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Table S1. Total Energies and Zero-Point Vibrational Energies (ZPVE's), in hartrees, of the Various Species

	B3-LYP/6-31G(d,p)	B3-LYP/6-311+G(2df,p) //B3-LYP/6-31G(d,p)	ZPVE B3-LYP/6-31G(d,p)
$H_2N\dot{C}HCOOH$	-283.80424	-283.91071	0.06707
O_2	-150.32004	-150.37834	0.00378
Gly—O–O$^{\bullet}$	-434.14620	-434.30539	0.07570
H_2N–CH($\dot{O}$)–COOH	-358.98190	-359.11448	0.07040
H_2N–$\dot{C}$OH–COOH	-359.02858	-359.16619	0.07179
OHC–COOH	-303.07508	-303.18932	0.04360
H_2N–CO–COOH	-358.46826	-358.60222	0.06147
NH_2–CHO	-169.89703	-169.96243	0.04541
H$^{\bullet}$	-0.50027	-0.50216	—
$^{\bullet}NH_2$	-55.87898	-55.90232	0.01897
O$\dot{C}$OH	-189.09529	-189.17120	0.02101
1 Gly—O–$\dot{O}$···HS—R	-912.17619	-912.38629	0.15205
2 Gly—O–OH···$\dot{S}$—R	-912.17421	-912.38524	0.15500
3 Gly—$\dot{O}$···H–SO—R	-912.18756	-912.41663	0.15297
4 Gly—$\dot{O}$···HO–S—R	-912.21455	-912.43087	0.15288
5 Gly—OH···$\dot{O}$–S—R	-912.25862	-912.48329	0.15505
TS**1**	-912.15723	-912.36662	0.14878
TS**2**	-912.12330	-912.34261	0.15160
TS**3**	-912.15518	-912.36666	0.15325
TS**4**	-912.21426	-912.43159	0.15219
TS**5**	-358.94693	-359.08204	0.06603
TS**6**	-358.95603	-359.09000	0.06672
TS**7**	-358.95510	-359.09085	0.06307
TS**8**	-358.97320	-359.10898	0.06831

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Table S2. Archive Entries for the B3-LYP/6-31G(d,p) Optimized Geometries

$H_2N\dot{C}HCOOH$

1\1\GINC-VANQC51\FOpt\UB3LYP\6-31G(d,p)\C2H4N1O2(2)\JAMES\15-Aug-1997\
1\\#P B3LYP/6-31G(D,P) GEOM=CHECK GUESS=READ FOPT=(READFC,Z-MATRIX,TIG
HT) TEST MAXDISK=786432000\\Glycine radical (H2N-C.H-COOH)\\0,2\C\C,1,
r1\N,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3b,1,a2b,2,d1b,0\H,1,r4,3,a3,2,
d2,0\O,2,r5,1,a4,3,d3,0\O,2,r6,1,a5,3,d4,0\H,8,r7,2,a6,1,d5,0\\r1=1.43
104184\r2=1.36310855\a1=117.42501205\r3=1.01293173\a2=115.11832332\d1=
-10.89261026\r3b=1.00759413\a2b=120.17184185\d1b=160.52686362\r4=1.080
9777\a3=119.58516796\d2=183.44571505\r5=1.23221056\a4=124.03938647\d3=
3.99274984\r6=1.36618617\a5=113.52246121\d4=183.56372041\r7=0.97039162
\a6=105.11475278\d5=180.63675285\\DEC-AXP-OSF/1-G94RevB.1\HF=-283.8042
445\S2=0.754\S2-1=0.\S2A=0.75\RMSD=5.878e-09\RMSF=5.304e-06\Dipole=-0.
0249174,0.2402352,-0.9562173\PG=C01 [X(C2H4N1O2)]\\@

O_2

1\1\GINC-VANQC8\FOpt\UB3LYP\6-31G(d)\O2(3)\KVFYS\14-Aug-1997\1\\# B3LY
P/6-31G(D) GUESS=READ FOPT=(READFC,Z-MATRIX) FREQ=NORAMAN TEST\\O2\\0,
3\O\O,1,r1\\r1=1.21454837\\Version=DEC-AXP-OSF/1-G94RevB.1\State=3-SGG
\HF=-150.3200379\S2=2.007\S2-1=0.\S2A=2.\RMSD=9.531e-10\RMSF=6.560e-06
\Dipole=0.,0.,0.\PG=D*H [C*(O1.O1)]\\@

$Gly—O–\dot{O}^{\bullet}$

1\1\GINC-VANQC51\Freq\UB3LYP\6-31G(d,p)\C2H4N1O4(2)\JWG501\26-Aug-1997
\1\\# B3LYP/6-31G(D,P) GEOM=CHECK GUESS=READ FOPT=(CALCAL,Z-MATRIX,NOR
AMAN) TEST MAXDISK=26214400\\Glycine-peroxy: H2N-CH(OO.)-COOH\\0,2\C\C,
1,r1\N,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3b,1,a2b,2,-d1b,0\H,1,r4,3,a3,
2,d2,0\O,2,r5,1,a4,3,d3,0\O,2,r6,1,a5,3,d4,0\H,8,r7,2,a6,1,d5,0\O,1,r8,
2,a7,3,d6,0\O,10,r9,1,a8,2,d7,0\\r1=1.5224379\r2=1.39022721\a1=111.4427
5611\r3=1.01584234\a2=111.53023756\d1=41.93644406\r3b=1.01444182\a2b=11
1.45791889\d1b=192.7444889\r4=1.09123508\a3=113.19912104\d2=128.2397780
6\r5=1.20887111\a4=123.82739714\d3=-23.30465675\r6=1.34293257\a5=111.48
404427\d4=158.74634778\r7=0.97295101\a6=107.03587629\d5=176.47064067\a7
=102.01455647\d6=122.55549878\r9=1.30993618\a8=109.65960407\d7=-159.168
97107\r8=1.56296874\\DEC-AXP-OSF/1-G94RevB.1\HF=-434.1462015\S2=0.753\S
2-1=0.\S2A=0.75\RMSD=2.618e-09\RMSF=2.264e-05\Dipole=0.0441956,0.581689
1,0.3326694\PG=C01 [X(C2H4N1O4)]\NImag=0\\@

