

Electronic Supplementary Information (ESI)

Intramolecular Homolytic Substitution of Sulfinates and Sulfinamides – A Computational Study†

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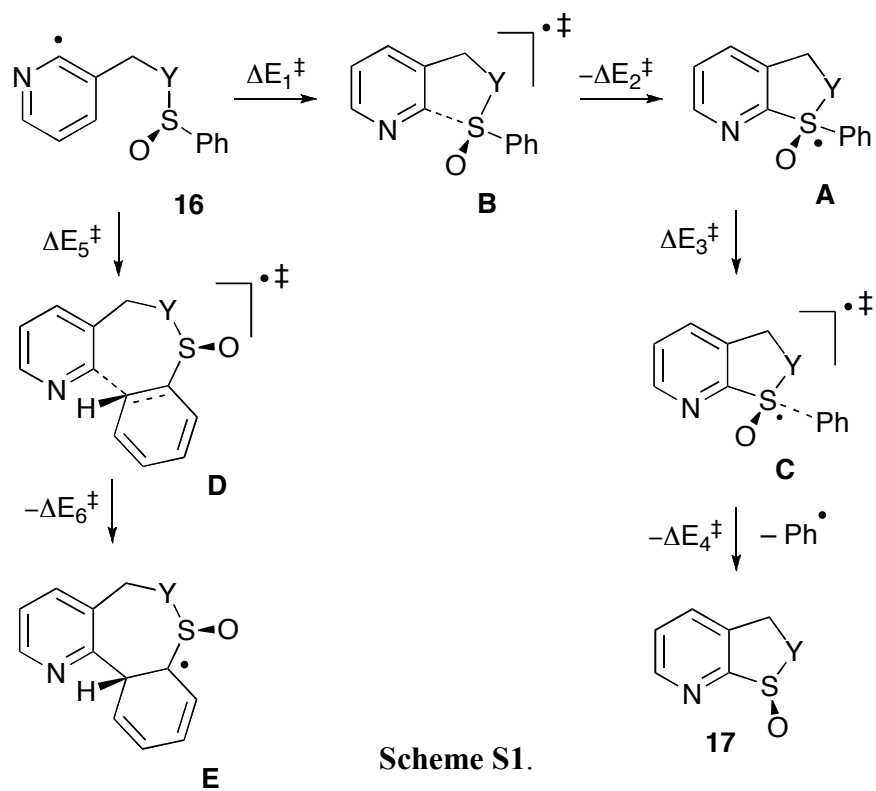
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Scheme S1, Figures S1 and S2, optimized geometries and energies for all structures in this study (Gaussian Archive Entries). (99 pages).



Scheme S1.

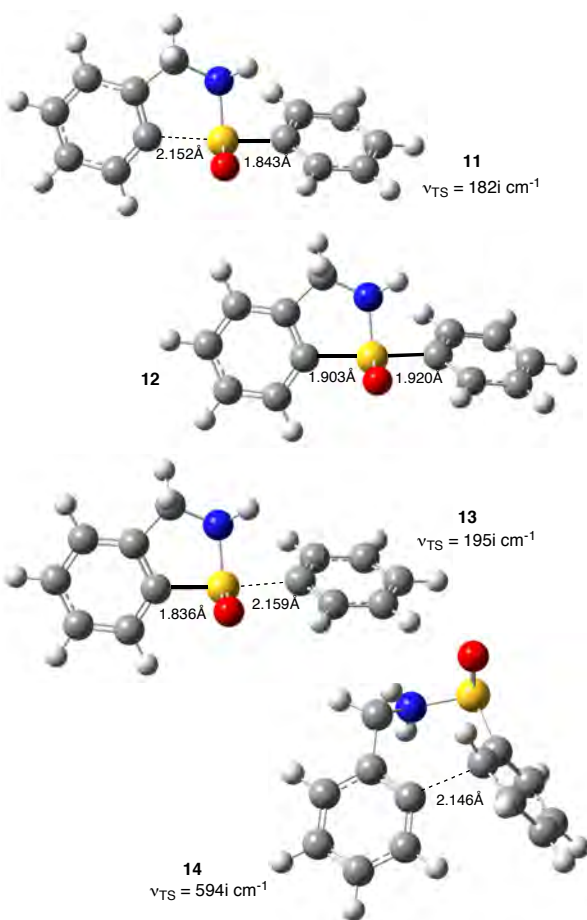


Figure S1. ROBHandHLYP/6-311++G(d,p) optimized structures 11 – 14 (Y = NH).

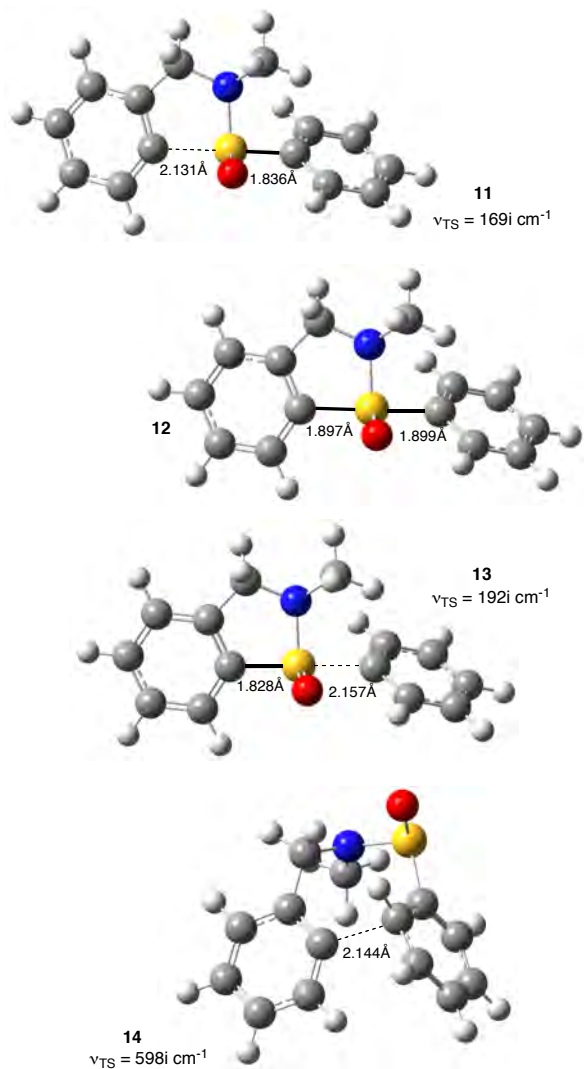


Figure S2. ROBHandHLYP/6-311++G(d,p) optimized structures 11 – 14 (Y = NMe).

Gaussian Archive Entries

Radical 6

ROHF/6-31G*

```
1\1\GINC-GOMBERG04\FOpt\ROHF\6-31G(d)\C4H9O2S1(2)\HMAITKEN\18-Jun-2010
1\1\#ROHF/6-31G* opt=(grad) geom=checkpoint guess=read\calc of 5 memb
ered starting material with Me attached\0,2\C\H,1,B1\H,1,B2,2,A1\C,1,
B3,2,A2,3,D1,0\H,4,B4,1,A3,2,D2,0\H,4,B5,1,A4,2,D3,0\C,4,B6,1,A5,2,D4,
0\H,7,B7,4,A6,1,D5,0\H,7,B8,4,A7,1,D6,0\O,7,B9,4,A8,1,D7,0\S,10,B10,7,
A9,4,D8,0\O,11,B11,10,A10,7,D9,0\C,11,B12,10,A11,7,D10,0\H,13,B13,11,A
12,10,D11,0\H,13,B14,11,A13,10,D12,0\H,13,B15,11,A14,10,D13,0\B1=1.07
580433\B2=1.0738411\B3=1.5004978\B4=1.08959424\B5=1.08482115\B6=1.5195
678\B7=1.08188768\B8=1.08634339\B9=1.42330322\B10=1.62741183\B11=1.459
55959\B12=1.78387693\B13=1.08221097\B14=1.08145714\B15=1.08168769\A1=1
16.59536481\A2=119.71075978\A3=110.75195226\A4=110.32443674\A5=111.892
96265\A6=111.07850515\A7=110.88559297\A8=107.57242072\A9=115.76834262\
A10=109.421311\A11=92.90603429\A12=107.61985732\A13=109.70477186\A14=1
08.20572895\A15=-156.96408578\A16=74.54646163\A17=-167.70080964\A18=-46.47
743767\A19=-62.08443958\A20=58.81957226\A21=178.31384673\A22=183.09895184\
A23=-71.59073282\A24=179.65534934\A25=-182.12513\A26=-61.99344388\A27=5
8.98891692\Version=AM64L-G03RevE.01\State=2-A\HF=-703.8249707\RMSE=8.
379e-09\RMSEF=2.024e-05\Thermal=0.\Dipole=0.4613583,1.2718741,0.1515527
\PG=C01 [X(C4H9O2S1)]\@
```

ROHF/6-311G**

```
1\1\GINC-GOMBERG04\FOpt\ROHF\6-311G(d,p)\C4H9O2S1(2)\HMAITKEN\18-Jun-2
010\1\1\#ROHF/6-311G** opt=(grad) geom=checkpoint guess=read\calc of 5
membered starting material with Me attached\0,2\C\H,1,B1\H,1,B2,2,A1
\C,1,B3,2,A2,3,D1,0\H,4,B4,1,A3,2,D2,0\H,4,B5,1,A4,2,D3,0\C,4,B6,1,A5,
2,D4,0\H,7,B7,4,A6,1,D5,0\H,7,B8,4,A7,1,D6,0\O,7,B9,4,A8,1,D7,0\S,10,B
10,7,A9,4,D8,0\O,11,B11,10,A10,7,D9,0\C,11,B12,10,A11,7,D10,0\H,13,B13
,11,A12,10,D11,0\H,13,B14,11,A13,10,D12,0\H,13,B15,11,A14,10,D13,0\B1
=1.07648473\B2=1.07439614\B3=1.49983668\B4=1.09019325\B5=1.08530309\B6
=1.51733179\B7=1.08309266\B8=1.08775295\B9=1.42166136\B10=1.62186998\B
11=1.45487139\B12=1.78266376\B13=1.08225313\B14=1.08152315\B15=1.08147
939\A1=116.85537823\A2=119.87701344\A3=110.55786551\A4=110.3171042\A5=
112.01734617\A6=111.04950822\A7=110.83458932\A8=107.62888668\A9=116.54
077156\A10=109.09362335\A11=93.04102301\A12=107.18946533\A13=109.56251
23\A14=107.40400005\A15=-158.31575906\A16=77.45990444\A17=-164.87798122\A
18=-43.55757379\A19=-61.56228301\A20=59.36046419\A21=178.89915942\A22=184.5
6073111\A23=-69.43460299\A24=182.18850295\A25=-181.66924992\A26=-61.437
26821\A27=59.56594743\Version=AM64L-G03RevE.01\State=2-A\HF=-703.9240
226\RMSE=8.300e-09\RMSEF=9.596e-06\Thermal=0.\Dipole=0.4374865,1.337833
4,0.0024141\PG=C01 [X(C4H9O2S1)]\@
```

ROBHandHLYP/6-311G**

```
1\1\GINC-GOMBERG05\FOpt\ROBHandHLYP\6-311G(d,p)\C4H9O2S1(2)\HMAITKEN\1
8-Jun-2010\1\1\#ROBHandHLYP/6-311G** opt=(grad) geom=checkpoint guess=r
ead\calc of 5 membered starting material with Me attached\0,2\C\H,1,
B1\H,1,B2,2,A1\C,1,B3,2,A2,3,D1,0\H,4,B4,1,A3,2,D2,0\H,4,B5,1,A4,2,D3,
0\C,4,B6,1,A5,2,D4,0\H,7,B7,4,A6,1,D5,0\H,7,B8,4,A7,1,D6,0\O,7,B9,4,A8
,1,D7,0\S,10,B10,7,A9,4,D8,0\O,11,B11,10,A10,7,D9,0\C,11,B12,10,A11,7,
D10,0\H,13,B13,11,A12,10,D11,0\H,13,B14,11,A13,10,D12,0\H,13,B15,11,A1
4,10,D13,0\B1=1.07619062\B2=1.07411054\B3=1.48504778\B4=1.09335762\B5
=1.0867014\B6=1.51295536\B7=1.08546286\B8=1.0897035\B9=1.42482886\B10=
1.65329122\B11=1.46666831\B12=1.79123984\B13=1.08257526\B14=1.08198673
\B15=1.0823577\A1=117.73643918\A2=120.63263675\A3=110.68530113\A4=110.
71868986\A5=112.32069618\A6=110.90686234\A7=110.63102059\A8=107.551020
92\A9=114.95688064\A10=109.46492222\A11=91.62095566\A12=107.1595016\A1
3=109.54756048\A14=106.93474218\A15=-168.78504071\A16=84.17745163\A17=-15
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8.52600239\D4=-36.55233205\D5=-62.18651876\D6=58.41179047\D7=178.14457
244\D8=185.00222059\D9=-70.83664981\D10=181.26694721\D11=-182.03662758
D12=-61.54326168\D13=59.25945908\\Version=AM64L-G03RevE.01\\State=2-A\
HF=-706.2606029\RMSD=2.856e-09\RMSF=1.986e-05\\Thermal=0.\\Dipole=0.2168
844,1.2293223,-0.1198376\PG=C01 [X(C4H9O2S1)]\\@

ROBHandHLYP/6-311++G**

1\1\GINC-GOMBERG04\FOpt\ROBHandHLYP\6-311++G(d,p)\C4H9O2S1(2)\HMAITKEN
\17-Aug-2010\1\\#ROBHandHLYP/6-311++G(d,p) opt=(grad) geom=checkpoint
guess=read\\calc of 5 membered starting material with Me attached\\0,2
\C\H,1,B1\H,1,B2,2,A1\C,1,B3,2,A2,3,D1,0\H,4,B4,1,A3,2,D2,0\H,4,B5,1,A
4,2,D3,0\C,4,B6,1,A5,2,D4,0\H,7,B7,4,A6,1,D5,0\H,7,B8,4,A7,1,D6,0\O,7,
B9,4,A8,1,D7,0\S,10,B10,7,A9,4,D8,0\O,11,B11,10,A10,7,D9,0\C,11,B12,10
,A11,7,D10,0\H,13,B13,11,A12,10,D11,0\H,13,B14,11,A13,10,D12,0\H,13,B1
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0944\B5=1.08666569\B6=1.51332915\B7=1.0855987\B8=1.08936065\B9=1.42616
702\B10=1.65263512\B11=1.46924092\B12=1.79124192\B13=1.0827801\B14=1.0
821884\B15=1.0825111\A1=117.76341706\A2=120.72737984\A3=110.53901835\A
4=110.63957953\A5=112.24632858\A6=110.87373133\A7=110.65761346\A8=107.
6271899\A9=115.22730424\A10=109.28845824\A11=92.03595359\A12=106.88242
841\A13=109.42306869\A14=107.54899903\D1=-169.55669343\D2=84.53558232\
D3=-158.23311869\D4=-36.17375628\D5=-63.18132928\D6=57.55316953\D7=177
.22143768\D8=183.24774218\D9=-72.26290393\D10=179.64517853\D11=-182.87
889114\D12=-62.7925868\D13=58.27989343\\Version=AM64L-G03RevE.01\\State
=2-A\HF=-706.2703908\RMSD=9.214e-09\RMSF=2.211e-05\\Thermal=0.\\Dipole=0
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QCISD/6-311++G**//BHandHLYP/6-311++G**

QCISD=-705.1215722

CCSD(T)/6-311++G**//BHandHLYP/6-311++G**

CCSD(T)=-705.1609797

QCISD/aug-cc-pVDZ//BHandHLYP/6-311++G**

QCISD=-705.0739566

CCSD(T)/aug-cc-pVDZ//BHandHLYP/6-311++G**

CCSD(T)=-705.1128661

ROMP2/6-311++G**//BHandHLYP/6-311++G**

MP2=-705.0575156

Transition state (7)

ROHF/6-31G*

```
1\1\GINC-GOMBERG01\FTS\ROHF\6-31G(d)\C4H9O2S1(2)\HMAITKEN\25-Jun-2010\
1\1\#ROHF/6-31G* opt=(grad,readfc,maxcyc=500,ts,noeigentest,nofreeze) g
eom=checkpoint guess=read\calc of 5 membered sulfinate ts with me\0,
2\S\O,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,1,B4,3,A3,2,D2,0\H,3,B5,2,
A4,1,D3,0\H,3,B6,2,A5,1,D4,0\H,4,B7,3,A6,2,D5,0\H,4,B8,3,A7,2,D6,0\H,5
,B9,4,A8,3,D7,0\H,5,B10,4,A9,3,D8,0\O,1,B11,2,A10,3,D9,0\C,1,B12,12,A1
1,2,D10,0\H,13,B13,1,A12,12,D11,0\H,13,B14,1,A13,12,D12,0\H,13,B15,1,A
14,12,D13,0\B2=1.42433283\B3=1.53052217\B5=1.08049301\B6=1.08252705\B
7=1.08453274\B8=1.08180726\B9=1.08433529\B10=1.07988341\B11=1.46088954
\B13=1.07920167\B14=1.07903285\B15=1.07887825\A1=117.26624518\A2=108.5
0940461\A3=62.27214887\A4=107.96253156\A5=106.72713247\A6=111.01347665
\A7=110.69420288\A8=112.55270761\A9=115.10615671\A10=112.51419632\A11=
98.37045212\A12=104.32039185\A13=105.04148008\A14=108.07738189\D1=1.91
978843\D2=152.5596453\D3=-120.6532523\D4=122.29269015\D5=149.74840801\
D6=-89.62630411\D7=73.90925618\D8=-158.32905026\D9=76.835488\D10=-90.6
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=-703.7708986\RMSD=3.149e-09\RMSF=2.281e-06\Thermal=0.\Dipole=0.535549
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```

ROHF/6-311G**

```
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10\1\1\#ROHF/6-311G** opt=(grad,readfc,maxcyc=500,ts,noeigentest,nofree
ze) geom=checkpoint guess=read\calc of 5 membered sulfinate ts with m
e\0,2\S\O,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,1,B4,3,A3,2,D2,0\H,3,
B5,2,A4,1,D3,0\H,3,B6,2,A5,1,D4,0\H,4,B7,3,A6,2,D5,0\H,4,B8,3,A7,2,D6,
0\H,5,B9,4,A8,3,D7,0\H,5,B10,4,A9,3,D8,0\O,1,B11,2,A10,3,D9,0\C,1,B12,
12,A11,2,D10,0\H,13,B13,1,A12,12,D11,0\H,13,B14,1,A13,12,D12,0\H,13,B1
5,1,A14,12,D13,0\B2=1.42361925\B3=1.53034491\B5=1.08094445\B6=1.08328
441\B7=1.08472313\B8=1.0821294\B9=1.0845955\B10=1.07962764\B11=1.45596
485\B13=1.0795699\B14=1.07922193\B15=1.07935036\A1=117.64831462\A2=108
.32889751\A3=62.28170687\A4=108.03783967\A5=106.79081975\A6=110.926693
5\A7=110.5196036\A8=112.81578328\A9=115.3066559\A10=112.06357527\A11=9
8.70436095\A12=104.10148359\A13=104.85952526\A14=107.7235424\D1=2.1454
455\D2=152.39167192\D3=-120.18054721\D4=122.54040808\D5=149.90986628\D
6=-89.42640938\D7=73.48047735\D8=-157.81161636\D9=76.56900072\D10=-90.
89470571\D11=-64.65503534\D12=54.12499301\D13=-185.02592138\B12=2.0104
0398\B4=1.88263507\B1=1.62450592\Version=AM64L-G03RevE.01\State=2-A\H
F=-703.8688938\RMSD=5.044e-09\RMSF=1.865e-05\Thermal=0.\Dipole=0.52884
19,1.2413043,0.6311836\PG=C01 [X(C4H9O2S1)]\@
```

ROBHandHLYP/6-311G**

```
1\1\GINC-GOMBERG02\FTS\ROBHandHLYP\6-311G(d,p)\C4H9O2S1(2)\HMAITKEN\25
-Jun-2010\1\1\#ROBHandHLYP/6-311G** opt=(grad,readfc,maxcyc=500,ts,noei
gentest,nofreeze) geom=checkpoint guess=read\calc of 5 membered sulfi
nate ts with me\0,2\S\O,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,1,B4,3,
A3,2,D2,0\H,3,B5,2,A4,1,D3,0\H,3,B6,2,A5,1,D4,0\H,4,B7,3,A6,2,D5,0\H,4
,B8,3,A7,2,D6,0\H,5,B9,4,A8,3,D7,0\H,5,B10,4,A9,3,D8,0\O,1,B11,2,A10,3
,D9,0\C,1,B12,12,A11,2,D10,0\H,13,B13,1,A12,12,D11,0\H,13,B14,1,A13,12
,D12,0\H,13,B15,1,A14,12,D13,0\B2=1.42770468\B3=1.52414369\B5=1.08296
87\B6=1.08571139\B7=1.08560115\B8=1.0836176\B9=1.08494991\B10=1.080317
77\B11=1.46828206\B13=1.07881377\B14=1.07818437\B15=1.07843775\A1=116.
77444866\A2=108.53967602\A3=61.5124533\A4=107.96495974\A5=107.02469553
\A6=110.90647782\A7=110.48734702\A8=113.21229616\A9=115.56832175\A10=1
12.32594448\A11=98.14063162\A12=102.6892623\A13=102.82635891\A14=106.7
9408419\D1=-1.13265018\D2=154.71955396\D3=-123.44704097\D4=119.2598992
6\D5=153.1789528\D6=-86.21058404\D7=71.47543145\D8=-158.75737904\D9=79
.02077801\D10=-88.85992886\D11=-64.09530772\D12=54.5955686\D13=-184.78
546105\B12=2.08709617\B4=1.89448187\B1=1.6562695\Version=AM64L-G03Rev
E.01\State=2-A\HF=-706.230947\RMSD=6.754e-09\RMSF=1.471e-05\Thermal=0.
```

\Dipole=0.6209249,1.1315631,0.5695035\PG=C01 [X(C4H9O2S1)]\@

ROBHandHLYP/6-311++G**

1\1\GINC-GOMBERG08\FTS\ROBHandHLYP\6-311++G(d,p)\C4H9O2S1(2)\HMAITKEN\09-Aug-2010\1\#\ROBHandHLYP\6-311++G(d,p) opt=(grad,readfc,maxcyc=500,ts,noeigentest,nofreeze) geom=checkpoint guess=read\calc of 5 membered sulfinate ts with me\0,2\S\O,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\C,1,B4,3,A3,2,D2,0\H,3,B5,2,A4,1,D3,0\H,3,B6,2,A5,1,D4,0\H,4,B7,3,A6,2,D5,0\H,4,B8,3,A7,2,D6,0\H,5,B9,4,A8,3,D7,0\H,5,B10,4,A9,3,D8,0\O,1,B11,2,A10,3,D9,0\C,1,B12,12,A11,2,D10,0\H,13,B13,1,A12,12,D11,0\H,13,B14,1,A13,12,D12,0\H,13,B15,1,A14,12,D13,0\B2=1.42736781\B3=1.52308985\B5=1.0831075\B6=1.08601619\B7=1.08570819\B8=1.08385512\B9=1.08502424\B10=1.08037099\B11=1.47048897\B13=1.07876083\B14=1.07828005\B15=1.07839213\A1=117.0099099\A2=108.52910212\A3=61.37902739\A4=107.79819092\A5=107.19861799\A6=110.7885061\A7=110.64216057\A8=113.04278442\A9=115.64060809\A10=112.31944374\A11=97.65138302\A12=102.22466\A13=102.77620569\A14=106.68108393\D1=-3.79727801\D2=157.66631477\D3=-126.10538583\D4=116.64000731\D5=153.93427689\D6=-85.62423727\D7=72.11312144\D8=-158.32389688\D9=81.67562761\D10=-88.62146114\D11=-62.68412703\D12=56.01338837\D13=-183.24055542\B12=2.09434407\B4=1.89366764\B1=1.65888298\Version=AM64L-G03RevE.01\State=2-A\HF=-706.2392127\RMSD=9.558e-10\RMSF=1.505e-05\Thermal=0.\Dipole=0.9916437,0.4176336,-1.00017\PG=C01 [X(C4H9O2S1)]\@

QCISD/6-311++G**//BHandHLYP/6-311++G**

QCISD=-705.094142

CCSD(T)/6-311++G**//BHandHLYP/6-311++G**

CCSD(T)=-705.1373979

QCISD/aug-cc-pVDZ//BHandHLYP/6-311++G**

QCISD=-705.0530823

CCSD(T)/aug-cc-pVDZ//BHandHLYP/6-311++G**

CCSD(T)=-705.0964686

ROMP2/6-311++G**//BHandHLYP/6-311++G**

MP2=-705.0370148

Sultine product (Scheme 4)

RHF/6-31G*

```
1\1\GINC-GOMBERG05\FOpt\RHF\6-31G(d)\C3H6O2S1\HMAITKEN\17-Aug-2010\1\
#HF/6-31G* opt=(grad) geom=checkpoint guess=read\calc of 5 membered s
ulfinate product\0,1\C\C,1,B1\C,2,B2,1,A1\H,1,B3,2,A2,3,D1,0\H,1,B4,2
,A3,3,D2,0\H,2,B5,1,A4,3,D3,0\H,2,B6,1,A5,3,D4,0\H,3,B7,2,A6,1,D5,0\H
,3,B8,2,A7,1,D6,0\H,3,B9,2,A8,1,D7,0\O,1,B10,2,A9,3,D8,0\O,10,B11,3,A10
,2,D9,0\B1=1.53588954\B2=1.52874036\B3=1.0798547\B4=1.08098996\B5=1.0
8290314\B6=1.08111973\B7=1.08403726\B8=1.0807197\B9=1.80178599\B10=1.4
3103498\B11=1.45904233\A1=105.19541496\A2=112.47303672\A3=112.26464899
\A4=111.49261422\A5=110.59492576\A6=112.406393\A7=113.98750622\A8=102.
44006418\A9=107.80519625\A10=105.04509523\D1=138.94935689\D2=-97.38778
947\D3=121.28069404\D4=-117.92154308\D5=76.84323329\D6=-157.20303406\D
7=-39.06132667\D8=19.1135048\D9=-69.53621414\Version=AM64L-G03RevE.01
\State=1-A\HF=-664.2639756\RMSD=3.840e-09\RMSF=1.787e-05\Thermal=0.\Di
pole=-0.5353669,1.6080707,0.5681313\PG=C01 [X(C3H6O2S1)]\@
```

RHF/6-311G**

```
1\1\GINC-GOMBERG04\FOpt\RHF\6-311G(d,p)\C3H6O2S1\HMAITKEN\17-Aug-2010\
1\#HF/6-311G** opt=(grad) geom=checkpoint guess=read\calc of 5 membe
red sulfinate product\0,1\C\C,1,B1\C,2,B2,1,A1\H,1,B3,2,A2,3,D1,0\H,1
,B4,2,A3,3,D2,0\H,2,B5,1,A4,3,D3,0\H,2,B6,1,A5,3,D4,0\H,3,B7,2,A6,1,D5
,0\H,3,B8,2,A7,1,D6,0\H,3,B9,2,A8,1,D7,0\O,1,B10,2,A9,3,D8,0\O,10,B11,
3,A10,2,D9,0\B1=1.53586921\B2=1.52810831\B3=1.08046863\B4=1.08167408\
B5=1.0829806\B6=1.08129753\B7=1.08431596\B8=1.08050023\B9=1.80289357\B
10=1.43017308\B11=1.45447657\A1=105.27485186\A2=112.30092994\A3=112.35
542006\A4=111.4762992\A5=110.36966125\A6=112.52107563\A7=114.28758414\
A8=102.24643428\A9=107.5835889\A10=104.80880165\D1=138.92134072\D2=-97
.32521431\D3=121.43954229\D4=-117.63028694\D5=76.4282363\D6=-156.84826
769\D7=-39.04674326\D8=19.22993431\D9=-69.1687898\Version=AM64L-G03Re
vE.01\State=1-A\HF=-664.3494102\RMSD=3.966e-09\RMSF=2.412e-05\Thermal=
0.\Dipole=-0.523685,1.6758028,0.5900314\PG=C01 [X(C3H6O2S1)]\@
```

BHandHLYP/6-311G**

```
1\1\GINC-GOMBERG06\FOpt\RBHandHLYP\6-311G(d,p)\C3H6O2S1\HMAITKEN\17-Au
g-2010\1\#BHandHLYP/6-311G** opt=(grad) geom=checkpoint guess=read\c
alc of 5 membered sulfinate product\0,1\C\C,1,B1\C,2,B2,1,A1\H,1,B3,2
,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,2,B5,1,A4,3,D3,0\H,2,B6,1,A5,3,D4,0\H
,3,B7,2,A6,1,D5,0\H,3,B8,2,A7,1,D6,0\H,3,B9,2,A8,1,D7,0\O,1,B10,2,A9,3
,D8,0\O,10,B11,3,A10,2,D9,0\B1=1.52746993\B2=1.51980975\B3=1.08242955\
B4=1.08420174\B5=1.08366716\B6=1.08286781\B7=1.08515302\B8=1.08140137\
B9=1.8168634\B10=1.43619265\B11=1.46639986\A1=105.20018219\A2=112.4310
1989\A3=112.14102111\A4=111.53383512\A5=110.36608533\A6=112.80656436\A
7=114.41280004\A8=101.92807546\A9=107.80074033\A10=104.71966388\D1=143
.73807282\D2=-92.68297075\D3=121.70099455\D4=-117.27020343\D5=73.06482
433\D6=-159.52881476\D7=-42.403053\D8=24.01527172\D9=-69.14386004\Ver
sion=AM64L-G03RevE.01\State=1-A\HF=-666.4297794\RMSD=3.259e-09\RMSF=6.
358e-05\Thermal=0.\Dipole=-0.4548234,1.601965,0.5197478\PG=C01 [X(C3H6
O2S1)]\@
```

