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ARTICLES

Towards an Improved Understanding of the Glutamate Mutase System

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SUPPORTING INFORMATION

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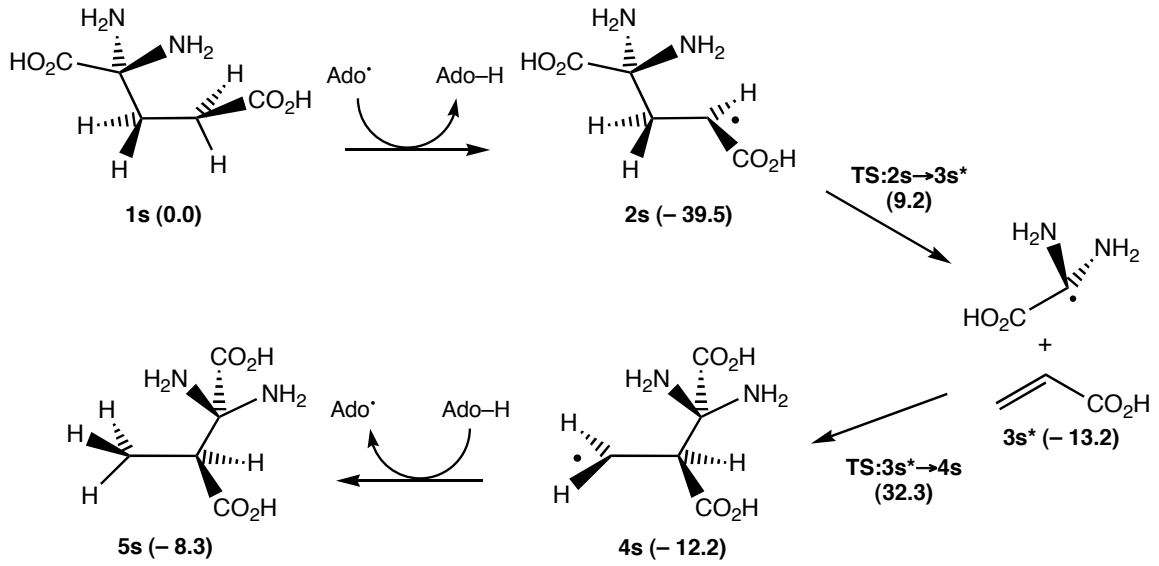
Hypothetical Isomerization of the Substrate Analogue 2,2-Diaminoglutaric Acid

The radical stabilization energies for the various substituted analogues of glycyl radical (Table 1) potentially allow us to predict beforehand which fragmentation products in a series of GM-catalyzed reactions are likely to be of higher energy and which are of lower energy. To illustrate the possible benefits of such an exercise, we have computed the energy requirements for the hypothetical isomerization of 2,2-diaminoglutaric acid (**1s**) to 2,2-diamino-3-methylsuccinic acid (**5s**) in a manner that is consistent with the catalytic pathway for GM (Scheme 2). The fragmentation step in this process involves the 2-aminoglycyl radical, $H_2N–•C(CO_2H)–NH_2$ (**3s**, Table 1), which we have found to be a strongly stabilized radical.

Scheme S1 shows the initial hydrogen abstraction by $Ado^{•}$ from 2,2-diaminoglutaric acid (**1s**) to form the substrate-derived radical **2s** to be exothermic by 39.5 kJ mol^{-1}. The barrier for fragmentation of the substrate-derived radical **2s** is calculated to be 48.7 kJ mol^{-1}, and the process is endothermic by only 26.3 kJ mol^{-1}.

Scheme S1. Schematic Energy Profile for the Hypothetical Conversion of 2,2-Diaminoglutaric Acid (**1s**) to 2,2-Diamino-3-Methylsuccinic Acid (**5s**) Catalyzed by Glutamate Mutase (energies relative to **1s** are given in parentheses, kJ mol^{-1})



Recombination of the fragments comprising **3s*** (with a barrier of 45.5 kJ mol^{-1}) yields the product-related radical **4s** in a reaction that is endothermic by 1.0 kJ mol^{-1}, leaving **4s** 27.4 kJ mol^{-1} higher in energy than the substrate-derived radical **2s**. Finally, we calculate that hydrogen re-abstraction by **4s** from Ado–H to generate the product 2,2-diamino-3-methylsuccinic acid (**5s**) and re-form Ado$^{\bullet}$ is slightly endothermic.

At this point, it is instructive to compare the results shown for the isomerization of 2,2-diaminoglutaric acid (**1s**) with those for (*S*)-glutamic acid (**1a**). In this context, it is pertinent to recall the data in Table 1, which show the RSE for **3s** to be 20.5 kJ mol^{-1} greater than that of glycyl radical (**3a**). A higher RSE for a particular radical might be expected to lead to lower energy demands for reactions involving that radical compared with those involving a radical with a lower RSE. Indeed, we observe the fragmentation barrier for **2s** to be 16.0 kJ mol^{-1} lower than that for **2a** (Scheme 2). Similarly, the

fragmentation enthalpy of **2s** is 11.7 kJ mol^{-1} lower than that for the **2a**. Furthermore, we observe a similar trend, albeit to a smaller degree, with the reverse fragmentation barrier of **4s**.

On the basis of a 20.5 kJ mol^{-1} difference in RSEs between **3s** and **3a**, one might expect larger energy differences along their respective reaction pathways than is actually observed in the explicit calculations. However, the relative stabilities of the substrate-derived and product-related radicals also contribute to the energy profile, and their contributions may not be trivial. Such a scenario is exemplified with **2s** and **4s** where intramolecular hydrogen bonds artificially stabilize these species. These artifacts of our truncated gas-phase models might potentially cancel in the enzyme environment. Hence, the use of RSEs to provide a qualitative indication of the propensity for the fragmentation process retains merit.

GAUSSIAN Archive Entries for the B3-LYP/6-31G(d,p) Optimized Geometries

1a


```
1\1\GINC-AC18\SP\ROMP2-FC\6-31G(d)\C5H9N1O4\GMS501\12-Sep-2005\0\\#ROM
 P2/6-31G* SCF=TIGHT\\glutamate from substrate radical conformer 1 b3ly
 p/6-31G**\\0,1\C,0,0.017296,-0.888529,-0.369755\C,0,0.945465,-0.013465
 ,0.490802\N,0,0.627195,1.427103,0.478173\H,0,-0.196326,1.61678,-0.0899
 25\H,0,0.44945,1.782766,1.411291\C,0,-1.405502,-1.089508,0.166793\C,0,
 -2.376322,0.03376,-0.126292\O,0,-3.633128,-0.292672,0.241185\H,0,-4.19
 4187,0.470389,0.020157\O,0,-2.113674,1.107116,-0.635076\H,0,0.503076,-
 1.864384,-0.446416\H,0,-0.027524,-0.476794,-1.38506\H,0,0.928165,-0.40
 1443,1.517987\C,0,2.406519,-0.211702,0.00365\O,0,3.021258,0.932249,-0.
 301195\O,0,2.920207,-1.305034,-0.082504\H,0,-1.406874,-1.254763,1.2523
 \H,0,2.318718,1.619018,-0.1384\H,0,-1.846899,-1.997885,-0.259608\\Vers
 ion=IA64L-G03RevC.02\State=1-A\HF=-548.5089535\MP2=-550.028034\RMSD=4.
 654e-09\PG=C01 [X(C5H9N1O4)]\\@
```


2a


```
1\1\GINC-AC18\SP\ROMP2-FC\6-31G(d)\C5H8N1O4(2)\GMS501\12-Sep-2005\0\\#
 ROMP2/6-31G* SCF=TIGHT\\glutamate from substrate radical conformer 1 b
 3lyp/6-31G**\\0,2\C,0,-0.008129,-0.910072,-0.35975\C,0,0.93037,-0.0265
 35,0.513878\N,0,0.587308,1.40351,0.507141\H,0,-0.189106,1.592641,-0.12
 64\H,0,0.313168,1.729499,1.427643\C,0,-1.392205,-1.024566,0.168259\C,0
 ,-2.388663,-0.021016,-0.139034\O,0,-3.626553,-0.333607,0.318057\H,0,-4
 .205904,0.40233,0.059751\O,0,-2.164233,1.026193,-0.745207\H,0,0.4642,-
 1.893409,-0.425213\H,0,-0.031313,-0.472488,-1.365132\H,0,0.924457,-0.4
 15649,1.538925\C,0,2.38509,-0.213394,0.001989\O,0,3.005639,0.940169,-0
 .247945\O,0,2.887433,-1.304728,-0.142294\H,0,-1.675742,-1.843905,0.821
 238\H,0,2.31203,1.625697,-0.053731\\Version=IA64L-G03RevC.02\State=2-A
 \HF=-547.8836873\MP2=-549.3824826\RMSD=4.055e-09\PG=C01 [X(C5H8N1O4)]\
 \@
```


C3-radical derived from 1a


```
1\1\GINC-AC31\SP\ROMP2-FC\6-31G(d)\C5H8N1O4(2)\GMS501\16-Nov-2005\0\\#
 ROMP2/6-31G* SCF=TIGHT\\C3 radical glutamate coords from 1I9C b3lyp/6-
 31G(d,p)\\0,2\N,0,2.012345,-1.773209,-0.222656\C,0,1.053292,-0.674493,
 -0.229603\C,0,1.744026,0.696901,-0.101655\O,0,2.890025,0.864935,0.2512
 18\C,0,0.045771,-0.858174,0.874607\C,0,-1.168141,-0.006633,1.0414\C,0,
 -2.162553,-0.089493,-0.11439\O,0,-1.958033,-0.556262,-1.212518\O,0,-3.
 347724,0.470787,0.229574\O,0,0.920353,1.727038,-0.418342\H,0,1.437591,
 2.540646,-0.286281\H,0,0.512012,-0.672239,-1.187626\H,0,2.558594,-1.74
 5991,-1.080379\H,0,2.683928,-1.605317,0.525425\H,0,0.138782,-1.776172,
 1.444876\H,0,-0.910882,1.059914,1.118186\H,0,-3.91394,0.409543,-0.5586
 88\H,0,-1.703842,-0.258564,1.961471\\Version=IA64L-G03RevC.02\State=2-
 A\HF=-547.8770052\MP2=-549.3684367\RMSD=4.163e-09\PG=C01 [X(C5H8N1O4)]
 \\@
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Acrylic acid


```
1\1\GINC-LC62\SP\ROMP2-FC\6-31G(d)\C3H4O2\GMS501\23-Feb-2005\0\\#ROMP2
 /6-31G* SCF=TIGHT\\acrlyic acid Cs symm romp2/6-31G*//b3lyp/6-31G(d,p)
 \\0,1\C,0,0.419826,-1.924138,0.\H,0,0.104497,-2.9622,0.\H,0,1.485032,-
 1.713793,0.\C,0,-0.461788,-0.922856,0.\H,0,-1.534159,-1.090009,0.\C,0,
 0.,0.48698,0.\O,0,1.155088,0.860929,0.\O,0,-1.04798,1.349702,0.\H,0,-0
 .660462,2.241031,0.\\Version=IA32L-G03RevC.02\State=1-A'\HF=-265.65143
 78\MP2=-266.3803828\RMSD=7.451e-09\PG=CS [SG(C3H4O2)]\\@
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TS:2a→3a*


```
1\1\GINC-AC41\SP\ROMP2-FC\6-31G(d)\C5H8N1O4(2)\GMS501\21-Feb-2006\0\\#
 romp2/6-31G* scf=tight\\glutamate coords from 1I9C b3lyp/6-31G(d,p)\\0
 ,2\C,0,0.204431,0.626568,1.174272\C,0,-1.209317,0.65442,-0.460819\H,0,
 -0.428385,0.714475,-1.209151\N,0,-2.040621,1.741117,-0.338195\H,0,-2.8
 09544,1.618795,0.309815\H,0,-1.627529,2.661617,-0.365326\C,0,-1.867621
 ,-0.632037,-0.20722\O,0,-2.914606,-0.74621,0.413512\O,0,-1.168654,-1.6
 89304,-0.68147\H,0,-1.659677,-2.480646,-0.404486\C,0,1.219899,-0.27745
 6,0.930116\C,0,2.285034,0.076724,0.001314\O,0,2.33613,1.106071,-0.6607
 17\O,0,3.252065,-0.878142,-0.083289\H,0,0.402577,1.671475,0.95779\H,0,
 -0.520718,0.427055,1.957349\H,0,1.199978,-1.28808,1.321113\H,0,3.89360
 9,-0.54115,-0.730003\\Version=IA64L-G03RevD.01\State=2-A\HF=-547.82953
 92\MP2=-549.3479478\RMSD=2.702e-09\Thermal=0.\PG=C01 [X(C5H8N1O4)]\\@
```