$H_2N–CH(\dot{O})–COOH$

1\1\GINC-VANQC8\FOpt\UB3LYP\6-31G(d,p)\C2H4N1O3(2)\KVFYS\28-Jan-1998\1
\\# B3LYP/6-31G(D,P) GEOM=CHECK GUESS=READ FOPT=(Z-MATRIX,READFC) FREQ
=NORAMAN TEST\\glycine: H2NCHO.COOH\\0,2\C\C,1,r1\N,1,r2,2,a1\H,3,r3,1
,a2,2,d1,0\H,3,r3b,1,a2b,2,-d1b,0\H,1,r4,3,a3,2,d2,0\O,2,r5,1,a4,3,d3,
0\O,2,r6,1,a5,3,d4,0\H,8,r7,2,a6,1,d5,0\O,1,r8,2,a7,3,d6,0\\r1=1.55474
854\r2=1.43760316\a1=109.14330965\r3=1.01686634\a2=109.83004046\d1=45.
35960272\r3b=1.01601753\a2b=109.38453341\d1b=195.57231908\r4=1.1114371
7\a3=110.19291638\d2=114.91280766\r5=1.20652005\a4=123.47703062\d3=-25
.9747483\r6=1.34077105\a5=111.58611156\d4=156.13536916\r7=0.97278817\a
6=106.94928447\d5=176.39337686\a7=107.87437011\d6=131.06484268\r8=1.36
604176\\Version=DEC-AXP-OSF/1-G94RevB.1\HF=-358.9818955\S2=0.754\S2-1=

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0.\S2A=0.75\RMSD=7.953e-09\RMSF=1.170e-05\Dipole=-0.1698285,0.2674038,
0.1677016\PG=C01 [X(C2H4N1O3)]\\@

H_2N-$\dot{C}$OH-COOH

1\1\GINC-FOX\FOpt\UB3LYP\6-31G(d,p)\C2H4N1O3(2)\JAMES\30-Oct-1997\1\\#
B3LYP/6-31G(D,P) FOPT=(CALCFC,Z-MATRIX) FREQ=NORAMAN TEST\\h2ncohcooh
\\0,2\C\C,1,r1\N,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3b,1,a2b,2,-d1b,0\O
,2,r5,1,a4,3,d3,0\O,2,r6,1,a5,3,d4,0\H,7,r7,2,a6,1,d5,0\O,1,r8,2,a7,3,
d6,0\H,9,r9,1,a8,2,d7,0\\r1=1.42112849\r2=1.36693675\a1=120.80167284\r
3=1.01183421\a2=113.00338132\d1=13.96362636\r3b=1.01149853\a2b=116.259
58362\d1b=208.75535842\r5=1.23415408\a4=125.39332012\d3=-4.92012504\r6
=1.38530884\a5=111.48585569\d4=175.52488291\r7=0.96883197\a6=105.75753
806\d5=179.29984728\a7=123.03209861\d6=183.25279893\r9=0.97013233\a8=1
06.8637758\d7=-360.87869805\r8=1.35236776\\Version=SGI-G94RevB.1\HF=-3
59.0285794\S2=0.754\S2-1=0.\S2A=0.75\RMSD=9.994e-09\RMSF=1.002e-05\Dip
ole=-0.3821594,-0.3520907,-0.4392936\PG=C01 [X(C2H4N1O3)]\\@

OHC-COOH

1\1\GINC-BALDER\Freq\RB3LYP\6-31G(d,p)\C2H2O3\JAMES\01-Jun-1999\1\\# B
3LYP/6-31G(D,P) FREQ=(NORAMAN) TEST\\OHCCOOH\\0,1\C\C,1,r1\O,1,r2,2,a1
\O,1,r3,2,a2,3,180.,0\H,4,r4,1,a3,2,0.,0\O,2,r2b,1,a1b,3,180.,0\H,2,r4
b,1,a3b,3,0.,0\\r3=1.33764505\a2=113.00385807\r1=1.53349753\r2=1.20578
842\a1=121.97014272\r2b=1.21217437\a1b=120.60434024\r4=0.97764483\a3=1
06.96071637\r4b=1.10382007\a3b=115.33566208\\Version=DEC-AXP-OSF/1-G98
RevA.6\State=1-A'\HF=-303.0750793\RMSD=9.435e-09\RMSF=1.389e-05\Dipole
=-0.2670286,0.,0.7205232\PG=CS[SG(C2H2O3)]\NImag=0\\@

H_2N-CO-COOH

1\1\GINC-VANQC8\FOpt\RB3LYP\6-31G(d,p)\C2H3N1O3\KVFYS\18-Aug-1997\1\\#
P B3LYP/6-31G(D,P) GUESS=READ FOPT=(Z-MATRIX) TEST\\H2NCOCOOH\\0,1\C\C
,1,r1\N,1,r2,2,a1\H,3,r3,1,a2,2,0.,0\H,3,r3b,1,a2b,2,-180.,0\O,1,r4,3,
a3,2,180.,0\O,2,r5,1,a4,3,0.,0\O,2,r6,1,a5,3,180.,0\H,8,r7,2,a6,1,180.
,0\\r1=1.54491802\r2=1.3546228\a1=110.65212622\r3=1.00867182\a2=119.76
413201\r3b=1.00750863\a2b=119.16883281\r4=1.21662138\a3=126.42684903\r
5=1.21417159\a4=123.27524194\r6=1.335508\a5=112.11268797\r7=0.97262842
\a6=106.58221911\\Version=DEC-AXP-OSF/1-G94RevB.1\State=1-A'\HF=-358.4
682638\RMSD=7.226e-09\RMSF=1.477e-05\Dipole=0.8345132,0.,0.2962454\PG=
CS [SG(C2H3N1O3)]\\@