BHandHLYP/6-311++G**

```
1\1\GINC-GOMBERG06\FOpt\RBHandHLYP\6-311++G(d,p)\C3H6O2S1\HMAITKEN\17-
Aug-2010\1\#BHandHLYP/6-311++G(d,p) opt=(grad) geom=checkpoint guess=
read\calc of 5 membered sulfinate product\0,1\C\C,1,B1\C,2,B2,1,A1\H
,1,B3,2,A2,3,D1,0\H,1,B4,2,A3,3,D2,0\H,2,B5,1,A4,3,D3,0\H,2,B6,1,A5,3
,D4,0\H,3,B7,2,A6,1,D5,0\H,3,B8,2,A7,1,D6,0\H,3,B9,2,A8,1,D7,0\O,1,B10
,2,A9,3,D8,0\O,10,B11,3,A10,2,D9,0\B1=1.52650613\B2=1.52001718\B3=1.08
25577\B4=1.08438828\B5=1.0839448\B6=1.0831514\B7=1.08528607\B8=1.08136
326\B9=1.81841133\B10=1.43605625\B11=1.46897779\A1=105.28324211\A2=112
.51967187\A3=112.10404243\A4=111.31238045\A5=110.61146522\A6=112.67844
906\A7=114.49489761\A8=102.49775897\A9=107.87723938\A10=104.92155194\D
1=144.16442363\D2=-92.23733927\D3=121.24556132\D4=-118.05346169\D5=73.
```

86235889\D6=-158.90744668\D7=-41.62725615\D8=24.55061853\D9=-70.944939
74\\Version=AM64L-G03RevE.01\State=1-A\HF=-666.4377986\RMSD=4.220e-09\
RMSF=3.678e-05\Thermal=0.\Dipole=-0.5078832,1.6777577,0.5419926\PG=C01
[X(C3H6O2S1)]\@

QCISD/6-311++G**//BHandHLYP/6-311++G**
QCISD=-665.3846376

CCSD(T)/6-311++G**//BHandHLYP/6-311++G**
CCSD(T)=-665.4213619

QCISD/aug-cc-pVDZ//BHandHLYP/6-311++G**
QCISD=-665.3455849

CCSD(T)/aug-cc-pVDZ//BHandHLYP/6-311++G**
CCSD(T)=-665.3815576

ROMP2/6-311++G(d,p)//BHandHLYP/6-311++G**
MP2=-665.3435476

Radical 8

ROHF/6-31G*

```
1\1\GINC-X127\FOpt\ROHF\6-31G(d)\C11H15O2S1(2)\SHK563\22-Apr-2010\1\#\n
ROHF/6-31G* opt=grad optcyc=300 scfcyc=300 geom=checkpoint guess=chec
k freq=noraman\Louis' starting radical t-butyl\0,2\C\S,1,B1\O,2,B2,1
,A1\O,2,B3,1,A2,3,D1,0\C,3,B4,2,A3,1,D2,0\C,5,B5,3,A4,2,D3,0\C,6,B6,5,
A5,3,D4,0\C,7,B7,6,A6,5,D5,0\C,8,B8,7,A7,6,D6,0\C,9,B9,8,A8,7,D7,0\C,1
0,B10,9,A9,8,D8,0\C,1,B11,2,A10,3,D9,0\C,1,B12,2,A11,3,D10,0\C,1,B13,2
,A12,3,D11,0\H,5,B14,3,A13,2,D12,0\H,5,B15,3,A14,2,D13,0\H,8,B16,7,A15
,6,D14,0\H,9,B17,8,A16,7,D15,0\H,10,B18,9,A17,8,D16,0\H,11,B19,10,A18
,9,D17,0\H,12,B20,1,A19,2,D18,0\H,12,B21,1,A20,2,D19,0\H,12,B22,1,A21,2
,D20,0\H,13,B23,1,A22,2,D21,0\H,13,B24,1,A23,2,D22,0\H,13,B25,1,A24,2,
D23,0\H,14,B26,1,A25,2,D24,0\H,14,B27,1,A26,2,D25,0\H,14,B28,1,A27,2,D
26,0\B1=1.82560889\B2=1.62649459\B3=1.4652569\B4=1.4262738\B5=1.50648
586\B6=1.37143941\B7=1.37444144\B8=1.38683504\B9=1.39058389\B10=1.3838
5155\B11=1.53192021\B12=1.53004354\B13=1.5358407\B14=1.0808674\B15=1.0
8362147\B16=1.07441578\B17=1.07570708\B18=1.07512634\B19=1.07533012\B2
0=1.0861851\B21=1.0818123\B22=1.08525695\B23=1.08176633\B24=1.08238679
\B25=1.08612074\B26=1.08278579\B27=1.08624738\B28=1.08483441\A1=95.311
47368\A2=107.06504315\A3=117.04097338\A4=110.154526\A5=121.82156616\A6
=125.57128086\A7=116.84882806\A8=120.05916636\A9=120.83038639\A10=108.
54245155\A11=110.07675208\A12=104.93177977\A13=107.63148708\A14=109.84
063317\A15=121.61921515\A16=119.95362549\A17=119.67142573\A18=120.4255
2155\A19=111.58610848\A20=111.55488244\A21=109.08887556\A22=111.482716
44\A23=110.81194543\A24=108.97483231\A25=111.2399109\A26=111.71010455\
A27=109.16129868\D1=-110.74589214\D2=178.31018482\D3=124.90080069\D4=1
25.48313796\D5=178.54492327\D6=0.21555821\D7=-0.06668972\D8=-0.0926117
4\D9=-63.08215381\D10=59.71302502\D11=-181.32645851\D12=-114.47249076\
D13=3.3302052\D14=179.98148924\D15=179.87741155\D16=179.98795397\D17=1
79.81200533\D18=-54.7239634\D19=66.83612762\D20=-173.52489945\D21=-65.
56734168\D22=55.6167883\D23=174.81005341\D24=-61.58605076\D25=59.76570
622\D26=178.82328667\Version=EM64L-G03RevE.01\State=2-A\HF=-972.39014
16\RMSD=7.993e-09\RMSF=8.634e-06\Thermal=0.\Dipole=-0.260635,-0.601885
8,0.6604322\PG=C01 [X(C11H15O2S1)]\@
```

ROHF/6-311G**

```
1\1\GINC-X82\FOpt\ROHF\6-311G(d,p)\C11H15O2S1(2)\SHK563\27-Apr-2010\1\
#\n ROHF/6-311G** opt=grad optcyc=300 scfcyc=300 geom=checkpoint guess=
check freq=noraman\Louis' starting radical t-butyl\0,2\C\S,1,B1\O,2,
B2,1,A1\O,2,B3,1,A2,3,D1,0\C,3,B4,2,A3,1,D2,0\C,5,B5,3,A4,2,D3,0\C,6,B
6,5,A5,3,D4,0\C,7,B7,6,A6,5,D5,0\C,8,B8,7,A7,6,D6,0\C,9,B9,8,A8,7,D7,0
\C,10,B10,9,A9,8,D8,0\C,1,B11,2,A10,3,D9,0\C,1,B12,2,A11,3,D10,0\C,1,B
13,2,A12,3,D11,0\H,5,B14,3,A13,2,D12,0\H,5,B15,3,A14,2,D13,0\H,8,B16,7
,A15,6,D14,0\H,9,B17,8,A16,7,D15,0\H,10,B18,9,A17,8,D16,0\H,11,B19,10,
A18,9,D17,0\H,12,B20,1,A19,2,D18,0\H,12,B21,1,A20,2,D19,0\H,12,B22,1,A
21,2,D20,0\H,13,B23,1,A22,2,D21,0\H,13,B24,1,A23,2,D22,0\H,13,B25,1,A2
4,2,D23,0\H,14,B26,1,A25,2,D24,0\H,14,B27,1,A26,2,D25,0\H,14,B28,1,A27
,2,D26,0\B1=1.82855184\B2=1.61995016\B3=1.46044269\B4=1.42452628\B5=1
.50608203\B6=1.3701034\B7=1.3734909\B8=1.38592322\B9=1.38977343\B10=1.
3829705\B11=1.53106969\B12=1.52901378\B13=1.53505871\B14=1.08101481\B1
5=1.08513361\B16=1.07444131\B17=1.07577623\B18=1.0751473\B19=1.0754937
9\B20=1.08669939\B21=1.08213924\B22=1.0858227\B23=1.08203175\B24=1.082
74286\B25=1.08668596\B26=1.08312647\B27=1.08675971\B28=1.08526667\A1=9
5.54927613\A2=106.8963067\A3=117.75307501\A4=110.47293593\A5=121.67229
664\A6=125.69142778\A7=116.77745836\A8=120.04623828\A9=120.8816225\A10
=108.26535283\A11=109.82516383\A12=104.71327078\A13=107.6002284\A14=10
9.74191887\A15=121.63906725\A16=119.94575187\A17=119.67536177\A18=120.
47921011\A19=111.5490241\A20=111.40177866\A21=109.14248375\A22=111.396
25201\A23=110.74177332\A24=108.93321736\A25=111.1827172\A26=111.691406
86\A27=109.07102548\D1=-110.64462333\D2=175.9243722\D3=121.61336845\D4
=127.06979296\D5=178.40527422\D6=0.21253368\D7=-0.04634981\D8=-0.08446
006\D9=-63.26407398\D10=59.48464334\D11=-181.51379593\D12=-117.8245175
```

8\D13=-0.06668332\D14=179.9597225\D15=179.87134858\D16=179.98116184\D17=179.81371008\D18=-54.47115956\D19=66.98735051\D20=-173.33078332\D21=-65.38003974\D22=55.69465476\D23=174.90998769\D24=-62.18785939\D25=59.12065309\D26=178.21465501\\Version=EM64L-G03RevE.01\\State=2-A\\HF=-972.5445492\\RMSD=3.697e-09\\RMSF=2.117e-05\\Thermal=0.\\Dipole=0.3894208,0.6793735,-0.6230239\\PG=C01 [X(C11H15O2S1)]\\@

ROBHandHLYP/6-311G**

1\\GINC-GOMBERG02\\FTS\\ROBHandHLYP\\6-311G(d,p)\\C11H15O2S1(2)\\CARLHS\\24-Jul-2010\\1\\#robhandhlyp/6-311G** opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpoint guess=read scfcyc=300\\t-Bu system\\0,2\\S\\C,1,r12\\O,1,r13,2,a213\\O,1,r14,2,a214,3,dih1,0\\C,3,r35,1,a135,2,dih2,0\\C,2,r26,1,a126,3,dih3,0\\C,6,r67,2,a267,1,dih4,0\\C,7,r78,6,a678,2,dih5,0\\C,8,r89,7,a789,6,dih6,0\\C,9,r910,8,a8910,7,dih7,0\\H,5,r511,6,a6511,2,dih8,0\\H,5,r512,6,a6512,2,dih9,0\\H,7,r713,6,a6713,2,dih10,0\\H,8,r814,7,a7814,6,dih11,0\\H,9,r915,8,a8915,7,dih12,0\\H,10,r1016,9,a91016,8,dih13,0\\C,1,r117,3,a2117,5,dih14,0\\C,17,r1718,1,a11718,2,dih15,0\\C,17,r1719,1,a11719,2,dih16,0\\C,17,r1720,1,a11720,2,dih17,0\\H,18,r1821,17,a171821,1,dih18,0\\H,18,r1822,17,a171822,1,dih19,0\\H,18,r1823,17,a171823,1,dih20,0\\H,19,r1924,17,a171924,1,dih21,0\\H,19,r1925,17,a171925,1,dih22,0\\H,19,r1926,17,a171926,1,dih23,0\\H,20,r2027,17,a172027,1,dih24,0\\H,20,r2028,17,a172028,1,dih25,0\\H,20,r2029,17,a172029,1,dih26,0\\r1718=1.51742156\\r1719=1.52084114\\r1720=1.51692573\\r1821=1.08743726\\r1822=1.08282498\\r1823=1.0871084\\r1924=1.08676101\\r1925=1.08713522\\r1926=1.08387541\\r2027=1.08866626\\r2028=1.08395601\\r2029=1.08256148\\a2117=91.58899464\\a1718=107.79851158\\a1719=103.36972152\\a1720=108.82726565\\a171821=109.37460032\\a171822=111.37116277\\a171823=111.52823324\\a171924=109.24868974\\a171925=111.6712248\\a171926=111.15574201\\a172027=109.08901709\\a172028=110.63239559\\a172029=111.3148497\\dih14=184.99490305\\dih15=374.06938183\\dih16=255.68945542\\dih17=137.04904637\\dih18=186.11182604\\dih19=66.30592892\\dih20=-55.06188335\\dih21=178.6675443\\dih22=59.67458592\\dih23=-61.69339112\\dih24=172.46105014\\dih25=53.26322631\\dih26=-67.76121304\\r13=1.65226184\\r14=1.46599775\\r35=1.42203022\\r26=1.36564668\\r67=1.387586\\r78=1.38476714\\r89=1.38798406\\r910=1.3881526\\r511=1.08326833\\r512=1.08685175\\r713=1.07825195\\r814=1.07632426\\r915=1.07699891\\r1016=1.07706128\\a213=83.53726648\\a214=99.61253863\\a135=118.38821664\\a126=103.90631648\\a267=118.65069965\\a678=119.09839735\\a789=120.8202626\\a8910=120.26265231\\a6511=112.48928516\\a6512=110.98495244\\a6713=120.69203321\\a7814=119.58058744\\a8915=119.81476609\\a91016=120.91285664\\dih1=109.95248015\\dih2=28.26401985\\dih3=-14.75933859\\dih4=180.94203439\\dih5=-0.32508469\\dih6=0.08076644\\dih7=0.03762607\\dih8=136.83701612\\dih9=-100.79678029\\dih10=179.80403602\\dih11=180.34594886\\dih12=180.07062626\\dih13=179.76826101\\r117=1.90969858\\r12=2.19333027\\\\Version=AM64L-G03RevE.01\\State=2-A\\HF=-976.4898988\\RMSD=9.526e-09\\RMSF=2.319e-05\\Thermal=0.\\Dipole=0.5201305,0.914865,0.2527115\\PG=C01 [X(C11H15O2S1)]\\@

ROBHandHLYP/6-311++G**

1\\GINC-GOMBERG02\\FTS\\ROBHandHLYP\\6-311++G(d,p)\\C11H15O2S1(2)\\CARLHS\\24-Jul-2010\\1\\#robhandhlyp/6-311++G** opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpoint guess=read scfcyc=300\\t-Bu system\\0,2\\S\\C,1,r12\\O,1,r13,2,a213\\O,1,r14,2,a214,3,dih1,0\\C,3,r35,1,a135,2,dih2,0\\C,2,r26,1,a126,3,dih3,0\\C,6,r67,2,a267,1,dih4,0\\C,7,r78,6,a678,2,dih5,0\\C,8,r89,7,a789,6,dih6,0\\C,9,r910,8,a8910,7,dih7,0\\H,5,r511,6,a6511,2,dih8,0\\H,5,r512,6,a6512,2,dih9,0\\H,7,r713,6,a6713,2,dih10,0\\H,8,r814,7,a7814,6,dih11,0\\H,9,r915,8,a8915,7,dih12,0\\H,10,r1016,9,a91016,8,dih13,0\\C,1,r117,3,a2117,5,dih14,0\\C,17,r1718,1,a11718,2,dih15,0\\C,17,r1719,1,a11719,2,dih16,0\\C,17,r1720,1,a11720,2,dih17,0\\H,18,r1821,17,a171821,1,dih18,0\\H,18,r1822,17,a171822,1,dih19,0\\H,18,r1823,17,a171823,1,dih20,0\\H,19,r1924,17,a171924,1,dih21,0\\H,19,r1925,17,a171925,1,dih22,0\\H,19,r1926,17,a171926,1,dih23,0\\H,20,r2027,17,a172027,1,dih24,0\\H,20,r2028,17,a172028,1,dih25,0\\H,20,r2029,17,a172029,1,dih26,0\\r1718=1.51794638\\r1719=1.52129697\\r1720=1.51723415\\r1821=1.08752117\\r1822=1.08306505\\r1823=1.08714768\\r1924=1.08687954\\r1925=1.08714185\\r1926=1.08405225\\r2027=1.08879739\\r2028=1.08409518\\r2029=1.08276766\\a2117=91.700263

2\ a11718=107.74468938\ a11719=103.35554648\ a11720=109.27071598\ a171821=
109.23846055\ a171822=111.41698798\ a171823=111.59198135\ a171924=109.118
48715\ a171925=111.7422087\ a171926=111.24428272\ a172027=108.86090749\ a1
72028=110.86961664\ a172029=111.4204211\ dih14=183.10022615\ dih15=374.71
855019\ dih16=256.55575306\ dih17=137.71612301\ dih18=186.91862278\ dih19=
67.20448409\ dih20=-54.3255693\ dih21=178.9503002\ dih22=60.03529371\ dih2
3=-61.51554649\ dih24=173.43891918\ dih25=54.36209779\ dih26=-66.98335906
\ r13=1.65265253\ r14=1.46718708\ r35=1.42234751\ r26=1.36547036\ r67=1.388
40552\ r78=1.38528731\ r89=1.38877028\ r910=1.38873154\ r511=1.08358454\ r5
12=1.08705026\ r713=1.07831409\ r814=1.07636119\ r915=1.0770505\ r1016=1.0
7712589\ a213=83.6135574\ a214=99.78553073\ a135=118.81820441\ a126=103.86
24807\ a267=118.60447457\ a678=119.10898753\ a789=120.81804002\ a8910=120.
2510035\ a6511=112.43049436\ a6512=111.02136775\ a6713=120.6996386\ a7814=
119.57539965\ a8915=119.82408094\ a91016=120.89753322\ dih1=110.00838688\
dih2=26.93879719\ dih3=-13.66571499\ dih4=180.62671643\ dih5=-0.38427341\
dih6=0.07964821\ dih7=0.05198025\ dih8=136.58068707\ dih9=-101.15282007\
dih10=179.7815977\ dih11=180.34997293\ dih12=180.08115271\ dih13=179.77254
472\ r117=1.90986759\ r12=2.19874478\ \Version=AM64L-G03RevE.01\State=2-A
\HF=-976.4987869\RMSE=7.059e-09\RMSE=1.906e-05\Thermal=0.\Dipole=0.531
1443,0.9450405,0.2109652\PG=C01 [X(C11H15O2S1)]\@

Transition State 9

ROHF/6-31G*

```
1\1\GINC-GOMBERG02\FTS\ROHF\6-31G(d)\C11H15O2S1(2)\CARLHS\24-Jul-2010\
1\#\rohff/6-31G* opt=(grad,ts,readfc,noeigentest,nofreeze) geom=checkpo
int guess=read scfcyc=300\t-Bu system\0,2\S\C,1,r12\O,1,r13,2,a213\O
,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,3,dih3,0
\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a789,6,dih6
,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r512,6,a651
2,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11,0\H,9,r
915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r117,3,a2117,5
,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,17,r1719,1,a11719,2,dih16,0\C
,17,r1720,1,a11720,2,dih17,0\H,18,r1821,17,a171821,1,dih18,0\H,18,r182
2,17,a171822,1,dih19,0\H,18,r1823,17,a171823,1,dih20,0\H,19,r1924,17,a
171924,1,dih21,0\H,19,r1925,17,a171925,1,dih22,0\H,19,r1926,17,a171926
,1,dih23,0\H,20,r2027,17,a172027,1,dih24,0\H,20,r2028,17,a172028,1,dih
25,0\H,20,r2029,17,a172029,1,dih26,0\|r1718=1.52842615\r1719=1.5315210
2\r1720=1.52856952\r1821=1.08611528\r1822=1.08197096\r1823=1.08646993\
r1924=1.08572491\r1925=1.08653966\r1926=1.08246125\r2027=1.08765926\r2
028=1.08221094\r2029=1.08173936\|a2117=92.29274561\|a1718=108.4742882\|a
11719=104.29000258\|a1720=110.26069369\|a171821=109.2834675\|a171822=111
.69436944\|a171823=111.56193524\|a171924=109.30189525\|a171925=111.640213
24\|a171926=111.30586681\|a172027=108.96449692\|a172028=110.91585755\|a172
029=111.53344563\|dih14=179.83063425\|dih15=379.28319991\|dih16=261.25618
201\|dih17=142.31642593\|dih18=186.81109258\|dih19=67.11244895\|dih20=-54.
42604303\|dih21=178.13743918\|dih22=59.22845568\|dih23=-62.1305444\|dih24=
173.74107708\|dih25=54.53710233\|dih26=-66.83621766\|r13=1.62705043\|r14=1
.45778978\|r35=1.42085326\|r26=1.3673763\|r67=1.38830558\|r78=1.38553212\|r
89=1.39105594\|r910=1.38718901\|r511=1.08106775\|r512=1.08313115\|r713=1.0
7692591\|r814=1.07527852\|r915=1.07569605\|r1016=1.07562033\|a213=84.97036
263\|a214=99.60357081\|a135=119.7089453\|a126=106.3782853\|a267=119.343301
64\|a678=118.85664513\|a789=120.78304977\|a8910=120.3104341\|a6511=112.876
09753\|a6512=111.7191683\|a6713=120.94185687\|a7814=119.6234153\|a8915=119
.68930309\|a91016=120.87191378\|dih1=110.76333573\|dih2=23.95556792\|dih3=
-11.67948521\|dih4=179.75377926\|dih5=-0.47625251\|dih6=0.07302381\|dih7=0
.0901951\|dih8=134.23860919\|dih9=-102.56901188\|dih10=179.65338076\|dih11
=180.34536614\|dih12=180.10501003\|dih13=179.8543613\|r117=1.88697889\|r12
=2.09316146\|Version=AM64L-G03RevE.01\|State=2-A\HF=-972.3480001\|RMSD=6
.331e-09\|RMSF=3.087e-05\|Thermal=0.\|Dipole=0.565304,1.0009128,0.404116\
PG=C01 [X(C11H15O2S1)]\|\@
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ROHF/6-311G**

```
1\1\GINC-GOMBERG02\FTS\ROHF\6-311G(d,p)\C11H15O2S1(2)\CARLHS\24-Jul-20
10\1\#\rohff/6-311G** opt=(grad,ts,readfc,noeigentest,nofreeze) geom=ch
eckpoint guess=read scfcyc=300\t-Bu system\0,2\S\C,1,r12\O,1,r13,2,a
213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,3,d
ih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a789,6
,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r512,6
,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11,0\
H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r117,3,a2
117,5,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,17,r1719,1,a11719,2,dih1
6,0\C,17,r1720,1,a11720,2,dih17,0\H,18,r1821,17,a171821,1,dih18,0\H,18
,r1822,17,a171822,1,dih19,0\H,18,r1823,17,a171823,1,dih20,0\H,19,r1924
,17,a171924,1,dih21,0\H,19,r1925,17,a171925,1,dih22,0\H,19,r1926,17,a1
71926,1,dih23,0\H,20,r2027,17,a172027,1,dih24,0\H,20,r2028,17,a172028
,1,dih25,0\H,20,r2029,17,a172029,1,dih26,0\|r1718=1.52713803\r1719=1.53
008236\r1720=1.52721046\r1821=1.08676937\r1822=1.08224492\r1823=1.0869
8511\r1924=1.08619445\r1925=1.08703459\r1926=1.08283493\r2027=1.088359
54\r2028=1.0825931\r2029=1.0819847\|a2117=92.43683003\|a11718=108.151629
57\|a11719=104.01542988\|a11720=109.81964248\|a171821=109.34652113\|a17182
2=111.54352839\|a171823=111.52235131\|a171924=109.25085099\|a171925=111.6
091589\|a171926=111.25485418\|a172027=108.94250111\|a172028=110.82750035\
a172029=111.43791796\|dih14=181.26277437\|dih15=378.84489749\|dih16=260.7
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4819243\dih17=141.81762342\dih18=186.83132009\dih19=67.0661331\dih20=-
54.36203536\dih21=177.76101631\dih22=58.84939183\dih23=-62.48472119\di
h24=173.5576008\dih25=54.30573474\dih26=-66.92828627\r13=1.62059793\r1
4=1.45282002\r35=1.4191619\r26=1.36596289\r67=1.38759149\r78=1.3846077
3\r89=1.3905225\r910=1.38621514\r511=1.08117559\r512=1.08402198\r713=1
.07690925\r814=1.07533417\r915=1.07574843\r1016=1.07572009\ a213=84.769
31042\ a214=99.44914072\ a135=119.87329019\ a126=106.45267176\ a267=119.28
967724\ a678=118.84130228\ a789=120.8144033\ a8910=120.3158169\ a6511=112.
80318886\ a6512=111.45929497\ a6713=120.94650434\ a7814=119.61567026\ a891
5=119.69602379\ a91016=120.95100958\ dih1=110.34789991\ dih2=24.90052448\
dih3=-12.55699023\ dih4=180.29158055\ dih5=-0.44940186\ dih6=0.07276013\ d
ih7=0.06954844\ dih8=134.03695312\ dih9=-102.62711505\ dih10=179.68326997
\ dih11=180.30179691\ dih12=180.08019203\ dih13=179.70458193\r117=1.89551
908\r12=2.08895746\ \Version=AM64L-G03RevE.01\State=2-A\HF=-972.5013565
\RMSD=7.795e-09\RMSF=1.558e-05\Thermal=0.\Dipole=0.5766925,1.0331186,0
.3676887\PG=C01 [X(C11H15O2S1)]\@

ROBHandHLYP/6-311G**

1\1\GINC-GOMBERG02\FTS\ROBHandHLYP\6-311G(d,p)\C11H15O2S1(2)\CARLHS\24
-Jul-2010\1\#\robhandhlyp/6-311G** opt=(grad,ts,readfc,noeigentest,nof
reeze) geom=checkpoint guess=read scfcyc=300\ \t-Bu system\ \0,2\S\C,1,r
12\O,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,
r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,
8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih
8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7
814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0
\C,1,r117,3,a2117,5,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,17,r1719,1
,a11719,2,dih16,0\C,17,r1720,1,a11720,2,dih17,0\H,18,r1821,17,a171821,
1,dih18,0\H,18,r1822,17,a171822,1,dih19,0\H,18,r1823,17,a171823,1,dih2
0,0\H,19,r1924,17,a171924,1,dih21,0\H,19,r1925,17,a171925,1,dih22,0\H,
19,r1926,17,a171926,1,dih23,0\H,20,r2027,17,a172027,1,dih24,0\H,20,r20
28,17,a172028,1,dih25,0\H,20,r2029,17,a172029,1,dih26,0\ \r1718=1.51742
156\r1719=1.52084114\r1720=1.51692573\r1821=1.08743726\r1822=1.0828249
8\r1823=1.0871084\r1924=1.08676101\r1925=1.08713522\r1926=1.08387541\r
2027=1.08866626\r2028=1.08395601\r2029=1.08256148\ a2117=91.58899464\ a1
1718=107.79851158\ a11719=103.36972152\ a11720=108.82726565\ a171821=109.
37460032\ a171822=111.37116277\ a171823=111.52823324\ a171924=109.2486897
4\ a171925=111.6712248\ a171926=111.15574201\ a172027=109.08901709\ a17202
8=110.63239559\ a172029=111.3148497\ dih14=184.99490305\ dih15=374.069381
83\ dih16=255.68945542\ dih17=137.04904637\ dih18=186.11182604\ dih19=66.3
0592892\ dih20=-55.06188335\ dih21=178.6675443\ dih22=59.67458592\ dih23=-
61.69339112\ dih24=172.46105014\ dih25=53.26322631\ dih26=-67.76121304\r1
3=1.65226184\r14=1.46599775\r35=1.42203022\r26=1.36564668\r67=1.387586
\r78=1.38476714\r89=1.38798406\r910=1.3881526\r511=1.08326833\r512=1.0
8685175\r713=1.07825195\r814=1.07632426\r915=1.07699891\r1016=1.077061
28\ a213=83.53726648\ a214=99.61253863\ a135=118.38821664\ a126=103.906316
48\ a267=118.65069965\ a678=119.09839735\ a789=120.8202626\ a8910=120.2626
5231\ a6511=112.48928516\ a6512=110.98495244\ a6713=120.69203321\ a7814=11
9.58058744\ a8915=119.81476609\ a91016=120.91285664\ dih1=109.95248015\ di
h2=28.26401985\ dih3=-14.75933859\ dih4=180.94203439\ dih5=-0.32508469\ di
h6=0.08076644\ dih7=0.03762607\ dih8=136.83701612\ dih9=-100.79678029\ dih
10=179.80403602\ dih11=180.34594886\ dih12=180.07062626\ dih13=179.768261
01\r117=1.90969858\r12=2.19333027\ \Version=AM64L-G03RevE.01\State=2-A\
HF=-976.4898988\RMSD=9.526e-09\RMSF=2.319e-05\Thermal=0.\Dipole=0.5201
305,0.914865,0.2527115\PG=C01 [X(C11H15O2S1)]\@

ROBHandHLYP/6-311++G**

1\1\GINC-GOMBERG02\FTS\ROBHandHLYP\6-311++G(d,p)\C11H15O2S1(2)\CARLHS\
24-Jul-2010\1\#\robhandhlyp/6-311++G** opt=(grad,ts,readfc,noeigentest
,nofreeze) geom=checkpoint guess=read scfcyc=300\ \t-Bu system\ \0,2\S\C
,1,r12\O,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\
C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,
0\C,8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2
,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,

