\23-Oct-1999\0\\#RO
MP2/6-31G(D) MAXDISK=5242880000\\4-glutamyl radical //B3-LYP/6-31G(d,p
)\\0,2\C,0,-0.1976884503,-0.8597519056,-0.1631935407\C,0,1.250239301,-
1.058874448,-0.4062484492\C,0,-0.6829086963,0.6258502644,-0.4708389051
\H,0,-0.7656035615,-1.5416899334,-0.8042560499\H,0,-0.4461311368,-1.06
06074226,0.8838855312\H,0,-0.3025214691,0.8876412494,-1.4650646244\N,0
,-0.2959228965,1.6216417185,0.502446028\H,0,0.6116275332,1.4032995654,
0.9057031741\H,0,-0.9756950084,1.6182276238,1.2597657058\H,0,1.6015704
322,-1.405008316,-1.3731033042\C,0,2.2434221073,-0.7277111743,0.591053
9086\O,0,2.0082909604,-0.1720886236,1.6620462188\O,0,3.5042227682,-1.0
801932519,0.2261385624\H,0,4.0816294693,-0.7995260507,0.9551817356\C,0
,-2.2029597438,0.5894980663,-0.5570800739\O,0,-2.9556108399,0.91887632
14,0.3322493915\O,0,-2.6309471364,0.0919330691,-1.7394049157\H,0,-3.60
16891092,0.0638863182,-1.6896260581\\Version=SGI-G98RevA.6\HF=-547.882
3371\MP2=-549.3774217\RMSD=8.908e-09\PG=C01 [X(C5H8N1O4)]\\@
```

TS:8→9

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@21\GINC-VPP10\SP\ROMP2-FC\6-31G(d)\C5H8N1O4(2)\SDW501\23-Oct-1999\0\\
#ROMP2/6-31G(D) MAXDISK=144179200\\fragmentation-recombination TS for
the rearrangement of 4-glutamyl radical //B3-LYP/6-31G(d,p)\\0,2\C,0,-
0.0288922203,-1.1141351205,-0.3601935665\C,0,1.3575030471,-1.117220738
2,-0.3513072468\C,0,-0.6901402745,0.9350818367,-0.3393901358\H,0,-0.53
65744166,-1.4623184371,-1.2546318153\H,0,-0.557522978,-1.26421867,0.57
54546305\H,0,0.0921045119,1.304772249,-0.990916743\N,0,-0.6760464838,1
.3623859718,0.9658834183\H,0,0.1850542729,1.1743698287,1.4747038551\H,
0,-1.5117768434,1.0935204789,1.4757387954\H,0,1.9271217871,-1.26428972
11,-1.2627758728\C,0,2.099685937,-0.800610725,0.8546374386\O,0,1.62850
52314,-0.3300122848,1.8906427379\O,0,3.4301721614,-1.0521378639,0.7425
304227\H,0,3.8205391066,-0.7859387242,1.5912924855\C,0,-2.0301482859,0
.7497822621,-0.9173251033\O,0,-3.0456592134,0.6147495583,-0.2546780273
\O,0,-2.0134384093,0.6733435133,-2.2719653495\H,0,-2.931307435,0.50247
27204,-2.5408158518\\Version=Fujitsu-VP-Unix-G98RevA.6\HF=-547.8299441
\MP2=-549.3512279\RMSD=5.392e-09\PG=C01 [X(C5H8N1O4)]\\@
```