H_2N-CHO

1\1\GINC-BALDER\Freq\RB3LYP\6-31G(d,p)\C1H3N1O1\JAMES\24-May-1999\1\\#
B3LYP/6-31G(D,P) FREQ=(NORAMAN) TEST\\H2NCHO\\0,1\N\C,1,r1\O,2,r2,1,a
1\H,1,r3,2,a2,3,180.,0\H,1,r4,2,a3,3,0.,0\H,2,r5,1,a4,3,180.,0\\r1=1.3
61392\r2=1.216116\a1=124.934\r3=1.007201\a2=121.681\r4=1.009393\a3=119
.002\r5=1.10884\a4=111.973\\Version=DEC-AXP-OSF/1-G98RevA.6\State=1-A'
\HF=-169.8970272\RMSD=3.411e-09\RMSF=8.460e-06\Dipole=-0.857593,0.,-1.
2344658\PG=CS [SG(C1H3N1O1)]\NImag=0\\

H$^{\bullet}$

1\1\GINC-WALT\SP\UB3LYP\6-31G(d,p)\H1(2)\JAMES\22-Nov-1999\0\\# B3LYP/
6-31G(D,P) SCF=TIGHT TEST\\H\\0,2\H\\Version=IBM-RS6000-G98RevA.4\HF=-

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0.5002728\S2=0.75\S2-1=0.\S2A=0.75\RMSD=1.238e-12\Dipole=0.,0.,0.\PG=K
H\\@

$^{\bullet}NH_2$

1\1\GINC-BALDER\Freq\UB3LYP\6-31G(d,p)\H2N1(2)\JAMES\01-Jun-1999\1\\#
B3LYP/6-31G(D,P) FREQ=(NORAMAN) TEST\\NH2 radical\\0,2\N\H,1,r1\H,1,r1
,2,a1\\r1=1.03331653\a1=101.83470877\\Version=DEC-AXP-OSF/1-G98RevA.6\
State=2-B1\HF=-55.8789805\S2=0.752701\S2-1=0.\S2A=0.750004\RMSD=7.430e
-09\RMSF=4.574e-06\Dipole=0.6008548,0.,0.4879994\DipoleDeriv=-0.062199
6,0.,0.0347679,0.,-0.6285852,0.,0.0347679,0.,-0.0767703,0.19792,0.,-0.
0945972,0.,0.3142926,0.,-0.0100829,0.,-0.128435,-0.1357203,0.,0.059829
2,0.,0.3142926,0.,-0.0246851,0.,0.2052054\Polar=8.7132606,0.,4.720447,
-1.2230569,0.,9.225827\PG=C02V [C2(N1),SGV(H2)]\NImag=0\\0.41744049,0.
,0.00001296,-0.06459407,0.,0.44451098,-0.03794457,0.,-0.03080479,0.044
23323,0.,-0.00000648,0.,0.,0.00000457,0.02382911,0.,-0.39303117,-0.015
71679,0.,0.40736823,-0.37949592,0.,0.09539887,-0.00628866,0.,-0.008112
33,0.38578458,0.,-0.00000648,0.,0.,0.00000192,0.,0.,0.00000457,0.04076
497,0.,-0.05147982,0.04652158,0.,-0.01433705,-0.08728655,0.,0.06581687
\\-0.00000305,0.,-0.00000247,-0.00000421,0.,0.00000829,0.00000725,0.,-
0.00000582\\\@

$O\dot{C}OH$

1\1\GINC-BALDER\FOpt\UB3LYP\6-31G(d,p)\C1H1O2(2)\JAMES\24-May-1999\1\\
B3LYP/6-31G(D,P) FOPT=(Z-MATRIX) FREQ=NORAMAN TEST\\OC(.)OH\\0,2\C\O
,1,r1\O,1,r2,2,a1\H,3,r3,1,a2,2,180.,0\\r1=1.18751058\r2=1.34799359\a1
=126.38856339\r3=0.96886598\a2=108.02093024\\Version=DEC-AXP-OSF/1-G98
RevA.6\State=2-A'\HF=-189.0952907\S2=0.752798\S2-1=0.\S2A=0.750006\RMS
D=3.084e-09\RMSF=1.112e-05\Dipole=0.0142381,0.,-1.1997499\PG=CS [SG(C1
H1O2)]\\@

1: Gly—O–$\dot{O}$···HS—R

1\1\GINC-LOKE\Freq\UB3LYP\6-31G(d,p)\C4H10N1O4S1(2)\JAMES\13-Feb-1999\
0\\# B3LYP/6-31G(D,P) OPT=(CALCAL,NORAMAN) TEST\\gl-o-o...hsch2ch3 .\\
0,2\C,-1.5572052827,-0.1955212089,-0.5432465031\C,-2.7433654971,0.5801
848512,0.0090596168\N,-0.5804501002,0.6514002928,-1.0257772184\H,-0.40
5975691,1.4273827309,-0.396668483\H,0.2797551971,0.1864255713,-1.30389
78506\H,-1.8512217784,-0.9869616535,-1.2326367761\O,-2.669285453,1.707
2593895,0.4398585171\O,-3.8654117557,-0.1610069004,0.0012422868\H,-4.5
60753959,0.3748649713,0.4203455523\O,-1.1235972586,-1.0805886217,0.699
9005871\O,-0.2144544183,-0.4743665982,1.4202821384\S,2.5772825651,-1.2
384725129,-0.734131088\H,1.8001502318,-1.443797213,0.3501694838\C,3.65
44909731,0.0604326639,0.0187497791\H,4.1389888386,-0.3712789406,0.8980
600197\H,4.4343594029,0.2298597153,-0.729061255\C,2.9317882471,1.35965
67811,0.3618858882\H,2.5193636654,1.8287926827,-0.5364480951\H,3.62858
05209,2.0682500624,0.8244108683\H,2.111123674,1.1833235532,1.063303551
3\\Version=DEC-AXP-OSF/1-G98RevA.1\HF=-912.1761916\S2=0.75392\S2-1=0.\
S2A=0.750011\RMSD=8.672e-09\RMSF=1.464e-06\Dipole=-0.1216401,0.2677244
,-0.1743761\PG=C01 [X(C4H10N1O4S1)]\NImag=0\\@