TS:3a*→4a


```
1\1\GINC-AC32\SP\ROMP2-FC\6-31G(d)\C5H8N1O4(2)\GMS501\21-Feb-2006\0\\#
 romp2/6-31G* scf=tight\\radical product glutamate coords from 1I9C TS
 recomb b3lyp/6-31G(d,p)\\0,2\C,0,-0.613377,0.335975,0.838379\C,0,0.562
 656,-0.10861,-0.794523\H,0,0.165442,0.651103,-1.463115\N,0,0.402565,-1
 .420548,-1.199827\H,0,-0.565439,-1.695669,-1.338797\H,0,0.90405,-2.066
 299,-0.598052\O,0,2.606257,-0.663527,0.298802\C,0,1.884157,0.180283,-0
 .19907\O,0,2.174965,1.504343,-0.192186\H,0,3.026338,1.590068,0.268398\
 C,0,-1.87454,0.191006,0.072957\O,0,-2.415609,-0.867559,-0.201325\O,0,-
 2.348984,1.379264,-0.377639\C,0,-0.38243,-0.587509,1.871814\H,0,-0.280
 152,1.361735,0.975683\H,0,0.402336,-0.425117,2.600497\H,0,-0.917851,-1
 .529541,1.892036\H,0,-3.144502,1.170528,-0.896423\\Version=IA64L-G03Re
 vD.01\State=2-A\HF=-547.8288671\MP2=-549.3432414\RMSD=8.006e-09\Therma
 l=0.\PG=C01 [X(C5H8N1O4)]\\@
```


4a


```
1\1\GINC-AC52\SP\ROMP2-FC\6-31G(d)\C5H8N1O4(2)\GMS501\02-Nov-2005\0\\#
 ROMP2/6-31G* SCF=TIGHT\\radical product glutamate coords from 1I9C b3l
 yp/6-31G(d,p)\\0,2\N,0,0.209647,0.30816,1.734875\C,0,-0.514031,0.14778
 9,-0.623407\C,0,-1.940692,-0.132109,-0.160249\O,0,-2.82053,0.686771,-0
 .031386\O,0,-2.133062,-1.453965,0.067033\C,0,0.484099,-0.35646,0.47545
 9\C,0,-0.328641,1.584102,-0.975426\C,0,1.930644,-0.1996,-0.002731\O,0,
 2.785193,0.441554,0.566406\O,0,2.167736,-0.886908,-1.146757\H,0,3.1045
 52,-0.743632,-1.365375\H,0,0.308605,-1.431305,0.597482\H,0,-0.333547,-
 0.488702,-1.502839\H,0,0.858737,-0.023145,2.444142\H,0,0.395509,1.3043
 ,1.632365\H,0,0.590979,1.910947,-1.447072\H,0,-1.124718,2.29575,-0.801
 769\H,0,-3.050605,-1.543275,0.374698\\Version=IA64L-G03RevC.02\State=2
 -A\HF=-547.8747605\MP2=-549.3687042\RMSD=7.441e-09\PG=C01 [X(C5H8N1O4)
 ]\\@
```


5a


```
1\1\GINC-AC50\SP\ROMP2-FC\6-31G(d)\C5H9N1O4\GMS501\02-Nov-2005\0\\#ROM
 P2/6-31G* SCF=TIGHT\\product glutamate coords from 1I9C b3lyp/6-31G(d,
 p)\\0,1\N,0,0.277691,-0.13686,1.781292\C,0,-0.511227,0.287347,-0.53055
 7\C,0,-1.935159,-0.132133,-0.18916\O,0,-2.862384,0.617529,0.013876\O,0
 ,-2.079691,-1.481824,-0.183401\C,0,0.49384,-0.474405,0.382123\C,0,-0.3
 68778,1.809777,-0.456212\C,0,1.927135,-0.207487,-0.083204\O,0,2.763729
 ,0.394757,0.553276\O,0,2.167764,-0.715716,-1.315192\H,0,3.087349,-0.48
 6547,-1.534052\H,0,0.30422,-1.542902,0.245167\H,0,-0.329428,-0.051752,
 -1.558643\H,0,0.708017,-0.843025,2.37236\H,0,0.768857,0.728934,1.99449
 4\H,0,0.636873,2.124125,-0.750548\H,0,-0.568703,2.168669,0.556416\H,0,
 -3.011203,-1.648392,0.037822\H,0,-1.090021,2.292364,-1.118464\\Version
 =IA64L-G03RevC.02\State=1-A\HF=-548.5115285\MP2=-550.0290212\RMSD=4.24
 8e-09\PG=C01 [X(C5H9N1O4)]\\@
```

1b

1\1\GINC-BAROSSA106\SP\ROMP2-FC\6-31G(d)\C5H8O5\SANDALG\30-Jun-2005\0\
\#ROMP2/6-31G* SCF=TIGHT\\2-OH-glutarate b3lyp/6-31G**\\0,1\C,0,0.9168
4,-0.016606,0.477438\C,0,2.380429,-0.194998,0.020482\O,0,2.925219,-1.2
74219,-0.005163\O,0,2.977247,0.945568,-0.345026\H,0,2.294222,1.641766,
-0.230864\C,0,0.011539,-0.911655,-0.383188\O,0,0.611491,1.370803,0.436
043\H,0,0.879188,-0.37572,1.518111\H,0,0.503159,-1.887133,-0.4276\H,0,
-0.012802,-0.519111,-1.406834\C,0,-1.418947,-1.118823,0.134844\C,0,-2.
349553,0.053698,-0.069545\H,0,-1.416688,-1.345779,1.209903\H,0,-1.8799
08,-1.987611,-0.346221\O,0,-2.016369,1.203918,-0.307678\O,0,-3.640833,
-0.296281,0.044844\H,0,-4.166701,0.513805,-0.073572\H,0,-0.296359,1.49
1771,0.092739\\Version=IA32L-G03RevC.02\State=1-A\HF=-568.3406207\MP2=
-569.8716786\RMSD=4.304e-09\PG=C01 [X(C5H8O5)]\\@

2b

1\1\GINC-BAROSSA021\SP\ROMP2-FC\6-31G(d)\C5H7O5(2)\SANDALG\30-Jun-2005
\0\\#ROMP2/6-31G* SCF=TIGHT\\radical 2-OH-glutarate b3lyp/6-31G**\\0,2
\C,0,0.880096,-0.030868,0.48114\C,0,2.355359,-0.194321,0.053785\O,0,2.
908774,-1.268353,0.036083\O,0,2.945639,0.953327,-0.297493\H,0,2.256302
,1.644666,-0.195636\C,0,0.001851,-0.92313,-0.442607\O,0,0.553013,1.345
676,0.437055\H,0,0.808856,-0.409317,1.510742\H,0,0.496281,-1.894867,-0
.501637\H,0,0.020575,-0.466961,-1.441778\C,0,-1.405491,-1.088219,0.014
783\C,0,-2.353411,-0.000745,-0.084118\H,0,-1.749611,-2.024642,0.441004
\O,0,-2.057579,1.157508,-0.394881\O,0,-3.623439,-0.355073,0.201109\H,0
,-4.162916,0.449284,0.119154\H,0,-0.35117,1.460865,0.075267\\Version=I
A32L-G03RevC.02\State=2-A\HF=-567.71377\MP2=-569.2246378\RMSD=9.024e-0
9\PG=C01 [X(C5H7O5)]\\@

C3-radical derived from 1b

1\1\GINC-AC42\SP\ROMP2-FC\6-31G(d)\C5H7O5(2)\GMS501\16-Nov-2005\0\\#RO
MP2/6-31G* SCF=TIGHT\\C2 radical 2-OH-glutarate b3lyp/6-31G**\\0,2\C,0
,0.964037,-0.654996,-0.171583\C,0,1.905821,0.554759,-0.151541\O,0,3.09
8116,0.4663,0.057444\C,0,-0.012149,-0.576553,0.968079\C,0,-1.232718,0.
283363,0.962195\C,0,-2.234137,-0.029841,-0.144758\O,0,-1.990741,-0.547
645,-1.211848\O,0,-3.47542,0.393526,0.192671\O,0,1.276492,1.725773,-0.
371298\H,0,1.953606,2.422232,-0.318841\H,0,0.40846,-0.62388,-1.121116\
H,0,0.247611,-1.142436,1.856194\H,0,-0.970167,1.344723,0.813356\H,0,-4
.044793,0.198758,-0.571578\H,0,-1.754436,0.231662,1.920889\O,0,1.73699
9,-1.831445,-0.094664\H,0,2.651032,-1.543534,0.068301\\Version=IA64L-G
03RevC.02\State=2-A\HF=-567.7049134\MP2=-569.2099635\RMSD=4.866e-09\PG
=C01 [X(C5H7O5)]\\@

TS:2b→3b*

1\1\GINC-AC41\SP\ROMP2-FC\6-31G(d)\C5H7O5(2)\GMS501\21-Feb-2006\0\\#ro
mp2/6-31G* scf=tight\\radical 2-OH-glutarate b3lyp/6-31G**\\0,2\C,0,-0
.234738,-0.814463,1.137035\C,0,1.239893,-0.653384,-0.492217\H,0,0.4842
06,-0.79401,-1.254814\O,0,2.077602,-1.692332,-0.307244\H,0,2.842813,-1
.328504,0.182728\O,0,2.899328,0.756867,0.383503\C,0,1.827089,0.653543,
-0.204227\O,0,1.0751,1.703497,-0.586857\H,0,1.545437,2.501821,-0.29413
8\C,0,-1.226702,0.122938,0.980238\C,0,-2.273095,-0.087427,-0.020614\O,
0,-2.304908,-1.004873,-0.827048\O,0,-3.232072,0.875124,0.018135\H,0,-0
.397889,-1.81712,0.756913\H,0,0.489526,-0.711401,1.938884\H,0,-1.21624
9,1.068942,1.509756\H,0,-3.862924,0.646774,-0.68453\\Version=IA64L-G03
RevD.01\State=2-A\HF=-567.6561304\MP2=-569.1834539\RMSD=5.516e-09\Ther
mal=0.\PG=C01 [X(C5H7O5)]\\@

TS:3b*→4b


```
1\1\GINC-AC46\SP\ROMP2-FC\6-31G(d)\C5H7O5(2)\GMS501\23-Feb-2006\0\\#ro
 mp2/6-31G* scf=(tight,noincfock,novaracc,maxcycle=5000,vshift=1500,nod
 iis) guess=read geom=check\\radical from product 2-OH-glutarate 21 b3l
 yp/6-31G**\\0,2\C,0,-0.654509,0.041397,0.905943\C,0,0.59571,0.279146,-
 0.78927\O,0,0.360765,-0.721841,-1.66553\H,0,0.97598,-1.440916,-1.42652
 4\H,0,0.206068,1.242321,-1.10015\C,0,1.901068,0.20182,-0.119708\O,0,2.
 245847,1.322769,0.549368\H,0,3.08687,1.129656,0.996483\O,0,2.562464,-0
 .825852,-0.112613\C,0,-1.932272,0.128609,0.140025\O,0,-2.632543,-0.805
 873,-0.182668\O,0,-2.231534,1.414228,-0.189506\C,0,-0.382588,-1.159033
 ,1.55243\H,0,-0.308915,0.97435,1.343935\H,0,0.420161,-1.24034,2.275825
 \H,0,-0.924279,-2.056494,1.276976\H,0,-3.060329,1.372343,-0.69546\\Ver
 sion=IA64L-G03RevD.01\State=2-A\HF=-567.6438831\MP2=-569.1760542\RMSD=
 9.634e-09\Thermal=0.\PG=C01 [X(C5H7O5)]\\@
```


4b


```
1\1\GINC-BAROSSA050\SP\ROMP2-FC\6-31G(d)\C5H7O5(2)\SANDALG\30-Jun-2005
 \0\\#ROMP2/6-31G* SCF=TIGHT\\radical from product 2-OH-glutarate 21 b3
 lyp/6-31G**\\0,2\H,0,0.093912,-0.03864,2.195561\C,0,0.424531,-0.840108
 ,1.545971\C,0,0.540989,-0.594164,0.072604\H,0,0.792702,-1.760803,1.979
 975\C,0,1.906299,0.038308,-0.196608\C,0,-0.558752,0.35066,-0.464887\H,
 0,0.483851,-1.540609,-0.473672\O,0,2.108959,1.23712,-0.299399\O,0,2.89
 2511,-0.870001,-0.27021\H,0,3.723667,-0.377512,-0.388287\O,0,-0.579794
 ,1.596592,0.211027\C,0,-1.938721,-0.304889,-0.312724\H,0,-0.397278,0.4
 94541,-1.54386\O,0,-2.17296,-1.411021,-0.736391\O,0,-2.853318,0.453682
 ,0.308293\H,0,-2.412929,1.288883,0.558091\H,0,0.306825,1.984327,0.0994
 93\\Version=IA32L-G03RevC.02\State=2-A\HF=-567.7032317\MP2=-569.212086
 1\RMSD=4.072e-09\PG=C01 [X(C5H7O5)]\\@
```


5b


```
1\1\GINC-BAROSSA088\SP\ROMP2-FC\6-31G(d)\C5H8O5\SANDALG\30-Jun-2005\0\
 \#ROMP2/6-31G* SCF=TIGHT\\product 2-OH-glutarate b3lyp/6-31G**\\0,1\H,
 0,0.399897,-0.237995,2.119603\C,0,0.419987,-1.079574,1.422608\H,0,1.25
 3633,-1.735811,1.682706\C,0,0.55266,-0.579121,-0.030867\H,0,-0.507311,
 -1.6473,1.530965\C,0,1.898748,0.091652,-0.223391\C,0,-0.560115,0.41178
 3,-0.428919\H,0,0.494272,-1.438289,-0.705923\O,0,2.085687,1.297933,-0.
 247804\O,0,2.908049,-0.788722,-0.339925\H,0,3.727584,-0.269842,-0.4181
 63\O,0,-0.581471,1.571831,0.389733\C,0,-1.941263,-0.25185,-0.345679\H,
 0,-0.416738,0.689358,-1.484812\O,0,-2.163727,-1.342047,-0.816925\O,0,-
 2.876305,0.484421,0.271164\H,0,-2.437402,1.299669,0.583731\H,0,0.28810
 2,1.995546,0.279443\\Version=IA32L-G03RevC.02\State=1-A\HF=-568.340916
 6\MP2=-569.873538\RMSD=4.647e-09\PG=C01 [X(C5H8O5)]\\@
```