acrylic acid

```
@24\GINC-VPP09\SP\ROMP2-FC\6-31G(d)\C3H4O2\SDW501\23-Oct-1999\0\\#ROMP
2/6-31G(D) MAXDISK=131072000\\ acrylic  acid  //B3-LYP/6-31G(d,p)\\0,1
\C,0,-1.7217530259,0.955352379,0.\C,0,-0.3877055423,0.9560799397,0.\H,
0,-2.2927173788,1.8777887349,0.\H,0,-2.2676130824,0.0167118158,0.\H,0,
0.1947720315,1.8720037863,0.\C,0,0.366036823,-0.3219112847,0.\O,0,-0.1
170514139,-1.4357076331,0.\O,0,1.705511638,-0.104238499,0.\H,0,2.11840
71078,-0.984061484,0.\\Version=Fujitsu-VP-Unix-G98RevA.6\State=1-A'\HF
=-265.6514474\MP2=-266.3803828\RMSD=8.895e-09\PG=CS [SG(C3H4O2)]\\@
```

glycine

```
@41\GINC-PC\SP\ROMP2-FC\6-31G(d)\C2H5N1O2\SDW501\26-Nov-1999\0\\#ROMP2
/6-31G(D) MAXDISK=5242880000\\glycine //B3-LYP/6-31G(d,p)\\0,1\C,0,-0.
580198,-0.858339,0.\C,0,0.,0.551764,0.\O,0,-0.972752,1.494354,0.\O,0,1
.180732,0.820976,0.\H,0,-0.520697,2.355248,0.\H,0,-1.237562,-0.949174,
0.873045\H,0,-1.237562,-0.949174,-0.873045\N,0,0.399025,-1.928715,0.\H
,0,1.009999,-1.819546,0.806627\H,0,1.009999,-1.819546,-0.806627\\Versi
on=SGI-G98RevA.6\State=1-A'\HF=-282.8280453\MP2=-283.6003943\RMSD=3.76
2e-09\PG=CS [SG(C2H1N1O2),X(H4)]\\@
```

2-glycyl radical

@25\GINC-PC\SP\ROMP2-FC\6-31G(d)\C2H4N1O2(2)\SDW501\24-Oct-1999\0\\#RO
MP2/6-31G(D) MAXDISK=5242880000\\2-glycyl radical //B3-LYP/6-31G(d,p
)\\0,2\C,0,0.6715304852,0.7242512752,-0.0002305128\H,0,1.7515416107,0.
760064278,0.0286827891\N,0,-0.0416023996,1.8854291809,0.0350436514\H,0
,0.3854465625,2.7508715772,-0.2545653452\H,0,-1.0382321053,1.782559366
8,-0.1137986002\C,0,-0.0657064739,-0.5022725419,0.0022394184\O,0,-1.29
55414356,-0.5678371751,-0.0375485231\O,0,0.7264050286,-1.6145364075,0.
0440081319\H,0,0.1106079177,-2.3643832272,0.0306452923\\Version=SGI-G9
8RevA.6\HF=-282.2134372\MP2=-282.9752382\RMSD=3.406e-09\PG=C01 [X(C2H4
N1O2)]\\@

TS:9→10

@23\GINC-VPP09\SP\ROMP2-FC\6-31G(d)\C5H8N1O4(2)\SDW501\23-Oct-1999\0\\
#ROMP2/6-31G(D) MAXDISK=144179200\\fragmentation-recombination TS for
3-methylaspartate related radical //B3-LYP/6-31G(d,p)\\0,2\C,0,-0.6219
14,0.34351,0.829236\C,0,-1.874529,0.194779,0.050724\C,0,0.570879,-0.11
5765,-0.787312\H,0,-0.288651,1.369797,0.962528\H,0,0.182196,0.639377,-
1.466007\N,0,0.412922,-1.430581,-1.184148\H,0,-0.554062,-1.705087,-1.3
31472\H,0,0.906568,-2.072429,-0.571775\C,0,1.886268,0.175515,-0.17974\
O,0,2.601379,-0.665626,0.332556\O,0,2.179354,1.499092,-0.180002\H,0,3.
025822,1.586941,0.289138\O,0,-2.414063,-0.865015,-0.221926\O,0,-2.3420
66,1.380357,-0.413903\H,0,-3.131999,1.168946,-0.940081\C,0,-0.403863,-
0.572271,1.87219\H,0,-0.94137,-1.513074,1.894187\H,0,0.373168,-0.40546
4,2.608132\\Version=Fujitsu-VP-Unix-G98RevA.6\HF=-547.8288612\MP2=-549
.3432479\RMSD=6.555e-09\PG=C01 [X(C5H8N1O4)]\\@