2: Gly—O–OH···$\dot{S}$—R

1\1\GINC-BALDER\Freq\UB3LYP\6-31G(d,p)\C4H10N1O4S1(2)\ROOT\07-Feb-1999

\1\\# B3LYP/6-31G(D,P) GEOM=CHECK GUESS=READ FOPT=(CALCAL,NORAMAN,Z-MA
TRIX) TEST\\complex2: gl-o-oh...s-ch2ch3\\0,2\C\C,1,r1\N,1,r2,2,a1\H,3
,r3,1,a2,2,d1,0\H,3,r3b,1,a2b,2,-d1b,0\H,1,r4,3,a3,2,d2,0\O,2,r5,1,a4,
3,d3,0\O,2,r6,1,a5,3,d4,0\H,8,r7,2,a6,1,d5,0\O,1,r8,2,a7,3,d6,0\O,10,r
9,1,a8,2,d7,0\H,11,r11,10,a10,1,d9,0\S,11,r10,10,a9,1,d8,0\C,13,r12,12
,a11,11,d10,0\H,14,r13,13,a12,12,d11,0\H,14,r14,13,a13,12,d12,0\C,14,r
15,13,a14,12,d13,0\H,17,r16,14,a15,13,d14,0\H,17,r17,14,a16,13,d15,0\H
,17,r18,14,a17,13,d16,0\\a10=99.64630066\d9=120.0566844\r11=0.98105323
\a7=102.1099044\r9=1.45495865\a8=105.62731104\r8=1.44744592\d6=123.777
89459\d7=-184.22925629\r10=3.38364999\r12=1.82272689\a11=104.28758245\
d10=-439.08696525\r1=1.53173731\r2=1.4237586\a1=108.77747065\r4=1.0930
7209\a3=110.09941344\d2=122.02744657\a9=99.18763283\d8=-232.0763687\r1
3=1.10061979\a12=103.55866286\d11=79.30190923\r14=1.09453341\a13=107.9
9030369\d12=191.73900581\r15=1.52836263\a14=115.50525817\d13=318.22633
481\r16=1.09433954\a15=110.93413708\d14=-62.93918862\r17=1.09546565\a1
6=109.58985127\d15=-181.58327588\r18=1.09207377\a17=111.56642257\d16=5
8.24973762\r3=1.01659716\a2=110.16652425\d1=53.58365191\r3b=1.014899\a
2b=109.89565064\d1b=185.26364762\r5=1.21040975\a4=123.51849013\d3=-46.
8296099\r6=1.3440426\a5=112.43650998\d4=133.57557702\r7=0.97319583\a6=
106.62405871\d5=179.2268053\\Version=DEC-AXP-OSF/1-G98RevA.3\HF=-912.1
742129\S2=0.752703\S2-1=0.\S2A=0.750003\RMSD=2.619e-09\RMSF=2.952e-05\
Dipole=0.2458962,-0.5928347,0.3780698\PG=C01 [X(C4H10N1O4S1)]\NImag=0\
\@

3: Gly—$\dot{O}$···H–SO—R

1\1\GINC-VANQC51\FOpt\UB3LYP\6-31G(d,p)\C4H10N1O4S1(2)\JAMES\23-Dec-19
98\1\\# B3LYP/6-31G(D,P) GEOM=CHECK GUESS=READ FOPT=(CALCFC,Z-MATRIX)
FREQ=NORAMAN TEST\\gl-o1-o2-s-ch2ch3 with h transfer directly from s t
o o1\\0,2\C\C,1,r1\N,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3b,1,a2b,2,-d1b
,0\H,1,r4,3,a3,2,d2,0\O,2,r5,1,a4,3,d3,0\O,2,r6,1,a5,3,d4,0\H,8,r7,2,a
6,1,d5,0\O,1,r8,2,a7,3,d6,0\O,10,r9,1,a8,2,d7,0\S,11,r10,10,a9,1,d8,0\
C,12,r12,11,a11,10,d10,0\H,13,r13,12,a12,11,d11,0\H,13,r14,12,a13,11,d
12,0\C,13,r15,12,a14,11,d13,0\H,16,r16,13,a15,12,d14,0\H,16,r17,13,a16
,12,d15,0\H,16,r18,13,a17,12,d16,0\H,10,r19,11,a18,12,d17,0\\r19=2.114
58294\a18=41.88655319\d17=-16.2997778\r10=1.53430255\a9=69.57326022\d8
=203.37131874\r12=1.84428616\a11=108.33440471\d10=280.91870712\r13=1.0
9336552\a12=105.62649389\d11=-67.99111171\r14=1.09275893\a13=106.18673
49\d12=47.70214506\r15=1.52629027\a14=110.95930171\d13=169.95897505\r1
6=1.09438818\a15=111.31071782\d14=-63.97389644\r17=1.09377061\a16=109.
79718108\d15=-182.96247595\r18=1.09465532\a17=111.81879687\d16=57.5938
5299\r1=1.53336817\r2=1.44838092\a1=109.01063605\r3=1.01751801\a2=110.
61111986\d1=45.35329619\r3b=1.03824568\a2b=114.08398977\d1b=184.564497
49\r4=1.09884245\a3=110.66845337\d2=122.32018272\r5=1.21053982\a4=124.
46282625\d3=-26.85291139\r6=1.34715889\a5=111.57373869\d4=156.47738711
\r7=0.97297109\a6=106.64166549\d5=175.39667618\a7=110.25590833\d6=109.
67972316\r9=3.42775679\a8=84.5142607\d7=-155.35374318\r8=1.37569768\\V
ersion=DEC-AXP-OSF/1-G98RevA.1\HF=-912.1875561\S2=0.75605\S2-1=0.\S2A=
0.750018\RMSD=5.033e-09\RMSF=1.132e-05\Dipole=-0.6775753,-0.8489739,-0
.0645265\PG=C01 [X(C4H10N1O4S1)]\\@