7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih
13,0\C,1,r117,3,a2117,5,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,17,r17
19,1,a11719,2,dih16,0\C,17,r1720,1,a11720,2,dih17,0\H,18,r1821,17,a171
821,1,dih18,0\H,18,r1822,17,a171822,1,dih19,0\H,18,r1823,17,a171823,1,
dih20,0\H,19,r1924,17,a171924,1,dih21,0\H,19,r1925,17,a171925,1,dih22,
0\H,19,r1926,17,a171926,1,dih23,0\H,20,r2027,17,a172027,1,dih24,0\H,20
,r2028,17,a172028,1,dih25,0\H,20,r2029,17,a172029,1,dih26,0\H,1718=1.5
1794638\r1719=1.52129697\r1720=1.51723415\r1821=1.08752117\r1822=1.083
06505\r1823=1.08714768\r1924=1.08687954\r1925=1.08714185\r1926=1.08405
225\r2027=1.08879739\r2028=1.08409518\r2029=1.08276766\ a2117=91.700263
2\ a11718=107.74468938\ a11719=103.35554648\ a11720=109.27071598\ a171821=
109.23846055\ a171822=111.41698798\ a171823=111.59198135\ a171924=109.118
48715\ a171925=111.7422087\ a171926=111.24428272\ a172027=108.86090749\ a1
72028=110.86961664\ a172029=111.4204211\ dih14=183.10022615\ dih15=374.71
855019\ dih16=256.55575306\ dih17=137.71612301\ dih18=186.91862278\ dih19=
67.20448409\ dih20=-54.3255693\ dih21=178.9503002\ dih22=60.03529371\ dih2
3=-61.51554649\ dih24=173.43891918\ dih25=54.36209779\ dih26=-66.98335906
\ r13=1.65265253\ r14=1.46718708\ r35=1.42234751\ r26=1.36547036\ r67=1.388
40552\ r78=1.38528731\ r89=1.38877028\ r910=1.38873154\ r511=1.08358454\ r5
12=1.08705026\ r713=1.07831409\ r814=1.07636119\ r915=1.0770505\ r1016=1.0
7712589\ a213=83.6135574\ a214=99.78553073\ a135=118.81820441\ a126=103.86
24807\ a267=118.60447457\ a678=119.10898753\ a789=120.81804002\ a8910=120.
2510035\ a6511=112.43049436\ a6512=111.02136775\ a6713=120.6996386\ a7814=
119.57539965\ a8915=119.82408094\ a91016=120.89753322\ dih1=110.00838688\
dih2=26.93879719\ dih3=-13.66571499\ dih4=180.62671643\ dih5=-0.38427341\
dih6=0.07964821\ dih7=0.05198025\ dih8=136.58068707\ dih9=-101.15282007\
dih10=179.7815977\ dih11=180.34997293\ dih12=180.08115271\ dih13=179.77254
472\ r117=1.90986759\ r12=2.19874478\ \Version=AM64L-G03RevE.01\State=2-A
\HF=-976.4987869\RMSD=7.059e-09\RMSF=1.906e-05\Thermal=0.\Dipole=0.531
1443,0.9450405,0.2109652\PG=C01 [X(C11H15O2S1)]\@

tert-Butyl Radical

ROHF/6-31G*

```
1\1\GINC-X129\FOpt\ROHF\6-31G(d)\C4H9(2)\SHK563\21-Apr-2010\1\1\# ROHF/
6-31G* opt=grad optcyc=300 scfcyc=300 geom=checkpoint guess=check freq
=noraman\Louis' leaving radical t-butyl\0,2\C\C,1,r1\C,1,r2,2,a1\C,1
,r3,2,a2,3,dih1,0\H,2,r4,1,a3,4,dih2,0\H,2,r5,1,a4,4,dih3,0\H,2,r6,1,a
5,4,dih4,0\H,3,r7,1,a6,4,dih5,0\H,3,r8,1,a7,4,dih6,0\H,3,r9,1,a8,4,dih
7,0\H,4,r10,1,a9,2,dih8,0\H,4,r11,1,a10,2,dih9,0\H,4,r12,1,a11,2,dih10
,0\|r1=1.50460444\r2=1.50461689\r3=1.50461681\r4=1.0919228\r5=1.085941
71\r6=1.08593965\r7=1.08593659\r8=1.09192346\r9=1.08594417\r10=1.08594
34\r11=1.09192389\r12=1.08593683\|a1=117.3699301\|a2=117.36908216\|a3=111
.39554378\|a4=111.45203996\|a5=111.45214512\|a6=111.45229656\|a7=111.39561
399\|a8=111.45247107\|a9=111.45287839\|a10=111.39562575\|a11=111.45182103\
\|dih1=148.31360076\|dih2=74.04929823\|dih3=-45.59323915\|dih4=193.69229727
\|dih5=45.56301897\|dih6=-74.08084693\|dih7=166.27761464\|dih8=45.59018379
\|dih9=-74.0521037\|dih10=166.3047035\|Version=EM64L-G03RevE.01\|State=2-
A\|HF=-156.6706486\|RMSD=3.819e-09\|RMSF=5.769e-05\|Thermal=0.\|Dipole=0.02
57507,-0.0907553,0.0156661\|PG=C01 [X(C4H9)]\|@
```

ROHF/6-311G**

```
1\1\GINC-X129\FOpt\ROHF\6-311G(d,p)\C4H9(2)\SHK563\21-Apr-2010\1\1\# RO
HF/6-311G** opt=grad optcyc=300 scfcyc=300 geom=checkpoint guess=check
freq=noraman\Louis' leaving radical t-butyl\0,2\C\C,1,r1\C,1,r2,2,a
1\C,1,r3,2,a2,3,dih1,0\H,2,r4,1,a3,4,dih2,0\H,2,r5,1,a4,4,dih3,0\H,2,r
6,1,a5,4,dih4,0\H,3,r7,1,a6,4,dih5,0\H,3,r8,1,a7,4,dih6,0\H,3,r9,1,a8,
4,dih7,0\H,4,r10,1,a9,2,dih8,0\H,4,r11,1,a10,2,dih9,0\H,4,r12,1,a11,2,
dih10,0\|r1=1.50351819\r2=1.503526\r3=1.50351024\r4=1.09308561\r5=1.08
63208\r6=1.08630156\r7=1.08631395\r8=1.09308804\r9=1.08630436\r10=1.08
631956\r11=1.09308364\r12=1.08630519\|a1=117.3620525\|a2=117.34810553\|a3
=111.26661595\|a4=111.40367981\|a5=111.4067777\|a6=111.40382305\|a7=111.26
8159\|a8=111.40551656\|a9=111.4036814\|a10=111.26554884\|a11=111.40694403\
\|dih1=148.23044292\|dih2=74.04274827\|dih3=-45.57384104\|dih4=193.66757492
\|dih5=45.56053874\|dih6=-74.05837703\|dih7=166.31853349\|dih8=45.57698704
\|dih9=-74.04004132\|dih10=166.33582303\|Version=EM64L-G03RevE.01\|State=
2-A\|HF=-156.7111036\|RMSD=2.463e-09\|RMSF=4.848e-05\|Thermal=0.\|Dipole=0.
0269539,-0.0946298,0.0163878\|PG=C01 [X(C4H9)]\|@
```

ROBHandHLYP/6-311G**

```
1\1\GINC-X132\FOpt\ROBHandHLYP\6-311G(d,p)\C4H9(2)\SHK563\21-Apr-2010\
1\1\# ROBHandHLYP/6-311G** opt=grad optcyc=300 scfcyc=300 geom=checkpoi
nt guess=check freq=noraman\Louis' leaving radical t-butyl\0,2\C\C,1
,r1\C,1,r2,2,a1\C,1,r3,2,a2,3,dih1,0\H,2,r4,1,a3,4,dih2,0\H,2,r5,1,a4,
4,dih3,0\H,2,r6,1,a5,4,dih4,0\H,3,r7,1,a6,4,dih5,0\H,3,r8,1,a7,4,dih6,
0\H,3,r9,1,a8,4,dih7,0\H,4,r10,1,a9,2,dih8,0\H,4,r11,1,a10,2,dih9,0\H,
4,r12,1,a11,2,dih10,0\|r1=1.4898746\r2=1.48985956\r3=1.48980535\r4=1.0
9564422\r5=1.08685231\r6=1.08688321\r7=1.08689684\r8=1.09565607\r9=1.0
8689597\r10=1.08691215\r11=1.09564788\r12=1.08690576\|a1=118.33609778\|a
2=118.35965989\|a3=111.57624446\|a4=111.62361346\|a5=111.62647306\|a6=111.
62808645\|a7=111.59155168\|a8=111.62976982\|a9=111.63947792\|a10=111.57786
144\|a11=111.63177262\|dih1=154.77467462\|dih2=77.32149431\|dih3=-42.07064
291\|dih4=196.70663275\|dih5=42.01420999\|dih6=-77.37854178\|dih7=163.2200
085\|dih8=42.0667795\|dih9=-77.33378347\|dih10=163.28922203\|Version=EM64
L-G03RevE.01\|State=2-A\|HF=-157.7286765\|RMSD=7.441e-09\|RMSF=4.104e-05\|T
hermal=0.\|Dipole=0.0192433,-0.0862817,0.0114009\|PG=C01 [X(C4H9)]\|@
```

ROBHandHLYP/6-311++G**

```
1\1\GINC-X139\FOpt\ROBHandHLYP\6-311++G(d,p)\C4H9(2)\SHK563\22-Apr-201
0\1\1\# ROBHandHLYP/6-311++G** opt=grad optcyc=300 scfcyc=300 geom=chec
kpoint guess=check freq=noraman\Louis' leaving radical t-butyl\0,2\C
\C,1,r1\C,1,r2,2,a1\C,1,r3,2,a2,3,dih1,0\H,2,r4,1,a3,4,dih2,0\H,2,r5,1
,a4,4,dih3,0\H,2,r6,1,a5,4,dih4,0\H,3,r7,1,a6,4,dih5,0\H,3,r8,1,a7,4,d
```

ih6,0\H,3,r9,1,a8,4,dih7,0\H,4,r10,1,a9,2,dih8,0\H,4,r11,1,a10,2,dih9,
0\H,4,r12,1,a11,2,dih10,0\\r1=1.48986737\r2=1.48985336\r3=1.4898013\r4
=1.09565246\r5=1.08685361\r6=1.08688349\r7=1.08689666\r8=1.09566419\r9
=1.08689587\r10=1.08691126\r11=1.09565663\r12=1.08690511\al=118.335670
16\al=118.35893135\al=111.57388695\al=111.62396805\al=111.62721778\al=111.6286539\al=111.58927886\al=111.62983767\al=111.63954002\al=111.57
60407\al=111.63184428\dih1=154.76865112\dih2=77.31869715\dih3=-42.072
03909\dih4=196.70315366\dih5=42.01635434\dih6=-77.37565261\dih7=163.22
420981\dih8=42.06956215\dih9=-77.32989768\dih10=163.29360897\\Version=
EM64L-G03RevE.01\State=2-A\HF=-157.7296818\RMSD=7.644e-09\RMSF=8.587e-
05\Thermal=0.\Dipole=0.0215299,-0.0965057,0.012769\PG=C01 [X(C4H9)]\@

Radical 10 (Y = O)

ROHF/6-31G*

```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET4\FOpt\ROHF\6-31G(d)\C13H11O2S1(2)
\CARLHS\10-Jan-2010\0\#\ROHF/6-31G* OPT=(GRAD,CARTESIAN,READFC) GEOM=C
HECKPOINT GUESS=READ OPTCYC=200 SCFCYC=300\\Louis' starting radical\\0
,2\S,-0.4921511991,0.6461086658,-1.5149158792\C,-1.0580773043,0.792979
4573,2.3434010075\O,0.4601760541,0.7265484761,-0.1995424819\O,-1.86285
0996,0.3718178629,-1.0878586435\C,0.377149461,1.9204623868,0.577129266
5\C,0.0351603075,1.5930736559,2.007476494\C,0.7668050745,2.0953059,3.0
534294329\C,0.5098017045,1.8792238927,4.385846098\C,-0.5820589682,1.08
03488615,4.6914771405\C,-1.3576725455,0.5417925186,3.6711068291\H,-0.3
691922019,2.5844051182,0.15498656\H,1.337433098,2.4133620208,0.5214900
211\H,-1.6608611608,0.3681876342,1.5611105983\H,1.127700586,2.30473155
39,5.1549488548\H,-0.8275074401,0.8760515002,5.7186814034\H,-2.2016604
123,-0.0780648567,3.9146599104\C,0.1895204363,-0.8961305712,-2.0899720
432\C,-0.6236910205,-2.0124931104,-2.1485790416\C,-0.1043078126,-3.199
7597687,-2.643888233\C,1.2088546816,-3.2556556353,-3.0774174438\C,2.0
150013411,-2.1262167606,-3.0214487423\C,1.5050674957,-0.9396838047,-2.
5298757221\H,-1.6394772629,-1.94491638,-1.8096316342\H,-0.7255867677,-
4.0756893864,-2.6900700335\H,1.607242518,-4.1771140978,-3.4625575564\H
,3.034347273,-2.1730531146,-3.3591036823\H,2.1240633864,-0.0620514882,
-2.4787580838\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-1045.7900369
\RMSD=5.068e-09\RMSF=9.153e-06\Dipole=0.9468455,-0.2963675,-0.2732265\
PG=C01 [X(C13H11O2S1)]\\@
```

ROHF/6-311G**

```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET4\FOpt\ROHF\6-311G(d,p)\C13H11O2S1
(2)\CARLHS\11-Jan-2010\0\#\ROHF/6-311G** OPT=(GRAD,CARTESIAN) GEOM=CHE
CKPOINT GUESS=READ OPTCYC=200 SCFCYC=300\\Louis' starting radical\\0,2
\S,0.9325237423,-1.003775239,1.0331219606\C,-2.5090906082,0.6879876104
,0.5061988482\O,-0.1126114787,-0.8578693885,-0.1952501148\O,0.51206140
08,-0.1086796522,2.1021626464\C,-1.3721249565,-1.5101057368,-0.0628344
241\C,-2.4950179292,-0.5154203934,-0.1985687944\C,-3.578232594,-0.7625
106801,-1.0008021041\C,-4.6622700491,0.0648412854,-1.1602151603\C,-4.6
509342935,1.2537542473,-0.4474569955\C,-3.5764846689,1.5585108707,0.37
88542361\H,-1.4290474389,-2.0099105626,0.8994685653\H,-1.4373973773,-2
.2595605086,-0.8391973094\H,-1.6792334917,0.9335078019,1.143933445\H,-
5.4779133832,-0.193844245,-1.810023285\H,-5.4734162057,1.9413587018,-0
.5366820662\H,-3.5723303039,2.4830044906,0.9276539715\C,2.270172664,-0
.1908072057,0.1820137208\C,2.6591687502,1.0706903712,0.5864675455\C,3.
7199408346,1.6855792837,-0.0603397119\C,4.3751769533,1.0357537832,-1.0
910309819\C,3.978570935,-0.2345920137,-1.4846272625\C,2.922234151,-0.8
538185286,-0.8456526945\H,2.1379057671,1.5495736195,1.3931223529\H,4.0
31882782,2.6685302361,0.2427614833\H,5.199175194,1.5153649067,-1.58835
08688\H,4.4910125513,-0.7369639708,-2.2847955742\H,2.6067275206,-1.837
4416812,-1.1451796647\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-1045
.9508245\RMSD=7.801e-09\RMSF=2.459e-05\Dipole=0.5699123,-0.2018642,-0.
9344001\PG=C01 [X(C13H11O2S1)]\\@
```

ROBHandHLYP/6-311G**

```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET4\FOpt\ROBHandHLYP\6-311G(d,p)\C13
H11O2S1(2)\CARLHS\12-Jan-2010\0\#\ROBHandHLYP/6-311G** OPT=(GRAD,CARTE
SIAN,READFC) GEOM=CHECKPOINT GUESS=READ OPTCYC=200 SCFCYC=300\\Louis'
starting radical\\0,2\S,0.8899922161,-0.9236304067,1.0442538879\C,-2.4
808556939,0.6546797175,0.4778464926\O,-0.0927873854,-0.8532226921,-0.2
795915288\O,0.4343312655,0.0604558355,2.0360464008\C,-1.3493722888,-1.
5219587194,-0.1616780703\C,-2.4852001346,-0.5442638287,-0.235081741\C,
-3.6015293458,-0.7902603707,-0.986942023\C,-4.6993520844,0.0170162647,
-1.0947382067\C,-4.6689702285,1.2033977319,-0.3726773379\C,-3.56309317
73,1.5129970403,0.4046589487\H,-1.3862734564,-2.0755015262,0.775234746
8\H,-1.4157228655,-2.2339913549,-0.9747902366\H,-1.6218138141,0.903897
5279,1.0781673099\H,-5.5431740955,-0.2438913231,-1.7094263016\H,-5.504
```

1748112,1.8815988674,-0.421444147\H,-3.543408324,2.4349006766,0.959563
6433\C,2.2694801407,-0.1718422053,0.1902875303\C,2.6776825486,1.087112
5684,0.5798279206\C,3.7668239997,1.6615168979,-0.0528658101\C,4.430839
4584,0.9731144733,-1.0526410707\C,4.0124780292,-0.2939673314,-1.428727
6706\C,2.9254821567,-0.87484988,-0.8049850415\H,2.1410255698,1.5916907
176,1.3635915273\H,4.0957467188,2.644512845,0.2360011778\H,5.279238747
7,1.4218802259,-1.53983078\H,4.5316566143,-0.8253991479,-2.2070792402\H,
2.5881929371,-1.8556302996,-1.0933924058\\Version=x86-Linux-G03RevB.
04\State=2-A\HF=-1050.2675361\RMSD=5.084e-09\RMSF=1.249e-05\Dipole=0.6
46816,-0.224444,-0.764897\PG=C01 [X(C13H11O2S1)]\\@

ROBHandHLYP/6-311++G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET13\FOpt\ROBHandHLYP\6-311++G(d,p)\
C13H11O2S1(2)\CARLHS\02-Oct-2004\0\#\ROBHANDHLYP/6-311++G** OPT=(GRAD,
CARTESIAN,READFC) GEOM=CHECKPOINT GUESS=READ OPTCYC=200 SCFCYC=300\\Lo
uis' starting radical\\0,2\S,0.8896511689,-0.8609292735,1.0560303957\C
, -2.5645664836,0.6022990584,0.5627793847\O,-0.0960005311,-0.8338328842
, -0.2684441828\O,0.4405020257,0.1616823326,2.0138748834\C,-1.347810211
6,-1.513147456,-0.132736023\C,-2.4966263682,-0.5521262607,-0.219110051
3\C,-3.5618780864,-0.7761734278,-1.0479033007\C,-4.6713343204,0.013245
3141,-1.1761607781\C,-4.7117845051,1.1555591342,-0.3862726994\C,-3.660
6649554,1.4417457471,0.4734829599\H,-1.3725651123,-2.0504306734,0.8135
866176\H,-1.4080750315,-2.2385162369,-0.9342260966\H,-1.7496611202,0.8
362120624,1.2281669233\H,-5.4712142459,-0.2288923197,-1.8540418975\H,-
5.5587330836,1.8182323744,-0.4458752203\H,-3.6964252049,2.3294564692,1
.0809266446\C,2.2778466011,-0.149493595,0.180272633\C,2.7418845646,1.0
88577703,0.5765962624\C,3.848258013,1.624072985,-0.0621889211\C,4.4777
693265,0.916198689,-1.0710359188\C,4.0072426142,-0.3321817213,-1.45010
0227\C,2.9030455478,-0.8740194206,-0.8203884124\H,2.2340854147,1.61237
85361,1.3671056849\H,4.2179048827,2.59137094,0.2306268128\H,5.33919612
99,1.3345370168,-1.5625897765\H,4.4994308725,-0.8799364405,-2.23473655
52\H,2.5273354202,-1.8396794367,-1.1122845218\\Version=x86-Linux-G03Re
vB.04\State=2-A\HF=-1050.2787035\RMSD=7.215e-09\RMSF=1.452e-06\Dipole=
0.6124412,-0.2643008,-0.7465417\PG=C01 [X(C13H11O2S1)]\\@

Intermediate 12 (Y = O)

ROHF/6-31G*

```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET4\FOpt\ROHF\6-31G(d)\C13H11O2S1(2)
\CARLHS\24-Dec-2009\1\#\ROHF/6-31G* OPT=GRAD SCFCYC=300\Louis' cycliz
ed product A (cyclic sultine) hypervalent intermediate - TS for rin\0
,2\S\C,1,r12\O,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,d
ih2,0\C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2
,dih5,0\C,8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a
6511,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8
,r814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016
,8,dih13,0\C,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C
,18,r1819,17,a171819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2
021,19,a192021,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823
,17,a171823,1,dih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a
192025,18,dih22,0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a21222
7,20,dih24,0\|r14=1.45406874\r35=1.41952024\r26=1.36892768\r67=1.38716
321\r78=1.38414371\r89=1.39270967\r910=1.3837827\r511=1.08145692\r512=
1.0828369\r713=1.07637572\r814=1.07516482\r915=1.07520699\r1016=1.0754
7172\|a213=87.97531334\|a214=101.36994487\|a135=119.28270254\|a126=111.427
30696\|a267=120.15582015\|a678=118.53550964\|a789=120.81770783\|a8910=120.
38048847\|a6511=113.10357762\|a6512=112.15921237\|a6713=121.0701829\|a7814
=119.64817444\|a8915=119.66619678\|a91016=120.91193413\|dih1=115.09402185
\|dih2=14.46677232\|dih3=-6.12334668\|dih4=178.71705118\|dih5=-0.50252641\
\|dih6=0.11306792\|dih7=0.07521096\|dih8=129.09800129\|dih9=-107.1198995\|di
h10=179.35543135\|dih11=180.32132909\|dih12=180.00170276\|dih13=179.62490
451\|a4117=101.76093371\|dih14=188.44275005\|r1718=1.38361984\|r1819=1.388
45712\|r1920=1.3840591\|r2021=1.38805297\|r2122=1.3832455\|a11718=119.0558
226\|a171819=119.24272862\|a181920=120.3245547\|a192021=119.98589771\|a202
122=120.02959483\|dih15=215.92597038\|dih16=173.07536399\|dih17=-0.762113
54\|dih18=-0.0386762\|dih19=0.00761809\|r1823=1.07231833\|r1924=1.07554655
\|r2025=1.07541779\|r2126=1.07551721\|r2227=1.07487007\|a171823=119.797701
4\|a181924=119.60909053\|a192025=120.05903613\|a202126=120.10940845\|a2122
27=120.08820213\|dih20=-7.9796343\|dih21=179.05958443\|dih22=180.07352527
\|dih23=179.98399685\|dih24=179.86247541\|r117=1.8765009\|r13=1.62770542\|r
12=1.87764851\|Version=x86-Linux-G03RevB.04\|State=2-A\|HF=-1045.7504567
\|RMSD=3.885e-09\|RMSF=7.028e-05\|Dipole=0.5617285,1.0150997,0.9332652\|PG
=C01 [X(C13H11O2S1)]\|@
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ROHF/6-311G**

```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET14\FOpt\ROHF\6-311G(d,p)\C13H11O2S
1(2)\CARLHS\25-Dec-2009\1\#\ROHF/6-311G** OPT=(GRAD,READFC) GEOM=CHECK
POINT GUESS=READ SCFCYC=300\Louis' cyclized product A (cyclic sultine
) hypervalent intermediate - TS for rin\0,2\S\C,1,r12\O,1,r13,2,a213\
O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,3,dih3,
0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a789,6,dih
6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r512,6,a65
12,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11,0\H,9,
r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r117,4,a4117,
2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a171819,1,dih16,
0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,18,dih18,0\C
,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,dih20,0\H,19,r1
924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,0\H,21,r2126,
20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\|r14=1.44781583
\r35=1.41834772\r26=1.36735557\r67=1.38663292\r78=1.38314625\r89=1.392
08781\r910=1.38285786\r511=1.08138071\r512=1.08366658\r713=1.07635788\
r814=1.07525681\r915=1.07526494\r1016=1.07561463\|a213=87.68224581\|a214
=101.23200057\|a135=119.35283819\|a126=111.06943258\|a267=120.05012195\|a6
78=118.55028691\|a789=120.83993458\|a8910=120.36777651\|a6511=113.0370910
6\|a6512=111.88203918\|a6713=121.05644362\|a7814=119.64224681\|a8915=119.6
7918165\|a91016=120.90582099\|dih1=114.26559101\|dih2=16.90351778\|dih3=-7
.73563751\|dih4=179.06308984\|dih5=-0.52238857\|dih6=0.07353229\|dih7=0.06
205962\|dih8=130.01278784\|dih9=-106.03099366\|dih10=179.44510928\|dih11=1
```

80.25990298\dih12=180.052637\dih13=179.60939148\ a4117=101.49668505\dih
14=187.62409902\r1718=1.38143727\r1819=1.38821124\r1920=1.38310588\r20
21=1.38752415\r2122=1.38221783\ a11718=119.5706683\ a171819=119.05674464
\ a181920=120.34853587\ a192021=120.03973606\ a202122=119.95772898\dih15=
207.49978717\dih16=173.97109251\dih17=-0.63427912\dih18=0.06021102\dih
19=-0.11395325\r1823=1.07253749\r1924=1.07559277\r2025=1.07546973\r212
6=1.07550848\r2227=1.0756833\ a171823=119.73905695\ a181924=119.58742407
\ a192025=120.02786942\ a202126=120.13608162\ a212227=120.07244965\dih20=
-6.79710343\dih21=179.27131911\dih22=180.11860125\dih23=179.91791843\d
ih24=179.88688588\r117=1.88332282\r13=1.61992173\r12=1.88785184\\Versi
on=x86-Linux-G03RevB.04\State=2-A\HF=-1045.9087577\RMSD=6.837e-09\RMSF
=5.038e-05\Dipole=0.5855725,1.018077,0.9090486\PG=C01 [X(C13H11O2S1)]\
\e

ROBHandHLYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET5\FOpt\ROBHandHLYP\6-311G(d,p)\C13
H11O2S1(2)\CARLHS\14-Sep-2004\1\#\ROBHANDHLYP/6-311G** OPT=(GRAD,READF
C) GEOM=CHECKPOINT GUESS=READ SCFCYC=300\\Louis' cyclized product A (c
yclic sultine) hypervalent intermediate - TS for rin\\0,2\S\C,1,r12\O,
1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1
,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89
,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H
,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6
,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,
r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a17
1819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,
18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,di
h20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,
0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\\r
14=1.46288723\r35=1.42108445\r26=1.36839762\r67=1.38493497\r78=1.38388
292\r89=1.38971087\r910=1.38380575\r511=1.08390699\r512=1.08648891\r71
3=1.07757957\r814=1.07623461\r915=1.07642698\r1016=1.07691224\ a213=87.
40754349\ a214=101.09342223\ a135=118.38606275\ a126=111.11507003\ a267=11
9.70429901\ a678=118.68077995\ a789=120.83857586\ a8910=120.38934664\ a651
1=112.83238317\ a6512=111.60914684\ a6713=120.92956399\ a7814=119.6141158
9\ a8915=119.7201867\ a91016=121.0154545\dih1=115.3384747\dih2=16.158757
89\dih3=-6.83528968\dih4=178.41907153\dih5=-0.72518096\dih6=0.16643505
\dih7=-0.05427879\dih8=131.22836885\dih9=-105.56005716\dih10=179.31637
278\dih11=180.37398356\dih12=180.01088303\dih13=179.72774274\ a4117=101
.43628551\r14=186.37528717\r1718=1.38051341\r1819=1.38626021\r1920=1
.38347962\r2021=1.3860881\r2122=1.38263835\ a11718=118.17742877\ a171819
=118.87378627\ a181920=120.31843151\ a192021=120.06546578\ a202122=120.07
54135\dih15=211.66054659\dih16=172.5908599\dih17=-0.80608248\dih18=0.0
0559969\dih19=-0.08175995\r1823=1.07477577\r1924=1.07673544\r2025=1.07
641432\r2126=1.07666636\r2227=1.07617899\ a171823=119.59429066\ a181924=
119.59992136\ a192025=120.00233492\ a202126=120.10710823\ a212227=120.409
00551\dih20=-8.74754934\dih21=178.90851217\dih22=180.08166029\dih23=17
9.83069024\dih24=179.54933915\r117=1.89400615\r13=1.65483499\r12=1.901
43498\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-1050.2512299\RMSD=6.
171e-09\RMSF=1.515e-05\Dipole=0.537022,0.9465863,0.8606784\PG=C01 [X(C
13H11O2S1)]\e

ROBHandHLYP/6-311++G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET5\FOpt\ROBHandHLYP\6-311++G(d,p)\C
13H11O2S1(2)\CARLHS\15-Sep-2004\1\#\ROBHANDHLYP/6-311++G** OPT=(GRAD,R
EADFC) GEOM=CHECKPOINT GUESS=READ SCFCYC=300\\Louis' cyclized product
A (cyclic sultine) hypervalent intermediate - TS for rin\\0,2\S\C,1,r1
2\O,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r
26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8
,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8
,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a78
14,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\
C,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17
,a171819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192

021,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,
1,dih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,di
h22,0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,
0\r14=1.46518829\r35=1.42079384\r26=1.36824637\r67=1.38566292\r78=1.3
8424069\r89=1.39062424\r910=1.38406036\r511=1.08436273\r512=1.08658423
\r713=1.07762087\r814=1.07627722\r915=1.07647504\r1016=1.07687579\ a213
=87.59993563\ a214=101.0229233\ a135=118.58372315\ a126=111.22826182\ a267
=119.66094677\ a678=118.68538832\ a789=120.8440428\ a8910=120.39237584\ a6
511=112.72760603\ a6512=111.70372794\ a6713=120.93263889\ a7814=119.61155
416\ a8915=119.72445353\ a91016=121.06549412\ dih1=115.60961083\ dih2=14.2
6506274\ dih3=-5.95314436\ dih4=178.51342867\ dih5=-0.5644094\ dih6=0.1227
0809\ dih7=-0.0321962\ dih8=129.80003841\ dih9=-107.10557419\ dih10=179.36
926023\ dih11=180.32359276\ dih12=179.98370039\ dih13=179.74957631\ a4117=
101.34546168\ dih14=186.5797263\ r1718=1.38106093\ r1819=1.38694824\ r1920
=1.3839964\ r2021=1.38666881\ r2122=1.38334373\ a11718=117.98912681\ a1718
19=118.86062255\ a181920=120.32984698\ a192021=120.04758206\ a202122=120.
0978617\ dih15=213.86227505\ dih16=172.45760874\ dih17=-0.83875294\ dih18=
-0.03451214\ dih19=-0.06627027\ r1823=1.07484875\ r1924=1.07677324\ r2025=
1.07645798\ r2126=1.0767066\ r2227=1.07606369\ a171823=119.74141881\ a1819
24=119.58794056\ a192025=120.01299626\ a202126=120.10587739\ a212227=120.
38217713\ dih20=-8.91025153\ dih21=178.87463819\ dih22=180.06557729\ dih23
=179.8774648\ dih24=179.74286488\ r117=1.89293508\ r13=1.65697358\ r12=1.8
9480758\ \Version=x86-Linux-G03RevB.04\State=2-A\HF=-1050.2637693\RMSE=
6.225e-09\RMSF=5.554e-05\Dipole=0.567855,0.9302124,0.8683781\PG=C01 [X
(C13H11O2S1)]\@

Transition state 11 (Y = O)

ROHF/6-31G*