H–HC(CO_2H)–H


```
1\1\GINC-SC107\SP\ROMP2-FC\6-31G(d)\C2H4O2\GMS501\16-Mar-2005\0\\# ROM
 P2/6-31G* SCF=TIGHT\\acetic acid romp2/6-31G*//b3lyp/6-31G**\\0,1\C,0,
 0.,0.155438,0.\O,0,0.194419,1.34993,0.\O,0,-1.247806,-0.380001,0.\H,0,
 -1.861038,0.374334,0.\C,0,1.059182,-0.917045,0.\H,0,2.044919,-0.454209
 ,0.\H,0,0.94406,-1.554957,0.88114\H,0,0.94406,-1.554957,-0.88114\\Vers
 ion=Al64T-G03RevC.02\State=1-A'\HF=-227.8081958\MP2=-228.418731\RMSD=2
 .623e-09\PG=CS [SG(C2H2O2),X(H2)]\\@
```


H–•C(CO_2H)–H


```
1\1\GINC-LC32\SP\ROMP2-FC\6-31G(d)\C2H3O2(2)\GMS501\26-Jul-2005\0\\#RO
 MP2/6-31G* SCF=TIGHT MAXDISK=39321600\\acetic acid radical Cs symm b3l
 yp/6-31G**\\0,2\C,0,0.,0.109383,0.\O,0,-0.245217,1.307656,0.\O,0,-0.98
 073,-0.836454,0.\H,0,-1.819634,-0.346964,0.\C,0,1.328875,-0.460244,0.\
 H,0,2.173961,0.214941,0.\H,0,1.480005,-1.532427,0.\\Version=IA32L-G03R
 evC.02\State=2-A"\HF=-227.1758341\MP2=-227.7644211\RMSD=3.815e-09\PG=C
 S [SG(C2H3O2)]\\@
```

H–HC(CO_2H)–NH_2

1\1\GINC-LC64\SP\ROMP2-FC\6-31G(d)\C2H5N1O2\GMS501\18-Feb-2005\0\\#ROM
P2/6-31G* SCF=TIGHT\\glycine Cs symm romp2/6-31G*//b3lyp/6-31G**\\0,1\
C,0,-0.580548,-0.858177,0.\C,0,0.,0.551593,0.\O,0,-0.972112,1.494684,0
.\O,0,1.180876,0.820624,0.\H,0,-0.519556,2.355343,0.\N,0,0.398539,-1.9
28701,0.\H,0,1.009427,-1.819593,0.806671\H,0,1.009427,-1.819593,-0.806
671\H,0,-1.237946,-0.9491,0.873037\H,0,-1.237946,-0.9491,-0.873037\\Ve
rsion=IA32L-G03RevC.02\State=1-A'\HF=-282.8280465\MP2=-283.6003968\RMS
D=6.032e-09\PG=CS [SG(C2H1N1O2),X(H4)]\\@

H–•C(CO_2H)–NH_2 (3a)

1\1\GINC-SC115\SP\ROMP2-FC\6-31G(d)\C2H4N1O2(2)\GMS501\15-Feb-2005\0\\
#ROMP2/6-31G* SCF=TIGHT\\glycyl radical C1 symm romp2/6-31G*//b3lyp/6-
31G**\\0,2\C,0,-0.71432,-0.681982,0.010147\H,0,-0.734036,-1.762793,0.0
11499\N,0,-1.885231,0.012381,-0.059922\H,0,-2.748024,-0.419205,0.23086
2\H,0,-1.798882,1.014253,0.061776\C,0,0.50125,0.073143,0.002227\O,0,0.
548358,1.304434,0.007943\O,0,1.625398,-0.703163,-0.003095\H,0,2.36593,
-0.076055,0.002285\\Version=Al64T-G03RevC.02\State=2-A\HF=-282.2134367
\MP2=-282.9752382\RMSD=7.657e-09\PG=C01 [X(C2H4N1O2)]\\@

H–HC(CO_2H)–SH

1\1\GINC-AC14\SP\ROMP2-FC\6-31G(d)\C2H4O2S1\GMS501\21-Sep-2005\0\\#ROM
P2/6-31G* SCF=TIGHT\\thiolgutarqate b3lyp/6-31G**\\0,1\H,0,0.208251,-1
.159987,1.272024\H,0,0.152291,-1.6743,-0.411879\C,0,0.241384,-0.801483
,0.237207\C,0,-0.955893,0.108395,0.032523\O,0,-0.947605,1.317046,0.075
029\O,0,-2.080249,-0.617435,-0.156767\H,0,-2.810022,0.021187,-0.232706
\S,0,1.844482,0.009038,-0.117917\H,0,1.447649,1.230125,0.294755\\Versi
on=IA64L-G03RevC.02\State=1-A\HF=-625.3094062\MP2=-626.0402713\RMSD=3.
578e-09\PG=C01 [X(C2H4O2S1)]\\@

H–•C(CO_2H)–SH (3c)

1\1\GINC-AC9\SP\ROMP2-FC\6-31G(d)\C2H3O2S1(2)\GMS501\20-Sep-2005\0\\#R
OMP2/6-31G* SCF=TIGHT\\thiolgutarqate b3lyp/6-31G**\\0,2\C,0,0.846964,
-0.377501,0.\O,0,0.44712,-1.536655,0.\O,0,2.168867,-0.060081,0.\H,0,2.
643159,-0.907598,0.\C,0,0.,0.793991,0.\S,0,-1.712372,0.632104,0.\H,0,-
1.672884,-0.72284,0.\H,0,0.417992,1.791722,0.\\Version=IA64L-G03RevC.0
2\State=2-A"\HF=-624.6900459\MP2=-625.4084624\RMSD=5.210e-09\PG=CS [SG
(C2H3O2S1)]\\@

H–HC(CO_2H)–S^-

1\1\GINC-AC52\SP\ROMP2-FC\6-31G(d)\C2H3O2S1(1-)\GMS501\16-May-2006\0\\
#romp2/6-31G* scf=tight\\thiolgutarqate b3lyp/6-31G**\\-1,1\H,0,0.2380
29,1.544579,0.875191\H,0,0.238029,1.544579,-0.875191\C,0,0.,0.924926,0
.\C,0,1.029087,-0.219264,0.\O,0,0.495038,-1.440351,0.\O,0,2.237089,-0.
032103,0.\S,0,-1.749938,0.356398,0.\H,0,-0.508583,-1.245871,0.\\Versio
n=IA64L-G03RevD.01\State=1-A'\HF=-624.7591961\MP2=-625.4947398\RMSD=3.
352e-09\Thermal=0.\PG=CS [SG(C2H1O2S1),X(H2)]\\@

H–•C(CO_2H)–S^- (3d)

1\1\GINC-AC39\SP\ROMP2-FC\6-31G(d)\C2H2O2S1(1-,2)\GMS501\16-May-2006\0
\\#romp2/6-31G* scf=tight\\thiolgutarqate b3lyp/6-31G**\\-1,2\C,0,0.,0
.817697,0.\C,0,0.980878,-0.241757,0.\O,0,0.471123,-1.518773,0.\O,0,2.2
05683,-0.080915,0.\S,0,-1.700577,0.556277,0.\H,0,-0.504413,-1.382377,0
.\H,0,0.413929,1.823811,0.\\Version=IA64L-G03RevD.01\State=2-A"\HF=-62
4.1565698\MP2=-624.8832045\RMSD=2.471e-09\Thermal=0.\PG=CS [SG(C2H2O2S
1)]\\@

H–HC(CO_2H)–OH

```
1\1\GINC-LC123\SP\ROMP2-FC\6-31G(d)\C2H4O3\GMS501\29-Jun-2005\0\\# ROM
 P2/6-31G* SCF=TIGHT MAXDISK=65536000\\cleavage product b3lyp/6-31G** 2
 -hydroxyglutarate\\0,1\H,0,-1.255717,-0.955056,0.882628\H,0,-1.255717,
 -0.955056,-0.882628\C,0,-0.604327,-0.867126,0.\C,0,0.,0.522897,0.\O,0,
 1.196821,0.72464,0.\O,0,-0.925548,1.498658,0.\H,0,-0.44473,2.344012,0.
 \O,0,0.396329,-1.848326,0.\H,0,1.241314,-1.368303,0.\\Version=IA32L-G0
 3RevC.02\State=1-A'\HF=-302.6535406\MP2=-303.4400314\RMSD=2.879e-09\PG
 =CS [SG(C2H2O3),X(H2)]\\@
```

H–•C(CO_2H)–OH (3b)

```
1\1\GINC-BAROSSA125\SP\ROMP2-FC\6-31G(d)\C2H3O3(2)\SANDALG\28-Jun-2005
 \0\\# ROMP2/6-31G* SCF=TIGHT\\cleavage product b3lyp/6-31G** 2-hydroxy
 glutarate\\0,2\C,0,0.,0.482886,0.\O,0,1.226805,0.615074,0.\O,0,-0.8674
 21,1.52345,0.\H,0,-0.322625,2.3271,0.\C,0,-0.611859,-0.813489,0.\O,0,0
 .209755,-1.868262,0.\H,0,1.11327,-1.486427,0.\H,0,-1.6726,-1.019147,0.
 \\Version=IA32L-G03RevC.02\State=2-A"\HF=-302.0362435\MP2=-302.8112572
 \RMSD=2.299e-09\PG=CS [SG(C2H3O3)]\\@
```

H–HC(CO_2H)–O^-

```
1\1\GINC-AC15\SP\ROMP2-FC\6-31G(d)\C2H3O3(1-)\GMS501\16-May-2006\0\\#r
 omp2/6-31G* scf=tight\\cleavage product b3lyp/6-31G** 2-hydroxyglutara
 te\\-1,1\H,0,-1.395673,-0.785409,0.884574\H,0,-1.395673,-0.785409,-0.8
 84574\C,0,-0.736388,-0.735882,0.\C,0,0.,0.647141,0.\O,0,1.26443,0.5248
 15,0.\O,0,-0.705767,1.675178,0.\O,0,0.213645,-1.784838,0.\H,0,1.031207
 ,-1.217975,0.\\Version=IA64L-G03RevD.01\State=1-A'\HF=-302.0898106\MP2
 =-302.8873519\RMSD=4.827e-09\Thermal=0.\PG=CS [SG(C2H1O3),X(H2)]\\@
```

H–•C(CO_2H)–O^-

```
1\1\GINC-AC2\SP\ROMP2-FC\6-31G(d)\C2H2O3(1-,2)\GMS501\16-May-2006\0\\#
  romp2/6-31G* scf=tight\\cleavage product b3lyp/6-31G** 2-hydroxygluta
 rate\\-1,2\C,0,0.,0.566305,0.\O,0,1.349738,0.223613,0.\O,0,-0.350572,1
 .757468,0.\C,0,-0.824729,-0.612994,0.\O,0,-0.299417,-1.793863,0.\H,0,-
 1.917316,-0.456667,0.\H,0,1.267704,-0.760943,0.\\Version=IA64L-G03RevD
 .01\State=2-A"\HF=-301.4687875\MP2=-302.261412\RMSD=2.926e-09\Thermal=
 0.\PG=CS [SG(C2H2O3)]\\@
```

H–HC(CO_2H)–F

```
1\1\GINC-BAROSSA084\SP\ROMP2-FC\6-31G(d)\C2H3F1O2\SANDALG\26-Jul-2005\
 0\\#ROMP2/6-31G* SCF=TIGHT\\cleavage product b3lyp/6-31G** fluoroaceti
 c1_b3p\\0,1\C,0,0.493638,-0.907277,0.\H,0,1.115377,-1.073411,0.888308\
 H,0,1.115377,-1.073411,-0.888308\F,0,-0.571901,-1.770392,0.\C,0,0.,0.5
 29688,0.\O,0,-1.151137,0.883716,0.\O,0,1.058789,1.375031,0.\H,0,0.6933
 01,2.275913,0.\\Version=IA32L-G03RevC.02\State=1-A'\HF=-326.6463023\MP
 2=-327.4227885\RMSD=3.817e-09\PG=CS [SG(C2H1F1O2),X(H2)]\\@
```

H–•C(CO_2H)–F

```
1\1\GINC-BAROSSA068\SP\ROMP2-FC\6-31G(d)\C2H2F1O2(2)\SANDALG\26-Jul-20
 05\0\\# ROMP2/6-31G* SCF=TIGHT\\cleavage product b3lyp/6-31G** fluoroa
 cetic1_b3p\\0,2\C,0,-0.78451,-0.637303,0.\H,0,-1.866571,-0.631665,0.\F
 ,0,-0.1968,-1.82717,0.\C,0,0.,0.570211,0.\O,0,-0.513336,1.680568,0.\O,
 0,1.337707,0.350528,0.\H,0,1.749867,1.229985,0.\\Version=IA32L-G03RevC
 .02\State=2-A"\HF=-326.0177543\MP2=-326.7783636\RMSD=5.344e-09\PG=CS [
 SG(C2H2F1O2)]\\@
```