4: Gly—$\dot{O}$···HO–S—R

1\1\GINC-BALDER\Freq\UB3LYP\6-31G(d,p)\C4H10N1O4S1(2)\ROOT\11-Feb-1999
\1\\# B3LYP/6-31G(D,P) GEOM=CHECK GUESS=READ FOPT=(CALCAL,NORAMAN,Z-MA
TRIX) TEST\\complex4: glycine-hydroperoxy...sch2ch3\\0,2\C\C,1,r1\N,1,

r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3b,1,a2b,2,-d1b,0\H,1,r4,3,a3,2,d2,0\O,
2,r5,1,a4,3,d3,0\O,2,r6,1,a5,3,d4,0\H,8,r7,2,a6,1,d5,0\O,1,r8,2,a7,3,d6
,0\O,10,r9,1,a8,2,d7,0\H,11,r11,10,a10,1,d9,0\S,11,r10,10,a9,1,d8,0\C,1
3,r12,12,a11,11,d10,0\H,14,r13,13,a12,12,d11,0\H,14,r14,13,a13,12,d12,0
\C,14,r15,13,a14,12,d13,0\H,17,r16,14,a15,13,d14,0\H,17,r17,14,a16,13,d
15,0\H,17,r18,14,a17,13,d16,0\\a10=22.28395829\d9=158.22694617\r11=0.97
799235\a7=107.79052881\r9=2.79140633\a8=99.89851574\r8=1.36474947\d6=13
2.14384583\d7=-140.54467976\r10=1.69349059\r12=1.82647465\a11=99.350803
64\d10=-455.88185203\r1=1.5630047\r2=1.42777216\a1=109.96658001\r4=1.11
518846\a3=110.03985856\d2=113.0991347\a9=126.0975955\d8=-158.51453372\r
13=1.0947893\a12=107.93749983\d11=82.52847321\r14=1.09747269\a13=103.70
331504\d12=196.07209789\r15=1.52656405\a14=114.52496519\d13=317.6756499
\r16=1.09367997\a15=111.14189846\d14=-61.56828247\r17=1.09585825\a16=11
0.63412208\d15=-182.17174764\r18=1.09425118\a17=110.72496267\d16=58.361
38741\r3=1.01535954\a2=111.70361676\d1=34.64340206\r3b=1.0179543\a2b=11
0.84957329\d1b=202.3882224\r5=1.20481447\a4=123.13805135\d3=-14.9399557
3\r6=1.33757214\a5=111.45858775\d4=165.69713996\r7=0.97287179\a6=107.12
724767\d5=178.27344514\\Version=DEC-AXP-OSF/1-G98RevA.3\HF=-912.2145485
\S2=0.754449\S2-1=0.\S2A=0.750013\RMSD=7.391e-09\RMSF=1.688e-05\Dipole=
-0.8102074,0.6998988,0.5347482\PG=C01 [X(C4H10N1O4S1)]\NImag=0\\@

5: Gly—OH···$\dot{O}$–S—R

1\1\GINC-VANQC51\FOpt\UB3LYP\6-31G(d,p)\C4H10N1O4S1(2)\JAMES\28-Dec-199
8\1\\# B3LYP/6-31G(D,P) GEOM=CHECK GUESS=READ FOPT=(CALCFC,Z-MATRIX)FRE
Q=NORAMAN TEST\\complex5: gly-OH...OS-R\\0,2\C\C,1,r1\N,1,r2,2,a1\H,3,r
3,1,a2,2,d1,0\H,3,r3b,1,a2b,2,-d1b,0\H,1,r4,3,a3,2,d2,0\O,2,r5,1,a4,3,d
3,0\O,2,r6,1,a5,3,d4,0\H,8,r7,2,a6,1,d5,0\O,1,r8,2,a7,3,d6,0\O,10,r9,1,
a8,2,d7,0\S,11,r10,10,a9,1,d8,0\C,12,r12,11,a11,10,d10,0\H,13,r13,12,a1
2,11,d11,0\H,13,r14,12,a13,11,d12,0\C,13,r15,12,a14,11,d13,0\H,16,r16,1
3,a15,12,d14,0\H,16,r17,13,a16,12,d15,0\H,16,r18,13,a17,12,d16,0\H,10,r
19,11,a18,12,d17,0\\r19=0.96884856\a18=127.9542518\d17=71.25749325\r10=
1.536366\a9=84.13766944\d8=183.88821447\r12=1.83763107\a11=106.82212141
\d10=308.0066502\r13=1.09481894\a12=106.88404747\d11=-57.97226612\r14=1
.09423312\a13=106.26818081\d12=58.23075136\r15=1.52832304\a14=110.04918
471\d13=180.28720162\r16=1.0945304\a15=111.55578647\d14=-60.87972721\r1
7=1.09376566\a16=109.70745017\d15=-180.01140971\r18=1.09467078\a17=111.
9498466\d16=60.45878028\r1=1.53134479\r2=1.40913063\a1=109.84495528\r3=
1.01482077\a2=111.14043495\d1=48.95140389\r3b=1.01785972\a2b=111.803033
07\d1b=185.98452626\r4=1.09740089\a3=110.1012493\d2=120.93263956\r5=1.2
078309\a4=126.06475823\d3=20.38356061\r6=1.35683057\a5=110.60270425\d4=
163.64097891\r7=0.9724463\a6=106.41920177\d5=175.46921322\a7=105.761198
87\d6=122.02708229\r9=3.65985561\a8=80.01726429\d7=162.73467668\r8=1.45
698565\\Version=DEC-AXP-OSF/1-G98RevA.1\HF=-912.2586185\S2=0.753716\S2-
1=0.\S2A=0.75001\RMSD=6.212e-09\RMSF=4.019e-06\Dipole=-1.1748454,-1.045
3085,-0.0273061\PG=C01 [X(C4H10N1O4S1)]\\@

TS1: TS for rarrangement of 1 to 2

1\1\ CENTER FOR PARALLEL COMPUTERS, CRAY J90-KALLSUP\Freq\UB3LYP\6-31G
(d,p)\C4H10N1O4S1(2)\LEIFAXEL\15-Nov-1998\1\\# B3LYP/6-31G(D,P) GUESS=
READ GEOM=CHECK FREQ=NORAMAN TEST\\glycine-peroxy<--h-->sch2ch3\\0,2\C
\C,1,r1\N,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3b,1,a2b,2,-d1b,0\H,1,r4,3
,a3,2,d2,0\O,2,r5,1,a4,3,d3,0\O,2,r6,1,a5,3,d4,0\H,8,r7,2,a6,1,d5,0\O,
1,r8,2,a7,3,d6,0\O,10,r9,1,a8,2,d7,0\H,11,r11,10,a10,1,d9,0\S,12,r10,1
1,a9,1,d8,0\C,13,r12,12,a11,11,d10,0\H,14,r13,13,a12,12,d11,0\H,14,r14
,13,a13,12,d12,0\C,14,r15,13,a14,12,d13,0\H,17,r16,14,a15,13,d14,0\H,1