```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET21\FTS\ROHF\6-31G(d)\C13H11O2S1(2)
\CARLHS\28-Dec-2009\1\#\ROHF/6-31G* OPT=(GRAD,TS,READFC,NOFREEZE,NOEIG
ENTEST) GEOM=CHECKPOINT GUESS=READ SCFCYC=300\Louis' cyclized product
A (cyclic sultine) hypervalent intermediate - TS for rin\0,2\S\C,1,r
12\O,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,
r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,
8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih
8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7
814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0
\C,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,1
7,a171819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a19
2021,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823
,1,dih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,d
ih22,0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24
,0\H,r14=1.45392654\r35=1.42240105\r26=1.36678282\r67=1.38866625\r78=1.
38509752\r89=1.39163539\r910=1.38657871\r511=1.08088248\r512=1.0828821
5\r713=1.07682766\r814=1.07522937\r915=1.07559678\r1016=1.07544163\
a213=85.66017071\
a214=99.93800279\
a135=119.8700037\
a126=106.70088871\
a267=119.32708278\
a678=118.81080128\
a789=120.82141253\
a8910=120.33362788\
a6511=112.92647738\
a6512=111.76632809\
a6713=120.94953022\
a7814=119.61389646\
a8915=119.67937696\
a91016=120.96487232\
dih1=112.17006484\
dih2=21.22685679\
dih3=-9.75981644\
dih4=178.99751649\
dih5=-0.51110915\
dih6=0.04942865\
dih7=0.08001544\
dih8=133.46194468\
dih9=-103.27097504\
dih10=179.58632103\
dih11=180.32029892\
dih12=180.11542481\
dih13=179.94009884\
a4117=104.06947546\
dih14=187.2376621\
r1718=1.38343022\
r1819=1.38809732\
r1920=1.38381553\
r2021=1.38845769\
r2122=1.38239474\
a11718=119.15945496\
a171819=119.2231463\
a181920=120.24305383\
a192021=120.11571531\
a202122=119.9883534\
dih15=209.88360405\
dih16=174.81100834\
dih17=-0.55995581\
dih18=-0.09980613\
dih19=0.04300541\
r1823=1.07253211\
r1924=1.0752634\
r2025=1.07534166\
r2126=1.07522162\
r2227=1.07487509\
a171823=119.66901187\
a181924=119.64959155\
a192025=120.00033349\
a202126=120.13172325\
a212227=120.19969788\
dih20=-5.93090099\
dih21=179.29138893\
dih22=180.06364145\
dih23=180.03074441\
dih24=179.7851465\
r117=1.82491063\
r13=1.62321677\
r12=2.075595\
Version=x86-Linux-G03RevB.04\
State=2-A\HF=-1045.7479671\
RMSD=4.398e-09\
RMSF=1.425e-05\
Dipole=0.5452233,1.0523486,0.4825091\
PG=C01 [X(C13H11O2S1)]\@
```

ROHF/6-311G**

```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET5\FTS\ROHF\6-311G(d,p)\C13H11O2S1(
2)\CARLHS\16-Sep-2004\1\#\ROHF/6-311G** OPT=(GRAD,TS,READFC,NOFREEZE,N
OEIGENTEST) GEOM=CHECKPOINT GUESS=READ SCFCYC=300\Louis' cyclized pro
duct A (cyclic sultine) hypervalent intermediate - TS for rin\0,2\S\C
,1,r12\O,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C
,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C
,8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih
8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a78
14,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C
,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a
171819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021
,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,dih
20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,0\
H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\H,r14
=1.44767073\r35=1.42090462\r26=1.36539801\r67=1.3879178\r78=1.38407547
\r89=1.3911143\r910=1.38546668\r511=1.08091156\r512=1.08370189\r713=1.
07678091\r814=1.07528935\r915=1.07563374\r1016=1.07554748\
a213=85.57392619\
a214=99.96561891\
a135=119.96524441\
a126=106.93079405\
a267=119.31534772\
a678=118.7881612\
a789=120.84548203\
a8910=120.33650129\
a6511=112.87356309\
a6512=111.55958557\
a6713=120.95417745\
a7814=119.60863721\
a8915=119.68848582\
a91016=121.00942336\
dih1=111.78147113\
dih2=22.19563725\
dih3=-10.63258915\
dih4=179.43209873\
dih5=-0.53813111\
dih6=0
```

```
.05844862\dih7=0.06843092\dih8=133.27903599\dih9=-103.21196199\dih10=1
79.59469359\dih11=180.28728403\dih12=180.09823974\dih13=179.78967446\
a4117=103.66923666\dih14=186.80773082\r1718=1.38155523\r1819=1.38759076
\r1920=1.38298543\r2021=1.3877584\r2122=1.38150868\al1718=119.40100222
\al71819=119.07291238\al181920=120.26905587\al192021=120.14734939\al20212
2=119.93956403\dih15=204.27898312\dih16=175.30299941\dih17=-0.47558852
\dih18=-0.07544141\dih19=0.02288643\r1823=1.07276159\r1924=1.07531376\
r2025=1.07541575\r2126=1.07523701\r2227=1.07544954\al71823=119.5951704
2\al181924=119.62687806\al192025=119.97857761\al202126=120.1559647\al21222
7=120.17533397\dih20=-5.28296936\dih21=179.39502679\dih22=180.06901202
\dih23=180.02705181\dih24=179.81278944\r117=1.83177597\r13=1.61611325\
r12=2.06363281\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-1045.907072
2\RMSE=9.359e-09\RMSF=6.410e-06\Dipole=0.5712874,1.0653624,0.4887652\PG
=C01 [X(C13H11O2S1)]\@
```

ROBHandHLYP/6-311G**

```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET5\FTS\ROBHandHLYP\6-311G(d,p)\C13H
11O2S1(2)\CARLHS\16-Sep-2004\1\#\ROBHANDHLYP/6-311G** OPT=(GRAD,TS,REA
DFC,NOFREEZE,NOEIGENTEST) GEOM=CHECKPOINT GUESS=READ SCFCYC=300\\Louis
' cyclized product A (cyclic sultine) hypervalent intermediate - TS fo
r rin\0,2\S\C,1,r12\0,1,r13,2,a213\0,1,r14,2,a214,3,dih1,0\C,3,r35,1,
a135,2,dih2,0\C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,
6,a678,2,dih5,0\C,8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,
r511,6,a6511,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih
10,0\H,8,r814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,
9,a91016,8,dih13,0\C,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,al1718,2,di
h15,0\C,18,r1819,17,a171819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0
\C,20,r2021,19,a192021,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,1
8,r1823,17,a171823,1,dih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r20
25,19,a192025,18,dih22,0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,2
1,a212227,20,dih24,0\r14=1.46145526\r35=1.4238999\r26=1.36499066\r67=
1.3876834\r78=1.38447445\r89=1.38847648\r910=1.38750903\r511=1.0831072
\r512=1.08656235\r713=1.07815282\r814=1.07628879\r915=1.07690705\r1016
=1.07693191\al213=84.589383\al214=100.05539268\al135=118.65329133\al126=10
4.72911822\al267=118.69878312\al678=119.0193325\al789=120.85456737\al8910=
120.29326315\al6511=112.56476304\al6512=111.09185285\al6713=120.73296067\
al7814=119.5701751\al8915=119.79717013\al91016=121.00075464\dih1=111.8152
2843\dih2=24.63494546\dih3=-11.87252547\dih4=179.38410764\dih5=-0.5039
6577\dih6=0.04543699\dih7=0.05575316\dih8=136.31482354\dih9=-101.15956
938\dih10=179.65121129\dih11=180.34255271\dih12=180.11374968\dih13=179
.85192873\al117=104.18667233\dih14=185.23365091\r1718=1.38080934\r1819
=1.38538994\r1920=1.38337009\r2021=1.38628991\r2122=1.38175299\al1718=
118.18049338\al171819=118.91032358\al181920=120.22686202\al192021=120.187
83113\al202122=120.05698184\dih15=206.3066457\dih16=174.65020522\dih17=
-0.65042737\dih18=0.03499508\dih19=-0.07511529\r1823=1.07518046\r1924=
1.07641405\r2025=1.07637461\r2126=1.07634942\r2227=1.07603228\al171823=
119.38038077\al181924=119.66281772\al192025=119.94756849\al202126=120.117
99417\al212227=120.52536623\dih20=-6.47348646\dih21=179.15504661\dih22=
180.11992262\dih23=179.83082401\dih24=179.48432101\r117=1.83099771\r13
=1.64848489\r12=2.15763157\\Version=x86-Linux-G03RevB.04\State=2-A\HF=
-1050.2490025\RMSE=8.729e-09\RMSF=9.800e-06\Dipole=0.5250718,0.9783494
,0.3527031\PG=C01 [X(C13H11O2S1)]\@
```

ROBHandHLYP/6-311++G**

```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET5\FTS\ROBHandHLYP\6-311++G(d,p)\C1
3H11O2S1(2)\CARLHS\16-Sep-2004\1\#\ROBHANDHLYP/6-311++G** OPT=(GRAD,TS
,READFC,NOFREEZE,NOEIGENTEST) GEOM=CHECKPOINT GUESS=READ SCFCYC=300\\L
ouis' cyclized product A (cyclic sultine) hypervalent intermediate - T
S for rin\0,2\S\C,1,r12\0,1,r13,2,a213\0,1,r14,2,a214,3,dih1,0\C,3,r3
5,1,a135,2,dih2,0\C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,
r78,6,a678,2,dih5,0\C,8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\
H,5,r511,6,a6511,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2
,dih10,0\H,8,r814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1
016,9,a91016,8,dih13,0\C,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,al1718,
```

2,dih15,0\C,18,r1819,17,a171819,1,dih16,0\C,19,r1920,18,a181920,17,dih
17,0\C,20,r2021,19,a192021,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0
\H,18,r1823,17,a171823,1,dih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20
,r2025,19,a192025,18,dih22,0\H,21,r2126,20,a202126,19,dih23,0\H,22,r22
27,21,a212227,20,dih24,0\\r14=1.46373348\r35=1.42397062\r26=1.36459162
\r67=1.38858504\r78=1.38493744\r89=1.38927939\r910=1.38808654\r511=1.0
8341889\r512=1.08673583\r713=1.0782115\r814=1.07632375\r915=1.07694509
\r1016=1.07693605\ a213=84.58762456\ a214=99.89180814\ a135=119.06531972\
a126=104.58581818\ a267=118.58623588\ a678=119.04010106\ a789=120.8650073
5\ a8910=120.28692446\ a6511=112.47265614\ a6512=111.12252538\ a6713=120.7
2840274\ a7814=119.56136177\ a8915=119.80955659\ a91016=121.01118624\ dih1
=111.73960318\ dih2=23.42466759\ dih3=-11.23071764\ dih4=179.48203285\ dih
5=-0.41040564\ dih6=-0.0162728\ dih7=0.08652432\ dih8=135.42982095\ dih9=-
102.18413507\ dih10=179.70321354\ dih11=180.29656302\ dih12=180.12415029\
dih13=179.85828713\ a4117=104.21701171\ dih14=185.15269658\ r1718=1.38109
433\ r1819=1.38618164\ r1920=1.38383429\ r2021=1.38687207\ r2122=1.3823674
6\ a11718=118.31894427\ a171819=118.89356483\ a181920=120.24003881\ a19202
1=120.17825122\ a202122=120.04882763\ dih15=205.11452832\ dih16=174.77357
226\ dih17=-0.63569195\ dih18=-0.06836664\ dih19=-0.05978621\ r1823=1.0752
8468\ r1924=1.07647111\ r2025=1.07644753\ r2126=1.0763911\ r2227=1.0762090
5\ a171823=119.51494101\ a181924=119.6498628\ a192025=119.95231247\ a20212
6=120.12686174\ a212227=120.45623209\ dih20=-6.17795332\ dih21=179.191837
56\ dih22=180.08057895\ dih23=179.96002439\ dih24=179.7360373\ r117=1.8300
1289\ r13=1.6499456\ r12=2.16555963\\Version=x86-Linux-G03RevB.04\State=
2-A\HF=-1050.2610616\RMSD=5.682e-09\RMSF=1.364e-05\Dipole=0.5446243,0.
9665687,0.3533734\PG=C01 [X(C13H11O2S1)]\\@

Transition state 13 (Y = O)

ROHF/6-31G*

```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET4\FTS\ROHF\6-31G(d)\C13H11O2S1(2)\
CARLHS\28-Dec-2009\1\#\ROHF/6-31G* OPT=(GRAD,TS,READFC,NOFREEZE,NOEIGE
NTEST) GEOM=CHECKPOINT GUESS=READ SCFCYC=300\Louis' cyclized product
A (cyclic sultine) hypervalent intermediate - TS for rin\0,2\S\C,1,r1
2\O,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r
26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8
,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8
,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a78
14,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\
C,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17
,a171819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192
021,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,
1,dih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,di
h22,0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,
0\r14=1.45491435\r35=1.42019237\r26=1.37289745\r67=1.38585588\r78=1.3
848406\r89=1.3916493\r910=1.38401519\r511=1.08106029\r512=1.08302304\r
713=1.07604785\r814=1.07511245\r915=1.07494353\r1016=1.07527071\
a213=88.93159241\
a214=103.18853161\
a135=117.80949473\
a126=111.64874181\
a267=120.09922795\
a678=118.58306483\
a789=120.89006058\
a8910=120.33715468\
a6511=113.21953345\
a6512=112.15335918\
a6713=121.04045978\
a7814=119.60089163\
a8915=119.72880005\
a91016=120.84445322\
dih1=113.75207379\
dih2=18.41028503\
dih3=-9.60151137\
dih4=180.68956362\
dih5=-0.45222502\
dih6=0.27670769\
dih7=0.02804818\
dih8=129.18197278\
dih9=-106.84041819\
dih10=179.58327113\
dih11=180.39665194\
dih12=179.95281972\
dih13=179.5452828\
a4117=98.73453754\
dih14=186.61415683\
r1718=1.3781832\
r1819=1.38974255\
r1920=1.38557826\
r2021=1.38773839\
r2122=1.38635439\
a11718=118.51002705\
a171819=118.32470771\
a181920=120.32618565\
a192021=120.19487231\
a202122=119.99334037\
dih15=208.58204063\
dih16=174.67978135\
dih17=-0.62171332\
dih18=-0.13909835\
dih19=0.02440515\
r1823=1.07289852\
r1924=1.0758932\
r2025=1.07550305\
r2126=1.0758638\
r2227=1.07547685\
a171823=120.35558378\
a181924=119.69066564\
a192025=119.9361202\
a202126=120.06893765\
a212227=120.49791021\
dih20=-6.14269229\
dih21=179.25011878\
dih22=180.04830454\
dih23=180.10134357\
dih24=179.98202458\
r13=1.62667198\
r12=1.82669885\
r117=2.07380162\
Version=x86-Linux-G03RevB.04\
State=2-A\HF=-1045.7476831\
RMSD=3.761e-09\
RMSF=3.719e-06\
Dipole=0.5492729,0.8579748,1.2887568\
PG=C01 [X(C13H11O2S1)]\@
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ROHF/6-311G**

```
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET21\FTS\ROHF\6-311G(d,p)\C13H11O2S1
(2)\CARLHS\29-Dec-2009\1\#\ROHF/6-311G** OPT=(GRAD,TS,READFC,NOFREEZE,
NOEIGENTEST) GEOM=CHECKPOINT GUESS=READ SCFCYC=300\Louis' cyclized pr
oduct A (cyclic sultine) hypervalent intermediate - TS for rin\0,2\S\
C,1,r12\O,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0
\C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5
,0\C,8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,
2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814
,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,di
h13,0\C,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1
819,17,a171819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,1
9,a192021,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a1
71823,1,dih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025
,18,dih22,0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,
dih24,0\r14=1.44876003\r35=1.41849447\r26=1.37092727\r67=1.38541907\r
78=1.38371483\r89=1.39120966\r910=1.38288443\r511=1.0810697\r512=1.083
82056\r713=1.07603814\r814=1.07522391\r915=1.07499995\r1016=1.07539574
\
a213=88.70365273\
a214=102.84560012\
a135=118.03023542\
a126=111.37706071\
a267=120.00135758\
a678=118.58886227\
a789=120.91222898\
a8910=120.32740758\
a6511=113.10828681\
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a6713=121.02987504\
a7814=119.59546441\
a8915=119.73661719\
a91016=120.86860531\
dih1=113.14063463\
dih2=19.57889318\
dih3=-10.51267287\
dih4=181.01144546\
dih5=-0.45086553\
dih
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h6=0.26085554\dih7=0.02641992\dih8=129.38566532\dih9=-106.49687791\dih10=179.6132762\dih11=180.35884592\dih12=179.9495777\dih13=179.43414314\aa117=98.58810212\dih14=186.13471455\r1718=1.37724575\r1819=1.38895786\r1920=1.38488613\r2021=1.38681931\r2122=1.38549757\aa11718=119.09185054\aa171819=118.22783808\aa181920=120.35948783\aa192021=120.21806974\aa202122=119.94180917\dih15=197.97779667\dih16=175.79448086\dih17=-0.46232021\dih18=-0.13200836\dih19=0.00929239\r1823=1.07303213\r1924=1.07593193\r2025=1.07552788\r2126=1.07584509\r2227=1.07609509\aa171823=120.23514346\aa181924=119.65627026\aa192025=119.91665335\aa202126=120.0967563\aa21227=120.43786623\dih20=-4.59872087\dih21=179.47657061\dih22=180.0578999\dih23=180.139999\dih24=180.07813446\r13=1.61846026\r12=1.83444195\r17=2.06136415\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-1045.9068136\RMSD=7.069e-09\RMSF=1.030e-06\Dipole=0.5788853,0.8721667,1.2509089\PG=C01 [X(C13H11O2S1)]\@

ROBHandHLYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET21\FTS\ROBHandHLYP\6-311G(d,p)\C13H11O2S1(2)\CARLHS\30-Dec-2009\1\#\ROBHANDHLYP/6-311G** OPT=(GRAD,TS,READFC,NOFREEZE,NOEIGENTEST) GEOM=CHECKPOINT GUESS=READ SCFCYC=300\\Louis' cyclized product A (cyclic sultine) hypervalent intermediate - TS for rin\0,2\S\C,1,r12\0,1,r13,2,a213\0,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a171819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,dih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\r14=1.4635061\r35=1.42221627\r26=1.37347701\r67=1.38356771\r78=1.3843002\r89=1.3887494\r910=1.38353634\r511=1.08351112\r512=1.08665236\r713=1.07717553\r814=1.07622346\r915=1.07609858\r1016=1.07658935\aa213=88.48762545\aa214=103.15033884\aa135=116.82226352\aa126=111.55689176\aa267=119.69058941\aa678=118.75643087\aa789=120.90602183\aa8910=120.33625473\aa6511=112.95621755\aa6512=111.68438092\aa6713=120.89499875\aa7814=119.56397081\aa8915=119.78327119\aa91016=120.93995787\dih1=113.49893194\dih2=20.18788624\dih3=-11.31835991\dih4=181.71158476\dih5=-0.50857957\dih6=0.33659483\dih7=0.03205911\dih8=129.74828623\dih9=-106.77713978\dih10=179.58801012\dih11=180.4511942\dih12=179.95934282\dih13=179.38674704\aa117=97.40488965\dih14=183.72787468\r1718=1.37212333\r1819=1.38909888\r1920=1.38480139\r2021=1.38578087\r2122=1.38705663\aa11718=117.29229534\aa171819=117.63299406\aa181920=120.29291042\aa192021=120.37003038\aa202122=120.00555106\dih15=195.68506532\dih16=175.55498526\dih17=-0.47544967\dih18=-0.06503782\dih19=-0.03477338\r1823=1.0754682\r1924=1.07718402\r2025=1.07649825\r2126=1.07711551\r2227=1.07704724\aa171823=120.42232724\aa181924=119.66957322\aa192025=119.83673705\aa202126=120.10176197\aa212227=120.79331811\dih20=-5.0080718\dih21=179.41438741\dih22=180.08753902\dih23=180.02492592\dih24=179.88310994\r13=1.65183888\r12=1.83501274\r117=2.16259891\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-1050.2484519\RMSD=1.931e-09\RMSF=2.034e-05\Dipole=0.519873,0.7567549,1.2579663\PG=C01 [X(C13H11O2S1)]\@

ROBHandHLYP/6-311++G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET21\FTS\ROBHandHLYP\6-311++G(d,p)\C13H11O2S1(2)\CARLHS\30-Dec-2009\1\#\ROBHANDHLYP/6-311++G** OPT=(GRAD,TS,READFC,NOFREEZE,NOEIGENTEST) GEOM=CHECKPOINT GUESS=READ SCFCYC=300\\Louis' cyclized product A (cyclic sultine) hypervalent intermediate - TS for rin\0,2\S\C,1,r12\0,1,r13,2,a213\0,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718

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Radical **15** (Y = O)

ROHF / 6-31G*

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1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET2\Fopt\ROHF\6-31G(d)\C13H11O2S1(2)
\CARLHS\01-Jan-2010\1\#\ROHF/6-31G* OPT=GRAD SCFCYC=300\Louis' biaryl
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,2,a217,3,dih4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r
910,8,a8910,7,dih7,0\C,10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,d
ih9,0\C,12,r1213,2,a21213,3,dih10,0\C,13,r1314,12,a121314,2,dih11,0\C
14,r1415,13,a131415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a
7817,1,dih14,0\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,
0\H,11,r1120,10,a101120,9,dih17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r
1322,12,a121322,2,dih19,0\H,14,r1423,13,a131423,12,dih20,0\H,15,r1524,
14,a141524,13,dih21,0\H,6,r625,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,d
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89=1.38660306\r910=1.37811673\r1011=1.38867622\r212=1.51057721\r1213=1.
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82557\r918=1.07507965\r1019=1.07541192\r1120=1.07243504\r1221=1.075931
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789=121.41781565\A8910=119.05684637\A91011=120.01228156\A3212=110.2984
9094\A21213=123.32723284\A121314=121.1313972\A131415=118.24673952\A321
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23=120.94402326\A141524=118.81607171\A7625=112.92719526\A7626=110.3045
8989\A3427=104.7261498\DIH1=79.88858934\DIH2=-59.30225216\DIH3=67.0042
6096\DIH4=-65.40272094\DIH5=181.2102243\DIH6=0.01211283\DIH7=-0.859744
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\DIH12=9.29717109\DIH13=-37.62034983\DIH14=180.37903306\DIH15=179.8437
7452\DIH16=180.7940302\DIH17=180.53631967\DIH18=166.4735988\DIH19=182.
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3=-176.66303346\DIH24=51.88835143\\Version=x86-Linux-G03RevB.04\State=
2-A\HF=-1045.799106\MSD=4.293e-09\RMSE=2.954e-05\Dipole=-0.4994554,-1.
4612811,-0.7017868\PG=C01 [X(C13H11O2S1)]\1\#\@

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ROHF / 6-311G**

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1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET21\Fopt\ROHF\6-311G(d,p)\C13H11O2S
1(2)\CARLHS\01-Jan-2010\1\#\ROHF/6-311G** OPT=(GRAD,READFC) GEOM=CHECK
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5,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,dih4,0\C,7,r78,1,a
178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910,7,dih7,0\C,10,r1
011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,r1213,2,a21213,3,
dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,13,a131415,12,dih12
,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih14,0\H,9,r918,8,a8
918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,11,r1120,10,a101120,9,dh
17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,12,a21322,2,dih19,0\H,
14,r1423,13,a131423,12,dih20,0\H,15,r1524,14,a141524,13,dih21,0\H,6,r6
25,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0\O,4,r427,3,a3427,2,dih
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1.42869696\r17=1.40204071\r78=1.38368115\r89=1.38604062\r910=1.3768971
6\r1011=1.38809208\r212=1.50958307\r1213=1.33239448\r1314=1.43620673\r
1415=1.43258905\r216=1.08725614\r817=1.07582207\r918=1.07508662\r1019=
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5763\ a217=120.61040856\ a178=119.68547322\ a789=121.41363307\ a8910=119.0
710263\ a91011=120.0018575\ a3212=110.29961566\ a21213=123.29085395\ a1213
14=121.15430755\ a131415=118.24693708\ a3216=107.34148044\ a7817=119.1526
7965\ a8918=120.19546246\ a91019=120.4484856\ a101120=118.61178227\ a21221
```

=116.53920541\al21322=120.09328195\al31423=120.95444939\al41524=118.93
641041\al7625=112.79058515\al7626=110.2666533\al3427=104.46807986\alh1=80
.25582041\alh2=-59.18849798\alh3=66.77645828\alh4=-65.73554534\alh5=18
0.98099502\alh6=0.17975175\alh7=-0.91065875\alh8=0.63902501\alh9=205.7
4907325\alh10=-15.65075817\alh11=3.68372435\alh12=9.45449756\alh13=-37
.20772503\alh14=180.52118658\alh15=179.80392921\alh16=180.77638194\alh
17=180.52185953\alh18=166.5393045\alh19=182.26175963\alh20=182.7470618
\alh21=167.50429246\alh22=-55.825759\alh23=-176.89851904\alh24=51.7816
0826\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-1045.9589007\RMSD=8.8
07e-09\RMSF=2.502e-05\Dipole=-0.4664123,-1.4918479,-0.7332983\PG=C01 [X(C13H11O2S1)]\@

ROBHandHLYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET21\FOpt\ROBHandHLYP\6-311G(d,p)\C1
3H11O2S1(2)\CARLHS\02-Jan-2010\1\#\ROBHANDHLYP/6-311G** OPT=(GRAD,READ
FC) GEOM=CHECKPOINT GUESS=READ SCFCYC=300\\Louis' biaryl intermediate
transition state\\0,2\C\C,1,r12\C,2,r23,1,al23\S,3,r34,2,a234,1,dih1,0
\O,4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,dih4
,\O,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910,7,
dih7,0\C,10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,r12
13,2,a21213,3,dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,13,a1
31415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih14,0
\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,11,r1120,1
0,a101120,9,dih17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,12,a12132
2,2,dih19,0\H,14,r1423,13,a131423,12,dih20,0\H,15,r1524,14,a141524,13,
dih21,0\H,6,r625,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0\O,4,r427
,3,a3427,2,dih24,0\\r12=1.5415406\r23=1.50246712\r34=1.77510752\r45=1.
64083624\r56=1.43407116\r17=1.39931475\r78=1.38484786\r89=1.38358432\r
910=1.37824997\r1011=1.38543241\r212=1.49829902\r1213=1.3455436\r1314=
1.41474787\r1415=1.4083338\r216=1.0913747\r817=1.07719188\r918=1.07614
201\r1019=1.07645899\r1120=1.07460629\r1221=1.07700658\r1322=1.0770166
2\r1423=1.07442172\r1524=1.07840424\r625=1.08526844\r626=1.08105964\r4
27=1.47462421\al23=111.43467499\al234=119.12554368\al345=100.33131475\al
56=117.42970491\al217=120.77593042\al178=119.49026319\al789=121.43352085\
a8910=119.14757573\al91011=119.93814677\al3212=110.64864609\al21213=122.7
1717028\al21314=121.29001595\al31415=119.04546865\al3216=107.34751861\al
7817=118.93689461\al8918=120.19964434\al91019=120.41900129\al101120=119.0
2799619\al21221=116.91082256\al21322=119.73505915\al31423=120.48467057\
al41524=119.43972359\al7625=112.83060445\al7626=110.32123543\al3427=104.0
6776153\alh1=181.45461651\alh2=-61.4072188\alh3=67.22246245\alh4=-65.78
862278\alh5=80.87947569\alh6=0.0430807\alh7=-0.93329218\alh8=0.724346
\alh9=206.74495409\alh10=-15.41904245\alh11=4.45779423\alh12=7.7597773
7\alh13=-35.30580292\alh14=180.42829324\alh15=179.84913415\alh16=180.9
0199513\alh17=180.52162596\alh18=167.43517743\alh19=182.83815768\alh20
=181.925648\alh21=169.20936269\alh22=-54.89099772\alh23=-175.90628877\
alh24=49.25575805\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-1050.291
8625\RMSD=5.766e-09\RMSF=3.603e-05\Dipole=-0.4983846,-1.3912844,-0.661
7467\PG=C01 [X(C13H11O2S1)]\@

ROBHandHLYP/6-311++G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET4\FOpt\ROBHandHLYP\6-311++G(d,p)\C
13H11O2S1(2)\CARLHS\03-Jan-2010\1\#\ROBHANDHLYP/6-311++G** OPT=(GRAD,R
EADFC) GEOM=CHECKPOINT GUESS=READ SCFCYC=300\\Louis' biaryl intermedia
te transition state\\0,2\C\C,1,r12\C,2,r23,1,al23\S,3,r34,2,a234,1,dih
1,0\O,4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,d
ih4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910
,7,dih7,0\C,10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,
r1213,2,a21213,3,dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,13
,al31415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih1
4,0\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,11,r112
0,10,a101120,9,dih17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,12,a12
1322,2,dih19,0\H,14,r1423,13,a131423,12,dih20,0\H,15,r1524,14,a141524,
13,dih21,0\H,6,r625,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0\O,4,r
427,3,a3427,2,dih24,0\\r12=1.54133809\r23=1.50306412\r34=1.77724337\r4

5=1.64082184\r56=1.4337477\r17=1.39914869\r78=1.38538396\r89=1.3842414
6\r910=1.37902507\r1011=1.38610925\r212=1.49846514\r1213=1.34613157\r1
314=1.41480067\r1415=1.40877368\r216=1.09162175\r817=1.07728364\r918=1
.07617592\r1019=1.07651777\r1120=1.07477994\r1221=1.07711082\r1322=1.0
7709091\r1423=1.07458011\r1524=1.07853521\r625=1.08550377\r626=1.08117
534\r427=1.47670407\ra123=111.52110149\ra234=119.60962794\ra345=100.57988
714\ra456=117.83028185\ra217=120.67963265\ra178=119.54250438\ra789=121.378
47779\ra8910=119.15893471\ra91011=119.94748785\ra3212=110.68829226\ra21213
=122.77352435\ra121314=121.2493792\ra131415=119.06997362\ra3216=107.56180
687\ra7817=118.99140093\ra8918=120.19721527\ra91019=120.41169221\ra101120=
119.01282433\ra21221=116.895359\ra121322=119.73674657\ra131423=120.506808
35\ra141524=119.36233189\ra7625=112.83285033\ra7626=110.38207673\ra3427=10
4.23706464\ dih1=80.82069252\ dih2=-59.90705871\ dih3=66.02815198\ dih4=-6
5.9715472\ dih5=180.9708498\ dih6=-0.05163969\ dih7=-0.90237505\ dih8=0.72
10712\ dih9=206.24628008\ dih10=-15.09175188\ dih11=4.12622262\ dih12=7.81
705655\ dih13=-35.89550637\ dih14=180.29951257\ dih15=179.84596536\ dih16=
180.88307698\ dih17=180.4517644\ dih18=167.59632746\ dih19=182.70454703\ d
ih20=182.05729002\ dih21=169.44374355\ dih22=-54.32763522\ dih23=-175.359
85481\ dih24=50.69835979\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-10
50.3030704\RMSD=5.208e-09\RMSF=4.328e-05\Dipole=-0.5238559,-1.4031054,
-0.6928954\PG=C01 [X(C13H11O2S1)]\@