10

@22\GINC-VPP10\SP\ROMP2-FC\6-31G(d)\C5H8N1O4(2)\SDW501\23-Oct-1999\0\\
#ROMP2/6-31G(D) MAXDISK=144179200\\3-methylaspartate related radical /
/B3-LYP/6-31G(d,p)\\0,2\C,0,0.263421856,-0.7719946852,-0.0869955872\C,
0,1.7877857908,-0.7680210109,-0.1557322391\C,0,-0.2528995884,0.7072436
749,-0.1569681536\H,0,-0.0955189254,-1.2550487012,-1.0085922692\H,0,0.
1067889664,1.1258574504,-1.1035138648\N,0,0.3067349693,1.4767955086,0.
9378942931\H,0,-0.0358081769,2.4333435703,0.892650048\H,0,-0.039011508
7,1.0999747405,1.8187918087\C,0,-1.7824806827,0.736893167,-0.214411148
6\O,0,-2.498162252,1.2901798487,0.5898463245\O,0,-2.2649994961,0.07797
98515,-1.2965061351\H,0,-3.2334332985,0.1580188089,-1.2594022251\O,0,2
.537821254,-1.2495578094,0.6607206761\O,0,2.22693012,-0.1753146817,-1.
2924280751\H,0,3.1974781419,-0.1964112399,-1.2495918156\C,0,-0.2247818
684,-1.5118099872,1.1109819221\H,0,0.4779774338,-1.9003762229,1.835907
2902\H,0,-1.2846074681,-1.7030915908,1.2341798921\\Version=Fujitsu-VP-
Unix-G98RevA.6\HF=-547.8747271\MP2=-549.3686707\RMSD=6.491e-09\PG=C01
[X(C5H8N1O4)]\\@

3-methylaspartate model (related to **10**)

@28\GINC-VPP07\SP\ROMP2-FC\6-31G(d)\C5H9N1O4\SDW501\28-Nov-1999\0\\#RO
MP2/6-31G(D) MAXDISK=131072000\\3-methylaspartate //B3-LYP/6-31G(d,p)\
\0,1\C,0,0.2660296808,-0.7343334858,-0.1294682208\C,0,1.7885534819,-0.
7526772838,-0.1710237494\C,0,-0.2385832127,0.7384806388,-0.1130476168\
H,0,-0.0734480362,-1.1767483341,-1.074865939\H,0,0.180559697,1.2296608
422,-0.9959510266\N,0,0.2335780168,1.4323275617,1.0758723157\H,0,0.155
2483693,2.4363475587,0.9376572314\H,0,-0.3861215103,1.2183515698,1.854
6602687\C,0,-1.7616362696,0.7691126231,-0.2593313818\O,0,-2.5348423912
,1.1388129115,0.5969660808\O,0,-2.1679899624,0.3181330538,-1.469747839
5\H,0,-3.1399095027,0.3562456042,-1.4671086697\O,0,2.5075145339,-1.393
1146116,0.5608875353\O,0,2.2774622273,0.0130935244,-1.1796388437\H,0,3
.2448796417,-0.0618193482,-1.1255314072\C,0,-0.2479392543,-1.569234832
6,1.0462792892\H,0,0.1200038369,-2.5945921375,0.9746245756\H,0,-1.3414
910965,-1.5939023321,1.0614272815\H,0,0.1095306655,-1.163321338,1.9957
960897\\Version=Fujitsu-VP-Unix-G98RevA.6\HF=-548.5115446\MP2=-550.029
044\RMSD=6.750e-09\PG=C01 [X(C5H9N1O4)]\\@

2-amino-5-methyltetrahydrofuran-3,4-diol (**III**)