7,r17,14,a16,13,d15,0\H,17,r18,14,a17,13,d16,0\\a9=158.79735353\d8=-32
.28695983\a10=108.61997702\d9=109.18906451\r12=1.83959328\a11=94.96221
075\d10=-265.94163238\r13=1.09723809\a12=106.43621526\d11=-27.31620049
\r14=1.09390377\a13=108.2954713\d12=87.4356883\r15=1.527024\a14=112.68
836186\d13=210.79702143\r16=1.09400658\a15=111.32850435\d14=-59.543804
86\r17=1.09557497\a16=110.04009714\d15=-179.08059097\r18=1.09390503\a1
7=111.34011901\d16=60.78512489\r1=1.53034138\r2=1.40423622\a1=109.8537
1258\r3=1.01516504\a2=111.841675\d1=45.27204575\r3b=1.01496777\a2b=113
.12681068\d1b=187.91385024\r4=1.09070569\a3=112.25578184\d2=125.691595
62\r5=1.20896366\a4=123.56690137\d3=-32.88732603\r6=1.34210661\a5=111.
78421532\d4=148.40911741\r7=0.97312092\a6=106.9955343\d5=177.73210794\
a7=102.29073475\d6=122.37250597\r9=1.37308104\a8=107.76211696\d7=-195.
36022645\r8=1.49606386\r11=1.24249555\r10=1.55145252\\Version=Cray-J90
-Unicos-G94RevE.2\HF=-912.1572319\S2=0.757\S2-1=0.\S2A=0.75\RMSD=9.600
e-10\RMSF=1.752e-05\Dipole=0.0701318,0.1645926,0.8171449\PG=C01 [X(C4H
10N1O4S1)]\NImag=1\\@

TS2: TS for rearrangement of 1 to 3

1\1\GINC-BALDER\FTS\UB3LYP\6-31G(d,p)\C4H10N1O4S1(2)\ROOT\27-Jan-1999\
1\\# B3LYP/6-31G(D,P) GEOM=CHECK GUESS=READ FOPT=(READFC,TS,NOEIGEN,Z-
MATRIX) SCFCYC=256 FREQ=NORAMAN TEST\\gl-o1-o2-hs-ch2ch3 with o2 trans
fer directly from s to o1\\0,2\C\C,1,r1\N,1,r2,2,a1\H,3,r3,1,a2,2,d1,0
\H,3,r3b,1,a2b,2,-d1b,0\H,1,r4,3,a3,2,d2,0\O,2,r5,1,a4,3,d3,0\O,2,r6,1
,a5,3,d4,0\H,8,r7,2,a6,1,d5,0\O,1,r8,2,a7,3,d6,0\H,10,r9,1,a8,2,d7,0\S
,11,r10,10,a9,1,d8,0\C,12,r12,11,a11,10,d10,0\H,13,r13,12,a12,11,d11,0
\H,13,r14,12,a13,11,d12,0\C,13,r15,12,a14,11,d13,0\H,16,r16,13,a15,12,
d14,0\H,16,r17,13,a16,12,d15,0\H,16,r18,13,a17,12,d16,0\O,10,r19,11,a1
8,12,d17,0\\r1=1.53524693\r2=1.43780361\a1=108.0854574\r3=1.0175305\a2
=109.1571719\d1=56.23924368\r3b=1.01562666\a2b=108.88319699\d1b=184.38
031252\r4=1.0951516\a3=108.97374197\d2=119.41776788\r5=1.21091641\a4=1
24.1948827\d3=-39.73772057\r6=1.34798268\a5=112.23431505\d4=142.029018
39\r7=0.97280857\a6=106.22199913\d5=177.26175092\r15=1.52417528\a14=10
9.5570789\d13=180.68069122\r16=1.09195685\a15=110.04789555\d14=-58.653
67541\r17=1.09395586\a16=109.17725922\d15=-177.38604051\r18=1.0942626\
a17=111.90218232\d16=62.93042747\r12=1.84152584\a11=97.11862094\d10=28
7.01162268\r13=1.09341164\a12=107.29410663\d11=-56.80292208\r14=1.0929
4624\a13=105.29309923\d12=61.25799395\r9=3.46159849\a8=97.47518464\d7=
-143.46434653\r19=1.66720436\a18=43.64268132\d17=-37.13826925\r10=1.35
599457\a9=64.95141223\d8=218.4612565\r8=1.41731854\a7=102.39769024\d6=
124.47841121\\Version=DEC-AXP-OSF/1-G98RevA.3\HF=-912.1233022\S2=0.762
798\S2-1=0.\S2A=0.750079\RMSD=6.115e-09\RMSF=4.311e-05\Dipole=0.184628
2,-1.2638736,-0.9926823\PG=C01 [X(C4H10N1O4S1)]\\@

TS3: TS for rearrangement of 2 to 4

1\1\GINC-FREJA\Freq\UB3LYP\6-31G(d,p)\C4H10N1O4S1(2)\JAMES\18-Jan-1999
\1\\# B3LYP/6-31G(D,P) GEOM=CHECK GUESS=READ FOPT=(CALCAL,NORAMAN,NOEI
GEN,TS,Z-MATRIX) TEST\\TS3: rearrangement of complex2 to complex4\\0,2
\C\C,1,r1\N,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3b,1,a2b,2,-d1b,0\H,1,r4
,3,a3,2,d2,0\O,2,r5,1,a4,3,d3,0\O,2,r6,1,a5,3,d4,0\H,8,r7,2,a6,1,d5,0\
O,1,r8,2,a7,3,d6,0\O,10,r9,1,a8,2,d7,0\H,11,r11,10,a10,1,d9,0\S,11,r10
,10,a9,1,d8,0\C,13,r12,12,a11,11,d10,0\H,14,r13,13,a12,12,d11,0\H,14,r
14,13,a13,12,d12,0\C,14,r15,13,a14,12,d13,0\H,17,r16,14,a15,13,d14,0\H
,17,r17,14,a16,13,d15,0\H,17,r18,14,a17,13,d16,0\\a10=94.03487561\d9=1
36.50188283\r11=0.97217125\a7=101.85377195\r9=1.66886986\a8=103.912663
02\r8=1.42344003\d6=124.65777069\d7=-192.96560891\r10=2.16545671\r12=1