Transition state 14 (Y = O)

ROHF/6-31G*

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1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET5\FTS\ROHF\6-31G(d)\C13H11O2S1(2)\
CARLHS\24-Sep-2004\1\#\ROHF/6-31G* OPT=(GRAD,TS,READFC,NOFREEZE,NOEIGE
NTEST) GEOM=CHECKPOINT GUESS=READ SCFCYC=300\\Louis' biaryl intermedia
te transition state\\0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234,1,dih
1,0\O,4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,d
ih4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910
,7,dih7,0\C,10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,
r1213,2,a21213,3,dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,13
,a131415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih1
4,0\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,11,r112
0,10,a101120,9,dih17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,12,a12
1322,2,dih19,0\H,14,r1423,13,a131423,12,dih20,0\H,15,r1524,14,a141524,
13,dih21,0\H,6,r625,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0\O,4,r
427,3,a3427,2,dih24,0\\r23=1.4231808\r34=1.77626933\r45=1.6205443\r56=
1.42825292\r17=1.38644067\r78=1.39010329\r89=1.38712652\r910=1.3818243
\r1011=1.39067058\r212=1.42005573\r1213=1.37493476\r1314=1.39244401\r1
415=1.39032862\r216=1.07487063\r817=1.07642879\r918=1.07508408\r1019=1
.07577912\r1120=1.07326589\r1221=1.07471195\r1322=1.0755956\r1423=1.07
422662\r1524=1.07590396\r625=1.0798629\r626=1.07935033\r427=1.46451524
\al23=102.60915635\al234=120.19305147\al345=100.47304379\al456=119.444258
97\al217=118.87563713\al178=117.26047999\al789=121.29869612\al8910=119.857
75546\al91011=119.91047711\al3212=116.35820588\al21213=120.56051202\al1213
14=120.82372644\al131415=119.55429047\al3216=117.40141642\al7817=119.2855
588\al8918=119.84094283\al91019=120.29100227\al101120=120.06742822\al21221
=119.00302224\al121322=119.6262963\al131423=120.28048105\al141524=120.001
29929\al7625=112.20244235\al7626=109.98434183\al3427=105.32937983\dih1=82
.67683178\dih2=-74.12046382\dih3=72.32333351\dih4=-60.26352138\dih5=18
0.6250797\dih6=0.01968068\dih7=-0.5095851\dih8=0.28118085\dih9=195.326
30155\dih10=-12.64614433\dih11=4.63940774\dih12=3.60475639\dih13=-16.5
8435928\dih14=180.23007017\dih15=179.964702\dih16=180.45053749\dih17=1
80.46270797\dih18=169.73045868\dih19=182.74944919\dih20=179.92075134\d
ih21=174.39301383\dih22=-57.75675719\dih23=-178.03257451\dih24=37.3543
5752\r12=2.04622775\\Version=x86-Linux-G03RevB.04\State=2-A\HF=-1045.7
453594\RMSD=4.487e-09\RMSF=1.191e-05\Dipole=-0.5145925,-1.4127297,-0.8
073642\PG=C01 [X(C13H11O2S1)]\\e
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ROHF/6-311G**

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1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET5\FTS\ROHF\6-311G(d,p)\C13H11O2S1(
2)\CARLHS\24-Sep-2004\1\#\ROHF/6-311G** OPT=(GRAD,TS,READFC,NOFREEZE,N
OEIGENTEST) GEOM=CHECKPOINT GUESS=READ SCFCYC=300\\Louis' biaryl inter
mediate transition state\\0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234,
1,dih1,0\O,4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a21
7,3,dih4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,
a8910,7,dih7,0\C,10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\
C,12,r1213,2,a21213,3,dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r14
15,13,a131415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1
,dih14,0\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,11
,r1120,10,a101120,9,dih17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,1
2,a121322,2,dih19,0\H,14,r1423,13,a131423,12,dih20,0\H,15,r1524,14,a14
1524,13,dih21,0\H,6,r625,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0\
O,4,r427,3,a3427,2,dih24,0\\r23=1.42167615\r34=1.77643122\r45=1.613161
39\r56=1.42720109\r17=1.38572904\r78=1.38890961\r89=1.38645027\r910=1.
38051327\r1011=1.39007756\r212=1.41904321\r1213=1.37391673\r1314=1.391
66986\r1415=1.38969161\r216=1.07469496\r817=1.07644854\r918=1.07509816
\r1019=1.07580774\r1120=1.07321271\r1221=1.07480491\r1322=1.07573735\r
1423=1.07424303\r1524=1.07592273\r625=1.08103841\r626=1.07912052\r427=
1.46005169\al23=102.35800337\al234=120.06168161\al345=100.45298806\al456=
120.10636536\al217=118.89210568\al178=117.24934945\al789=121.30785637\al89
10=119.86160102\al91011=119.90748021\al3212=116.30622487\al21213=120.5403
271\al121314=120.85557137\al131415=119.54096664\al3216=117.4034536\al7817=
```

119.24870271\ a8918=119.83593961\ a91019=120.3167831\ a101120=120.0310336
1\ a21221=119.0284041\ a121322=119.61247271\ a131423=120.29755515\ a141524
=120.07455888\ a7625=112.05496073\ a7626=109.93339464\ a3427=105.17102674
\ dih1=82.97557856\ dih2=-74.14473005\ dih3=72.15947336\ dih4=-60.52015693
\ dih5=180.43136554\ dih6=0.15840691\ dih7=-0.5511588\ dih8=0.25805055\ dih
9=195.49866013\ dih10=-12.59249805\ dih11=4.52034858\ dih12=3.73394492\ di
h13=-16.29377897\ dih14=180.35968514\ dih15=179.94533539\ dih16=180.45069
207\ dih17=180.44421609\ dih18=169.72932145\ dih19=182.65799837\ dih20=179
.98585401\ dih21=174.38756316\ dih22=-58.05518684\ dih23=-178.39040289\ di
h24=37.15228535\ r12=2.04705626\ \ Version=x86-Linux-G03RevB.04\ State=2-A
\ HF=-1045.9051535\ RMSD=5.253e-09\ RMSF=3.303e-05\ Dipole=-0.4817648,-1.4
491139,-0.8563415\ PG=C01 [X(C13H11O2S1)]\ \ @

ROBHandHLYP/6-311G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET5\FTS\ROBHandHLYP\6-311G(d,p)\C13H
11O2S1(2)\CARLHS\25-Sep-2004\1\ \#ROBHANDHLYP/6-311G** OPT=(GRAD,TS,REA
DFC,NOFREEZE,NOEIGENTEST) GEOM=CHECKPOINT GUESS=READ SCFCYC=300\ \Louis
' biaryl intermediate transition state\ \0,2\C\C,1,r12\C,2,r23,1,a123\S
,3,r34,2,a234,1,dih1,0\O,4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0
\C,1,r17,2,a217,3,dih4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6
,0\C,9,r910,8,a8910,7,dih7,0\C,10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a
3212,4,dih9,0\C,12,r1213,2,a21213,3,dih10,0\C,13,r1314,12,a121314,2,di
h11,0\C,14,r1415,13,a131415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,
r817,7,a7817,1,dih14,0\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91019,
8,dih16,0\H,11,r1120,10,a101120,9,dih17,0\H,12,r1221,2,a21221,3,dih18,
0\H,13,r1322,12,a121322,2,dih19,0\H,14,r1423,13,a131423,12,dih20,0\H,1
5,r1524,14,a141524,13,dih21,0\H,6,r625,7,a7625,1,dih22,0\H,6,r626,7,a7
626,1,dih23,0\O,4,r427,3,a3427,2,dih24,0\ \r23=1.41044505\ r34=1.7833680
1\ r45=1.64592306\ r56=1.43246683\ r17=1.37957657\ r78=1.39100203\ r89=1.38
461749\ r910=1.38161366\ r1011=1.38966302\ r212=1.40970073\ r1213=1.375611
69\ r1314=1.39022576\ r1415=1.3874241\ r216=1.07608771\ r817=1.07802068\ r9
18=1.07616674\ r1019=1.0770241\ r1120=1.07588073\ r1221=1.0760452\ r1322=1
.07669157\ r1423=1.07551338\ r1524=1.0772902\ r625=1.08477666\ r626=1.0817
9093\ r427=1.47302468\ a123=100.99236598\ a234=119.69272424\ a345=100.0751
8817\ a456=118.22303406\ a217=119.33271253\ a178=116.74159552\ a789=121.22
193558\ a8910=120.04798685\ a91011=119.84525306\ a3212=116.96936713\ a2121
3=120.39105732\ a121314=120.78205135\ a131415=119.66303481\ a3216=117.834
76537\ a7817=119.06685564\ a8918=119.79052481\ a91019=120.31345311\ a10112
0=120.43316492\ a21221=119.20674065\ a121322=119.65865061\ a131423=120.22
615412\ a141524=120.34563721\ a7625=111.98278036\ a7626=110.04757068\ a342
7=104.79645883\ dih1=82.82411495\ dih2=-78.5147853\ dih3=74.78595295\ dih4
=-58.07302665\ dih5=179.07208674\ dih6=0.20089341\ dih7=-0.58223264\ dih8=
0.22018454\ dih9=193.25012002\ dih10=-10.54822735\ dih11=3.87309282\ dih12
=2.9727639\ dih13=-13.41379874\ dih14=180.34385401\ dih15=179.93973731\ di
h16=180.46778029\ dih17=180.60715336\ dih18=171.50238348\ dih19=182.14204
08\ dih20=179.86324938\ dih21=175.32651679\ dih22=-57.2150941\ dih23=-177.
53184482\ dih24=32.72577236\ r12=2.14206834\ \ Version=x86-Linux-G03RevB.0
4\ State=2-A\ HF=-1050.2478894\ RMSD=7.697e-09\ RMSF=2.587e-05\ Dipole=-0.4
298173,-1.3898186,-0.6758432\ PG=C01 [X(C13H11O2S1)]\ \ @

ROBHandHLYP/6-311++G**

1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET5\FTS\ROBHandHLYP\6-311++G(d,p)\C1
3H11O2S1(2)\CARLHS\26-Sep-2004\1\ \#ROBHANDHLYP/6-311++G** OPT=(GRAD,TS
,READFC,NOFREEZE,NOEIGENTEST) GEOM=CHECKPOINT GUESS=READ SCFCYC=300\ \L
ouis' biaryl intermediate transition state\ \0,2\C\C,1,r12\C,2,r23,1,a1
23\S,3,r34,2,a234,1,dih1,0\O,4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,di
h3,0\C,1,r17,2,a217,3,dih4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,
dih6,0\C,9,r910,8,a8910,7,dih7,0\C,10,r1011,9,a91011,8,dih8,0\C,2,r212
,3,a3212,4,dih9,0\C,12,r1213,2,a21213,3,dih10,0\C,13,r1314,12,a121314,
2,dih11,0\C,14,r1415,13,a131415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H
,8,r817,7,a7817,1,dih14,0\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91
019,8,dih16,0\H,11,r1120,10,a101120,9,dih17,0\H,12,r1221,2,a21221,3,di
h18,0\H,13,r1322,12,a121322,2,dih19,0\H,14,r1423,13,a131423,12,dih20,0
\ H,15,r1524,14,a141524,13,dih21,0\H,6,r625,7,a7625,1,dih22,0\H,6,r626,

7,a7626,1,dih23,0\0,4,r427,3,a3427,2,dih24,0\\r23=1.41083996\r34=1.785
24357\r45=1.64631483\r56=1.43186416\r17=1.37932206\r78=1.39151176\r89=
1.38535399\r910=1.38238406\r1011=1.39041201\r212=1.4097257\r1213=1.376
13359\r1314=1.3905242\r1415=1.38817896\r216=1.07615085\r817=1.07808152
\r918=1.07620635\r1019=1.07707263\r1120=1.07602785\r1221=1.07614748\r1
322=1.07679017\r1423=1.07561541\r1524=1.0774362\r625=1.0850072\r626=1.
08191632\r427=1.47485914\|a123=101.01830353\|a234=120.0417276\|a345=100.3
7183133\|a456=118.67700258\|a217=118.85417462\|a178=116.75715855\|a789=121
.16331194\|a8910=120.07334947\|a91011=119.85249304\|a3212=117.02992685\|a2
1213=120.41624343\|a121314=120.74470081\|a131415=119.66941676\|a3216=118.
11671372\|a7817=119.12400488\|a8918=119.78258459\|a91019=120.30540242\|a10
1120=120.44082906\|a21221=119.19577119\|a121322=119.67734049\|a131423=120
.25409449\|a141524=120.26314242\|a7625=112.04187834\|a7626=110.08298009\|a
3427=104.87082773\|dih1=82.82660076\|dih2=-76.94228621\|dih3=73.32189485\
dih4=-59.02193127\|dih5=179.20244521\|dih6=0.16083937\|dih7=-0.55995977\|d
ih8=0.21318851\|dih9=193.25600973\|dih10=-10.40968246\|dih11=3.73268512\|d
ih12=2.98272289\|dih13=-13.14556851\|dih14=180.27987653\|dih15=179.935785
42\|dih16=180.45258627\|dih17=180.51820945\|dih18=171.63409151\|dih19=182.
07796541\|dih20=179.88792114\|dih21=175.36372511\|dih22=-56.50851396\|dih2
3=-176.80706605\|dih24=34.20857936\r12=2.14461963\\Version=x86-Linux-G0
3RevB.04\|State=2-A\|HF=-1050.2589893\|RMSD=5.240e-09\|RMSF=2.488e-05\|Dipo
le=-0.4515867,-1.4053159,-0.7175555\|PG=C01 [X(C13H11O2S1)]\|@

Sultine 4 (Y = O)

RHF/6-31G*

```
N-N= 6.124145641616D+02 E-N=-3.149865882875D+03 KE= 8.148347366921D+02
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET4\FOpt\RHF\6-31G(d)\C7H6O2S1\CARLH
S\14-Dec-2009\1\1\#RHF/6-31G* OPT=(GRAD,READFC) GEOM=CHECKPOINT GUESS=R
EAD\\Louis' cyclized product A (cyclic sultine)\\0,1\S\C,1,r12\O,1,r13
,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126
,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a7
89,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r5
12,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih1
1,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\\r12=1.78
515071\r13=1.63147961\r14=1.45470947\r35=1.42030481\r26=1.37800364\r67
=1.38435176\r78=1.38584667\r89=1.39017232\r910=1.38456874\r511=1.08074
46\r512=1.08317047\r713=1.07564757\r814=1.07505738\r915=1.07461892\r10
16=1.07501995\ a213=89.85424177\ a214=106.66132605\ a135=116.01975691\ a12
6=111.12205861\ a267=119.82195223\ a678=118.71368928\ a789=121.01767212\ a
8910=120.23693826\ a6511=113.08692227\ a6512=112.06367482\ a6713=120.9712
6861\ a7814=119.51758721\ a8915=119.83175342\ a91016=120.75202156\ dihl=11
1.56239372\ dih2=23.31232338\ dih3=-14.24329526\ dih4=183.41465978\ dih5=-
0.35246986\ dih6=0.45819275\ dih7=0.11014377\ dih8=129.01036386\ dih9=-107
.04719583\ dihl0=179.89002928\ dihl1=180.530867\ dihl2=179.92890997\ dihl3
=179.26604801\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-815.7350696\
RMSD=3.279e-09\RMSF=5.184e-05\Dipole=0.5406941,0.6869658,1.8773623\PG=
C01 [X(C7H6O2S1)]\\@
```

RHF/6-311G**

```
N-N= 6.136005875079D+02 E-N=-3.153373389177D+03 KE= 8.159668677956D+02
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET4\FOpt\RHF\6-311G(d,p)\C7H6O2S1\CA
RLHS\14-Dec-2009\1\1\#RHF/6-311G** OPT=(GRAD,READFC) GEOM=CHECKPOINT GU
ESS=READ\\Louis' cyclized product A (cyclic sultine)\\0,1\S\C,1,r12\O,
1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1
,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89
,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H
,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6
,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\\r12
=1.78697119\r13=1.62317453\r14=1.44921992\r35=1.41838676\r26=1.3761671
\r67=1.3838454\r78=1.38463953\r89=1.38985681\r910=1.38319687\r511=1.08
076113\r512=1.0839061\r713=1.07561738\r814=1.07518588\r915=1.07463626\
r1016=1.07504851\ a213=89.74362861\ a214=106.13038286\ a135=116.16075293\
a126=110.85826094\ a267=119.70783118\ a678=118.7239831\ a789=121.05274394
\ a8910=120.21396178\ a6511=112.95634813\ a6512=111.7541319\ a6713=120.960
69568\ a7814=119.50439877\ a8915=119.84315515\ a91016=120.82892369\ dihl=1
11.02486883\ dih2=24.25924478\ dih3=-15.3395479\ dih4=184.26396269\ dih5=-
0.08615976\ dih6=0.43652856\ dih7=0.0901941\ dih8=128.62001785\ dih9=-107.
28596301\ dihl0=180.05650162\ dihl1=180.45637941\ dihl2=179.81499406\ dihl
3=179.19082422\\Version=x86-Linux-G03RevB.04\State=1-A\HF=-815.8457626
\RMSD=6.351e-09\RMSF=5.710e-05\Dipole=0.5517094,0.706033,1.9015995\PG=
C01 [X(C7H6O2S1)]\\@
```

BHandHLYP/6-311G**

```
N-N= 6.115435530106D+02 E-N=-3.151961631367D+03 KE= 8.172233473927D+02
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET10\FOpt\RBHandHLYP\6-311G(d,p)\C7H
6O2S1\CARLHS\14-Dec-2009\1\1\#BHANDHLYP/6-311G** OPT=(GRAD,READFC) GEOM
=CHECKPOINT GUESS=READ\\Louis' cyclized product A (cyclic sultine)\\0,
1\S\C,1,r12\O,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,di
h2,0\C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,
dih5,0\C,8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6
511,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,
r814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,
8,dih13,0\\r12=1.795844\r13=1.6537331\r14=1.46313981\r35=1.42340446\r2
6=1.37826714\r67=1.38230658\r78=1.38484027\r89=1.38771243\r910=1.38362
942\r511=1.08319774\r512=1.08658483\r713=1.07683769\r814=1.07623457\r9
```

15=1.07583799\r1016=1.07629342\ a213=89.17228883\ a214=105.7102994\ a135=
115.15920386\ a126=111.02623979\ a267=119.53249534\ a678=118.87700685\ a78
9=120.98375941\ a8910=120.25742817\ a6511=112.90374541\ a6512=111.6306789
2\ a6713=120.84821416\ a7814=119.50734633\ a8915=119.85701799\ a91016=120.
8542048\ dih1=111.43933534\ dih2=25.12536704\ dih3=-16.55487382\ dih4=185.
52440164\ dih5=-0.25110605\ dih6=0.49253906\ dih7=0.28395416\ dih8=128.690
29454\ dih9=-107.72113838\ dih10=179.87527548\ dih11=180.55513125\ dih12=1
79.91166713\ dih13=178.91374441\ \Version=x86-Linux-G03RevB.04\State=1-A
\HF=-818.7895813\RMSD=9.684e-09\RMSF=5.811e-05\Dipole=0.480105,0.60581
21,1.7921702\PG=C01 [X(C7H6O2S1)]\@

BHandHLYP/6-311++G**

N-N= 6.111216712952D+02 E-N=-3.150599823335D+03 KE= 8.170738639736D+02
1\1\ CHEMISTRY CLUSTER KIRKLAND-KNET12\FOpt\RBHandHLYP\6-311++G(d,p)\C
7H6O2S1\CARLHS\18-Sep-2004\1\#\BHANDHLYP/6-311++G** OPT=(GRAD,READFC)
GEOM=CHECKPOINT GUESS=READ\Louis' cyclized product A (cyclic sultine)
\0,1\S\C,1,r12\O,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,
2,dih2,0\C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a67
8,2,dih5,0\C,8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,
6,a6511,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\
H,8,r814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91
016,8,dih13,0\ r12=1.79548544\ r13=1.65462386\ r14=1.46575619\ r35=1.4238
4941\ r26=1.37823291\ r67=1.38299785\ r78=1.3850869\ r89=1.38848879\ r910=1
.38387547\ r511=1.08342571\ r512=1.08663283\ r713=1.07687149\ r814=1.07627
427\ r915=1.07589373\ r1016=1.07629426\ a213=89.33349836\ a214=105.8659526
9\ a135=115.3924123\ a126=111.06049772\ a267=119.50063867\ a678=118.875102
02\ a789=120.98886954\ a8910=120.26971318\ a6511=112.91366914\ a6512=111.7
4601067\ a6713=120.83706419\ a7814=119.50378716\ a8915=119.86245402\ a9101
6=120.83437387\ dih1=111.53317535\ dih2=23.89247287\ dih3=-15.50647043\ di
h4=185.19867812\ dih5=-0.38926164\ dih6=0.63066045\ dih7=0.10902085\ dih8=
128.41199158\ dih9=-107.93931845\ dih10=179.91264322\ dih11=180.56182109\
dih12=179.87475455\ dih13=179.03875826\ \Version=x86-Linux-G03RevB.04\St
ate=1-A\HF=-818.8002861\RMSD=9.290e-09\RMSF=2.435e-05\Dipole=0.5028611
,0.6274739,1.8352895\PG=C01 [X(C7H6O2S1)]\@

Radical 10 (Y = NH)

ROHF/6-31G*

```
1\1\GINC-GOMBERG04\FOpt\ROHF\6-31G(d)\C13H12N1O1S1(2)\CARLHS\11-Jun-20
10\0\0\#rohff/6-31G* opt=(grad, cartesian, readfc) optcyc=200 scfcyc=300 g
eom=checkpoint guess=read\\Louis' starting radical with nitrogen\\0,2\
S,-0.1121895429,-0.2054686423,-0.0918916102\C,-0.6090985308,0.47350194
65,3.5685460589\N,1.1047101592,0.0184766264,1.0268323947\O,-1.33827122
72,-0.7567268795,0.5186765456\C,1.101992862,1.2481415162,1.8215766928\
C,0.5997779434,1.0933648299,3.2440018805\C,1.3247427811,1.5890946389,4
.3009426556\C,0.9623914757,1.5305279595,5.6238865861\C,-0.2443274903,0
.91011031,5.915892949\C,-1.0193537744,0.3859320277,4.8895327101\H,0.50
77373791,1.9839557292,1.2904749916\H,2.1147145956,1.6302803095,1.85141
53122\H,-1.2200426516,0.0535557983,2.7897243153\H,1.5847955432,1.94169
98475,6.3972732435\H,-0.5771667403,0.8335374636,6.9359333733\H,-1.9526
344563,-0.0957043272,5.119660587\C,0.6532876019,-1.5769338723,-0.95190
13996\C,-0.0419957426,-2.7677567491,-1.0530391708\C,0.5160109692,-3.82
03680154,-1.7662116657\C,1.7478278114,-3.6700091755,-2.3768031784\C,2.
4338560457,-2.4657503242,-2.2795757107\C,1.887559016,-1.4144247439,-1.
5688329403\H,-0.9989510274,-2.8603931968,-0.5770915558\H,-0.01504271,-
4.751823938,-1.8437065366\H,2.1758473728,-4.4859238323,-2.9311634502\H
,3.3906528173,-2.3499745249,-2.7558021081\H,2.4156460222,-0.4829247704
,-1.4816125335\H,1.3062090033,-0.8053402313,1.5623135917\\Version=AM64
L-G03RevE.01\State=2-A\HF=-1025.9643587\RMSD=6.644e-09\RMSF=5.869e-06\
Thermal=0.\Dipole=1.1093006,-0.3207383,-0.1462209\PG=C01 [X(C13H12N1O1
S1)]\\@
```

ROHF/6-311G**

```
1\1\GINC-GOMBERG02\FOpt\ROHF\6-311G(d,p)\C13H12N1O1S1(2)\CARLHS\11-Jun
-2010\0\0\#rohff/6-311G** opt=(grad, cartesian, readfc) optcyc=200 scfcyc=
300 geom=checkpoint guess=read\\Louis' starting radical with nitrogen\
\0,2\S,-0.0567107407,-0.1191885327,-0.1388596817\C,-0.5760934789,0.413
2154203,3.5395274102\N,1.1364774577,0.0633345633,1.0066000127\O,-1.309
8431326,-0.6153057109,0.452919234\C,1.1265078062,1.2762237039,1.826638
0885\C,0.6090322061,1.0872792334,3.2391800404\C,1.29287403,1.606187681
9,4.3107065597\C,0.9126348521,1.5241033999,5.6262320088\C,-0.270039636
3,0.8503933157,5.8940905388\C,-1.0032679536,0.2996055266,4.8523732729\
H,0.5327389913,2.0241220776,1.3106637436\H,2.1374700574,1.6607225678,1
.8771851684\H,-1.1549007254,-0.0268705028,2.7470304685\H,1.5041621559,
1.957054519,6.4119100716\H,-0.6161292389,0.7530933748,6.9079841281\H,-
1.9187385279,-0.223203697,5.0635435811\C,0.6702547926,-1.531688276,-0.
9681131667\C,-0.0267199357,-2.7235333248,-0.9794580962\C,0.507071182,-
3.8113906017,-1.6564007453\C,1.7152532982,-3.6932440125,-2.3169955263\
C,2.4031317965,-2.4866769308,-2.3069642831\C,1.8817274592,-1.400716384
1,-1.632733365\H,-0.9672836676,-2.7852670908,-0.4664597376\H,-0.025593
9549,-4.74508521,-1.6673020332\H,2.1237741592,-4.5368572848,-2.8440663
478\H,3.3417296277,-2.3962871339,-2.8232006729\H,2.4106126637,-0.46526
78044,-1.61388989\H,1.318553962,-0.7720971069,1.5269112468\\Version=AM
64L-G03RevE.01\State=2-A\HF=-1026.1232213\RMSD=8.526e-09\RMSF=1.664e-0
5\Thermal=0.\Dipole=1.1779431,-0.4150906,-0.1632031\PG=C01 [X(C13H12N1
O1S1)]\\@
```

ROBHandHLYP/6-311G**

```
1\1\GINC-GOMBERG02\FOpt\ROBHandHLYP\6-311G(d,p)\C13H12N1O1S1(2)\CARLHS
\11-Jun-2010\0\0\#robhandhlyp/6-311G** opt=(grad, cartesian, readfc) optc
yc=200 scfcyc=300 geom=checkpoint guess=read\\Louis' starting radical
with nitrogen\\0,2\S,-0.0674873126,-0.0970010481,-0.1164079858\C,-0.51
53243324,-0.3468298413,3.5046329725\N,1.1806815863,0.0935986886,0.98925
01349\O,-1.3128274202,-0.6140304084,0.5058454629\C,1.1730808391,1.2870
832524,1.8287969076\C,0.634543307,1.0882371399,3.2253724998\C,1.251504
194,1.6557120212,4.3091537812\C,0.8502576239,1.5700679828,5.612271448\
C,-0.2982780129,0.8275072394,5.8593411824\C,-0.968006996,0.2230032801,
4.8075629183\H,0.594699917,2.0485816324,1.3108378856\H,2.1874942024,1.1
```

6648872784,1.8980761705\H,-1.0461005738,-0.1340964158,2.69859212\H,1.3
92785802,2.0462852568,6.4104108687\H,-0.6623655431,0.7219256127,6.8674
006977\H,-1.8565313095,-0.3523574657,5.0020752951\C,0.6636559014,-1.51
4683425,-0.9484732193\C,-0.0471770318,-2.6975292167,-0.9507528644\C,0.
4710369391,-3.7911589337,-1.625513888\C,1.6766806031,-3.6863897893,-2.
2944685413\C,2.3757804192,-2.4885376478,-2.2916783188\C,1.8707585254,-
1.3939262241,-1.6172177272\H,-0.9857179955,-2.7396586653,-0.4268386355
\H,-0.0705084732,-4.7211539564,-1.6302306172\H,2.0736656701,-4.5362918
315,-2.8223278336\H,3.313670581,-2.4097432152,-2.8135248729\H,2.409137
876,-0.4625464115,-1.5993693962\H,1.4095765192,-0.7519587912,1.4862355
831\\Version=AM64L-G03RevE.01\State=2-A\HF=-1030.4053471\RMSD=6.141e-0
9\RMSF=1.623e-06\Thermal=0.\Dipole=1.0965237,-0.4461522,-0.190601\PG=C
01 [X(C13H12N1O1S1)]\@

ROBHandHLYP/6-311++G**

1\1\GINC-GOMBERG01\FOpt\ROBHandHLYP\6-311++G(d,p)\C13H12N1O1S1(2)\CARL
HS\12-Jun-2010\0\#\robhandhlyp\6-311++G** opt=(grad, cartesian, readfc)
optcyc=200 scfcyc=300 geom=checkpoint guess=read\\Louis' starting radi
cal with nitrogen\\0,2\S,-0.0976918006,-0.1568572377,-0.0903801181\C,-
0.5465180524,0.3908120405,3.5325189988\N,1.1548021368,0.0718811669,1.0
031360033\O,-1.3220272173,-0.7112793178,0.5471461232\C,1.1330865743,1.
2823152235,1.8201005713\C,0.6183372209,1.0992419181,3.2275973928\C,1.2
734583666,1.6484603506,4.298285415\C,0.898744511,1.5746960486,5.610726
3461\C,-0.2655872639,0.8655730181,5.8826644358\C,-0.9752793828,0.28030
24531,4.8450432944\H,0.5315731283,2.0212156577,1.2960577657\H,2.140590
0997,1.6808960286,1.8683382572\H,-1.1087786727,-0.0753612754,2.7392093
759\H,1.4718202341,2.0353922056,6.3965497671\H,-0.6110054713,0.7703676
825,6.8983354666\H,-1.8757349561,-0.2691393577,5.0588541929\C,0.658605
8442,-1.5513830011,-0.939107399\C,-0.0636306805,-2.7255132363,-1.02139
82995\C,0.470476658,-3.7969767346,-1.720350804\C,1.7021434969,-3.67851
92705,-2.3384623007\C,2.4109877292,-2.4885391258,-2.2600612191\C,1.890
6544857,-1.4167944696,-1.5597020968\H,-1.0217775503,-2.7845919474,-0.5
359212281\H,-0.0796631289,-4.719787846,-1.7839362288\H,2.1116436013,-4
.510604881,-2.8849637244\H,3.3689136056,-2.3978683379,-2.7422235712\H,
2.4375940692,-0.4933356269,-1.485338805\H,1.3929479204,-0.7619463481,1
.5163344164\\Version=AM64L-G03RevE.01\State=2-A\HF=-1030.41543\RMSD=5.
482e-09\RMSF=1.297e-06\Thermal=0.\Dipole=1.0903529,-0.3768814,-0.21922
14\PG=C01 [X(C13H12N1O1S1)]\@

Intermediate 12 (Y = NH)

ROHF/6-31G*