HO–HC(CO_2H)–NH_2


```
1\1\GINC-BAROSSA104\SP\ROMP2-FC\6-31G(d)\C2H5N1O3\SANDALG\28-Jun-2005\
 0\\#ROMP2/6-31G* SCF=TIGHT\\hydroxyglycine1 b3lyp/6-31G**\\0,1\N,0,-1.
 266603,-1.157469,-0.176466\C,0,-0.684501,0.053878,0.374945\O,0,-1.2767
 37,1.23712,-0.091013\C,0,0.824,0.070067,0.049498\H,0,-0.77015,-0.02587
 5,1.471967\O,0,1.423741,1.109262,-0.116062\O,0,1.39028,-1.137644,-0.00
 2299\H,0,0.642649,-1.774564,0.034614\H,0,-1.435477,-1.018952,-1.171963
 \H,0,-2.166406,-1.351811,0.25284\H,0,-0.539663,1.85991,-0.223854\\Vers
 ion=IA32L-G03RevC.02\State=1-A\HF=-357.682297\MP2=-358.6369511\RMSD=6.
 812e-09\PG=C01 [X(C2H5N1O3)]\\@
```


HO–·C(CO_2H)–NH_2


```
1\1\GINC-LC34\SP\ROMP2-FC\6-31G(d)\C2H4N1O3(2)\GMS501\12-Feb-2005\0\\#
 ROMP2/6-31G* SCF=TIGHT\\hydroxyglycyl_rad9 from hydroxyglutamate romp2
 /6-31G*//b3lyp/6-31G**\\0,2\C,0,0.74693,-0.083648,-0.00285\O,0,1.34775
 3,-1.170807,0.003289\O,0,1.381784,1.132734,0.004957\H,0,2.329905,0.930
 524,0.01608\C,0,-0.670001,-0.006729,-0.001638\N,0,-1.406835,1.143873,-
 0.07666\H,0,-0.900202,1.98804,0.149237\H,0,-2.343633,1.090523,0.301376
 \O,0,-1.358722,-1.164361,0.002751\H,0,-0.666325,-1.854466,0.008879\\Ve
 rsion=IA32L-G03RevC.02\State=2-A\HF=-357.0710324\MP2=-358.0142463\RMSD
 =3.062e-09\PG=C01 [X(C2H4N1O3)]\\@
```


H_2N–HC(CO_2H)–NH_2


```
1\1\GINC-BAROSSA125\SP\ROMP2-FC\6-31G(d)\C2H6N2O2\SANDALG\27-Jul-2005\
 0\\# ROMP2/6-31G* SCF=TIGHT\\cleavage product b3lyp/6-31G** two-aminoc
 leav-nonrad1\\0,1\C,0,-0.674622,0.047584,0.362352\H,0,-0.742454,0.0294
 92,1.463631\N,0,-1.187913,-1.251091,-0.100923\H,0,-1.997064,-1.541959,
 0.439591\H,0,-1.497601,-1.136364,-1.065307\N,0,-1.315303,1.192971,-0.2
 51105\H,0,-2.100017,1.523593,0.301339\H,0,-0.632688,1.945599,-0.317139
 \C,0,0.842753,0.105416,0.053553\O,0,1.452849,1.148121,-0.017867\O,0,1.
 402725,-1.098746,-0.080577\H,0,0.638952,-1.726522,-0.065793\\Version=I
 A32L-G03RevC.02\State=1-A\HF=-337.849773\MP2=-338.7914059\RMSD=7.075e-
 09\PG=C01 [X(C2H6N2O2)]\\@
```


H_2N–·C(CO_2H)–NH_2 (3s)


```
1\1\GINC-BAROSSA148\SP\ROMP2-FC\6-31G(d)\C2H5N2O2(2)\SANDALG\29-Apr-20
 05\0\\# ROMP2/6-31G* SCF=TIGHT\\2-aminoglut cleavage product b3lyp/6-3
 1G**\\0,2\C,0,0.662044,0.027842,0.001724\C,0,-0.753001,-0.15091,0.0042
 52\O,0,-1.320317,-1.248935,0.019466\O,0,-1.450609,1.038491,-0.019693\H
 ,0,-2.385269,0.781743,-0.01318\N,0,1.271908,1.266358,0.092176\N,0,1.47
 3045,-1.08763,-0.096172\H,0,2.266322,-1.092567,0.536912\H,0,0.921589,-
 1.937389,-0.038693\H,0,0.617799,2.034896,0.021673\H,0,2.078032,1.38418
 6,-0.512781\\Version=IA32L-G03RevC.02\State=2-A\HF=-337.2452657\MP2=-3
 38.1732395\RMSD=3.250e-09\PG=C01 [X(C2H5N2O2)]\\@
```


F–HC(CO_2H)–NH_2


```
1\1\GINC-BAROSSA089\SP\ROMP2-FC\6-31G(d)\C2H4F1N1O2\SANDALG\26-Jul-200
 5\0\\# ROMP2/6-31G* SCF=TIGHT\\cleavage product b3lyp/6-31G** fluorogl
 ycine1_b3p\\0,1\C,0,0.673446,-0.281416,-0.354887\H,0,0.688206,-0.92723
 8,-1.236019\C,0,-0.747455,0.170273,-0.012442\O,0,-1.003226,1.139282,0.
 66447\O,0,-1.673968,-0.665348,-0.515061\H,0,-2.538982,-0.339354,-0.211
 319\N,0,1.482474,0.851395,-0.536149\H,0,1.369202,1.507506,0.230924\H,0
 ,2.458721,0.614834,-0.67015\F,0,1.056349,-1.104459,0.738701\\Version=I
 A32L-G03RevC.02\State=1-A\HF=-381.681326\MP2=-382.6238889\RMSD=5.046e-
 09\PG=C01 [X(C2H4F1N1O2)]\\@
```

F–•C(CO_2H)–NH_2

```
1\1\GINC-BAROSSA125\SP\ROMP2-FC\6-31G(d)\C2H3F1N1O2(2)\SANDALG\27-Jul-
 2005\0\\# ROMP2/6-31G* SCF=TIGHT\\cleavage product b3lyp/6-31G** fluor
 oglycine1_b3p\\0,2\C,0,0.652748,-0.078481,0.019786\C,0,-0.751888,0.165
 894,0.005728\O,0,-1.218073,1.308242,0.022925\O,0,-1.513947,-0.96213,-0
 .015034\H,0,-2.431688,-0.646916,-0.010681\N,0,1.55675,0.935917,-0.0928
 39\H,0,1.135376,1.849307,0.025197\H,0,2.453708,0.801367,0.356247\F,0,1
 .155151,-1.316505,0.006988\\Version=IA32L-G03RevC.02\State=2-A\HF=-381
 .0566943\MP2=-381.9872276\RMSD=2.183e-09\PG=C01 [X(C2H3F1N1O2)]\\@
```

HO–HC(CO_2H)–OH

```
1\1\GINC-SC96\SP\ROMP2-FC\6-31G(d)\C2H4O4\GMS501\26-Feb-2005\0\\#ROMP2
 /6-31G* SCF=TIGHT\\23S dihydroxyacetic acid romp2/6-31G*//b3lyp/6-31G(
 d,p)\\0,1\C,0,0.693928,-0.219972,0.374686\H,0,0.744485,-0.678566,1.370
 493\C,0,-0.75397,0.143604,0.018974\O,0,-1.045483,1.173045,-0.54944\O,0
 ,-1.635339,-0.797844,0.382599\H,0,-2.51119,-0.498674,0.082321\O,0,1.08
 5629,-1.129514,-0.632346\H,0,2.022255,-1.320877,-0.482578\O,0,1.468037
 ,0.933801,0.417318\H,0,1.121941,1.520422,-0.277252\\Version=Al64T-G03R
 evC.02\State=1-A\HF=-377.5125308\MP2=-378.4778289\RMSD=5.884e-09\PG=C0
 1 [X(C2H4O4)]\\@
```

HO–•C(CO_2H)–OH (3f)

```
1\1\GINC-LC18\SP\ROMP2-FC\6-31G(d)\C2H3O4(2)\GMS501\24-Feb-2005\0\\#RO
 MP2/6-31G* SCF=TIGHT\\Cs dihydroxyacetic acid radical romp2/6-31G*//b3
 lyp/6-31G(d,p)\\0,2\O,0,-1.113176,-1.358496,0.\C,0,0.109833,-0.729663,
 0.\O,0,1.19646,-1.321465,0.\C,0,0.,0.685771,0.\O,0,1.101474,1.437276,0
 .\O,0,-1.14702,1.373473,0.\H,0,-0.931067,-2.310554,0.\H,0,1.84087,0.80
 0312,0.\H,0,-1.870704,0.7273,0.\\Version=IA32L-G03RevC.02\State=2-A"\H
 F=-376.8931509\MP2=-377.8504176\RMSD=7.570e-09\PG=CS [SG(C2H3O4)]\\@
```

O=HC(CO_2H)

```
1\1\GINC-BAROSSA063\SP\ROMP2-FC\6-31G(d)\C2H2O3\SANDALG\28-Jun-2005\0\
 \#ROMP2/6-31G* SCF=TIGHT\\formylformic b3lyp/6-31G(d,p)\\0,1\C,0,0.,0.
 584127,0.\C,0,-0.75137,-0.752687,0.\H,0,-1.852485,-0.675527,0.\O,0,-0.
 578795,1.641904,0.\O,0,-0.144285,-1.801869,0.\O,0,1.329466,0.436391,0.
 \H,0,1.509617,-0.52452,0.\\Version=IA32L-G03RevC.02\State=1-A'\HF=-301
 .4758172\MP2=-302.2562192\RMSD=5.320e-09\PG=CS [SG(C2H2O3)]\\@
```

O=•C(CO_2H) (3e)

```
1\1\GINC-SC64\SP\ROMP2-FC\6-31G(d)\C2H1O3(2)\GMS501\27-Feb-2005\0\\#RO
 MP2/6-31G* SCF=TIGHT\\formylformic radical romp2/6-31G*//b3lyp/6-31G(d
 ,p)\\0,2\C,0,0.472635,0.114325,0.02283\O,0,0.963847,1.21624,-0.041598\
 O,0,1.128187,-1.057177,-0.043558\H,0,2.069882,-0.849059,-0.17744\C,0,-
 0.971281,-0.098853,0.404952\O,0,-1.976784,-0.064534,-0.2135\\Version=A
 l64T-G03RevC.02\State=2-A\HF=-300.848153\MP2=-301.6192816\RMSD=9.793e-
 09\PG=C01 [X(C2H1O3)]\\@
```