@36\GINC-VPP09\SP\ROMP2-FC\6-31G(d)\C5H11N1O3\SDW501\18-Feb-2000\0\\#R
OMP2/6-31G(D) MAXDISK=131072000\\model 5'-deoxyadenosine molecule //B3
-LYP/6-31G(d,p)\\0,1\C,0,0.,0.,0.\C,0,0.,0.,1.52032\O,0,1.353994,0.,1.
997293\C,0,-0.654958,1.226808,2.18286\O,0,-2.048196,1.089537,2.437594\
C,0,0.082848,1.290733,3.527101\O,0,-0.430973,0.323958,4.424336\C,0,1.4
98652,0.885582,3.106363\N,0,2.232259,2.063513,2.641215\H,0,-0.511973,-
0.89693,1.899902\H,0,-0.439757,2.133607,1.603435\H,0,0.062406,2.299376
,3.964452\H,0,1.995754,0.327319,3.913884\H,0,3.05513,1.739173,2.137826
\H,0,2.568378,2.598001,3.441109\H,0,-2.505588,0.940666,1.60071\H,0,-1.
389815,0.310661,4.27984\H,0,0.492896,0.898956,-0.382511\H,0,-1.024767,
-0.03394,-0.390154\H,0,0.530864,-0.874992,-0.385116\\Version=Fujitsu-V
P-Unix-G98RevA.7\HF=-474.7470103\MP2=-476.0961474\RMSD=3.104e-09\PG=C0
1 [X(C5H11N1O3)]\\@

model 5'-deoxyadenosyl radical (related to **III**)

@37\GINC-VPP11\SP\ROMP2-FC\6-31G(d)\C5H10N1O3(2)\SDW501\18-Feb-2000\0\
\#ROMP2/6-31G(D) MAXDISK=131072000\\model for 5'-deoxyadenosine radica
l //B3-LYP/6-31G(d,p)\\0,2\C,0,0.,0.,0.\C,0,0.,0.,1.479312\O,0,1.34697
2,0.,1.983621\C,0,-0.640527,1.252831,2.145187\O,0,-2.04791,1.179391,2.
297862\C,0,0.018224,1.226891,3.527681\O,0,-0.579836,0.240306,4.348388\
C,0,1.443824,0.791406,3.169968\N,0,2.257774,1.962954,2.848578\H,0,-0.5
4002,-0.87639,1.868346\H,0,-0.331012,2.156675,1.607197\H,0,0.007556,2.
215588,4.008595\H,0,1.857463,0.152492,3.9654\H,0,3.0884,1.638946,2.357
804\H,0,2.578196,2.405142,3.708857\H,0,-2.446553,1.105522,1.421172\H,0
,-1.532422,0.289205,4.174098\H,0,-0.728245,-0.571491,-0.56411\H,0,0.73
0087,0.597583,-0.534587\\Version=Fujitsu-VP-Unix-G98RevA.7\HF=-474.109
1379\MP2=-475.4348737\RMSD=9.172e-09\PG=C01 [X(C5H10N1O3)]\\@