```
1\1\GINC-GOMBERG01\FOpt\ROHF\6-31G(d)\C13H12N1O1S1(2)\CARLHS\12-Jun-20
10\1\1\#rohff/6-31G* opt=grad scfcyc=300\Louis' cyclized product A (cyc
lic sultine) hypervalent intermediate - TS for rin\0,2\S\C,1,r12\N,1,
r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a
126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7
,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5
,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,d
ih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r1
17,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a1718
19,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,18
,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,dih2
0,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,0\
H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\H,3,
r328,1,a1328,4,dih25,0\H,r14=1.46531969\r35=1.45820949\r26=1.3730483\r6
7=1.38703953\r78=1.38456732\r89=1.39151385\r910=1.38439908\r511=1.0838
3737\r512=1.08707245\r713=1.07651668\r814=1.0752951\r915=1.0753398\r10
16=1.07559628\r328=0.9991177\A213=86.73213297\A214=101.14214554\A135=1
17.84170545\A126=111.91068446\A267=119.81950577\A678=118.87257119\A789
=120.73952285\A8910=120.2848486\A6511=112.02834854\A6512=110.83703508\
A6713=120.81027062\A7814=119.6643827\A8915=119.73599253\A91016=120.833
01084\A1328=112.19345882\dih1=116.72671841\dih2=21.76902766\dih3=-10.8
2673665\dih4=179.26358626\dih5=-0.212263\dih6=0.05869063\dih7=-0.08382
189\dih8=133.86049271\dih9=-105.13969371\dih10=179.76998259\dih11=180.
25485539\dih12=179.97690909\dih13=179.88988641\A4117=100.43611239\dih1
4=189.86169628\r1718=1.38504728\r1819=1.3883788\r1920=1.38465342\r2021
=1.38781441\r2122=1.38414124\A11718=119.51611183\A171819=119.38295972\
A181920=120.30582935\A192021=119.99962287\A202122=119.99312897\dih15=2
15.64828849\dih16=173.54561325\dih17=-0.78564089\dih18=-0.20937271\dih
19=0.14688564\r1823=1.07238337\r1924=1.07567076\r2025=1.07550036\r2126
=1.07562552\r2227=1.07517055\A171823=119.57726058\A181924=119.66544265
\A192025=120.04526942\A202126=120.10669674\A212227=120.16130898\dih20=
-7.1064247\dih21=179.14701932\dih22=180.09894055\dih23=180.35746484\di
h24=180.26160087\dih25=59.33956508\r117=1.89808299\r13=1.67311979\r12=
1.8871441\Version=AM64L-G03RevE.01\State=2-A\HF=-1025.9224267\RMSD=8.
351e-09\RMSF=3.503e-05\Thermal=0.\Dipole=0.9923515,0.7497653,0.3650747
\PG=C01 [X(C13H12N1O1S1)]\@
```

ROHF/6-311G**

```
1\1\GINC-GOMBERG01\FOpt\ROHF\6-311G(d,p)\C13H12N1O1S1(2)\CARLHS\12-Jun
-2010\1\1\#rohff/6-311G** opt=(grad,readfc) geom=checkpoint guess=read s
cfcyc=300 optcyc=300\Louis' cyclized product A (cyclic sultine) hyper
valent intermediate - TS for rin\0,2\S\C,1,r12\N,1,r13,2,a213\O,1,r14
,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,3,dih3,0\C,6,r
67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a789,6,dih6,0\C,9
,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r512,6,a6512,2,di
h9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11,0\H,9,r915,8,
a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r117,4,a4117,2,dih14
,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a171819,1,dih16,0\C,19,
r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,18,dih18,0\C,21,r212
2,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,dih20,0\H,19,r1924,18,
a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,0\H,21,r2126,20,a202
126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\H,3,r328,1,a1328,4,dih
25,0\H,r14=1.45993795\r35=1.45845343\r26=1.37115542\r67=1.38653199\r78=
1.3835509\r89=1.39098367\r910=1.38338336\r511=1.08384814\r512=1.087699
12\r713=1.07651805\r814=1.0753749\r915=1.07537499\r1016=1.07569815\r32
8=0.99719572\A213=86.74087844\A214=101.06522743\A135=117.61548987\A126
=111.6410543\A267=119.73612259\A678=118.86876901\A789=120.7641382\A891
0=120.28339374\A6511=111.91389996\A6512=110.56540908\A6713=120.8147600
3\A7814=119.66046758\A8915=119.74339062\A91016=120.86199753\A1328=112.
10239754\dih1=116.09872981\dih2=22.733611\dih3=-11.56481741\dih4=179.4
```

6075227\ dih5=-0.28590634\ dih6=-0.04542051\ dih7=-0.00509063\ dih8=134.30
946018\ dih9=-104.59978473\ dih10=179.75549587\ dih11=180.17075076\ dih12=
180.09591587\ dih13=179.78676109\ a4117=100.1507232\ dih14=189.42606763\ r
1718=1.38328773\ r1819=1.3881231\ r1920=1.38367889\ r2021=1.38732447\ r212
2=1.38316682\ a11718=119.71773368\ a171819=119.23574666\ a181920=120.3185
2314\ a192021=120.04083471\ a202122=119.95635676\ dih15=211.01701876\ dih1
6=173.98559491\ dih17=-0.65815616\ dih18=-0.15925961\ dih19=0.06786957\ r1
823=1.0727384\ r1924=1.07571666\ r2025=1.07554548\ r2126=1.07563198\ r2227
=1.07571142\ a171823=119.50460945\ a181924=119.6460747\ a192025=120.02135
213\ a202126=120.1204386\ a212227=120.13918596\ dih20=-6.36887951\ dih21=1
79.34973678\ dih22=180.12059931\ dih23=180.32262741\ dih24=180.18715593\ d
ih25=60.11906912\ r117=1.90739017\ r13=1.66797464\ r12=1.89117913\ \Versio
n=AM64L-G03RevE.01\ State=2-A\ HF=-1026.0795396\ RMSD=4.366e-09\ RMSF=2.20 9e-
05\ Thermal=0.\ Dipole=1.0321165,0.8003218,0.364255\ PG=C01 [X(C13H12N
1O1S1)]\ \@

ROBHandHLYP/6-311G**

1\1\GINC-GOMBERG03\FOpt\ROBHandHLYP\6-311G(d,p)\C13H12N1O1S1(2)\CARLHS
\12-Jun-2010\1\1\#robhandhlyp/6-311G** opt=(grad,readfc) geom=checkpoin
t guess=read scfcyc=300 optcyc=300\Louis' cyclized product A (cyclic
sultine) hypervalent intermediate - TS for rin\0,2\S\C,1,r12\N,1,r13,
2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,
3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a78
9,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r51
2,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11
0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r117,4
a4117,2,dih14,0\C,17,r1718,1,a1718,2,dih15,0\C,18,r1819,17,a171819,1
dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,18,dih
18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,dih20,0\H
19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,0\H,21
r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\H,3,r328
1,a1328,4,dih25,0\ r14=1.47454719\ r35=1.45521033\ r26=1.37205444\ r67=1
.38490388\ r78=1.3840536\ r89=1.38890753\ r910=1.38422215\ r511=1.08582231
\ r512=1.08987634\ r713=1.07776044\ r814=1.07632559\ r915=1.07653653\ r1016
=1.07701834\ r328=1.00289512\ a213=86.18423556\ a214=100.85944093\ a135=11
7.63261362\ a126=111.46284329\ a267=119.45037785\ a678=118.96280144\ a789=
120.76186269\ a8910=120.3181986\ a6511=111.70646695\ a6512=110.40716878\ a
6713=120.70143983\ a7814=119.63354967\ a8915=119.76867493\ a91016=120.964
74213\ a1328=111.79483079\ dih1=117.11915144\ dih2=22.54452468\ dih3=-11.1
5097592\ dih4=179.10823657\ dih5=-0.37215859\ dih6=-0.05341343\ dih7=-0.05
366287\ dih8=135.0879796\ dih9=-104.36366257\ dih10=179.66815255\ dih11=18
0.21019457\ dih12=180.10205383\ dih13=179.88387334\ a4117=100.18334624\ di
h14=188.16823517\ r1718=1.38185652\ r1819=1.38625135\ r1920=1.38407703\ r2
021=1.38595374\ r2122=1.38351869\ a11718=118.58581019\ a171819=119.027644
61\ a181920=120.30066514\ a192021=120.07552754\ a202122=120.03369117\ dih1
5=212.19258142\ dih16=172.72840035\ dih17=-0.82389639\ dih18=-0.14358402\
dih19=0.00706958\ r1823=1.07505367\ r1924=1.07688598\ r2025=1.07649329\ r2
126=1.07680259\ r2227=1.07676746\ a171823=119.26924232\ a181924=119.66693
92\ a192025=119.99587526\ a202126=120.09598859\ a212227=120.43300953\ dih2
0=-8.07296667\ dih21=179.069358\ dih22=180.16036131\ dih23=180.26352904\ d
ih24=180.22788898\ dih25=60.60190295\ r117=1.91845107\ r13=1.68495972\ r12
=1.90891941\ Version=AM64L-G03RevE.01\ State=2-A\ HF=-1030.3872043\ RMSD=
6.877e-09\ RMSF=2.805e-05\ Thermal=0.\ Dipole=1.0152207,0.7190942,0.34472
25\ PG=C01 [X(C13H12N1O1S1)]\ \@

ROBHandHLYP/6-311++G**

1\1\GINC-GOMBERG03\FOpt\ROBHandHLYP\6-311++G(d,p)\C13H12N1O1S1(2)\CARL
HS\13-Jun-2010\1\1\#robhandhlyp/6-311++G** opt=(grad,readfc) geom=check
point guess=read scfcyc=300 optcyc=300\Louis' cyclized product A (cyc
lic sultine) hypervalent intermediate - TS for rin\0,2\S\C,1,r12\N,1,
r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a
126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7
a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5
r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,d

ih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r1
17,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a1718
19,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,18
,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,dih2
0,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,0\
H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\H,3,
r328,1,a1328,4,dih25,0\|r14=1.47707636\r35=1.45546971\r26=1.37204412\r
67=1.38558075\r78=1.3845975\r89=1.3897678\r910=1.38466117\r511=1.08591
689\r512=1.0897591\r713=1.07780363\r814=1.07636071\r915=1.07658188\r10
16=1.07702892\r328=1.00320195\|a213=86.34054933\|a214=100.90035928\|a135=
117.64201907\|a126=111.53311701\|a267=119.39396594\|a678=118.95827599\|a78
9=120.77484784\|a8910=120.32182014\|a6511=111.65342351\|a6512=110.4438546
3\|a6713=120.71784496\|a7814=119.62731407\|a8915=119.76861628\|a91016=121.
00503578\|a1328=111.86328192\|dih1=117.23975611\|dih2=22.01411625\|dih3=-1
1.01428846\|dih4=179.3962903\|dih5=-0.21327941\|dih6=-0.06376759\|dih7=-0.
0208449\|dih8=134.46195814\|dih9=-104.99649111\|dih10=179.72114739\|dih11=
180.1893731\|dih12=180.04184067\|dih13=179.85210885\|a4117=100.07010259\|d
ih14=188.48913245\r1718=1.38223317\r1819=1.38714798\r1920=1.38450358\r
2021=1.38659586\r2122=1.38420452\|a11718=118.56102972\|a171819=119.02113
67\|a181920=120.31722252\|a192021=120.05052617\|a202122=120.04605661\|dih1
5=213.65683578\|dih16=172.72575954\|dih17=-0.81136563\|dih18=-0.2373863\|d
ih19=0.06998404\r1823=1.07513661\r1924=1.07692235\r2025=1.07653074\r21
26=1.07682859\r2227=1.07677927\|a171823=119.42884963\|a181924=119.644320
02\|a192025=120.01216571\|a202126=120.10391835\|a212227=120.37887411\|dih2
0=-8.0492425\|dih21=179.0711837\|dih22=180.13211157\|dih23=180.35330565\|d
ih24=180.49908363\|dih25=60.02282008\r117=1.91976588\r13=1.68555507\r12
=1.90336886\|Version=AM64L-G03RevE.01\|State=2-A\|HF=-1030.3987347\|RMSD=
5.891e-09\|RMSF=2.138e-05\|Thermal=0.\|Dipole=1.0191896,0.7135137,0.35928
02\|PG=C01 [X(C13H12N1O1S1)]\|@

Transition state 11 (Y = NH)

ROHF/6-31G*

```
1\1\GINC-GOMBERG03\FTS\ROHF\6-31G(d)\C13H12N1O1S1(2)\CARLHS\13-Jun-201
0\1\#rohff/6-31G* opt=(grad,ts,readfc,nofreeze,noeigentest) optcyc=400
scfcyc=300 geom=checkpoint guess=read\Louis' cyclized product A (cyc
lic sultam) hypervalent intermediate - TS TS2\0,2\S\C,1,r12\N,1,r13,2
,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,3
,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a789
,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r512
,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11
,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r117,4
,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a171819,1
,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,18,dih1
8,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,dih20,0\H
,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,0\H,21
,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\H,3,r328
,5,a5328,6,dih25,0\H,r328=1.00042041\ a5328=113.8316292\ dih25=197.1070276
2\ r14=1.4662798\ r35=1.46203277\ r26=1.369366\ r67=1.38892338\ r78=1.38493
438\ r89=1.3912969\ r910=1.38624529\ r511=1.08374539\ r512=1.08701234\ r713
=1.07690109\ r814=1.07534844\ r915=1.07568236\ r1016=1.07555898\ a213=84.9
8231891\ a214=100.1568067\ a135=118.70898988\ a126=108.2311262\ a267=119.1
1651709\ a678=119.06432629\ a789=120.75939664\ a8910=120.24852537\ a6511=1
11.780668\ a6512=110.41117019\ a6713=120.73413025\ a7814=119.63289031\ a89
15=119.73020801\ a91016=120.93659991\ dih1=114.35792381\ dih2=23.10383506
\ dih3=-10.96544826\ dih4=178.70521815\ dih5=-0.27652797\ dih6=-0.07643082
\ dih7=0.02785139\ dih8=136.17814479\ dih9=-103.45836641\ dih10=179.768217
03\ dih11=180.20355601\ dih12=180.11355974\ dih13=180.06429984\ a4117=102.
80896273\ dih14=189.15504097\ r1718=1.38481746\ r1819=1.38821235\ r1920=1.
38401388\ r2021=1.388359\ r2122=1.38300618\ a11718=119.16284384\ a171819=1
19.38077741\ a181920=120.25492146\ a192021=120.06299239\ a202122=120.0231
0066\ dih15=212.92276175\ dih16=174.80815121\ dih17=-0.72002727\ dih18=-0.
13258376\ dih19=0.13308309\ r1823=1.07248272\ r1924=1.07538\ r2025=1.07539
962\ r2126=1.07534771\ r2227=1.07466586\ a171823=119.46808676\ a181924=119
.6568316\ a192025=120.02416105\ a202126=120.11859654\ a212227=120.2807409
1\ dih20=-5.69874562\ dih21=179.28870444\ dih22=180.13304289\ dih23=180.26
753492\ dih24=180.01426625\ r117=1.83948803\ r13=1.67471111\ r12=2.0602878
5\ Version=AM64L-G03RevE.01\ State=2-A\ HF=-1025.9207288\ RMSD=3.589e-09\
RMSF=2.373e-06\ Thermal=0.\ Dipole=0.9636349,0.8385744,-0.0016781\ PG=C01
[X(C13H12N1O1S1)]\ \e
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ROHF/6-311G**

```
1\1\GINC-GOMBERG04\FTS\ROHF\6-311G(d,p)\C13H12N1O1S1(2)\CARLHS\13-Jun-
2010\1\#rohff/6-311G** opt=(grad,ts,readfc,nofreeze,noeigentest) optcy
c=400 scfcyc=300 geom=checkpoint guess=read\Louis' cyclized product A
(cyclic sultam) hypervalent intermediate - TS TS2\0,2\S\C,1,r12\N,1,r13,2
,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a
126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7
,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5
,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,d
ih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r1
17,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a1718
19,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,18
,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,dih2
0,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,0\
H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\H,3,
r328,5,a5328,6,dih25,0\H,r328=0.99846039\ a5328=114.02904491\ dih25=196.6
255868\ r14=1.46065234\ r35=1.46202396\ r26=1.36782066\ r67=1.38824251\ r78
=1.38392884\ r89=1.39077528\ r910=1.3851755\ r511=1.08379749\ r512=1.08764
704\ r713=1.07689501\ r814=1.07540201\ r915=1.07571352\ r1016=1.07566544\ a
213=85.10842128\ a214=100.10586493\ a135=118.45091125\ a126=108.33809743\
a267=119.09943696\ a678=119.04294672\ a789=120.77850266\ a8910=120.259662
49\ a6511=111.6754709\ a6512=110.2061454\ a6713=120.74377881\ a7814=119.63
```

299491\ a8915=119.7374115\ a91016=120.98488013\ dih1=114.06456247\ dih2=23.76111101\ dih3=-11.49600183\ dih4=178.77394481\ dih5=-0.34224398\ dih6=-0.08856146\ dih7=0.01074363\ dih8=136.42010589\ dih9=-103.05684739\ dih10=179.74558456\ dih11=180.16786548\ dih12=180.12982199\ dih13=179.96214552\ a4117=102.41593777\ dih14=188.95131227\ r1718=1.38309775\ r1819=1.38789543\ r1920=1.38302369\ r2021=1.38786505\ r2122=1.3819675\ a11718=119.31825059\ a171819=119.2532852\ a181920=120.27080663\ a192021=120.09416368\ a202122=119.98641333\ dih15=209.25549365\ dih16=175.03800255\ dih17=-0.63897177\ dih18=-0.08547274\ dih19=0.0801504\ r1823=1.07280206\ r1924=1.07542678\ r2025=1.07546415\ r2126=1.07536366\ r2227=1.07517378\ a171823=119.3735282\ a181924=119.63688783\ a192025=120.00658249\ a202126=120.13349056\ a212227=120.25312271\ dih20=-5.27109021\ dih21=179.41183669\ dih22=180.16026545\ dih23=180.25123901\ dih24=179.99315548\ r117=1.84680678\ r13=1.67005406\ r12=2.04963133\ \Version=AM64L-G03RevE.01\ State=2-A\ HF=-1026.0783084\ RMSD=1.163e-09\ RMSF=4.772e-06\ Thermal=0.\ Dipole=1.0045907,0.888227,0.0054833\ PG=C01 [X(C13H12N1O1S1)]\ \@

ROBHandHLYP/6-311G**

1\1\GINC-GOMBERG07\FTS\ROBHandHLYP\6-311G(d,p)\C13H12N1O1S1(2)\CARLHS\13-Jun-2010\1\#\robhandhlyp/6-311G** opt=(grad,ts,readfc,nofreeze,noeigentest) optcyc=400 scfcyc=300 geom=checkpoint guess=read\Louis' cyclized product A (cyclic sultam) hypervalent intermediate - TS TS2\0,2\ S\ C,1,r12\N,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\ C,3,r35,1,a135,2,dih2,0\ C,2,r26,1,a126,3,dih3,0\ C,6,r67,2,a267,1,dih4,0\ C,7,r78,6,a678,2,dih5,0\ C,8,r89,7,a789,6,dih6,0\ C,9,r910,8,a8910,7,dih7,0\ H,5,r511,6,a6511,2,dih8,0\ H,5,r512,6,a6512,2,dih9,0\ H,7,r713,6,a6713,2,dih10,0\ H,8,r814,7,a7814,6,dih11,0\ H,9,r915,8,a8915,7,dih12,0\ H,10,r1016,9,a91016,8,dih13,0\ C,1,r117,4,a4117,2,dih14,0\ C,17,r1718,1,a11718,2,dih15,0\ C,18,r1819,17,a171819,1,dih16,0\ C,19,r1920,18,a181920,17,dih17,0\ C,20,r2021,19,a192021,18,dih18,0\ C,21,r2122,20,a202122,19,dih19,0\ H,18,r1823,17,a171823,1,dih20,0\ H,19,r1924,18,a181924,17,dih21,0\ H,20,r2025,19,a192025,18,dih22,0\ H,21,r2126,20,a202126,19,dih23,0\ H,22,r2227,21,a212227,20,dih24,0\ H,3,r328,5,a5328,6,dih25,0\ r328=1.00472401\ a5328=113.72535892\ dih25=195.08146976\ r14=1.47427542\ r35=1.45983566\ r26=1.36713913\ r67=1.38793669\ r78=1.38420039\ r89=1.38841396\ r910=1.38704825\ r511=1.08562003\ r512=1.08981909\ r713=1.07826548\ r814=1.07636964\ r915=1.07698017\ r1016=1.0770566\ a213=83.89068483\ a214=100.28492935\ a135=118.48457039\ a126=106.20205821\ a267=118.55177148\ a678=119.22544831\ a789=120.79130213\ a8910=120.23551007\ a6511=111.31203927\ a6512=109.83949425\ a6713=120.55024313\ a7814=119.59584888\ a8915=119.81966536\ a91016=120.98800172\ dih1=114.33765592\ dih2=25.06316031\ dih3=-11.93146697\ dih4=178.54768898\ dih5=-0.33747667\ dih6=-0.10568523\ dih7=0.008995\ dih8=138.38727386\ dih9=-101.90783238\ dih10=179.78996029\ dih11=180.21039097\ dih12=180.13739561\ dih13=180.01000082\ a4117=103.07061379\ dih14=187.50536101\ r1718=1.38210277\ r1819=1.38556133\ r1920=1.38352622\ r2021=1.38631981\ r2122=1.38229369\ a1718=118.17307194\ a171819=119.0812499\ a181920=120.23870331\ a192021=120.13278903\ a202122=120.0828669\ dih15=208.68425729\ dih16=174.65200706\ dih17=-0.75349329\ dih18=-0.01624566\ dih19=0.01019956\ r1823=1.07531159\ r1924=1.07653437\ r2025=1.07641821\ r2126=1.07648212\ r2227=1.07611081\ a171823=119.055527\ a181924=119.67396763\ a192025=119.97826507\ a202126=120.10349043\ a212227=120.59375849\ dih20=-6.05761083\ dih21=179.22844324\ dih22=180.21583004\ dih23=180.14320708\ dih24=179.87719932\ r117=1.84378872\ r13=1.68618731\ r12=2.14453126\ \Version=AM64L-G03RevE.01\ State=2-A\ HF=-1030.3855057\ RMSD=6.688e-09\ RMSF=6.710e-06\ Thermal=0.\ Dipole=0.9925391,0.8182944,-0.0845009\ PG=C01 [X(C13H12N1O1S1)]\ \@

ROBHandHLYP/6-311++G**

1\1\GINC-GOMBERG05\FTS\ROBHandHLYP\6-311++G(d,p)\C13H12N1O1S1(2)\CARLHS\14-Jun-2010\1\#\robhandhlyp/6-311++G** opt=(grad,ts,readfc,nofreeze,noeigentest) optcyc=400 scfcyc=300 geom=checkpoint guess=read\Louis' cyclized product A (cyclic sultam) hypervalent intermediate - TS TS2\0,2\ S\ C,1,r12\N,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\ C,3,r35,1,a135,2,dih2,0\ C,2,r26,1,a126,3,dih3,0\ C,6,r67,2,a267,1,dih4,0\ C,7,r78,6,a678,2,dih5,0\ C,8,r89,7,a789,6,dih6,0\ C,9,r910,8,a8910,7,dih7,0\ H,5,r511,6,

a6511,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,
8,r814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a9101
6,8,dih13,0\C,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C
,18,r1819,17,a171819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r
2021,19,a192021,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823
,17,a171823,1,dih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a
192025,18,dih22,0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a2122
27,20,dih24,0\H,3,r328,5,a5328,6,dih25,0\|r328=1.00518765\|a5328=113.54
981226\|dih25=195.54306843\|r14=1.47707578\|r35=1.46035133\|r26=1.36685362
\r67=1.38872854\r78=1.38483019\r89=1.38916374\r910=1.38775901\r511=1.0
8567872\r512=1.08976364\r713=1.0783175\r814=1.07639633\r915=1.07702437
\r1016=1.0770852\|a213=83.83010227\|a214=100.22356194\|a135=118.49849376\
a126=105.99934104\|a267=118.44481622\|a678=119.23354361\|a789=120.8087334
\a8910=120.22849735\|a6511=111.25724675\|a6512=109.85479299\|a6713=120.56
379638\|a7814=119.5851413\|a8915=119.82888633\|a91016=121.00714119\|dih1=1
14.16498004\|dih2=25.14730996\|dih3=-12.27664657\|dih4=179.00836297\|dih5=
-0.18505027\|dih6=-0.12398798\|dih7=0.01592728\|dih8=137.8945505\|dih9=-10
2.43080039\|dih10=179.89022191\|dih11=180.18310794\|dih12=180.10234993\|di
h13=179.96530687\|a4117=103.1246793\|dih14=187.62977207\r1718=1.3825595\
r1819=1.38635005\r1920=1.38395301\r2021=1.38687657\r2122=1.38294276\|a1
1718=118.19219709\|a171819=119.09331953\|a181920=120.25120774\|a192021=12
0.10621485\|a202122=120.09689298\|dih15=209.80767844\|dih16=174.6321888\|d
ih17=-0.76455916\|dih18=-0.11661098\|dih19=0.0913953\r1823=1.07541558\r1
924=1.07658001\r2025=1.07647216\r2126=1.07652198\r2227=1.07616459\|a171
823=119.20690436\|a181924=119.65464692\|a192025=119.99325885\|a202126=120
.10833455\|a212227=120.51805074\|dih20=-6.04129411\|dih21=179.21963995\|di
h22=180.18917972\|dih23=180.23891385\|dih24=180.08863174\r117=1.8429432\
r13=1.68681767\r12=2.15227508\|Version=AM64L-G03RevE.01\|State=2-A\|HF=-
1030.3968016\|RMSD=4.310e-09\|RMSF=8.923e-06\|Thermal=0.\|Dipole=0.9868514
,0.8215326,-0.0838449\|PG=C01 [X(C13H12N1O1S1)]\|\\@

Transition state 13 (Y = NH)

ROHF/6-31G*

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1\1\GINC-GOMBERG05\FTS\ROHF\6-31G(d)\C13H12N1O1S1(2)\CARLHS\12-Jun-201
0\1\#rohff/6-31G* opt=(grad,ts,readfc,nofreeze,noeigentest) optcyc=400
scfcyc=300 geom=checkpoint guess=read\Louis' cyclized product A (cyc
lic sultam) hypervalent intermediate - TS TS2\0,2\S\C,1,r12\N,1,r13,2
,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,3
,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a789
,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r512
,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11
,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r117,4
,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a171819,1
,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,18,dih1
8,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,dih20,0\H
,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,0\H,21
,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\H,3,r328
,1,a1328,2,dih25,0\H,r328=0.99903725\al328=112.18521412\dih25=162.633868
39\r14=1.46667437\r35=1.45845404\r26=1.37681185\r67=1.38554745\r78=1.3
8536116\r89=1.39048721\r910=1.38461496\r511=1.08355565\r512=1.08719444
\r713=1.07614796\r814=1.07523675\r915=1.07504223\r1016=1.07531563\r213
=87.3704779\al214=103.3708827\al35=116.31537474\al26=112.37592669\al267=
119.76956383\al678=118.88772469\al789=120.83333193\al8910=120.249901\al651
1=112.14140775\al6512=110.82708668\al6713=120.79875978\al7814=119.6067667
7\al8915=119.79990452\al91016=120.81187437\dih1=115.35521972\dih2=25.313
47591\dih3=-14.14715368\dih4=181.21623503\dih5=-0.13292141\dih6=0.0627
112\dih7=0.02196583\dih8=133.83397607\dih9=-104.95075703\dih10=179.907
93842\dih11=180.25957325\dih12=180.04623799\dih13=179.71534763\al4117=9
8.23874545\dih14=188.35989683\r1718=1.38079898\r1819=1.38925159\r1920=
1.38606939\r2021=1.38746742\r2122=1.38685887\al11718=118.68222901\al1718
19=118.65254943\al181920=120.29039463\al192021=120.17842939\al202122=119.
96796252\dih15=211.80316455\dih16=174.21632496\dih17=-0.78166958\dih18
=-0.21997073\dih19=0.0828137\r1823=1.07309799\r1924=1.07596702\r2025=1
.07557116\r2126=1.07593541\r2227=1.07565131\al171823=120.05965169\al1819
24=119.75369321\al192025=119.93833287\al202126=120.06524489\al212227=120.
46479254\dih20=-6.41117323\dih21=179.22221568\dih22=180.1055133\dih23=
180.35654755\dih24=180.3519348\r13=1.67516818\r12=1.8312005\r117=2.071
6037\Version=AM64L-G03RevE.01\State=2-A\HF=-1025.9207722\RMSD=8.856e-
09\RMSF=2.135e-05\Thermal=0.\Dipole=0.9596764,0.6448195,0.730011\PG=C0
1 [X(C13H12N1O1S1)]\e
```

ROHF/6-311G**