1c

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1\1\GINC-AC27\SP\ROMP2-FC\6-31G(d)\C5H8O4S1\GMS501\23-Feb-2006\0\\#rom
 p2/6-31G* scf=tight\\Xtal thiolgutarqate b3lyp/6-31G**\\0,1\C,0,0.7918
 63,-0.33608,-0.13791\C,0,1.224174,1.116277,-0.034897\O,0,1.389963,1.71
 4824,1.007899\C,0,-0.149204,-0.745586,1.001142\C,0,-1.468773,0.035048,
 1.036318\C,0,-2.368842,-0.223585,-0.152482\O,0,-2.116667,-0.939194,-1.
 098846\O,0,-3.536585,0.452965,-0.045485\O,0,1.417509,1.679909,-1.24560
 6\H,0,1.739277,2.582596,-1.080254\H,0,0.318616,-0.50839,-1.106048\H,0,
```

-0.354315,-1.814357,0.901408\H,0,0.365216,-0.589255,1.953961\H,0,-1.29
3018,1.114602,1.109668\H,0,-4.050743,0.234883,-0.841531\H,0,-2.036418,
-0.224978,1.937609\S,0,2.320955,-1.381415,-0.195192\H,0,2.767045,-1.03
695,1.031533\\Version=IA64L-G03RevD.01\State=1-A\HF=-890.995765\MP2=-8
92.4689081\RMSD=8.696e-09\Thermal=0.\PG=C01 [X(C5H8O4S1)]\\@

2c

1\1\GINC-AC49\SP\ROMP2-FC\6-31G(d)\C5H7O4S1(2)\GMS501\23-Feb-2006\0\\#
romp2/6-31G* scf=tight\\thiolgutarqate b3lyp/6-31G**\\0,2\C,0,0.810598
,-0.334837,-0.157185\C,0,1.2719,1.109656,-0.05946\O,0,1.444071,1.70437
4,0.983366\C,0,-0.188897,-0.690833,0.970645\C,0,-1.432468,0.127897,0.8
91824\C,0,-2.460641,-0.209317,-0.074067\O,0,-2.381366,-1.128795,-0.88\
O,0,-3.542695,0.611855,-0.008919\O,0,1.486648,1.659564,-1.271361\H,0,1
.822774,2.558168,-1.1119\H,0,0.350954,-0.511661,-1.13155\H,0,-0.432825
,-1.751053,0.859099\H,0,0.302795,-0.531376,1.933571\H,0,-1.559564,1.01
3359,1.504828\H,0,-4.156229,0.299667,-0.694375\S,0,2.304215,-1.426887,
-0.152287\H,0,2.748431,-1.038288,1.061695\\Version=IA64L-G03RevD.01\St
ate=2-A\HF=-890.3690124\MP2=-891.8210819\RMSD=9.384e-09\Thermal=0.\PG=
C01 [X(C5H7O4S1)]\\@

C3-radical derived from 1c

1\1\GINC-AC13\SP\ROMP2-FC\6-31G(d)\C5H7O4S1(2)\GMS501\25-Aug-2006\0\\#
romp2/6-31G* scf=tight\\thiolgutarqate b3lyp/6-31G**\\0,2\C,0,-0.70190
3,0.026798,-0.114492\C,0,-1.959118,-0.766951,0.188461\O,0,-2.512493,-0
.798031,1.2667\C,0,0.230439,0.050817,1.023993\C,0,1.651231,0.487713,0.
886765\C,0,2.478302,-0.30408,-0.117119\O,0,2.054847,-0.988799,-1.02223
7\O,0,3.80123,-0.121088,0.099924\O,0,-2.405878,-1.434035,-0.894182\H,0
,-3.225492,-1.881272,-0.622348\H,0,-0.230581,-0.331303,-1.030516\H,0,-
0.197571,-0.048614,2.015943\H,0,2.167178,0.464229,1.85004\H,0,4.262774
,-0.619304,-0.596314\H,0,1.704821,1.536708,0.544835\S,0,-1.270073,1.78
7397,-0.59739\H,0,-1.855315,2.051053,0.589303\\Version=IA64L-G03RevD.0
1\State=2-A\HF=-890.361583\MP2=-891.8122843\RMSD=7.462e-09\Thermal=0.\
PG=C01 [X(C5H7O4S1)]\\@

TS:2c→3c*

1\1\GINC-AC38\SP\ROMP2-FC\6-31G(d)\C5H7O4S1(2)\GMS501\23-Feb-2006\0\\#
romp2/6-31G* scf=tight\\thiolgutarqate b3lyp/6-31G**\\0,2\C,0,-0.36043
2,-0.734033,1.181428\C,0,1.091873,-0.295157,-0.406591\H,0,0.397113,-0.
578845,-1.188498\S,0,2.45759,-1.374639,-0.2074\H,0,3.179541,-0.490457,
0.518733\C,0,1.325669,1.13889,-0.179979\O,0,2.254788,1.608742,0.456796
\O,0,0.347857,1.903599,-0.721193\H,0,0.557563,2.821204,-0.479072\C,0,-
1.473911,0.052772,0.998926\C,0,-2.464174,-0.314087,-0.015568\O,0,-2.35
7267,-1.242899,-0.801372\O,0,-3.542869,0.511334,-0.010225\H,0,-0.38161
7,-1.751828,0.808801\H,0,0.322388,-0.528671,1.998728\H,0,-1.604368,0.9
96832,1.515708\H,0,-4.126279,0.189473,-0.717354\\Version=IA64L-G03RevD
.01\State=2-A\HF=-890.3072549\MP2=-891.7807069\RMSD=9.843e-09\Thermal=
0.\PG=C01 [X(C5H7O4S1)]\\@

TS:3c*→4c

1\1\GINC-AC44\SP\ROMP2-FC\6-31G(d)\C5H7O4S1(2)\GMS501\23-Feb-2006\0\\#
romp2/6-31G* scf=tight\\thiolgutarqate b3lyp/6-31G**\\0,2\C,0,0.732906
,-0.975045,0.452071\C,0,-0.594199,0.292768,-0.58858\C,0,-1.863035,-0.3
54906,-0.197825\H,0,-1.302695,1.955947,0.838827\O,0,-2.602305,0.01833,
0.693812\O,0,-2.084856,-1.492412,-0.904967\H,0,-2.904144,-1.875184,-0.
548548\H,0,-0.221229,0.049244,-1.577939\S,0,-0.421759,1.999107,-0.1841
9\C,0,1.998582,-0.353019,-0.037684\O,0,2.7128,0.392658,0.596103\O,0,2.

264188,-0.703445,-1.324199\C,0,0.496753,-0.940046,1.823569\H,0,0.38859
4,-1.831115,-0.121895\H,0,-0.291533,-1.532095,2.273221\H,0,1.044256,-0
.243545,2.447873\H,0,3.090223,-0.248526,-1.559805\\Version=IA64L-G03Re
vD.01\State=2-A\HF=-890.2967519\MP2=-891.7726792\RMSD=3.472e-09\Therma
l=0.\PG=C01 [X(C5H7O4S1)]\\@

4c

1\1\GINC-AC11\SP\ROMP2-FC\6-31G(d)\C5H7O4S1(2)\GMS501\23-Feb-2006\0\\#
romp2/6-31G* scf=tight\\thiolgutarqate b3lyp/6-31G**\\0,2\C,0,-1.88116
6,-0.38517,-0.132216\C,0,-0.478707,0.114078,-0.451172\S,0,-0.338566,1.
929337,-0.218274\H,0,-0.869881,1.942917,1.020213\O,0,-2.594014,0.01006
1,0.761973\C,0,0.567472,-0.718038,0.368241\C,0,1.993543,-0.399405,-0.0
82042\O,0,2.938874,-0.221132,0.648572\O,0,2.099095,-0.388471,-1.432509
\C,0,0.425195,-0.601947,1.846107\O,0,-2.22633,-1.401749,-0.95601\H,0,-
3.106681,-1.701807,-0.670151\H,0,-0.28684,-0.055574,-1.51094\H,0,0.399
381,-1.764958,0.049383\H,0,-0.548557,-0.709371,2.306775\H,0,1.301228,-
0.438739,2.45861\H,0,3.029386,-0.188633,-1.631226\\Version=IA64L-G03Re
vD.01\State=2-A\HF=-890.3522126\MP2=-891.8065922\RMSD=9.289e-09\Therma
l=0.\PG=C01 [X(C5H7O4S1)]\\@

5c

1\1\GINC-AC41\SP\ROMP2-FC\6-31G(d)\C5H8O4S1\GMS501\23-Feb-2006\0\\#rom
p2/6-31G* scf=tight\\thiolgutarqate b3lyp/6-31G**\\0,1\C,0,-1.884808,-
0.351661,-0.226348\C,0,-0.48039,0.192792,-0.454624\S,0,-0.345043,1.946
57,0.085879\H,0,-1.164314,1.816666,1.148368\C,0,0.564271,-0.764915,0.1
94041\C,0,1.987419,-0.351153,-0.167854\O,0,2.933717,-0.372435,0.583997
\O,0,2.100039,0.005541,-1.471737\C,0,0.419536,-0.935086,1.70728\O,0,-2
.665012,0.003029,0.627538\O,0,-2.148484,-1.359292,-1.089966\H,0,-3.034
33,-1.691922,-0.864072\H,0,-0.298593,0.206944,-1.529916\H,0,0.414609,-
1.738777,-0.296469\H,0,-0.570501,-1.319308,1.965032\H,0,0.566722,0.018
645,2.219725\H,0,3.034005,0.237373,-1.60932\H,0,1.174843,-1.629352,2.0
78949\\Version=IA64L-G03RevD.01\State=1-A\HF=-890.9891783\MP2=-892.467
7628\RMSD=5.714e-09\Thermal=0.\PG=C01 [X(C5H8O4S1)]\\@

1d

1\1\GINC-AC14\SP\ROMP2-FC\6-31G(d)\C5H7O4S1(1-)\GMS501\16-May-2006\0\\
#romp2/6-31G* scf=tight\\Xtal thiolgutarqate b3lyp/6-31G**\\-1,1\C,0,0
.762867,-0.392984,-0.24331\C,0,1.256509,0.957593,0.187895\O,0,1.336387
,1.384117,1.332876\C,0,-0.197118,-0.991679,0.79029\C,0,-1.475485,-0.15
7859,1.104811\C,0,-2.408191,-0.057206,-0.069799\O,0,-3.231485,-0.88593
5,-0.410403\O,0,-2.236649,1.092398,-0.783177\O,0,1.625576,1.759038,-0.
858794\H,0,1.990517,2.546354,-0.423737\H,0,0.258556,-0.275616,-1.21040
8\H,0,-0.484891,-1.98977,0.447752\H,0,0.355039,-1.113271,1.726029\H,0,
-1.177893,0.838727,1.438685\H,0,-2.828687,1.003327,-1.548668\H,0,-2.03
1932,-0.653667,1.90689\S,0,2.271073,-1.456264,-0.449993\\Version=IA64L
-G03RevD.01\State=1-A\HF=-890.4359841\MP2=-891.9097322\RMSD=5.264e-09\
Thermal=0.\PG=C01 [X(C5H7O4S1)]\\@

2d

1\1\GINC-AC17\SP\ROMP2-FC\6-31G(d)\C5H6O4S1(1-,2)\GMS501\16-May-2006\0
\\#romp2/6-31G* scf=tight\\thiolgutarqate b3lyp/6-31G**\\-1,2\C,0,0.93
3913,-0.369889,-0.242247\C,0,1.520813,0.996494,-0.006013\O,0,1.572622,
1.608429,1.047037\C,0,-0.255804,-0.626375,0.784863\C,0,-1.39033,0.2927
67,0.576204\C,0,-2.602097,-0.112103,-0.051873\O,0,-2.912792,-1.236873,
-0.458232\O,0,-3.525072,0.922853,-0.176737\O,0,2.027897,1.553718,-1.14
8289\H,0,2.421857,2.388238,-0.845542\H,0,0.524829,-0.402897,-1.256001\

H,0,-0.568576,-1.663662,0.65849\H,0,0.19147,-0.497409,1.774416\H,0,-1.
279142,1.343953,0.822452\H,0,-4.282349,0.48606,-0.596633\S,0,2.278231,
-1.595291,-0.064563\\Version=IA64L-G03RevD.01\State=2-A\HF=-889.809475
9\MP2=-891.2653911\RMSD=8.865e-09\Thermal=0.\PG=C01 [X(C5H6O4S1)]\\@

C3-radical derived from 1d

1\1\GINC-AC22\SP\ROMP2-FC\6-31G(d)\C5H6O4S1(1-,2)\GMS501\25-Aug-2006\0
\\#romp2/6-31G* scf=tight\\thiolgutarqate b3lyp/6-31G**\\-1,2\C,0,-1.1
16731,-0.29845,0.660952\C,0,-1.518482,0.98014,-0.014279\O,0,-1.004689,
1.539566,-0.970655\C,0,0.326168,-0.626805,0.681262\C,0,1.230199,-0.507
718,-0.519614\C,0,2.597835,-0.043585,-0.080008\O,0,3.569771,-0.744316,
0.139275\O,0,2.671425,1.308569,0.097528\O,0,-2.623616,1.540478,0.57624
9\H,0,-2.833092,2.293398,-0.000114\H,0,-1.513744,-0.276139,1.679208\H,
0,0.624639,-1.356818,1.430937\H,0,0.802959,0.212775,-1.219778\H,0,3.57
4847,1.458035,0.422246\H,0,1.365257,-1.471823,-1.027147\S,0,-2.002371,
-1.689706,-0.274651\\Version=IA64L-G03RevD.01\State=2-A\HF=-889.803237
6\MP2=-891.2551402\RMSD=5.080e-09\Thermal=0.\PG=C01 [X(C5H6O4S1)]\\@

TS:2d→3d*

1\1\GINC-AC14\SP\ROMP2-FC\6-31G(d)\C5H6O4S1(1-,2)\GMS501\16-May-2006\0
\\#romp2/6-31G* scf=tight\\thiolgutarqate b3lyp/6-31G**\\-1,2\C,0,-0.2
27268,-0.753192,0.976038\C,0,1.238448,-0.330151,-0.415723\H,0,0.606941
,-0.525356,-1.280522\S,0,2.582595,-1.38457,-0.160543\C,0,1.360168,1.11
5408,-0.128904\O,0,1.995085,1.673845,0.749658\O,0,0.572072,1.859446,-0
.980489\H,0,0.656399,2.765061,-0.640377\C,0,-1.375844,0.040745,0.87646
7\C,0,-2.470792,-0.320231,0.02749\O,0,-2.601468,-1.329592,-0.667608\O,
0,-3.501994,0.613264,0.049702\H,0,-0.306757,-1.783653,0.646145\H,0,0.4
43223,-0.588445,1.813047\H,0,-1.425747,1.009507,1.363025\H,0,-4.153408
,0.224832,-0.554925\\Version=IA64L-G03RevD.01\State=2-A\HF=-889.769743
2\MP2=-891.2571276\RMSD=4.372e-09\Thermal=0.\PG=C01 [X(C5H6O4S1)]\\@

TS:3d*→4d

1\1\GINC-AC11\SP\ROMP2-FC\6-31G(d)\C5H6O4S1(1-,2)\GMS501\16-May-2006\0
\\#romp2/6-31G* scf=tight\\thiolgutarqate b3lyp/6-31G**\\-1,2\C,0,0.60
5423,-0.951635,0.254504\C,0,-0.541568,0.406122,-0.43316\C,0,-1.860833,
-0.235542,-0.141785\O,0,-2.513824,-0.234389,0.882098\O,0,-2.312296,-0.
963431,-1.231341\H,0,-3.142153,-1.354618,-0.911768\H,0,-0.294706,0.248
627,-1.485059\S,0,-0.302152,2.047878,0.12797\C,0,1.938718,-0.400593,-0
.104824\O,0,2.756432,0.098949,0.643015\O,0,2.190665,-0.485797,-1.45211
3\C,0,0.434466,-1.271718,1.639362\H,0,0.297322,-1.730799,-0.446101\H,0
,-0.420658,-1.858094,1.956668\H,0,0.947855,-0.676748,2.385321\H,0,3.02
1714,0.003112,-1.564425\\Version=IA64L-G03RevD.01\State=2-A\HF=-889.76
39468\MP2=-891.2302109\RMSD=5.022e-09\Thermal=0.\PG=C01 [X(C5H6O4S1)]\
\@

4d

1\1\GINC-AC11\SP\ROMP2-FC\6-31G(d)\C5H6O4S1(1-,2)\GMS501\16-May-2006\0
\\#romp2/6-31G* scf=tight\\thiolgutarqate b3lyp/6-31G**\\-1,2\C,0,1.82
5618,0.329894,-0.384801\C,0,0.472368,-0.308318,-0.239953\S,0,0.516927,
-1.404927,1.250436\O,0,2.198782,1.425127,0.009894\C,0,-0.658271,0.7643
42,-0.145953\C,0,-2.012691,0.115344,-0.375435\O,0,-3.015067,0.244012,0
.297238\O,0,-2.050021,-0.61411,-1.53081\C,0,-0.648392,1.555301,1.12033
9\O,0,2.70273,-0.469325,-1.07268\H,0,3.543738,0.011933,-1.011834\H,0,0
.306753,-0.907209,-1.141025\H,0,-0.531811,1.441844,-1.01681\H,0,0.2859
63,1.992734,1.440361\H,0,-1.494571,1.506657,1.792113\H,0,-2.944082,-0.
992122,-1.544094\\Version=IA64L-G03RevD.01\State=2-A\HF=-889.7966406\M
P2=-891.2487478\RMSD=9.711e-09\Thermal=0.\PG=C01 [X(C5H6O4S1)]\\@

5d

1\1\GINC-AC11\SP\ROMP2-FC\6-31G(d)\C5H7O4S1(1-)\GMS501\16-May-2006\0\\
#romp2/6-31G* scf=tight\\thiolgutarqate b3lyp/6-31G**\\-1,1\C,0,1.8385
7,0.27499,-0.414566\C,0,0.483496,-0.340019,-0.19767\S,0,0.540221,-1.27
1436,1.403422\C,0,-0.65909,0.717857,-0.286695\C,0,-2.000697,0.013854,-
0.396491\O,0,-3.002098,0.24088,0.251957\O,0,-2.031743,-0.904758,-1.408
578\C,0,-0.690082,1.744219,0.847195\O,0,2.220664,1.404105,-0.141333\O,
0,2.710013,-0.596557,-1.017418\H,0,3.552876,-0.114827,-1.01024\H,0,0.3
30495,-1.053001,-1.012344\H,0,-0.541076,1.245799,-1.249931\H,0,0.23089
9,2.327594,0.831058\H,0,-0.75247,1.214465,1.799984\H,0,-2.916655,-1.29
8951,-1.344968\H,0,-1.555471,2.407128,0.744019\\Version=IA64L-G03RevD.
01\State=1-A\HF=-890.4341585\MP2=-891.9107639\RMSD=5.423e-09\Thermal=0
.\PG=C01 [X(C5H7O4S1)]\\@

1e

1\1\GINC-BAROSSA105\SP\ROMP2-FC\6-31G(d)\C5H6O5\SANDALG\28-Jun-2005\0\
\#ROMP2/6-31G* SCF=TIGHT\\ketoglutarate b3lyp/6-31G(d,p)\\0,1\O,0,-1.0
30302,-1.27474,1.253115\C,0,-1.48686,-0.637806,0.331668\C,0,-1.017619,
0.787429,-0.048526\O,0,-1.668793,1.380063,-0.891199\O,0,-2.480075,-1.0
59915,-0.451486\H,0,-2.657541,-0.325098,-1.075834\C,0,0.118116,1.42438
7,0.722708\H,0,0.383146,2.337671,0.183662\H,0,-0.289782,1.726069,1.696
512\C,0,1.347701,0.536734,0.962308\H,0,1.113631,-0.246781,1.689565\H,0
,2.178894,1.12231,1.364467\C,0,1.78394,-0.163467,-0.301977\O,0,1.06711
3,-0.354577,-1.264861\O,0,3.058345,-0.593996,-0.243398\H,0,3.229673,-1
.072527,-1.072828\\Version=IA32L-G03RevC.02\State=1-A\HF=-567.1753291\
MP2=-568.6965741\RMSD=7.545e-09\PG=C01 [X(C5H6O5)]\\@

2e

1\1\GINC-BAROSSA124\SP\ROMP2-FC\6-31G(d)\C5H5O5(2)\SANDALG\29-Jun-2005
\0\\#ROMP2/6-31G* SCF=TIGHT\\ketoglutarate substrate radical b3lyp/6-3
1G(d,p)\\0,2\O,0,-2.332793,-1.236453,-0.325062\H,0,-2.634545,-0.548614
,-0.953597\C,0,-1.338271,-0.689542,0.374076\O,0,-0.742743,-1.243048,1.
267881\C,0,-1.056956,0.770546,-0.05215\O,0,-1.804298,1.28701,-0.85972\
C,0,0.049082,1.507789,0.685866\H,0,0.189819,2.462446,0.160021\H,0,-0.3
29828,1.747634,1.687822\C,0,1.328961,0.753818,0.802647\H,0,1.952018,0.
840729,1.684234\C,0,1.751745,-0.082345,-0.297471\O,0,1.060459,-0.29185
9,-1.29204\O,0,2.979122,-0.625603,-0.133966\H,0,3.137201,-1.184172,-0.
913045\\Version=IA32L-G03RevC.02\State=2-A\HF=-566.54683\MP2=-568.0472
184\RMSD=8.187e-09\PG=C01 [X(C5H5O5)]\\@

C3-radical derived from 1e

1\1\GINC-AC7\SP\ROMP2-FC\6-31G(d)\C5H5O5(2)\GMS501\14-Jul-2005\0\\#ROM
P2/6-31G* SCF=TIGHT\\C2 rad bent ketoglutarate b3lyp/6-31G(d,p)\\0,2\O
,0,0.543721,-1.490185,-0.727425\C,0,1.379622,-0.775096,-0.222853\C,0,1
.233728,0.748566,-0.042878\O,0,2.22519,1.355113,0.412105\O,0,2.5599,-1
.210668,0.220563\H,0,3.030923,-0.415325,0.549337\C,0,0.035578,1.432185
,-0.404397\H,0,0.081981,2.510591,-0.280135\C,0,-1.238997,0.797285,-0.8
43867\H,0,-1.063488,0.079462,-1.652385\H,0,-1.949339,1.546972,-1.20470
1\C,0,-1.904945,0.008304,0.283375\O,0,-1.473106,-0.122985,1.404212\O,0
,-3.068289,-0.526388,-0.139408\H,0,-3.429313,-1.02828,0.611229\\Versio
n=IA64L-G03RevC.02\State=2-A\HF=-566.5462927\MP2=-568.050455\RMSD=2.54
1e-09\PG=C01 [X(C5H5O5)]\\@

TS:2e→3e*