11

@35\GINC-PC\SP\ROMP2-FC\6-31G(d)\C5H7N1O4(1+,2)\SDW501\17-Feb-2000\0\\
#ROMP2/6-31G(D) MAXDISK=5242880000\\radical cation formed by hydride i
on removal from 4-glutamyl radical without twisted radical center\\1,2
\C,0,-0.3636320334,-1.0501676367,0.9927852386\C,0,0.9960561172,-0.6016
925469,0.5931176371\C,0,1.0133762833,0.8909984154,0.4299229028\H,0,1.7
39723792,-0.9342894518,1.329866202\H,0,1.2449255304,-1.0340330872,-0.3
872016741\C,0,1.4332201892,1.4268434226,-0.8692037464\H,0,0.7561481029
,1.5557846318,1.2481142858\C,0,-1.5987416137,-0.935700543,0.0864370716
\N,0,-0.6428917448,-1.5617332431,2.1449278905\H,0,-1.6171051357,-1.820
2130857,2.3309244543\H,0,0.0607464639,-1.7242739201,2.8605642092\O,0,-
2.677119111,-1.2889804633,0.4967226288\O,0,-1.286494222,-0.4539397278,
-1.1036328892\H,0,-2.0823193875,-0.4182804501,-1.6675706038\O,0,1.7198
836372,0.7091960864,-1.8129695707\O,0,1.4621030374,2.7669644871,-0.876
9531539\H,0,1.7694624587,3.0598283378,-1.7528828483\\Version=SGI-G98Re
vA.6\HF=-547.0606799\MP2=-548.5395313\RMSD=5.658e-09\PG=C01 [X(C5H7N1O
4)]\\@

TS:11→12

@32\GINC-PC\SP\ROMP2-FC\6-31G(d)\C5H7N1O4(1+,2)\SDW501\15-Dec-1999\0\\
#ROMP2/6-31G(D) MAXDISK=5242880000\\addition-elimination TS for rearra
ngement of radical cation formed by hydride ion removal from 4-glutamy
l radical //B3-LYP/6-31G(d,p)\\1,2\C,0,-0.72451612,0.3076994359,0.0913
976094\C,0,0.9887476017,0.2779541331,0.1329756825\C,0,0.2230046664,1.5
218127504,0.1084549172\H,0,0.2250856937,2.0938274814,-0.8156235721\H,0
,0.1492099233,2.0906364765,1.0311531228\C,0,1.6193876986,-0.2103523371
,-1.1429665664\H,0,1.3355029441,-0.1306113813,1.0771871936\C,0,-1.4513
803807,-0.1741627557,1.3308409407\N,0,-1.3075015725,-0.1017870323,-1.0
550953134\H,0,-2.1216225124,-0.7138748179,-0.9688063977\H,0,-0.8350010
246,0.0525664501,-1.9508228834\O,0,-2.4420904124,-0.8556692693,1.23481
61779\O,0,-0.8609044935,0.2432445516,2.4489277399\H,0,-1.3597011066,-0
.0876471775,3.2188493546\O,0,1.1472755631,0.0102471964,-2.2423401745\O
,0,2.7397431592,-0.8718770655,-0.8910734644\H,0,3.1553857629,-1.137658
4697,-1.7331273556\\Version=SGI-G98RevA.6\HF=-547.038682\MP2=-548.5385
348\RMSD=8.642e-09\PG=C01 [X(C5H7N1O4)]\\@

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@34\GINC-PC\SP\ROMP2-FC\6-31G(d)\C5H7N1O4(1+,2)\SDW501\27-Jan-2000\0\\
#ROMP2/6-31G(D) MAXDISK=5242880000\\cyclic cation radical intermediate
 along rearrangement pathway of radical formed via hydride ion removal
 from 4-glutamyl radical\\1,2\C,0,-0.6271060169,0.270698279,0.13744654
75\C,0,0.958355044,0.1300453992,0.0829236008\C,0,0.4216108926,1.487776
0456,0.1395475169\H,0,0.3960612448,2.0792900884,-0.7704489883\H,0,0.41
71293012,2.0201592503,1.0853719358\C,0,1.5197523159,-0.3583769751,-1.2
320090194\H,0,1.3565451901,-0.3093811421,0.9932323253\C,0,-1.399471842
4,-0.0501463711,1.400506109\N,0,-1.349577931,0.0562010256,-0.992743557
4\H,0,-2.3139847024,-0.2627599387,-0.8750425098\H,0,-0.8752294374,0.09
41881208,-1.9038125994\O,0,-2.541200262,-0.434755682,1.3403586644\O,0,
-0.6699917461,0.1515634609,2.4960261478\H,0,-1.2033926282,-0.067202315
5,3.2825369814\O,0,0.9948220516,-0.1275531033,-2.3058876811\O,0,2.6444
343958,-1.0299754708,-1.0458274678\H,0,3.006558676,-1.3019131466,-1.91
04780787\\Version=SGI-G98RevA.6\HF=-547.043489\MP2=-548.5379156\RMSD=3
.513e-09\PG=C01 [X(C5H7N1O4)]\\@