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.82304189\a11=113.66636562\d10=-362.81109788\r1=1.53940172\r2=1.427030
03\a1=109.12201816\r4=1.09548508\a3=110.03901424\d2=119.8066612\a9=149
.32052473\d8=-113.07992232\r13=1.09431449\a12=108.10108367\d11=51.9746
7699\r14=1.0973117\a13=104.5737383\d12=165.89313344\r15=1.52818634\a14
=113.89344419\d13=287.23232757\r16=1.09338086\a15=111.00619666\d14=-59
.63504093\r17=1.09618393\a16=110.04810222\d15=-179.69230172\r18=1.0930
9579\a17=110.87420432\d16=60.4743536\r3=1.01665782\a2=109.93372613\d1=
53.61579899\r3b=1.01513933\a2b=110.00439761\d1b=185.63232754\r5=1.2082
7945\a4=124.17007216\d3=-32.74900275\r6=1.34616075\a5=111.61256827\d4=
148.66162922\r7=0.97283349\a6=106.58040277\d5=177.27049465\\Version=DE
C-AXP-OSF/1-G98RevA.1\HF=-912.155181\S2=0.783877\S2-1=0.\S2A=0.750155\
RMSD=5.846e-09\RMSF=1.898e-05\Dipole=-0.3200704,0.3334236,-0.2298026\P
G=C01 [X(C4H10N1O4S1)]\NImag=1\\@

TS4: TS for rearrangement of 4 to 5

1\1\GINC-BALDER\Freq\UB3LYP\6-31G(d,p)\C4H10N1O4S1(2)\ROOT\20-Feb-1999
\1\\# B3LYP/6-31G(D,P) GUESS=READ FOPT=(CALCAL,NORAMAN,TS,NOEIGEN,Z-MA
TRIX) TEST\\TS4: complex4 <--> complex5\\0,2\C\C,1,r1\N,1,r2,2,a1\H,3,r
3,1,a2,2,d1,0\H,3,r3b,1,a2b,2,-d1b,0\H,1,r4,3,a3,2,d2,0\O,2,r5,1,a4,3,d
3,0\O,2,r6,1,a5,3,d4,0\H,8,r7,2,a6,1,d5,0\O,1,r8,2,a7,3,d6,0\O,10,r9,1,
a8,2,d7,0\H,11,r11,10,a10,1,d9,0\S,11,r10,10,a9,1,d8,0\C,13,r12,12,a11,
11,d10,0\H,14,r13,13,a12,12,d11,0\H,14,r14,13,a13,12,d12,0\C,14,r15,13,
a14,12,d13,0\H,17,r16,14,a15,13,d14,0\H,17,r17,14,a16,13,d15,0\H,17,r18
,14,a17,13,d16,0\\a10=16.82382819\d9=143.22035442\r11=0.99283707\a7=105
.77861233\r9=2.61593646\a8=102.58575272\r8=1.37347226\d6=128.81696154\d
7=-153.2535045\r10=1.67651123\r12=1.82640405\a11=101.64537897\d10=-450.
63455543\r1=1.56047552\r2=1.43358676\a1=109.29172615\r4=1.1081173\a3=10
9.38926715\d2=114.29594159\a9=121.43653141\d8=-169.15696056\r13=1.09463
514\a12=107.66746885\d11=82.28229117\r14=1.09712801\a13=104.1072572\d12
=196.13012742\r15=1.52687099\a14=113.82642681\d13=317.98725249\r16=1.09
359171\a15=111.14123859\d14=-63.81760512\r17=1.0956608\a16=110.49031298
\d15=-184.3251146\r18=1.09378595\a17=110.68317518\d16=56.06555071\r3=1.
01604256\a2=111.21265044\d1=44.2639635\r3b=1.01701797\a2b=110.31169682\
d1b=194.03872301\r5=1.2051486\a4=123.30193437\d3=-18.87632006\r6=1.3389
5916\a5=111.49196079\d4=162.08712973\r7=0.9729504\a6=107.06203829\d5=17
7.87277029\\Version=DEC-AXP-OSF/1-G98RevA.3\HF=-912.2142584\S2=0.754809
\S2-1=0.\S2A=0.750014\RMSD=7.866e-09\RMSF=1.778e-05\Dipole=-0.8343783,0
.4532627,0.2809355\PG=C01 [X(C4H10N1O4S1)]\NImag=1\\@

TS5: TS for rearrangement of $H_2N-CH(\dot{O})-COOH$ to $H_2N-\dot{C}OH-COOH$

1\1\GINC-WOLF\FTS\UB3LYP\6-31G(d,p)\C2H4N1O3(2)\JAMES\29-Oct-1998\1\\#
B3LYP/6-31G(D,P) GUESS=READ FOPT=(EF,TS,READFC,Z-MATRIX) FREQ=(NORAMA
N) TEST\\h2nchocooh radical <-> h2ncohcooh radical\\0,2\C\C,1,r1\N,1,r
2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3b,1,a2b,2,-d1b,0\H,1,r4,3,a3,2,d2,0\O,
2,r5,1,a4,3,d3,0\O,2,r6,1,a5,3,d4,0\H,8,r7,2,a6,1,d5,0\O,1,r8,2,a7,3,d
6,0\\r1=1.49846949\r2=1.37779117\a1=113.98559714\r3=1.01107704\a2=116.
14432763\d1=6.75197823\r3b=1.00899162\a2b=115.8802377\d1b=208.31735493
\r5=1.21851201\a4=122.83294039\d3=7.43775047\r6=1.34692137\a5=113.1156
7717\d4=185.00455652\r7=0.97157579\a6=105.96419271\d5=182.36121307\a7=
121.72721383\r8=1.37299914\r4=1.26598819\a3=123.8462757\d2=134.2253709
1\d6=155.98841692\\Version=SGI-G94RevD.4\HF=-358.9469302\S2=0.757\S2-1
=0.\S2A=0.75\RMSD=7.502e-09\RMSF=3.286e-05\Dipole=0.3445895,0.0752776,
0.0491826\PG=C01 [X(C2H4N1O3)]\\@