```
1\1\GINC-AC12\SP\ROMP2-FC\6-31G(d)\C5H5O5(2)\GMS501\22-Feb-2006\0\\#ro
 mp2/6-31G* scf=tight\\TS intra ketoglutarate substrate radical b3lyp/6
 -31G(d,p)\\0,2\C,0,0.577728,-0.572256,1.520253\C,0,-1.239777,0.737548,
 0.550461\O,0,-1.05099,1.817822,0.08778\C,0,-2.147338,-0.336401,-0.1358
 12\O,0,-2.059397,-1.515099,0.069948\O,0,-3.104409,0.22243,-0.896735\H,
 0,-2.915778,1.171236,-1.00045\C,0,1.184283,-0.88217,0.354944\C,0,2.271
 401,-0.029685,-0.174346\O,0,2.698195,0.981903,0.346084\O,0,2.757993,-0
 .515407,-1.344288\H,0,0.93206,0.26768,2.108884\H,0,-0.175403,-1.225213
 ,1.944376\H,0,0.885918,-1.743789,-0.23253\H,0,3.464284,0.094676,-1.615
 599\\Version=IA64L-G03RevD.01\State=2-A\HF=-566.4817604\MP2=-567.99305
 51\RMSD=6.742e-09\Thermal=0.\PG=C01 [X(C5H5O5)]\\@
```


TS:3e*→4e


```
1\1\GINC-AC12\SP\ROMP2-FC\6-31G(d)\C5H5O5(2)\GMS501\22-Feb-2006\0\\#ro
 mp2/6-31G* scf=tight\\TS intra ketoglutarate substrat b3lyp/6-31G(d,p)
 \\0,2\C,0,0.902407,0.927959,0.105698\C,0,-0.708343,-0.628674,-0.00302\
 O,0,-0.607195,-1.582605,-0.7145\O,0,-2.101937,1.273028,0.628985\C,0,-2
 .034286,0.140677,0.230665\O,0,-3.107858,-0.653159,0.061862\H,0,-2.8223
 95,-1.485728,-0.353151\C,0,0.583168,1.553346,-1.059441\C,0,2.053791,-0
 .021246,0.143296\O,0,2.659537,-0.427727,-0.824049\O,0,2.349994,-0.3854
 4,1.41232\H,0,1.069129,1.258607,-1.983926\H,0,-0.180522,2.321175,-1.08
 6596\H,0,0.514622,1.28345,1.053624\H,0,3.098418,-1.002656,1.349926\\Ve
 rsion=IA64L-G03RevD.01\State=2-A\HF=-566.4709307\MP2=-567.9885714\RMSD
 =6.354e-09\Thermal=0.\PG=C01 [X(C5H5O5)]\\@
```


4e


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1\1\GINC-LC146\SP\ROMP2-FC\6-31G(d)\C5H5O5(2)\GMS501\29-Jun-2005\0\\#R
 OMP2/6-31G* SCF=TIGHT MAXDISK=72089600\\rotate COOH ketoglutarate prod
 uct radical b3lyp/6-31G(d,p)\\0,2\C,0,-1.503052,1.865012,-0.465689\H,0
 ,-1.121805,2.676605,0.140209\H,0,-2.480654,1.938336,-0.923975\C,0,-0.7
 48924,0.581121,-0.54464\H,0,-0.72762,0.18343,-1.569104\C,0,0.684645,0.
 694939,-0.053102\C,0,1.587785,-0.536963,-0.285215\O,0,1.163487,1.67636
 2,0.478593\O,0,1.216128,-1.510895,-0.893928\O,0,2.80853,-0.384117,0.23
 1598\H,0,2.829351,0.501421,0.646291\C,0,-1.429347,-0.497994,0.316855\O
 ,0,-2.531442,-0.982421,-0.283507\O,0,-1.047383,-0.837129,1.413328\H,0,
 -2.920469,-1.630867,0.328655\\Version=IA32L-G03RevC.02\State=2-A\HF=-5
 66.5333546\MP2=-568.0317895\RMSD=7.562e-09\PG=C01 [X(C5H5O5)]\\@
```


5e


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1\1\GINC-LC9\SP\ROMP2-FC\6-31G(d)\C5H6O5\GMS501\29-Jun-2005\0\\#ROMP2/
 6-31G* SCF=TIGHT MAXDISK=72089600\\ketoglutarate product b3lyp/6-31G(d
 ,p)\\0,1\C,0,-1.531987,1.864389,-0.372924\C,0,-0.747279,0.551375,-0.51
 5633\H,0,-0.726942,0.223323,-1.561444\C,0,0.689349,0.684115,-0.045956\
 C,0,1.608929,-0.538144,-0.271524\O,0,1.167582,1.683465,0.454164\O,0,1.
 243904,-1.529175,-0.856205\O,0,2.836165,-0.355067,0.220405\H,0,2.84770
 8,0.539813,0.615484\C,0,-1.393574,-0.561402,0.300403\O,0,-2.442757,-1.
 111332,-0.340309\O,0,-1.041824,-0.881626,1.414434\H,0,-1.560407,2.1844
 28,0.67127\H,0,-1.054047,2.655706,-0.954759\H,0,-2.55432,1.731317,-0.7
 33087\H,0,-2.809176,-1.786693,0.256425\\Version=IA32L-G03RevC.02\State
 =1-A\HF=-567.1714878\MP2=-568.693486\RMSD=4.941e-09\PG=C01 [X(C5H6O5)]
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3e'

1\1\GINC-AC52\SP\ROMP2-FC\6-31G(d)\C5H5O5(2)\GMS501\22-Jul-2005\0\\#RO
MP2/6-31G* SCF=TIGHT\\TS intra ketoglutarate substrate radical b3lyp/6
-31G(d,p)\\0,2\C,0,0.151325,-0.699915,1.512551\C,0,0.612356,-0.703702,
0.131091\C,0,1.970332,-0.109336,-0.1445\O,0,2.66754,0.440867,0.673925\
O,0,2.301941,-0.263139,-1.442552\O,0,-2.798923,0.793221,-0.412722\H,0,
-2.30828,1.628341,-0.267183\C,0,-1.92062,-0.194906,-0.218189\O,0,-2.18
6614,-1.371151,-0.311764\C,0,-0.5328,0.342199,0.130111\O,0,-0.351466,1
.579156,0.21484\H,0,0.653069,-0.055374,2.224036\H,0,-0.60473,-1.402414
,1.837758\H,0,0.346552,-1.567563,-0.474589\H,0,3.170011,0.159338,-1.56
0216\\Version=IA64L-G03RevC.02\State=2-A\HF=-566.4965811\MP2=-568.0249
365\RMSD=4.258e-09\PG=C01 [X(C5H5O5)]\\@