TS:12→13

@31\GINC-PC\SP\ROMP2-FC\6-31G(d)\C5H7N1O4(1+,2)\SDW501\15-Dec-1999\0\\
#ROMP2/6-31G(D) MAXDISK=5242880000\\addition-elimination TS for rearra
ngement of radical cation formed by hydride ion removal from 3-methyla
spartate derived radical //B3-LYP/6-31G(d,p)\\1,2\C,0,-0.3407643959,-0
.5407859204,-0.0967243667\C,0,1.5632731958,-0.489204855,-0.1304304656\
C,0,0.6024901034,0.637470819,-0.0749341862\H,0,1.9485729875,-0.9141325
916,0.7906720198\H,0,1.9344936554,-0.8457075363,-1.0842186566\C,0,0.61
18703608,1.4513803082,1.2138774849\H,0,0.5496243307,1.234140298,-0.983
8724396\C,0,-0.8755125506,-1.143429139,-1.384237699\N,0,-0.8766624234,
-1.047727915,1.0049405598\H,0,-1.5277278704,-1.8255009726,0.9011980882
\H,0,-0.6525815149,-0.6253015911,1.9111033557\O,0,-1.7143956901,-2.008
3278113,-1.3514927305\O,0,-0.3156561964,-0.5969365857,-2.462826091\H,0
,-0.6998324812,-1.0011335726,-3.2629020884\O,0,0.3651863824,0.97282864
22,2.3035336462\O,0,0.9456391942,2.7094192323,0.9747522151\H,0,0.96975
80547,3.2032762745,1.8163948797\\Version=SGI-G98RevA.6\HF=-547.0356428
\MP2=-548.5369177\RMSD=3.971e-09\PG=C01 [X(C5H7N1O4)]\\@

13

@30\GINC-PC\SP\ROMP2-FC\6-31G(d)\C5H7N1O4(1+,2)\SDW501\09-Dec-1999\0\\
#ROMP2/6-31G(D) MAXDISK=5242880000\\radical cation formed by hydride i
on removal from 3-methylaspartate derived radical\\1,2\C,0,0.448734485
3,-1.0775963378,1.4267543565\C,0,0.6033577855,-0.5490292907,0.02340430
26\C,0,1.9468645248,0.1704833616,-0.1619572482\C,0,-0.5942078363,0.355
7987621,-0.0513553303\H,0,0.5021620208,-1.3605848674,-0.7003520437\N,0
,-0.5291231771,1.6344281387,0.1202904971\H,0,0.4021924755,2.0696341426
,0.1985692133\H,0,-1.4013392447,2.1667789229,0.1374937554\C,0,-2.01010
10858,-0.1850097455,-0.2422921863\O,0,-2.9525788917,0.5660000738,-0.21
74896345\O,0,-2.0161133418,-1.4972473323,-0.4491741565\H,0,-2.93345398
82,-1.7985747889,-0.5893330437\O,0,2.1089164014,1.3640933224,0.0101253
264\O,0,2.8955357554,-0.6928434049,-0.4882154492\H,0,3.7482457565,-0.2
241287642,-0.5618769139\H,0,0.7188764201,-0.4479170945,2.2675825672\H,
0,0.0132121725,-2.0541062901,1.59659093\\Version=SGI-G98RevA.6\HF=-547
.0551995\MP2=-548.5380744\RMSD=4.619e-09\PG=C01 [X(C5H7N1O4)]\\@