```
1\1\GINC-GOMBERG03\FTS\ROHF\6-311G(d,p)\C13H12N1O1S1(2)\CARLHS\13-Jun-
2010\1\#rohff/6-311G** opt=(grad,ts,readfc,nofreeze,noeigentest) optcy
c=400 scfcyc=300 geom=checkpoint guess=read\Louis' cyclized product A
(cyclic sultam) hypervalent intermediate - TS TS2\0,2\S\C,1,r12\N,1,r13,2
,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,3
,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7
,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5
,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,d
ih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r1
17,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a1718
19,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,18
,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,dih2
0,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,0\
H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\H,3,
r328,1,a1328,2,dih25,0\H,r328=0.9971326\al328=112.15215499\dih25=163.06
844038\r14=1.46115933\r35=1.45852413\r26=1.37446368\r67=1.38514293\r78
=1.38425575\r89=1.39005813\r910=1.38352182\r511=1.08360952\r512=1.0877
7927\r713=1.07618418\r814=1.07534191\r915=1.07509661\r1016=1.07543645\
al213=87.36588956\al214=103.00512806\al35=116.24591349\al26=112.10131181
\al267=119.68881849\al678=118.88236926\al789=120.85018558\al8910=120.24826
616\al6511=111.98930861\al6512=110.58633535\al6713=120.80112936\al7814=119
```

.60826774\ a8915=119.80145167\ a91016=120.85511576\ dih1=114.93769712\ dih2=25.73982573\ dih3=-14.53428806\ dih4=181.26614933\ dih5=-0.18595317\ dih6=0.02152364\ dih7=0.02690001\ dih8=134.04949181\ dih9=-104.65753362\ dih10=179.89023196\ dih11=180.21771629\ dih12=180.08533645\ dih13=179.6454159\ a4117=98.13751745\ dih14=188.26720755\ r1718=1.37993642\ r1819=1.38884516\ r1920=1.38497418\ r2021=1.38693926\ r2122=1.38563396\ a11718=118.95947767\ a171819=118.60854095\ a181920=120.31046662\ a192021=120.18561647\ a202122=119.95191068\ dih15=207.85154249\ dih16=174.43178199\ dih17=-0.69404447\ dih18=-0.17342897\ dih19=0.0303348\ r1823=1.07334058\ r1924=1.07599454\ r2025=1.07559239\ r2126=1.07592587\ r2227=1.07602303\ a171823=119.92271661\ a181924=119.71559953\ a192025=119.93519388\ a202126=120.07645601\ a212227=120.4078356\ dih20=-5.94450269\ dih21=179.36874177\ dih22=180.12531419\ dih23=180.34384383\ dih24=180.29524639\ r13=1.66945736\ r12=1.83792724\ r117=2.05976807\ \Version=AM64L-G03RevE.01\ State=2-A\ HF=-1026.0784458\ R MSD=4.814e-09\ RMSF=4.897e-06\ Thermal=0.\ Dipole=1.0041325,0.7037976,0.7021095\ PG=C01 [X(C13H12N1O1S1)]\ \@

ROBHandHLYP/6-311G**

1\1\GINC-GOMBERG07\FTS\ROBHandHLYP\6-311G(d,p)\C13H12N1O1S1(2)\CARLHS\13-Jun-2010\1\ \#robhandhlyp/6-311G** opt=(grad,ts,readfc,nofreeze,noeigentest) optcyc=400 scfcyc=300 geom=checkpoint guess=read\ \Louis' cyclized product A (cyclic sultam) hypervalent intermediate - TS TS2\ \0,2\ S\ C,1,r12\ N,1,r13,2,a213\ O,1,r14,2,a214,3,dih1,0\ C,3,r35,1,a135,2,dih2,0\ C,2,r26,1,a126,3,dih3,0\ C,6,r67,2,a267,1,dih4,0\ C,7,r78,6,a678,2,dih5,0\ C,8,r89,7,a789,6,dih6,0\ C,9,r910,8,a8910,7,dih7,0\ H,5,r511,6,a6511,2,dih8,0\ H,5,r512,6,a6512,2,dih9,0\ H,7,r713,6,a6713,2,dih10,0\ H,8,r814,7,a7814,6,dih11,0\ H,9,r915,8,a8915,7,dih12,0\ H,10,r1016,9,a91016,8,dih13,0\ C,1,r117,4,a4117,2,dih14,0\ C,17,r1718,1,a11718,2,dih15,0\ C,18,r1819,17,a171819,1,dih16,0\ C,19,r1920,18,a181920,17,dih17,0\ C,20,r2021,19,a192021,18,dih18,0\ C,21,r2122,20,a202122,19,dih19,0\ H,18,r1823,17,a171823,1,dih20,0\ H,19,r1924,18,a181924,17,dih21,0\ H,20,r2025,19,a192025,18,dih22,0\ H,21,r2126,20,a202126,19,dih23,0\ H,22,r2227,21,a212227,20,dih24,0\ H,3,r328,1,a1328,2,dih25,0\ \r328=1.00289601\ a1328=111.85935698\ dih25=164.58825971\ r14=1.47597788\ r35=1.45555752\ r26=1.37694305\ r67=1.38326617\ r78=1.38460712\ r89=1.38797527\ r910=1.38395839\ r511=1.08550802\ r512=1.08999256\ r713=1.07730988\ r814=1.07630532\ r915=1.07617228\ r1016=1.07658325\ a213=86.77641041\ a214=103.42522653\ a135=115.93620791\ a126=112.1878382\ a267=119.44024075\ a678=118.99969772\ a789=120.84873977\ a8910=120.28845046\ a6511=111.85923087\ a6512=110.46609369\ a6713=120.68439747\ a7814=119.58299143\ a8915=119.82394905\ a91016=120.95383713\ dih1=115.3430578\ dih2=26.96998582\ dih3=-15.84526793\ dih4=182.37477857\ dih5=-0.19182092\ dih6=0.04702707\ dih7=0.05760407\ dih8=134.05780247\ dih9=-105.08399563\ dih10=179.90984827\ dih11=180.26242693\ dih12=180.11057694\ dih13=179.57905473\ a4117=97.27309695\ dih14=185.75809362\ r1718=1.37500105\ r1819=1.38849938\ r1920=1.38523272\ r2021=1.38568304\ r2122=1.38736058\ a11718=117.08508382\ a171819=118.03748603\ a181920=120.24743013\ a192021=120.34194641\ a202122=119.99121593\ dih15=204.56537132\ dih16=174.32833776\ dih17=-0.71560327\ dih18=-0.15239563\ dih19=-0.02154826\ r1823=1.07591398\ r1924=1.07724727\ r2025=1.0765597\ r2126=1.07720231\ r2227=1.07732904\ a171823=120.03891462\ a181924=119.75181702\ a192025=119.85131234\ a202126=120.0815119\ a212227=120.74451538\ dih20=-6.23555484\ dih21=179.30164217\ dih22=180.16704025\ dih23=180.29778445\ dih24=180.32254429\ r13=1.68627475\ r12=1.83670895\ r117=2.16127462\ \Version=AM64L-G03RevE.01\ State=2-A\ HF=-1030.3854642\ RMSD=5.338e-09\ RMSF=8.843e-06\ Thermal=0.\ Dipole=0.9729095,0.5970588,0.7475579\ PG=C01 [X(C13H12N1O1S1)]\ \@

ROBHandHLYP/6-311++G**

1\1\GINC-GOMBERG02\FTS\ROBHandHLYP\6-311++G(d,p)\C13H12N1O1S1(2)\CARLHS\14-Jun-2010\1\ \#robhandhlyp/6-311++G** opt=(grad,ts,readfc,nofreeze,noeigentest) optcyc=400 scfcyc=300 geom=checkpoint guess=read\ \Louis' cyclized product A (cyclic sultam) hypervalent intermediate - TS TS2\ \0,2\ S\ C,1,r12\ N,1,r13,2,a213\ O,1,r14,2,a214,3,dih1,0\ C,3,r35,1,a135,2,dih2,0\ C,2,r26,1,a126,3,dih3,0\ C,6,r67,2,a267,1,dih4,0\ C,7,r78,6,a678,2,dih5,0\ C,8,r89,7,a789,6,dih6,0\ C,9,r910,8,a8910,7,dih7,0\ H,5,r511,6,

a6511,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a171819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,dih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\H,3,r328,1,a1328,2,dih25,0\|r328=1.00317631\|a1328=111.91634616\dih25=163.99207868\r14=1.47854392\r35=1.4559494\r26=1.37692846\r67=1.38395395\r78=1.3851014\r89=1.38877568\r910=1.38441631\r511=1.08561147\r512=1.08991659\r713=1.07737623\r814=1.07635947\r915=1.0762443\r1016=1.07664133\|a213=86.92168518\|a214=103.41409441\|a135=116.02847002\|a126=112.18284225\|a267=119.40358087\|a678=118.99382487\|a789=120.85537836\|a8910=120.29088259\|a6511=111.82905278\|a6512=110.49581893\|a6713=120.69787522\|a7814=119.57817549\|a8915=119.82660975\|a91016=120.95915965\dih1=115.49398688\dih2=26.26004138\dih3=-15.36057801\dih4=182.35512851\dih5=-0.08722741\dih6=0.07758024\dih7=0.03798589\dih8=133.70615749\dih9=-105.45030716\dih10=179.94010177\dih11=180.24207409\dih12=180.0257785\dih13=179.52579296\|a4117=97.07939444\|dih14=185.97592188\r1718=1.37541205\r1819=1.38939918\r1920=1.38564347\r2021=1.38629528\r2122=1.38803346\|a11718=117.15049338\|a171819=118.0410987\|a181920=120.26571878\|a192021=120.31133673\|a202122=120.00237334\dih15=204.93556459\dih16=174.44931594\dih17=-0.72579236\dih18=-0.23310159\dih19=0.05855435\r1823=1.07595579\r1924=1.0772696\r2025=1.07658533\r2126=1.07720834\r2227=1.0773566\|a171823=120.17571273\|a181924=119.72069476\|a192025=119.86811242\|a202126=120.09487086\|a212227=120.67367038\dih20=-6.06478109\dih21=179.2894849\dih22=180.15786062\dih23=180.37693606\dih24=180.53408763\r13=1.6867708\r12=1.83618571\r117=2.15881839\|Version=AM64L-G03RevE.01\|State=2-A\|HF=-1030.3970998\RMSD=4.405e-09\RMSF=8.305e-06\Thermal=0.\|Dipole=0.9756375,0.6018752,0.7413029\PG=C01 [X(C13H12N1O1S1)]\|\\@

Sulfinamide 4 (Y = NH)

ROHF/6-31G*

```
1\1\GINC-GOMBERG01\FOpt\RHF\6-31G(d)\C7H7N1O1S1\CARLHS\11-Jun-2010\1\
#RHF/6-31G* opt=(grad,readfc) geom=checkpoint guess=read\\Louis' cycli
zed product N (cyclic sultam)\\0,1\S\C,1,r12\N,1,r13,2,a213\O,1,r14,2,
a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,3,dih3,0\C,6,r67,
2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a789,6,dih6,0\C,9,r9
10,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r512,6,a6512,2,dih9,
0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11,0\H,9,r915,8,a89
15,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\H,3,r317,1,a1317,2,dih14,0\
\r12=1.78479163\r13=1.68934983\r14=1.46960127\r35=1.46155209\r26=1.381
89875\r67=1.38382862\r78=1.38652414\r89=1.38900119\r910=1.38519633\r51
1=1.08323738\r512=1.08716354\r713=1.07569274\r814=1.07519308\r915=1.07
470124\r1016=1.0750154\r317=1.00085165\ a213=87.92186296\ a214=107.57135
159\ a135=113.99458581\ a126=112.1652568\ a267=119.56348606\ a678=118.9678
3192\ a789=120.98338335\ a8910=120.14986859\ a6511=112.09706253\ a6512=110
.71283657\ a6713=120.7735654\ a7814=119.51145809\ a8915=119.90264742\ a910
16=120.73725174\ a1317=111.24707293\ di h1=112.01497759\ di h2=30.13072775\
di h3=-18.82142337\ di h4=183.76172313\ di h5=0.06168688\ di h6=0.17691702\ di
h7=0.05350936\ di h8=133.99326182\ di h9=-104.71237619\ di h10=180.31546509\
di h11=180.33525828\ di h12=180.01430575\ di h13=179.54349893\ di h14=162.455
55653\\Version=AM64L-G03RevE.01\State=1-A\HF=-795.9058157\RMSE=5.815e-
09\RMSEF=3.972e-05\Thermal=0.\Dipole=0.9538785,0.5088626,1.2198438\PG=C
01 [X(C7H7N1O1S1)]\\@
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ROHF/6-311G**

```
1\1\GINC-GOMBERG05\FOpt\RHF\6-311G(d,p)\C7H7N1O1S1\CARLHS\11-Jun-2010\
1\#RHF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\\Louis'
cyclized product N (cyclic sultam)\\0,1\S\C,1,r12\N,1,r13,2,a213\O,1,r
14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,3,dih3,0\C,6
,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a789,6,dih6,0\C
,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r512,6,a6512,2,
dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11,0\H,9,r915,
8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\H,3,r317,1,a1317,2,dih
14,0\\r12=1.78584071\r13=1.68345817\r14=1.46524348\r35=1.46156507\r26=
1.38008386\r67=1.38303351\r78=1.38564269\r89=1.38834072\r910=1.3842087
4\r511=1.08326784\r512=1.08765669\r713=1.07568569\r814=1.07532359\r915
=1.07471608\r1016=1.07506883\r317=0.99900576\ a213=87.92401438\ a214=106
.94185064\ a135=113.70179719\ a126=111.85139663\ a267=119.4750659\ a678=11
8.96816205\ a789=121.00816218\ a8910=120.13794136\ a6511=112.00787069\ a65
12=110.3929249\ a6713=120.77703149\ a7814=119.50679677\ a8915=119.9134445
6\ a91016=120.80215816\ a1317=111.28335791\ di h1=111.48558255\ di h2=31.180
43774\ di h3=-19.88966182\ di h4=184.49391454\ di h5=0.14013135\ di h6=0.18937
075\ di h7=0.05284289\ di h8=134.13881098\ di h9=-104.41160785\ di h10=180.357
29895\ di h11=180.3198989\ di h12=179.95862298\ di h13=179.47515198\ di h14=16
3.34214167\\Version=AM64L-G03RevE.01\State=1-A\HF=-796.0149845\RMSE=3.
210e-09\RMSEF=6.768e-05\Thermal=0.\Dipole=1.0022428,0.567897,1.2264007\
PG=C01 [X(C7H7N1O1S1)]\\@
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ROBHandHLYP/6-311G**

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1\1\GINC-GOMBERG05\FOpt\RBHandHLYP\6-311G(d,p)\C7H7N1O1S1\CARLHS\11-Ju
n-2010\1\#BHandHLYP/6-311G** opt=(grad,readfc) geom=checkpoint guess=
read\\Louis' cyclized product N (cyclic sultam)\\0,1\S\C,1,r12\N,1,r13
,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126
,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a7
89,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r5
12,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih1
1,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\H,3,r317,
1,a1317,2,dih14,0\\r12=1.79509205\r13=1.69997832\r14=1.4783108\r35=1.4
59741\r26=1.38141521\r67=1.38175429\r78=1.3853131\r89=1.38688409\r910=
1.38415491\r511=1.08518508\r512=1.08978018\r713=1.07692796\r814=1.0763
1787\r915=1.07590546\r1016=1.07628596\r317=1.00461511\ a213=87.00724039
```

\a214=106.50551274\ a135=113.63338191\ a126=111.98660004\ a267=119.370685
32\ a678=119.07417019\ a789=120.93032119\ a8910=120.21693074\ a6511=111.91
549497\ a6512=110.33831889\ a6713=120.67522608\ a7814=119.53199808\ a8915=
119.8921224\ a91016=120.85767669\ a1317=111.11572641\ dih1=111.99509851\ d
ih2=32.02581146\ dih3=-21.08275537\ dih4=185.76077439\ dih5=0.19765874\ di
h6=0.11979105\ dih7=0.21022341\ dih8=133.76965297\ dih9=-105.17509313\ dih
10=180.39432594\ dih11=180.29371709\ dih12=180.060794\ dih13=179.34101432
\dih14=164.24346123\\Version=AM64L-G03RevE.01\State=1-A\HF=-798.923656
8\RMSD=8.005e-09\RMSF=1.813e-05\Thermal=0.\Dipole=0.9657139,0.4866721,
1.1331573\PG=C01 [X(C7H7N1O1S1)]\\@

ROBHandHLYP/6-311++G**

1\1\GINC-GOMBERG04\FOpt\RBHandHLYP\6-311++G(d,p)\C7H7N1O1S1\CARLHS\11-
Jun-2010\1\#\BHandHLYP/6-311++G** opt=(grad,readfc) geom=checkpoint gu
ess=read\\Louis' cyclized product N (cyclic sultam)\\0,1\S\C,1,r12\N,1
,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,
a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,
7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,
5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,
dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\H,3,r
317,1,a1317,2,dih14,0\\r12=1.79449708\r13=1.69932673\r14=1.48168222\r3
5=1.45971552\r26=1.38126805\r67=1.38254199\r78=1.38561579\r89=1.387743
55\r910=1.38437771\r511=1.08531374\r512=1.08970668\r713=1.07697071\r81
4=1.07637166\r915=1.07596452\r1016=1.07631707\r317=1.00443833\ a213=87.
22110732\ a214=106.58969642\ a135=114.03037402\ a126=112.05593464\ a267=11
9.3202689\ a678=119.07189232\ a789=120.93887464\ a8910=120.22604046\ a6511
=111.82891701\ a6512=110.51247555\ a6713=120.67093715\ a7814=119.52385934
\ a8915=119.89858745\ a91016=120.85620507\ a1317=111.49680204\ dih1=112.31
213335\ dih2=30.66198212\ dih3=-20.1281004\ dih4=185.57604109\ dih5=0.1248
3036\ dih6=0.2373128\ dih7=0.13314003\ dih8=132.94220946\ dih9=-106.010183
58\ dih10=180.35550097\ dih11=180.30490483\ dih12=180.0078931\ dih13=179.2
5558121\ dih14=164.05827837\\Version=AM64L-G03RevE.01\State=1-A\HF=-798
.9342664\RMSD=2.616e-09\RMSF=3.348e-05\Thermal=0.\Dipole=0.9963281,0.5
154721,1.1791368\PG=C01 [X(C7H7N1O1S1)]\\@

Radical **15** (Y = NH)

ROHF/6-31G*

```

1\1\GINC-GOMBERG02\Fopt\ROHF\6-31G(d)\C13H12N1O1S1(2)\CARLHS\12-Jun-20
10\1\1\#rohlf/6-31G* opt=grad scfcyc=300\\Louis' biaryl intermediate tra
nsition state\\0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234,1,dih1,0\N,
4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,dih4,0\
C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910,7,dih
7,0\C,10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,r1213
2,a21213,3,dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,13,a1314
15,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih14,0\H,
9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,11,r1120,10,a
101120,9,dih17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,12,a21322,2,
dih19,0\H,14,r1423,13,a131423,12,dih20,0\H,15,r1524,14,a141524,13,dih
21,0\H,6,r625,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0\O,4,r427,3,
a3427,2,dih24,0\H,5,r528,4,a4528,27,dih25,0\\r528=1.00126562\ a4528=111
.90368659\dih25=172.35321811\r12=1.54579596\r23=1.5166365\r34=1.779719
37\r45=1.67063197\r56=1.46006639\r17=1.40405129\r78=1.38639591\r89=1.3
8670247\r910=1.37821449\r1011=1.38843578\r212=1.5106637\r1213=1.333661
28\r1314=1.43620907\r1415=1.43296915\r216=1.08709687\r817=1.07626269\r
918=1.07524361\r1019=1.07543078\r1120=1.07250351\r1221=1.07606677\r132
2=1.07581914\r1423=1.0723726\r1524=1.07686651\r625=1.08111624\r626=1.0
8238777\r427=1.47543154\ a123=111.9060116\ a234=119.52472183\ a345=103.83
691037\ a456=118.98832354\ a217=120.81730718\ a178=119.43765602\ a789=121.
60882046\ a8910=119.05642322\ a91011=119.9072437\ a3212=110.45156392\ a212
13=123.27192849\ a121314=121.06912483\ a131415=118.23528074\ a3216=107.28
181237\ a7817=119.06612103\ a8918=120.20040808\ a91019=120.49354793\ a1011
20=118.61358445\ a21221=116.47370875\ a121322=120.17766124\ a131423=120.8
983666\ a141524=118.75853076\ a7625=112.47344769\ a7626=109.41984818\ a342
7=104.32421065\ dihl=80.4250719\ dih2=-56.08318249\ dih3=58.94736227\ dih4
=-68.17928971\ dih5=181.47169168\ dih6=-0.33761437\ dih7=-0.60510415\ dih8
=0.70760259\ dih9=205.74475427\ dih10=-16.1450316\ dih11=3.90893723\ dih12
=9.53259888\ dih13=-37.13905117\ dih14=179.77336452\ dih15=179.84919945\ d
ih16=180.65181588\ dih17=180.19816766\ dih18=166.29249503\ dih19=182.4200
2188\ dih20=182.43120545\ dih21=166.99529621\ dih22=-54.71125932\ dih23=-1
73.0522732\ dih24=53.52616925\\Version=AM64L-G03RevE.01\State=2-A\HF=-1
025.96639\RMSD=6.367e-09\RMSF=2.357e-05\Thermal=0.\Dipole=0.0079654,-1
.6406251,-1.1790754\PG=C01 [X(C13H12N1O1S1)]\\e

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ROHF/6-311G**

```
1\1\GINC-GOMBERG05\Fopt\ROHF\6-311G(d,p)\C13H12N1O1S1(2)\CARLHS\12-Jun
-2010\1\#\rohff/6-311G** opt=(grad,readfc) geom=checkpoint guess=read s
cfccyc=300\Louis' biaryl intermediate transition state\0,2\C\C,1,r12\
C,2,r23,1,a123\S,3,r34,2,a234,1,dih1,0\N,4,r45,3,a345,2,dih2,0\C,5,r56
,4,a456,3,dih3,0\C,1,r17,2,a217,3,dih4,0\C,7,r78,1,a178,2,dih5,0\C,8,r
89,7,a789,1,dih6,0\C,9,r910,8,a8910,7,dih7,0\C,10,r1011,9,a91011,8,dih
8,0\C,2,r212,3,a3212,4,dih9,0\C,12,r1213,2,a21213,3,dih10,0\C,13,r1314
,12,a121314,2,dih11,0\C,14,r1415,13,a131415,12,dih12,0\H,2,r216,3,a321
6,4,dih13,0\H,8,r817,7,a7817,1,dih14,0\H,9,r918,8,a8918,7,dih15,0\H,10
,r1019,9,a91019,8,dih16,0\H,11,r1120,10,a101120,9,dih17,0\H,12,r1221,2
,a1221,3,dih18,0\H,13,r1322,12,a21322,2,dih19,0\H,14,r1423,13,a13142
3,12,dih20,0\H,15,r1524,14,a141524,13,dih21,0\H,6,r625,7,a7625,1,dih22
,0\H,6,r626,7,a7626,1,dih23,0\O,4,r427,3,a3427,2,dih24,0\H,5,r528,4,a4
528,27,dih25,0\#r528=0.99913094#a4528=111.90193609\dih25=172.86171641\
r12=1.5451065\r23=1.51542813\r34=1.78097843\r45=1.66579765\r56=1.46079
76\r17=1.40344512\r78=1.38537881\r89=1.38615746\r910=1.37693809\r1011=
1.38788225\r212=1.50978853\r1213=1.33244577\r1314=1.43615491\r1415=1.4
3287717\r216=1.08686506\r817=1.07627675\r918=1.07524745\r1019=1.075428
9\r1120=1.07247565\r1221=1.0763384\r1322=1.07591982\r1423=1.07238996\r
1524=1.0769784\r625=1.08164107\r626=1.08217485\r427=1.47215609#a123=11
1.7913343#a234=119.29674298#a345=103.97126413#a456=118.88964846#a217=1
20.78800705#a178=119.42185662#a789=121.61598336#a8910=119.06680271#a91
011=119.89152295#a3212=110.43461404#a21213=123.25524889#a121314=121.09
```

```
303554\al31415=118.23649407\as3216=107.20292477\aw7817=119.05260293\aw891
8=120.18936768\aw91019=120.50989445\aw101120=118.58594969\aw21221=116.549
47309\aw121322=120.12205463\aw131423=120.90953887\aw141524=118.87150235\aw
7625=112.30684142\aw7626=109.3173765\aw3427=103.92104429\dih1=80.6523747
8\dih2=-56.38842978\dih3=58.97547084\dih4=-68.2385292\dih5=181.3512062
4\dih6=-0.24555777\dih7=-0.60813565\dih8=0.67192052\dih9=206.05070109\
dih10=-15.95158901\dih11=3.74565765\dih12=9.64238573\dih13=-36.8829094
2\dih14=179.80066405\dih15=179.79854382\dih16=180.59540979\dih17=180.1
6387637\dih18=166.37204106\dih19=182.29263378\dih20=182.52771691\dih21
=166.91085628\dih22=-54.65918961\dih23=-172.89264604\dih24=53.02126223
\Version=AM64L-G03RevE.01\State=2-A\HF=-1026.1250424\RMSD=7.274e-09\R
MSF=1.976e-05\Thermal=0.\Dipole=0.0493206,-1.6371372,-1.2202327\PG=C01
[X(C13H12N1O1S1)]\@
```

ROBHandHLYP/6-311G**

```
1\1\GINC-GOMBERG01\FOpt\ROBHandHLYP\6-311G(d,p)\C13H12N1O1S1(2)\CARLHS
\13-Jun-2010\1\1\#robhandhlyp/6-311G** opt=(grad,readfc) geom=checkpoin
t guess=read scfcyc=300\Louis' biaryl intermediate transition state\
0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234,1,dih1,0\N,4,r45,3,a345,2,
dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,dih4,0\C,7,r78,1,a178,
2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910,7,dih7,0\C,10,r1011,
9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,r1213,2,a21213,3,dih1
0,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,13,a131415,12,dih12,0\H
,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih14,0\H,9,r918,8,a8918,
7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,11,r1120,10,a101120,9,dih17,
0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,12,a121322,2,dih19,0\H,14,r
1423,13,a131423,12,dih20,0\H,15,r1524,14,a141524,13,dih21,0\H,6,r625,7
,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0\O,4,r427,3,a3427,2,dih24,0
\H,5,r528,4,a4528,27,dih25,0\r528=1.00530829\aw4528=111.80728776\dih25
=174.44285974\r12=1.54153329\r23=1.50284717\r34=1.78233482\r45=1.68391
232\r56=1.45840597\r17=1.40043589\r78=1.38624075\r89=1.38380663\r910=1
.37830882\r1011=1.38531961\r212=1.49863786\r1213=1.34544332\r1314=1.41
504239\r1415=1.40831072\r216=1.09097002\r817=1.07768518\r918=1.0762814
9\r1019=1.07646312\r1120=1.0746858\rl1221=1.07713146\r1322=1.07711645\r
1423=1.07455438\r1524=1.07858242\r625=1.08507534\r626=1.08427291\r427=
1.4848609\aw123=111.42902061\aw234=119.0285558\aw345=103.81060494\aw456=11
7.87496427\aw217=120.86849269\aw178=119.27520952\aw789=121.59745903\aw8910
=119.14204251\aw91011=119.85088703\aw3212=110.79326498\aw21213=122.677027
13\aw121314=121.24727672\aw131415=119.03318142\aw3216=107.1893282\aw7817=1
18.85392092\aw8918=120.19595773\aw91019=120.46058974\aw101120=119.0441729
1\aw21221=116.91802868\aw121322=119.7595403\aw131423=120.44612984\aw141524
=119.38410486\aw7625=112.37328187\aw7626=109.42302882\aw3427=103.5092749\
dih1=81.74127266\dih2=-57.65921467\dih3=58.87723365\dih4=-68.54346666\
dih5=181.24155179\dih6=-0.41382055\dih7=-0.58069365\dih8=0.74307387\di
h9=206.8960072\dih10=-15.63508877\dih11=4.52244356\dih12=7.84542651\di
h13=-35.10084186\dih14=179.64214662\dih15=179.83978286\dih16=180.68156
429\dih17=180.10992706\dih18=167.3543097\dih19=182.85391963\dih20=181.
71585158\dih21=168.74157307\dih22=-53.55536786\dih23=-171.73529014\dih
24=50.9466417\Version=AM64L-G03RevE.01\State=2-A\HF=-1030.4226504\RMS
D=8.145e-09\RMSF=1.254e-05\Thermal=0.\Dipole=0.0218154,-1.5049869,-1.1
670452\PG=C01 [X(C13H12N1O1S1)]\@
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ROBHandHLYP/6-311++G**

```
1\1\GINC-GOMBERG05\FOpt\ROBHandHLYP\6-311++G(d,p)\C13H12N1O1S1(2)\CARL
HS\13-Jun-2010\1\1\#robhandhlyp/6-311++G** opt=(grad,readfc) geom=check
point guess=read scfcyc=300\Louis' biaryl intermediate transition sta
te\0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234,1,dih1,0\N,4,r45,3,a34
5,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,dih4,0\C,7,r78,1,a
178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910,7,dih7,0\C,10,r1
011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,r1213,2,a21213,3,
dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,13,a131415,12,dih12
,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih14,0\H,9,r918,8,a8
918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,11,r1120,10,a101120,9,di
h17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,12,a121322,2,dih19,0\H,
```

14,r1423,13,a131423,12,dih20,0\H,15,r1524,14,a141524,13,dih21,0\H,6,r6
25,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0\O,4,r427,3,a3427,2,dih
24,0\H,5,r528,4,a4528,27,dih25,0\r528=1.00562705\ a4528=111.76312665\d
ih25=171.6142404\r12=1.54108302\r23=1.50359587\r34=1.78462607\r45=1.68
375491\r56=1.45850916\r17=1.40003451\r78=1.38670415\r89=1.38452701\r91
0=1.37913596\r1011=1.38596267\r212=1.49889064\r1213=1.34594543\r1314=1
.41523509\r1415=1.40862867\r216=1.09119377\r817=1.07776321\r918=1.0763
1695\r1019=1.07650642\r1120=1.07488114\r1221=1.07724981\r1322=1.077179
53\r1423=1.07469045\r1524=1.07864199\r625=1.08519355\r626=1.08426652\r
427=1.4868669\ a123=111.41898153\ a234=119.65508135\ a345=104.14491218\ a4
56=118.45677877\ a217=120.738304\ a178=119.32310974\ a789=121.53631791\ a8
910=119.15781755\ a91011=119.85771524\ a3212=110.83109489\ a21213=122.731
07671\ a121314=121.21396108\ a131415=119.06987134\ a3216=107.51200922\ a78
17=118.91640564\ a8918=120.19144362\ a91019=120.44769821\ a101120=119.038
09742\ a21221=116.90063556\ a121322=119.75879677\ a131423=120.4618037\ a14
1524=119.32778989\ a7625=112.31745967\ a7626=109.5237146\ a3427=103.73559
882\ dihl=80.9311099\ dihl2=-55.4371844\ dihl3=56.96760739\ dihl4=-69.0233719
\ dihl5=181.30138161\ dihl6=-0.50121331\ dihl7=-0.52319991\ dihl8=0.70914277\ d
ih9=206.16261921\ dihl10=-15.28323701\ dihl11=4.19652505\ dihl12=7.82534999\
dihl13=-35.87058837\ dihl14=179.51909982\ dihl15=179.83875557\ dihl16=180.650
17887\ dihl17=180.05329779\ dihl18=167.55655549\ dihl19=182.73224386\ dihl20=1
81.82972651\ dihl21=169.09759898\ dihl22=-52.96992935\ dihl23=-171.13434868\
dihl24=53.35860645\\ Version=AM64L-G03RevE.01\ State=2-A\ HF=-1030.4332406
\ RMSD=5.956e-09\ RMSF=2.949e-05\ Thermal=0.\ Dipole=-0.0380938,-1.4932541 , -
1.2129011\ PG=C01 [X(C13H12N1O1S1)]\ \@