1f

1\1\GINC-SC96\SP\ROMP2-FC\6-31G(d)\C5H8O6\GMS501\26-Feb-2005\0\\#ROMP2
/6-31G* SCF=TIGHT\\hydrate of ketoglutarate romp2/6-31G*//b3lyp/6-31G(
d,p)\\0,1\C,0,-0.802516,-0.222059,0.095193\C,0,-2.304559,0.116924,-0.0
2771\O,0,-3.162923,-0.47182,0.593279\O,0,-2.564736,1.093113,-0.91378\H
,0,-3.532415,1.185917,-0.949001\C,0,0.08477,1.041917,0.11058\O,0,-0.57
9297,-1.053931,-1.009742\O,0,-0.612899,-0.875284,1.325277\H,0,-0.41590
9,1.802944,0.717182\H,0,0.140016,1.432815,-0.90848\C,0,1.484365,0.8465
72,0.711078\C,0,2.446818,0.032016,-0.116872\H,0,1.399201,0.344716,1.68
1955\H,0,1.953373,1.816389,0.904253\O,0,2.162328,-0.739124,-1.018259\O
,0,3.724354,0.227395,0.260372\H,0,4.270196,-0.358902,-0.291561\H,0,0.3
88537,-1.116309,-1.137092\H,0,-1.390884,-1.442592,1.451954\\Version=Al
64T-G03RevC.02\State=1-A\HF=-643.2068855\MP2=-644.9160472\RMSD=3.219e-
09\PG=C01 [X(C5H8O6)]\\@

2f

1\1\GINC-SC32\SP\ROMP2-FC\6-31G(d)\C5H7O6(2)\GMS501\26-Feb-2005\0\\#RO
MP2/6-31G* SCF=TIGHT\\hydrate of ketoglutarate romp2/6-31G*//b3lyp/6-3
1G(d,p)\\0,2\C,0,-0.772771,0.206236,0.118174\C,0,-2.284201,-0.049514,-
0.069406\O,0,-3.115953,0.818676,0.078434\O,0,-2.579316,-1.324848,-0.37
0891\H,0,-3.549277,-1.385168,-0.414371\C,0,0.085297,-0.525469,-0.95964
5\O,0,-0.527389,-0.250095,1.414361\O,0,-0.539111,1.579131,-0.049457\H,
0,-0.410553,-0.426168,-1.927995\H,0,0.086454,-1.587552,-0.690516\C,0,1
.475444,0.000132,-1.074968\C,0,2.442927,-0.139105,-0.010334\H,0,1.7883
12,0.535212,-1.964112\O,0,2.201854,-0.574585,1.118219\O,0,3.686012,0.2
63589,-0.358995\H,0,4.242023,0.147268,0.429396\H,0,0.440499,-0.366039,
1.518272\H,0,-1.286413,2.033822,0.373034\\Version=Al64T-G03RevC.02\Sta
te=2-A\HF=-642.5792009\MP2=-644.26761\RMSD=7.705e-09\PG=C01 [X(C5H7O6)
]\\@

C3-radical derived from 1f

1\1\GINC-AC22\SP\ROMP2-FC\6-31G(d)\C5H7O6(2)\GMS501\23-Feb-2006\0\\#ro
mp2/6-31G* scf=tight\\Xtal hydrate of ketoglutarate b3lyp/6-31G(d,p)\\
0,2\O,0,1.399795,-1.645085,0.785773\C,0,0.912039,-0.50466,0.137175\C,0
,2.113842,0.455834,-0.091348\O,0,3.267,0.091963,-0.027601\C,0,-0.15332
4,0.083365,1.014755\C,0,-1.27476,0.901214,0.462821\C,0,-2.423558,0.043
369,-0.059416\O,0,-2.301068,-1.013046,-0.651704\O,0,-3.626824,0.593912
,0.183349\O,0,1.74383,1.712871,-0.392134\H,0,2.561415,2.21306,-0.55850
3\O,0,0.458701,-0.746701,-1.176939\H,0,-0.128523,-0.177209,2.066837\H,
0,-0.92532,1.490099,-0.395492\H,0,-4.290189,-0.000233,-0.209498\H,0,-1
.671644,1.597183,1.206041\H,0,2.300169,-1.786021,0.448208\H,0,-0.42281
1,-1.16293,-1.107461\\Version=IA64L-G03RevD.01\State=2-A\HF=-642.57172
66\MP2=-644.257867\RMSD=7.899e-09\Thermal=0.\PG=C01 [X(C5H7O6)]\\@

TS:2f→3f*


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1\1\GINC-AC13\SP\ROMP2-FC\6-31G(d)\C5H7O6(2)\GMS501\22-Feb-2006\0\\#ro
 mp2/6-31G* scf=tight\\Xtal hydrate of ketoglutarate b3lyp/6-31G(d,p)\\
 0,2\C,0,0.260126,0.011755,1.385336\C,0,-1.083842,0.630401,-0.220786\O,
 0,-0.272262,0.789412,-1.263183\H,0,0.594644,1.178987,-0.985186\O,0,-1.
 631756,1.751864,0.307403\H,0,-2.419775,1.451548,0.800905\O,0,-3.0014,-
 0.532356,0.504739\C,0,-1.992121,-0.539142,-0.19052\O,0,-1.570779,-1.59
 6111,-0.901243\H,0,-2.221737,-2.301698,-0.749654\C,0,1.305541,-0.73051
 6,0.872895\C,0,2.337283,-0.070438,0.095791\O,0,2.251667,1.071315,-0.37
 4566\O,0,3.443576,-0.818203,-0.099262\H,0,0.395194,1.08094,1.515247\H,
 0,-0.454789,-0.456175,2.055279\H,0,1.354899,-1.809017,0.969398\H,0,4.0
 37276,-0.284313,-0.653394\\Version=IA64L-G03RevD.01\State=2-A\HF=-642.
 5157941\MP2=-644.2290304\RMSD=2.547e-09\Thermal=0.\PG=C01[X(C5H7O6)]\@
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TS:3f*→4f


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1\1\GINC-AC20\SP\ROMP2-FC\6-31G(d)\C5H7O6(2)\GMS501\21-Feb-2006\0\\#ro
 mp2/6-31G* scf=tight\\radical from 24 hydketo_prod1 hydrate of ketoglu
 tarate b3lyp/6-31G**\\0,2\C,0,-0.641918,0.638582,-0.77392\C,0,0.582343
 ,-0.611811,0.342938\O,0,0.394598,-1.81965,-0.204654\H,0,-0.578493,-1.9
 59705,-0.304761\O,0,0.192899,-0.486486,1.643489\H,0,0.677456,0.284687,
 1.991967\C,0,1.88655,0.057763,0.067329\O,0,2.437733,-0.259247,-1.11370
 5\H,0,3.237319,0.287388,-1.197701\O,0,2.332119,0.898884,0.830796\C,0,-
 1.889179,-0.010417,-0.301889\O,0,-2.693873,0.779526,0.430135\O,0,-2.17
 2911,-1.188854,-0.50674\C,0,-0.428886,2.008444,-0.550387\H,0,-0.276918
 ,0.2045,-1.70162\H,0,0.352025,2.537804,-1.083487\H,0,-0.965749,2.54331
 2,0.222766\H,0,-3.423626,0.213249,0.733836\\Version=IA64L-G03RevD.01\S
 tate=2-A\HF=-642.5113856\MP2=-644.2226512\RMSD=2.431e-09\Thermal=0.\PG
 =C01 [X(C5H7O6)]\\@
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4f


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1\1\GINC-SC30\SP\ROMP2-FC\6-31G(d)\C5H7O6(2)\GMS501\26-Feb-2005\0\\#RO
 MP2/6-31G* SCF=TIGHT\\radical from 24 hydketo_prod1 hydrate of ketoglu
 tarate romp2/6-31G*//b3lyp/6-31G**\\0,2\C,0,0.675409,-0.755356,0.46127
 4\C,0,1.762453,0.183738,-0.036557\O,0,1.63503,1.390889,-0.192305\O,0,2
 .928838,-0.432668,-0.244729\H,0,3.565017,0.247306,-0.529483\C,0,-0.656
 224,-0.573139,-0.341226\C,0,0.503656,-0.582252,1.938049\H,0,0.984089,-
 1.778634,0.234575\H,0,0.46519,0.41044,2.372485\H,0,0.302326,-1.439666,
 2.566624\O,0,-1.43515,-1.703893,-0.14931\O,0,-0.272712,-0.426732,-1.69
 9674\C,0,-1.526328,0.658466,0.075888\O,0,-2.709372,0.480747,0.30593\O,
 0,-0.964624,1.852221,0.105637\H,0,0.00886,1.79836,-0.088545\H,0,-1.013
 645,-0.755705,-2.229094\H,0,-2.32172,-1.355365,0.084475\\Version=Al64T
 -G03RevC.02\State=2-A\HF=-642.5615826\MP2=-644.2534107\RMSD=6.747e-09\
 PG=C01 [X(C5H7O6)]\\@
```


5f


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1\1\GINC-SC122\SP\ROMP2-FC\6-31G(d)\C5H8O6\GMS501\26-Feb-2005\0\\#ROMP
 2/6-31G* SCF=TIGHT\\24 hydketo_prod1 hydrate of ketoglutarate romp2/6-
 31G*//b3lyp/6-31G**\\0,1\C,0,0.681033,-0.800791,0.268351\C,0,1.752503,
 0.216976,-0.06362\O,0,1.610805,1.433202,-0.055544\O,0,2.939894,-0.3434
 09,-0.318443\H,0,3.568786,0.381433,-0.483049\C,0,-0.663905,-0.504236,-
 0.436598\C,0,0.528581,-0.929977,1.795734\H,0,1.002436,-1.761028,-0.143
 126\H,0,0.256958,0.026758,2.251103\H,0,1.460048,-1.276669,2.250094\H,0
 ,-0.255548,-1.658909,2.011431\O,0,-1.44001,-1.656033,-0.380946\O,0,-0.
 333249,-0.155921,-1.773017\C,0,-1.528708,0.65012,0.176185\O,0,-2.7083,
 0.436564,0.396044\O,0,-0.968851,1.828328,0.373446\H,0,0.001096,1.80688
 5,0.150166\H,0,-1.126356,-0.309629,-2.306561\H,0,-2.326754,-1.343241,-
 0.102688\\Version=Al64T-G03RevC.02\State=1-A\HF=-643.1994194\MP2=-644.
 9158228\RMSD=4.219e-09\PG=C01 [X(C5H8O6)]\\@
```