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TS6: TS for cleavage of C—N bond in $H_2N-CH(\dot{O})-COOH$

1\1\GINC-BALDER\Freq\UB3LYP\6-31G(d,p)\C2H4N1O3(2)\JAMES\03-Jun-1999\1
\\# B3LYP/6-31G(D,P) GUESS=READ FOPT=(Z-MATRIX,EF,TS,CALCAL,NORAMAN) T
EST\\ts: h2nchocooh <--> h2n + ohccooh\\0,2\C\C,1,r1\N,1,r2,2,a1\H,3,r
3,1,a2,2,d1,0\H,3,r3b,1,a2b,2,-d1b,0\H,1,r4,3,a3,2,d2,0\O,2,r5,1,a4,3,
d3,0\O,2,r6,1,a5,3,d4,0\H,8,r7,2,a6,1,d5,0\O,1,r8,2,a7,3,d6,0\\r1=1.53
640213\r2=2.11020386\a1=92.74769453\r3=1.02970408\a2=99.30240576\d1=65
.94020588\r3b=1.02916212\a2b=102.28779045\d1b=187.09220814\r4=1.103017
21\a3=94.5250758\d2=114.98437186\r5=1.20648179\a4=124.85726462\d3=-74.
85401164\r6=1.34855712\a5=110.30002251\d4=105.96938474\r7=0.97263183\a
6=106.90419886\d5=179.95630477\a7=120.64863396\d6=97.16375935\r8=1.228
18963\\Version=DEC-AXP-OSF/1-G98RevA.6\HF=-358.9560305\S2=0.764996\S2-
1=0.\S2A=0.750071\RMSD=7.410e-09\RMSF=3.886e-06\Dipole=0.3943926,0.726
4905,0.0314529\PG=C01 [X(C2H4N1O3)]\NImag=1\\@

TS7: TS for cleavage of C_α—H bond in $H_2N-CH(\dot{O})-COOH$

1\1\GINC-VANQC51\FTS\UB3LYP\6-31G(d,p)\C2H4N1O3(2)\JAMES\08-Jul-1998\1
\\# B3LYP/6-31G(D,P) GEOM=CHECK GUESS=READ FOPT=(EF,TS,CALCFC,Z-MATRIX
) FREQ=NORAMAN TEST\\TS for cleavage of Ca-H bond in h2nchocooh. //b31
yp/6-31G(d,p)\\0,2\C\C,1,r1\N,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r3b,1,a
2b,2,-d1b,0\H,1,r4,3,a3,2,d2,0\O,2,r5,1,a4,3,d3,0\O,2,r6,1,a5,3,d4,0\H
,8,r7,2,a6,1,d5,0\O,1,r8,2,a7,3,d6,0\\r1=1.55475007\r2=1.37095476\a1=1
10.26733665\r3=1.00938776\a2=118.30399292\d1=-20.72843737\r3b=1.008178
55\a2b=117.5795849\d1b=176.03992635\r4=1.65707208\a3=105.51607845\d2=9
2.71480259\r5=1.2121213\a4=123.03253682\d3=11.04392477\r6=1.33537252\a
5=111.95861347\d4=191.22543247\r7=0.97248834\a6=106.56952462\d5=180.08
740206\a7=122.35163398\d6=161.60545531\r8=1.24109124\\Version=DEC-AXP-
OSF/1-G94RevB.1\HF=-358.9550984\S2=0.767\S2-1=0.\S2A=0.75\RMSD=7.489e-
09\RMSF=7.025e-06\Dipole=0.6845433,0.3383826,0.2920404\PG=C01 [X(C2H4N
1O3)]\\@

TS8: TS for cleavage of C—C bond in $H_2N-CH(\dot{O})-COOH$

1\1\ CENTER FOR PARALLEL COMPUTERS, CRAY J90-KALLSUP\FTS\UB3LYP\6-31G(
d,p)\C2H4N1O3(2)\LEIFAXEL\27-Oct-1998\1\\# B3LYP/6-31G(D,P) GUESS=READ
 FOPT=(EF,TS,READFC,Z-MATRIX) FREQ=NORAMAN TEST\\ts8: ts for h2nchocoo
h <-> h2ncho + ocoh\\0,2\C\C,1,r1\N,1,r2,2,a1\H,3,r3,1,a2,2,d1,0\H,3,r
3b,1,a2b,2,-d1b,0\H,1,r4,3,a3,2,d2,0\O,2,r5,1,a4,3,d3,0\O,2,r6,1,a5,3,
d4,0\H,8,r7,2,a6,1,d5,0\O,1,r8,2,a7,3,d6,0\\r2=1.39351633\a1=107.51052
23\r3=1.01354331\a2=113.22996146\d1=73.61288278\r3b=1.01251266\a2b=115
.71259755\d1b=58.85707078\r4=1.10835076\a3=111.82662789\d2=100.9896276
7\r5=1.1943162\a4=121.21585501\d3=-18.47544723\r6=1.32703292\a5=109.27
82494\d4=165.66219347\r7=0.97707509\a6=108.37429466\d5=174.18519836\a7
=95.01952116\d6=124.9598105\r8=1.26352084\r1=1.96790431\\Version=Cray-
J90-Unicos-G94RevE.2\HF=-358.9731981\S2=0.764\S2-1=0.\S2A=0.75\RMSD=8.
205e-09\RMSF=2.684e-05\Dipole=0.3922223,0.8554688,0.8505015\PG=C01 [X(
C2H4N1O3)]\\@