2-aminoethyl cation

@39\GINC-PC\SP\ROMP2-FC\6-31G(d)\C2H6N1(1+)\SDW501\13-Mar-2000\0\\#ROM
P2/6-31G(D) SCF=TIGHT MAXDISK=5242880000\\aminoethyl cation //B3-LYP/6
-31G(d,p)\\1,1\C,0,0.,0.,0.\H,0,0.,0.,1.090227\N,0,1.156843,0.,-0.5694
34\C,0,-1.279351,0.,-0.725107\H,0,2.019964,0.,-0.029872\H,0,1.252531,0
.,-1.583824\H,0,-1.863088,-0.874679,-0.406892\H,0,-1.863088,0.874679,-
0.406892\H,0,-1.166988,0.,-1.810764\\Version=SGI-G98RevA.6\State=1-A'\
HF=-133.4415955\MP2=-133.8489182\RMSD=3.439e-09\PG=CS [SG(C2H4N1),X(H2
)]\\@

transition structure for hydride ion removal (See Equation 3)

@38\GINC-PC\SP\ROMP2-FC\6-31G(d)\C5H14N2(1+,2)\SDW501\12-Mar-2000\0\\#
ROMP2/6-31G(D) SCF=TIGHT MAXDISK=5242880000\\TS for hydride ion remova
l from the aminopropyl radical by the ethylamine cation //B3-LYP/6-31G
(d,p)\\1,2\H,0,-0.3931713204,0.0422173891,0.0437809074\C,0,0.805464477
7,0.3885153531,-0.2880550813\C,0,1.651881697,-0.693812292,0.4037033585
\C,0,3.0094416415,-0.7535470344,-0.209027197\N,0,1.0634930437,1.687170
2091,0.0493685552\H,0,0.7004089503,0.2479950773,-1.3680839546\H,0,1.13
93984863,-1.6556836468,0.3055447869\H,0,1.7028402447,-0.4564557303,1.4
76523331\H,0,3.2849863044,-1.5622001467,-0.8749568727\H,0,3.7124387695
,0.0583012748,-0.0629472628\H,0,0.8388077135,2.4493494872,-0.571383012
9\H,0,1.3690613315,1.9323074658,0.9799578077\C,0,-1.704218231,-0.27825
64125,0.3713245601\H,0,-1.5047371459,-0.3276959636,1.4440995554\N,0,-2
.0576858939,-1.4669360654,-0.1671588045\C,0,-2.4041343792,0.9636664861
,-0.1171387499\H,0,-1.8169748164,-2.3405434733,0.2776698955\H,0,-2.445
4259886,-1.522220488,-1.0987740812\H,0,-3.4006107888,1.0138944164,0.33
54544379\H,0,-1.8566361283,1.8616097822,0.177719624\H,0,-2.5216468958,
0.958088948,-1.2049147586\\Version=SGI-G98RevA.6\HF=-306.0525838\MP2=-
307.0217931\RMSD=2.847e-09\PG=C01 [X(C5H14N2)]\\@

ethylamine

@40\GINC-PC\SP\ROMP2-FC\6-31G(d)\C2H7N1\SDW501\13-Mar-2000\0\\#ROMP2/6
-31G(D) SCF=TIGHT MAXDISK=5242880000\\aminoethyl radical //B3-LYP/6-31
G(d,p)\\0,1\C,0,0.,0.,0.\N,0,0.,0.,1.466029\C,0,1.378684,0.,-0.672775\
H,0,0.512843,-0.8118,1.805817\H,0,1.292463,0.,-1.765629\H,0,-0.570606,
-0.876069,-0.331977\H,0,0.512843,0.8118,1.805817\H,0,1.95739,-0.885291
,-0.383464\H,0,1.95739,0.885291,-0.383464\H,0,-0.570606,0.876069,-0.33
1977\\Version=SGI-G98RevA.6\State=1-A'\HF=-134.2466425\MP2=-134.675464
7\RMSD=1.441e-09\PG=CS [SG(C2H1N1),X(H6)]\\@