1s

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1\1\GINC-AC16\SP\ROMP2-FC\6-31G(d)\C5H10N2O4\GMS501\18-Sep-2005\0\\# R
 OMP2/6-31G* SCF=TIGHT\\two-aminoglut consistent b3p\\0,1\C,0,-0.115638
 ,-0.754035,-0.650489\C,0,-1.506084,-1.024288,-0.062236\C,0,-2.477954,0
 .124065,-0.205903\C,0,0.88122,-0.087569,0.319521\O,0,-2.204436,1.27085
 ,-0.509601\O,0,-3.745804,-0.259339,0.053916\N,0,1.016281,-0.917146,1.5
 26897\N,0,0.501752,1.270368,0.750461\C,0,2.267685,0.005645,-0.391767\O
 ,0,2.855391,1.199182,-0.274553\O,0,2.776811,-0.948805,-0.939695\H,0,-1
 .968451,-1.899343,-0.530097\H,0,-4.299681,0.533874,-0.045293\H,0,0.114
 413,1.225855,1.689857\H,0,-0.237607,1.637272,0.151412\H,0,0.33782,-1.6
 94281,-0.975274\H,0,-0.200762,-0.129111,-1.545879\H,0,-1.423492,-1.263
 435,1.005662\H,0,1.416658,-1.813311,1.252632\H,0,1.704199,-0.489397,2.
 14713\H,0,2.179601,1.741316,0.21306\\Version=IA64L-G03RevC.02\State=1-
 A\HF=-603.535457\MP2=-605.2233003\RMSD=5.221e-09\PG=C01 [X(C5H10N2O4)]
 \\@
```

2s

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1\1\GINC-AC11\SP\ROMP2-FC\6-31G(d)\C5H9N2O4(2)\GMS501\18-Sep-2005\0\\#
  ROMP2/6-31G* SCF=TIGHT\\two-aminoglut consistent b3p\\0,2\C,0,-0.1300
 63,-0.737886,-0.702044\C,0,-1.49548,-0.969388,-0.166116\C,0,-2.490157,
 0.079904,-0.228776\C,0,0.857682,-0.100211,0.321392\O,0,-2.271823,1.229
 324,-0.610383\O,0,-3.718821,-0.315604,0.188343\N,0,0.962646,-0.960561,
 1.505859\N,0,0.463754,1.240014,0.776888\C,0,2.253741,0.010519,-0.36867
 8\O,0,2.863265,1.181508,-0.16298\O,0,2.752009,-0.915942,-0.969941\H,0,
 -4.295511,0.462005,0.107212\H,0,-0.004843,1.15393,1.675767\H,0,-0.2182
 61,1.647925,0.136931\H,0,0.323171,-1.672258,-1.045337\H,0,-0.183585,-0
 .060176,-1.561309\H,0,-1.76198,-1.901541,0.318406\H,0,1.334935,-1.8637
 1,1.216559\H,0,1.658813,-0.566613,2.13927\H,0,2.191079,1.712349,0.3382
 79\\Version=IA64L-G03RevC.02\State=2-A\HF=-602.9097783\MP2=-604.576313
 \RMSD=4.054e-09\PG=C01 [X(C5H9N2O4)]\\@
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TS:2s→3s*

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1\1\GINC-AC49\SP\ROMP2-FC\6-31G(d)\C5H9N2O4(2)\GMS501\21-Feb-2006\0\\#
  romp2/6-31G* scf=tight\\two-aminoglut Xtal COOH b3p\\0,2\C,0,0.182605
 ,0.208054,1.314029\C,0,-1.158626,0.64167,-0.194458\N,0,-0.432288,0.938
 574,-1.350011\H,0,-0.059907,0.098036,-1.776417\H,0,0.342536,1.57305,-1
 .161668\N,0,-1.846227,1.73218,0.359327\H,0,-2.63818,1.424845,0.914272\
 H,0,-2.120501,2.404923,-0.348447\C,0,-1.88247,-0.659967,-0.153083\O,0,
 -1.297039,-1.612978,-0.918786\H,0,-1.801241,-2.430321,-0.772418\O,0,-2
 .855366,-0.873126,0.54796\C,0,1.238884,-0.601936,0.891638\C,0,2.337598
 ,-0.027082,0.142743\O,0,2.396494,1.127024,-0.283125\O,0,3.35453,-0.906
 687,-0.076692\H,0,0.379198,1.271738,1.40332\H,0,-0.510268,-0.189432,2.
 051474\H,0,1.239068,-1.675554,1.043106\H,0,4.022006,-0.410856,-0.57849
 4\\Version=IA64L-G03RevD.01\State=2-A\HF=-602.8609156\MP2=-604.5503894
 \RMSD=8.466e-09\Thermal=0.\PG=C01 [X(C5H9N2O4)]\\@
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TS:3s*→4s

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1\1\GINC-AC36\SP\ROMP2-FC\6-31G(d)\C5H9N2O4(2)\GMS501\21-Feb-2006\0\\#
  romp2/6-31G* scf=tight\\two-aminoglut Xtal COOH b3p\\0,2\H,0,0.914414
 ,-2.077118,-0.930899\C,0,-0.614506,0.628602,-0.735664\C,0,0.574898,-0.
 589867,0.39523\N,0,0.071542,-0.405593,1.704828\H,0,0.491359,-1.075117,
 2.345371\H,0,0.265108,0.537523,2.027447\N,0,0.471514,-1.917883,-0.0342
 66\H,0,-0.493157,-2.23555,-0.040358\O,0,2.39304,-0.345229,-1.117841\C,
 0,1.868928,0.083392,0.063115\H,0,3.191324,0.187594,-1.269497\O,0,2.360
 839,0.982092,0.713611\C,0,-1.943615,0.18733,-0.221489\O,0,-2.67477,0.8
 1348,0.513085\O,0,-2.28125,-1.06384,-0.665871\C,0,-0.335491,2.00285,-0
 .581685\H,0,-0.3146,0.153807,-1.668294\H,0,0.488255,2.470651,-1.106752
```

\H,0,-0.884832,2.588842,0.145315\H,0,-3.143412,-1.252164,-0.257177\\Ve
rsion=IA64L-G03RevD.01\State=2-A\HF=-602.8565296\MP2=-604.538541\RMSD=
9.167e-09\Thermal=0.\PG=C01 [X(C5H9N2O4)]\\@

4s

1\1\GINC-AC16\SP\ROMP2-FC\6-31G(d)\C5H9N2O4(2)\GMS501\18-Sep-2005\0\\#
 ROMP2/6-31G* SCF=TIGHT\\two-aminoglut consistent b3p\\0,2\C,0,-0.5442
41,0.496662,-0.444156\C,0,0.536364,-0.461812,0.22458\N,0,0.392572,-1.8
60742,-0.12075\H,0,-0.562238,-2.187887,-0.006607\H,0,0.703804,-2.0166,
-1.076016\C,0,-0.399108,1.938021,-0.076954\C,0,-1.950375,0.046233,-0.0
71641\O,0,-2.317059,-0.254885,1.049743\O,0,-2.784765,0.042872,-1.12877
9\N,0,0.558743,-0.248843,1.67571\C,0,1.902266,0.001311,-0.35803\O,0,2.
257051,-0.295079,-1.477309\O,0,2.59849,0.780444,0.468633\H,0,-0.416515
,0.374395,-1.522304\H,0,-3.664153,-0.200961,-0.789696\H,0,2.05396,0.80
1639,1.296363\H,0,-0.391759,-0.131624,2.022569\H,0,0.930741,-1.098061,
2.098216\H,0,0.077081,2.633314,-0.756603\H,0,-0.689288,2.283574,0.9082
59\\Version=IA64L-G03RevC.02\State=2-A\HF=-602.8966263\MP2=-604.564477
2\RMSD=3.663e-09\PG=C01 [X(C5H9N2O4)]\\@

5s

1\1\GINC-AC11\SP\ROMP2-FC\6-31G(d)\C5H10N2O4\GMS501\18-Sep-2005\0\\# R
OMP2/6-31G* SCF=TIGHT\\two-aminoglut consistent b3p\\0,1\C,0,-0.553697
,0.552196,-0.247018\C,0,0.551467,-0.519842,0.035811\N,0,0.455237,-1.71
6514,-0.787477\H,0,-0.490396,-2.087864,-0.785617\H,0,0.740051,-1.50118
5,-1.739578\C,0,-0.441246,1.839111,0.602781\C,0,-1.947027,-0.025619,-0
.072783\O,0,-2.258635,-0.927867,0.683218\O,0,-2.85518,0.608893,-0.8421
66\N,0,0.597264,-0.853033,1.467327\C,0,1.904864,0.153115,-0.339391\O,0
,2.247818,0.312673,-1.48923\O,0,2.609083,0.569492,0.715371\H,0,-0.4438
58,0.829338,-1.300206\H,0,-3.720737,0.216471,-0.632863\H,0,2.075797,0.
271013,1.495724\H,0,-0.352115,-0.953878,1.821032\H,0,1.028945,-1.77383
9,1.538291\H,0,-1.206613,2.558374,0.300822\H,0,0.536618,2.305178,0.462
231\H,0,-0.566048,1.623933,1.66728\\Version=IA64L-G03RevC.02\State=1-A
\HF=-603.5345056\MP2=-605.2255805\RMSD=5.249e-09\PG=C01 [X(C5H10N2O4)]
\\@

Tetrahydro-5-methylfuran-3,4-diol

1\1\GINC-AC17\SP\ROMP2-FC\6-31G(d)\C5H10O3\GMS501\19-Oct-2005\0\\# ROM
P2/6-31G* SCF=TIGHT\\5'-deoxyadenosine molecule b3lyp/6-31G(d,p)\\0,1\
O,0,0.612579,-1.23887,-0.598293\C,0,1.009655,0.149528,-0.446837\C,0,-0
.066469,0.811322,0.472128\C,0,-1.136214,-0.302405,0.590076\C,0,-0.2781
57,-1.551706,0.476988\H,0,0.953324,0.607787,-1.440696\H,0,0.36562,1.02
2705,1.458089\H,0,-1.733438,-0.237247,1.502583\H,0,-0.843796,-2.447372
,0.206498\H,0,0.26477,-1.744836,1.415783\C,0,2.432436,0.245149,0.08802
\H,0,2.735988,1.29439,0.169233\H,0,3.131815,-0.268387,-0.577205\H,0,2.
510162,-0.209289,1.081995\O,0,-2.045487,-0.19437,-0.509022\H,0,-1.5839
73,-0.567128,-1.276995\O,0,-0.592877,2.018909,-0.025505\H,0,-1.361695,
1.752695,-0.558969\\Version=IA64L-G03RevC.02\State=1-A\HF=-419.7152713
\MP2=-420.903483\RMSD=9.710e-09\PG=C01 [X(C5H10O3)]\\@

Tetrahydro-5-methylfuran-3,4-diol radical

1\1\GINC-AC51\SP\ROMP2-FC\6-31G(d)\C5H9O3(2)\GMS501\20-Oct-2005\0\\# R
OMP2/6-31G* SCF=TIGHT\\5'-deoxyadenosine molecule b3lyp/6-31G(d,p)\\0,
2\O,0,0.704577,-1.148106,-0.664716\C,0,1.059722,0.240116,-0.441669\C,0
,-0.082571,0.843742,0.461459\C,0,-1.038515,-0.369579,0.626295\C,0,-0.0
83299,-1.541505,0.463736\H,0,1.010698,0.738716,-1.422591\H,0,0.332513,
1.137285,1.431885\H,0,-1.595832,-0.356915,1.565692\H,0,-0.582991,-2.48
3664,0.225081\H,0,0.538416,-1.67698,1.362271\C,0,2.420349,0.350182,0.1

46949\H,0,2.773767,1.305337,0.521922\H,0,3.128205,-0.461541,0.02332\O,
0,-2.003342,-0.349024,-0.429445\H,0,-1.540587,-0.677406,-1.217382\O,0,
-0.728673,1.964176,-0.089524\H,0,-1.498803,1.601058,-0.56134\\Version=
IA64L-G03RevC.02\State=2-A\HF=-419.077168\MP2=-420.2425664\RMSD=7.189e
-09\PG=C01 [X(C5H9O3)]\\@

G3(MP2)-RAD//B3-LYP/6-31G(d,p) Total Energies (Hartrees) at 0 K

Species	Energy
1a	– 550.89286
2a	– 550.24423
C3-radical derived from 1a	– 550.23289
Acrylic acid	– 266.80264
TS:2a→3a*	– 550.21768
TS:3a*→4a	– 550.21570
4a	– 550.23331
5a	– 550.89481
1b	– 570.76300
2b	– 570.11309
C3-radical derived from 1b	– 570.10170
TS:2b→3b*	– 570.07996
TS:3b*→4b	– 570.07644
4b	– 570.10206
5b	– 570.76468
H–HC(CO_2H)–H	– 228.78251
H–•C(CO_2H)–H	– 228.12559
H–HC(CO_2H)–NH_2	– 284.05429
H–•C(CO_2H)–NH_2 (3a)	– 283.42520
H–HC(CO_2H)–SH	– 625.53324
H–•C(CO_2H)–SH (3c)	– 625.89922
H–HC(CO_2H)–S^-	– 626.00569
H–•C(CO_2H)–S^- (3d)	– 625.38884
H–HC(CO_2H)–OH	– 303.92173
H–•C(CO_2H)–OH (3b)	– 303.28623

H–HC(CO_2H)–O^-	– 303.38913
H–•C(CO_2H)–O^-	– 302.75587
H–HC(CO_2H)–F	– 327.93119
H–•C(CO_2H)–F	– 327.28255
HO–HC(CO_2H)–NH_2	– 359.20574
HO–•C(CO_2H)–NH_2	– 358.57986
H_2N–HC(CO_2H)–NH_2	– 339.33471
H_2N–•C(CO_2H)–NH_2 (3s)	– 338.71341
F–HC(CO_2H)–NH_2	– 383.22059
F–•C(CO_2H)–NH_2	– 382.58038
HO–HC(CO_2H)–OH	– 379.07336
HO–•C(CO_2H)–OH (3f)	– 378.44154
O=HC(CO_2H)	– 302.71673
O=•C(CO_2H) (3e)	– 302.07118
1c	– 893.37477
2c	– 892.72400
C3-radical derived from 1c	– 892.71671
TS:2c→3c*	– 892.69179
TS:3c*→4c	– 892.68685
4c	– 892.71068
5c	– 893.37281
1d	– 892.83179
2d	– 892.18547
C3-radical derived from 1d	– 892.17755
TS:2d→3d*	– 892.17629
TS:3d*→4d	– 892.15740
4d	– 892.17174
5d	– 892.83335

1e	– 569.56684
2e	– 568.91588
C3-radical derived from 1e	– 568.91789
TS:2e→3e*	– 568.86684
TS:3e*→4e	– 568.86375
4e	– 568.90205
5e	– 569.56473
3e'	– 568.88922
1f	– 645.92179
2f	– 645.27083
C3-radical derived from 1f	– 645.26136
TS:2f→3f*	– 645.23853
TS:3f*→4f	– 645.23516
4f	– 645.26025
5f	– 645.92313
1s	– 606.17731
2s	– 605.52800
TS:2s→3s*	– 605.50751
TS:3s*→4s	– 605.49869
4s	– 605.51747
5s	– 606.17948
Tetrahydro -5-methylfuran-3,4-diol	– 421.58926
Tetrahydro -5-methylfuran-3,4-diol radical	– 420.92686

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