Transition state 14 (Y = NH)

ROHF/6-31G*

```
1\1\GINC-GOMBERG06\FTS\ROHF\6-31G(d)\C13H12N1O1S1(2)\CARLHS\13-Jun-201
0\1\#rohff/6-31G* opt=(grad,ts,readfc,nofreeze,noeigentest) optcyc=400
scfcyc=300 geom=checkpoint guess=read\Biaryl TS with nitrogen (sulta
m)\0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234,1,dih1,0\N,4,r45,3,a34
5,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,dih4,0\C,7,r78,1,a
178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910,7,dih7,0\C,10,r1
011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,r1213,2,a21213,3,
dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,13,a131415,12,dih12
,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih14,0\H,9,r918,8,a8
918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,11,r1120,10,a101120,9,di
h17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,12,a21322,2,dih19,0\H,
14,r1423,13,a131423,12,dih20,0\H,15,r1524,14,a141524,13,dih21,0\H,6,r6
25,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0\O,4,r427,3,a3427,2,dih
24,0\H,5,r528,4,a4528,27,dih25,0\|r528=1.00085874\|a4528=112.2286747\|di
h25=173.71878369\r23=1.42408876\r34=1.78324674\r45=1.67252217\r56=1.45
857178\r17=1.38728331\r78=1.39142739\r89=1.38721429\r910=1.38189316\r1
011=1.3905003\r212=1.41963181\r1213=1.37546487\r1314=1.39176208\r1415=
1.39138246\r216=1.07478694\r817=1.07682115\r918=1.07524261\r1019=1.075
8141\r1120=1.07332434\r1221=1.07479881\r1322=1.07566726\r1423=1.074392
1\r1524=1.07623965\r625=1.08077125\r626=1.08288441\r427=1.47467758\|a12
3=102.86800878\|a234=120.33363327\|a345=103.9360205\|a456=119.94941604\|a2
17=119.06478949\|a178=117.07371982\|a789=121.45540513\|a8910=119.84955225
\|a91011=119.81490471\|a3212=116.51416114\|a21213=120.5817897\|a121314=120
.74312404\|a131415=119.53542653\|a3216=117.25229994\|a7817=119.19670659\|a
8918=119.84422143\|a91019=120.33352386\|a101120=120.03720584\|a21221=118.
9938449\|a121322=119.66049987\|a131423=120.28086143\|a141524=119.86980698
\|a7625=111.82918461\|a7626=109.04556077\|a3427=104.97574869\|dih1=82.9159
8928\|dih2=-70.2841268\|dih3=63.58963117\|dih4=-63.41109048\|dih5=181.2307
4325\|dih6=-0.22030106\|dih7=-0.28442914\|dih8=0.32102014\|dih9=195.672293
57\|dih10=-12.76659226\|dih11=4.7538136\|dih12=3.65367342\|dih13=-16.29794
477\|dih14=179.7689909\|dih15=179.95940655\|dih16=180.32470146\|dih17=180.
14402872\|dih18=169.68893598\|dih19=182.7942103\|dih20=179.68817528\|dih21
=173.72945708\|dih22=-56.82224123\|dih23=-174.48187743\|dih24=39.60260989
\r12=2.04805058\|Version=AM64L-G03RevE.01\|State=2-A\|HF=-1025.9127274\R
MSD=2.715e-09\RMSF=8.831e-06\Thermal=0.\|Dipole=-0.0109284,-1.6443598,-
1.2360104\|PG=C01 [|X(C13H12N1O1S1)]\|
```

ROHF/6-311G**

```
1\1\GINC-GOMBERG03\FTS\ROHF\6-311G(d,p)\C13H12N1O1S1(2)\CARLHS\13-Jun-
2010\1\#rohff/6-311G** opt=(grad,ts,readfc,nofreeze,noeigentest) optcy
c=400 scfcyc=300 geom=checkpoint guess=read\Biaryl TS with nitrogen (
sultam)\0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234,1,dih1,0\N,4,r45,
3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,dih4,0\C,7,r7
8,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910,7,dih7,0\C,
10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,r1213,2,a212
13,3,dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,13,a131415,12,
dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih14,0\H,9,r918
,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,11,r1120,10,a101120
,9,dih17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,12,a21322,2,dih19
,0\H,14,r1423,13,a131423,12,dih20,0\H,15,r1524,14,a141524,13,dih21,0\H
,6,r625,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0\O,4,r427,3,a3427,
2,dih24,0\H,5,r528,4,a4528,27,dih25,0\|r528=0.99861934\|a4528=112.35537
243\|dih25=173.67325158\r23=1.42263389\r34=1.78401742\r45=1.66702308\r5
6=1.45902017\r17=1.38675496\r78=1.3904536\r89=1.38658929\r910=1.380593
1\r1011=1.38993246\r212=1.41866901\r1213=1.37443463\r1314=1.39102333\r
1415=1.39084326\r216=1.07458327\r817=1.07685615\r918=1.07525413\r1019=
1.0758298\r1120=1.07328298\r1221=1.0749089\r1322=1.07579378\r1423=1.07
440758\r1524=1.07627666\r625=1.08136547\r626=1.0827186\r427=1.47113847
\|a123=102.58194652\|a234=120.19381894\|a345=104.0447578\|a456=119.9162361
4\|a217=119.12383469\|a178=117.05980551\|a789=121.46745086\|a8910=119.8528
```

6204\ a91011=119.80970134\ a3212=116.45191524\ a21213=120.56584913\ a12131
4=120.76755802\ a131415=119.52944972\ a3216=117.23015653\ a7817=119.17132
323\ a8918=119.83611747\ a91019=120.36098546\ a101120=119.99127539\ a21221
=119.01720953\ a121322=119.65149737\ a131423=120.29278704\ a141524=119.91
865725\ a7625=111.66509212\ a7626=108.95321752\ a3427=104.68729186\ dih1=8
3.14455564\ dih2=-70.79890141\ dih3=63.59389992\ dih4=-63.30643106\ dih5=1
81.0263146\ dih6=-0.13056275\ dih7=-0.2941989\ dih8=0.29009143\ dih9=195.7
6617169\ dih10=-12.79503538\ dih11=4.68957021\ dih12=3.7674871\ dih13=-16.
12521399\ dih14=179.79066926\ dih15=179.91381071\ dih16=180.28978846\ dih1
7=180.10724155\ dih18=169.62247492\ dih19=182.71473719\ dih20=179.7256183
\ dih21=173.70161803\ dih22=-56.85314303\ dih23=-174.38790172\ dih24=38.96
953689\ r12=2.04893556\ \Version=AM64L-G03RevE.01\ State=2-A\ HF=-1026.071
4043\ RMSD=3.414e-09\ RMSF=2.268e-05\ Thermal=0.\ Dipole=0.036982,-1.64836
05,-1.2953609\ PG=C01 [X(C13H12N1O1S1)]\ \e

ROBHandHLYP/6-311G**

1\1\GINC-GOMBERG07\FTS\ROBHandHLYP\6-311G(d,p)\C13H12N1O1S1(2)\CARLHS\
13-Jun-2010\1\ \#robhandhlyp/6-311G** opt=(grad,ts,readfc,nofreeze,noei
gentest) optcyc=400 scfcyc=300 geom=checkpoint guess=read\Biaryl TS w
ith nitrogen (sultam)\0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234,1,d
ih1,0\N,4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3
,dih4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a89
10,7,dih7,0\C,10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,1
2,r1213,2,a21213,3,dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,
13,a131415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,di
h14,0\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,11,r1
120,10,a101120,9,dih17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,12,a
121322,2,dih19,0\H,14,r1423,13,a131423,12,dih20,0\H,15,r1524,14,a14152
4,13,dih21,0\H,6,r625,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0\O,4
,r427,3,a3427,2,dih24,0\H,5,r528,4,a4528,27,dih25,0\ \r528=1.0044605\ a4
528=112.57865994\ dih25=175.81810793\ r23=1.41093388\ r34=1.79207992\ r45=
1.68391816\ r56=1.4559996\ r17=1.38033986\ r78=1.39224311\ r89=1.38486581\
r910=1.38168229\ r1011=1.38954379\ r212=1.40944497\ r1213=1.37599901\ r131
4=1.3897698\ r1415=1.38834326\ r216=1.07608967\ r817=1.07845901\ r918=1.07
630674\ r1019=1.0770461\ r1120=1.07603532\ r1221=1.07614627\ r1322=1.07674
685\ r1423=1.07568038\ r1524=1.07774905\ r625=1.08477206\ r626=1.08496221\
r427=1.48287789\ a123=101.19106808\ a234=119.86302052\ a345=103.964641\ a4
56=119.33231674\ a217=119.51058541\ a178=116.60481819\ a789=121.34792674\
a8910=120.03752507\ a91011=119.76054739\ a3212=117.14310166\ a21213=120.4
0909966\ a121314=120.69670494\ a131415=119.64448361\ a3216=117.64429216\ a
7817=119.0087559\ a8918=119.79240587\ a91019=120.34251611\ a101120=120.41
909888\ a21221=119.20076217\ a121322=119.69892574\ a131423=120.21440061\ a
141524=120.19301374\ a7625=111.6211835\ a7626=109.06104255\ a3427=104.338
71023\ dih1=82.846646\ dih2=-74.19645182\ dih3=65.64889356\ dih4=-61.42164
616\ dih5=180.14773566\ dih6=-0.19858565\ dih7=-0.27817268\ dih8=0.3026864
4\ dih9=193.37529297\ dih10=-10.66801721\ dih11=4.02454127\ dih12=2.946922
18\ dih13=-13.38221332\ dih14=179.69656089\ dih15=179.9462873\ dih16=180.3
1993813\ dih17=180.16373626\ dih18=171.46394134\ dih19=182.15766785\ dih20
=179.55002645\ dih21=174.61670661\ dih22=-56.32144483\ dih23=-173.7680978
9\ dih24=34.99647185\ r12=2.14325712\ \Version=AM64L-G03RevE.01\ State=2-A
\ HF=-1030.3786828\ RMSD=8.866e-09\ RMSF=2.568e-05\ Thermal=0.\ Dipole=0.08
88872,-1.5861957,-1.1211974\ PG=C01 [X(C13H12N1O1S1)]\ \e

ROBHandHLYP/6-311++G**

1\1\GINC-GOMBERG04\FTS\ROBHandHLYP\6-311++G(d,p)\C13H12N1O1S1(2)\CARLH
S\14-Jun-2010\1\ \#robhandhlyp/6-311++G** opt=(grad,ts,readfc,nofreeze,
noeigentest) optcyc=400 scfcyc=300 geom=checkpoint guess=read\Biaryl
TS with nitrogen (sultam)\0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234
,1,dih1,0\N,4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a2
17,3,dih4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8
,a8910,7,dih7,0\C,10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0
\C,12,r1213,2,a21213,3,dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1
415,13,a131415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,
1,dih14,0\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,1

1,r1120,10,a101120,9,dih17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,
12,a121322,2,dih19,0\H,14,r1423,13,a131423,12,dih20,0\H,15,r1524,14,a1
41524,13,dih21,0\H,6,r625,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0
\0,4,r427,3,a3427,2,dih24,0\H,5,r528,4,a4528,27,dih25,0\|r528=1.005035
14\|a4528=112.40278994\|dih25=173.40030189\r23=1.41130902\r34=1.7941608\
r45=1.68435266\r56=1.45653232\r17=1.37999138\r78=1.39272701\r89=1.3856
8323\r910=1.38243172\r1011=1.39031153\r212=1.40961841\r1213=1.37642712
\r1314=1.39015502\r1415=1.38908893\r216=1.07616727\r817=1.07853245\r91
8=1.07634442\r1019=1.07708544\r1120=1.07618949\r1221=1.07625317\r1322=
1.0768321\r1423=1.07577197\r1524=1.07779103\r625=1.08480242\r626=1.084
94667\r427=1.48466591\|a123=101.18489903\|a234=120.31500986\|a345=104.316
17992\|a456=119.84394001\|a217=119.01481124\|a178=116.61048404\|a789=121.2
9522491\|a8910=120.06069809\|a91011=119.76295498\|a3212=117.19360202\|a212
13=120.43589759\|a121314=120.65761929\|a131415=119.65390838\|a3216=117.99
35925\|a7817=119.0753301\|a8918=119.78168651\|a91019=120.33438436\|a101120
=120.42531425\|a21221=119.18872556\|a121322=119.72001795\|a131423=120.239
65289\|a141524=120.14249317\|a7625=111.61336442\|a7626=109.13600828\|a3427
=104.50439381\|dih1=82.7680399\|dih2=-72.23948598\|dih3=63.65704176\|dih4=
-62.31976008\|dih5=180.07777761\|dih6=-0.24908785\|dih7=-0.24803243\|dih8=
0.27737457\|dih9=193.28445569\|dih10=-10.55072817\|dih11=3.87411084\|dih12
=3.00993625\|dih13=-13.1790662\|dih14=179.58913019\|dih15=179.93660945\|di
h16=180.3075731\|dih17=180.11446138\|dih18=171.56904869\|dih19=182.105896
69\|dih20=179.60067897\|dih21=174.69157566\|dih22=-55.4147316\|dih23=-172.
84299733\|dih24=37.0865063\r12=2.14554221\|Version=AM64L-G03RevE.01\Sta
te=2-A\HF=-1030.3891065\RMSD=6.104e-09\RMSF=2.799e-05\Thermal=0.\Dipol
e=0.0430476,-1.5765999,-1.1739608\PG=C01 [X(C13H12N1O1S1)]\|@

Radical 10 (Y = NMe)

ROHF/6-31G*

```
1\1\GINC-GOMBERG02\FOpt\ROHF\6-31G(d)\C14H14N1O1S1(2)\CARLHS\14-Jun-20
10\0\0\#rohff/6-31G* opt=(grad, cartesian) optcyc=200 scfcyc=300\Louis'
starting radical\0,2\S,-0.1234654807,-0.3118490762,-0.1604203113\C,-0
.6613798774,0.2997084327,3.5915272284\N,1.0444267766,0.3042690813,0.85
24462661\O,-1.4076570855,-0.5317868246,0.5381068579\C,0.7307677077,1.4
191011237,1.7522067875\C,0.4517454025,1.0465344974,3.197227371\C,1.284
5080164,1.4613984953,4.2078736863\C,1.1147729258,1.2099604222,5.547835
955\C,0.0012048911,0.4651154558,5.9082067482\C,-0.8771962021,0.0148908
127,4.9300846006\H,-0.1165407775,1.9499180449,1.3418278278\H,1.5742394
38,2.0997962776,1.7292884854\H,-1.3442669736,-0.0590639828,2.843357318
1\H,1.8110183239,1.5717642876,6.2820445334\H,-0.1816766575,0.236751321
8,6.9434690168\H,-1.739360099,-0.5615806442,5.2139385344\C,-0.39726938
75,1.1358446872,-1.1817799844\C,-1.6847465528,1.6187100118,-1.32952342
91\C,-1.9146236499,2.6935965062,-2.1781824808\C,-0.8659175404,3.264949
3082,-2.875665124\C,0.4227218723,2.7662833452,-2.7306020293\C,0.659689
0571,1.6988101945,-1.8860012641\H,-2.4848873987,1.1577853516,-0.783526
3187\H,-2.9119517369,3.0784744848,-2.2919252898\H,-1.0472923008,4.0954
23396,-3.5341826888\H,1.2371361769,3.2101811592,-3.2741842372\H,1.6551
280496,1.3129832133,-1.7633540864\C,2.0292454472,-0.6576451857,1.33199
00019\H,2.9122205692,-0.1151300369,1.6479741384\H,2.3094616289,-1.3192
35396,0.5234236787\H,1.6728775678,-1.2497129382,2.1680889257\Version=
AM64L-G03RevE.01\State=2-A\HF=-1064.9907661\RMSD=6.503e-09\RMSF=7.203e
-06\Thermal=0.\Dipole=0.8675693,0.7351025,-0.3618237\PG=C01 [X(C14H14N
1O1S1)]\@
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ROHF/6-311G**

```
1\1\GINC-GOMBERG02\FOpt\ROHF\6-311G(d,p)\C14H14N1O1S1(2)\CARLHS\14-Jun
-2010\0\0\#rohff/6-311G** opt=(grad, cartesian, readfc) geom=checkpoint gu
ess=read optcyc=200 scfcyc=300\Louis' starting radical\0,2\S,-0.1071
764493,-0.3134808447,-0.1560113168\C,-0.6654471023,0.2993910042,3.5771
896309\N,1.0553288636,0.3009166318,0.8547830971\O,-1.385653921,-0.5305
551068,0.545696411\C,0.7441113985,1.4178148076,1.751887511\C,0.4503132
146,1.0468182983,3.19440254\C,1.2701233549,1.4632222958,4.212972636\C,
1.0876010458,1.2136593193,5.5507425231\C,-0.0281996948,0.4682675649,5.
8995479476\C,-0.8949715855,0.0163569869,4.9129421616\H,-0.0977276165,1
.9556201102,1.3383456566\H,1.5919341099,2.0938219763,1.7376300027\H,-1
.3386566043,-0.0606403523,2.8204672326\H,1.7757636197,1.5775012875,6.2
915590056\H,-0.2218130982,0.2408603494,6.933128848\H,-1.7597473283,-0.
5605738863,5.1878018875\C,-0.3920175562,1.1320418965,-1.179628302\C,-1
.6745043556,1.6322849838,-1.2911633326\C,-1.9107878531,2.7088272313,-2
.1352424423\C,-0.873792849,3.2626502943,-2.8616338463\C,0.4103204139,2
.7452107968,-2.7510847227\C,0.6538631831,1.6766385221,-1.9116016176\H,
-2.4646052881,1.1817323596,-0.7217581611\H,-2.9051225115,3.1080554718,
-2.2228933946\H,-1.0607380294,4.0946081665,-3.5168228255\H,1.215960767
3,3.1754338123,-3.3182463458\H,1.6462762773,1.2750176404,-1.8159656868
\C,2.0541026938,-0.6524723318,1.3246201154\H,2.9402098993,-0.103149613
9,1.6220384731\H,2.3246002454,-1.3194203691,0.516353719\H,1.7133848868
,-1.2402134762,2.1715133126\Version=AM64L-G03RevE.01\State=2-A\HF=-10
65.1574115\RMSD=8.720e-09\RMSF=1.277e-05\Thermal=0.\Dipole=0.9278042,0
.7646841,-0.402113\PG=C01 [X(C14H14N1O1S1)]\@
```

ROBHandHLYP/6-311G**

```
1\1\GINC-GOMBERG04\FOpt\ROBHandHLYP\6-311G(d,p)\C14H14N1O1S1(2)\CARLHS
\15-Jun-2010\0\0\#robhandhlyp/6-311G** opt=(grad, cartesian, readfc) geom
=checkpoint guess=read optcyc=200 scfcyc=300\Louis' starting radical\
0,2\S,-0.0805955118,-0.3648956232,-0.1651887861\C,-0.6395286728,0.317
507292,3.4829917188\N,1.112548575,0.2588460452,0.8291654378\O,-1.36360
74938,-0.6027329536,0.5494964984\C,0.8332488045,1.400892751,1.69917512
32\C,0.487158382,1.0647861054,3.131496545\C,1.2587728981,1.4988164173,
4.1757817573\C,1.0300682757,1.2781000786,5.5059237096\C,-0.0976548028,
```

0.532307727,5.8240500915\C,-0.9203119544,0.0582551525,4.8130733869\H,0
.0284079436,1.9719908844,1.2514455778\H,1.7133189008,2.0374316609,1.69
76314712\H,-1.2768552397,-0.0609233657,2.6999937606\H,1.6856888855,1.6
576066312,6.270329666\H,-0.3294577696,0.3236622829,6.8550000337\H,-1.7
928637082,-0.5199259968,5.0638354519\C,-0.3822578737,1.1137990653,-1.1
456400872\C,-1.6716371386,1.6012904555,-1.2184210693\C,-1.9322314817,2
.6988091988,-2.023661177\C,-0.9122553926,3.2840686705,-2.7507785576\C,
0.3769267347,2.7775699345,-2.6774444364\C,0.6467797508,1.6865099337,-1
.8747642556\H,-2.4425623273,1.1188268199,-0.6442792432\H,-2.9323038527
,3.0920505431,-2.0827369025\H,-1.1186370457,4.1338453104,-3.3783603285
\H,1.1691425013,3.2345777167,-3.2447650136\H,1.6449705078,1.2911935531
, -1.8011687825\C,2.0684631273,-0.7124350468,1.3387408374\H,2.996964414
2,-0.1981378418,1.56663057\H,2.2695062294,-1.4532662719,0.5744834013\H
,1.7237264656,-1.2141813035,2.2395343185\\Version=AM64L-G03RevE.01\Sta
te=2-A\HF=-1069.6941007\RMSD=4.890e-09\RMSF=8.433e-06\Thermal=0.\Dipol
e=0.8251568,0.7335924,-0.3694323\PG=C01 [X(C14H14N1O1S1)]\@

ROBHandHLYP/6-311++G**

1\1\GINC-GOMBERG04\FOpt\ROBHandHLYP\6-311++G(d,p)\C14H14N1O1S1(2)\CARL
HS\16-Jun-2010\0\#\robhandhlyp/6-311++G** opt=(grad, cartesian, readfc)
geom=checkpoint guess=read optcyc=200 scfcyc=300\\Louis' starting radi
cal\\0,2\S,-0.1052292411,-0.3590001237,-0.1671398373\C,-0.6206632688,0
.2997135445,3.5001873257\N,1.0938604201,0.2467437124,0.8307203823\O,-1
.3929219314,-0.5829808206,0.5481705248\C,0.8318959242,1.3916660289,1.7
018697656\C,0.4943812213,1.05948876,3.1373980172\C,1.2628102711,1.5129
804055,4.1760059333\C,1.0432181895,1.300902261,5.5094779011\C,-0.07310
42513,0.541655287,5.8385589827\C,-0.893212906,0.0478998955,4.834141587
9\H,0.0277845533,1.9696944459,1.2612225428\H,1.7172481506,2.0208581653
,1.6931563025\H,-1.2573592315,-0.0941804901,2.7243644779\H,1.696622528
5,1.6961424128,6.2678454545\H,-0.2982581974,0.3386909652,6.8721408612\
H,-1.7569375882,-0.5399857731,5.0930760389\C,-0.393028621,1.1254606938
, -1.1452540568\C,-1.6886657195,1.5879286461,-1.2673730773\C,-1.9408232
27,2.6838398283,-2.0785851431\C,-0.906234152,3.2920391401,-2.766011727
1\C,0.3890620756,2.8091952445,-2.6466432013\C,0.6499739789,1.719876246
6,-1.8374282324\H,-2.4731137191,1.0920715957,-0.7235793768\H,-2.945788
04,3.0572822156,-2.1734476094\H,-1.1056666984,4.1404554084,-3.39779075
61\H,1.1931885293,3.2828122003,-3.1828690035\H,1.6529371885,1.34443246
39,-1.730934731\C,2.0428173399,-0.735416186,1.3327568278\H,2.979650080
3,-0.232215525,1.5518868591\H,2.2287319973,-1.480229966,0.5683522995\H
,1.6997564753,-1.2315748563,2.2372953852\\Version=AM64L-G03RevE.01\Sta
te=2-A\HF=-1069.7034529\RMSD=4.238e-09\RMSF=1.462e-06\Thermal=0.\Dipol
e=0.8461388,0.7186383,-0.3907072\PG=C01 [X(C14H14N1O1S1)]\@

Intermediate 12 (Y = NMe)

ROHF/6-31G*

```
1\1\GINC-GOMBERG02\FOpt\ROHF\6-31G(d)\C14H14N1O1S1(2)\CARLHS\14-Jun-20
10\1\1\#rohff/6-31G* opt=(grad,readfc,nofreeze) geom=checkpoint guess=re
ad scfcyc=300 optcyc=300\Louis' cyclized product NMe (cyclic sultam)
hypervalent intermediate - TS for ri\0,2\S\C,1,r12\N,1,r13,2,a213\O,1
,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,3,dih3,0\C
,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a789,6,dih6,0
\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r512,6,a6512
,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11,0\H,9,r91
5,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r117,4,a4117,2,d
ih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a171819,1,dih16,0\C
,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,18,dih18,0\C,21
,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,dih20,0\H,19,r1924
,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,0\H,21,r2126,20
,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\C,3,r328,1,a1328,4
,dih25,0\H,28,r2829,3,a32829,5,dih26,0\H,28,r2830,3,a32830,5,dih27,0\H
,28,r2831,3,a32831,5,dih28,0\H,r2829=1.08350657\r2830=1.08639983\r2831=
1.0773025\A32829=108.01108424\A32830=111.671223\A32831=110.94479643\di
h26=-55.37969311\diH27=64.42454107\diH28=-173.75461946\r14=1.4653956\r
35=1.46263058\r26=1.3695442\r67=1.38842748\r78=1.38346505\r89=1.393169
98\r910=1.38293161\r511=1.08509732\r512=1.08839534\r713=1.07659833\r81
4=1.07529422\r915=1.0753969\r1016=1.07561875\r328=1.45838204\A213=88.8
4714562\A214=102.52657786\A135=116.79731335\A126=111.84598506\A267=119
.88901005\A678=118.82223192\A789=120.71947778\A8910=120.31868409\A6511
=112.28548644\A6512=110.11517818\A6713=120.84621293\A7814=119.70320687
\A8915=119.69153736\A91016=120.92965247\A1328=117.22796156\diH1=115.78
724296\diH2=9.521062\diH3=-1.09657047\diH4=174.94495194\diH5=-0.138806
23\diH6=-0.0830064\diH7=-0.25931372\diH8=133.13855603\diH9=-106.936195
73\diH10=179.58750907\diH11=180.05647093\diH12=179.90744286\diH13=180.
2475926\A4117=101.11061474\diH14=195.72090528\r1718=1.38514613\r1819=1
.3887901\r1920=1.38416923\r2021=1.38851671\r2122=1.38328852\A11718=119
.46206505\A171819=119.45972654\A181920=120.32986209\A192021=119.910948
49\A202122=120.05533531\diH15=229.25095413\diH16=170.53380554\diH17=-0
.70482269\diH18=-0.22874972\diH19=0.03901112\r1823=1.07264783\r1924=1.
07571846\r2025=1.07545751\r2126=1.07568264\r2227=1.07529928\A171823=11
9.58072546\A181924=119.63846114\A192025=120.09902306\A202126=120.07022
118\A212227=120.19784866\diH20=-10.14933381\diH21=179.17111803\diH22=1
80.04830696\diH23=180.24681041\diH24=180.2160731\diH25=44.81335747\r11
7=1.88786044\r13=1.68419994\r12=1.88340418\Version=AM64L-G03RevE.01\S
tate=2-A\HF=-1064.9464833\RMSE=5.187e-09\RMSEF=1.876e-05\Thermal=0.\Dip
ole=0.9768729,0.8174015,0.3788397\PG=C01 [X(C14H14N1O1S1)]\@
```

ROHF/6-311G**

```
1\1\GINC-GOMBERG01\FOpt\ROHF\6-311G(d,p)\C14H14N1O1S1(2)\CARLHS\14-Jun
-2010\1\1\#rohff/6-311G** opt=(grad,readfc,nofreeze) geom=checkpoint gue
ss=read scfcyc=300 optcyc=300\Louis' cyclized product NMe (cyclic sul
tam) hypervalent intermediate - TS for ri\0,2\S\C,1,r12\N,1,r13,2,a21
3\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,3,dih
3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a789,6,d
ih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r512,6,a
6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11,0\H,
9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r117,4,a411
7,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a171819,1,dih1
6,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,18,dih18,0\
C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,dih20,0\H,19,
r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,0\H,21,r212
6,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\C,3,r328,1,a1
328,4,dih25,0\H,28,r2829,3,a32829,5,dih26,0\H,28,r2830,3,a32830,5,dih2
7,0\H,28,r2831,3,a32831,5,dih28,0\H,r2829=1.08382641\r2830=1.0872019\r2
831=1.07797931\A32829=108.03962779\A32830=111.59132853\A32831=110.9641
2532\diH26=-53.12638159\diH27=66.76394342\diH28=-171.49115364\r14=1.46
```

048868\r35=1.46326906\r26=1.36741228\r67=1.38818993\r78=1.38222363\r89
=1.39289126\r910=1.38169198\r511=1.08526937\r512=1.08899061\r713=1.076
60445\r814=1.07536688\r915=1.07544156\r1016=1.07569452\r328=1.45969795
\a213=88.94432878\xa214=102.43218573\xa135=116.62912313\xa126=111.5853256
1\xa267=119.80293443\xa678=118.82665638\xa789=120.73839299\xa8910=120.3178
128\xa6511=112.06036787\xa6512=109.92399335\xa6713=120.84714995\xa7814=119
.70278096\xa8915=119.69826981\xa91016=120.96748185\xa1328=116.589784\dih1
=115.3270934\dih2=10.14823849\dih3=-1.4113757\dih4=174.75038984\dih5=-
0.27169874\dih6=-0.0970758\dih7=-0.27846302\dih8=133.67179327\dih9=-10
6.34480325\dih10=179.52918417\dih11=180.02803277\dih12=179.96862946\di
h13=180.23603498\xa4117=100.81255819\dih14=195.49102419\r1718=1.3834522
3\r1819=1.3883249\r1920=1.38332172\r2021=1.38786804\r2122=1.38245938\ a
11718=119.63380907\ a171819=119.33202816\ a181920=120.34518573\ a192021=1
19.93365742\ a202122=120.03289109\ di h15=226.55299023\ di h16=170.89175896
\ di h17=-0.60680704\ di h18=-0.21746281\ di h19=-0.01722372\r1823=1.0729488
\ r1924=1.07578048\r2025=1.07549122\r2126=1.07570242\r2227=1.07569944\ a
171823=119.5212437\ a181924=119.62127439\ a192025=120.08198959\ a202126=1
20.08149581\ a212227=120.1781683\ di h20=-9.68576505\ di h21=179.2847172\ di
h22=180.02425808\ di h23=180.24694513\ di h24=180.18919413\ di h25=44.342568
76\r117=1.89253533\r13=1.68032543\r12=1.8883967\\Version=AM64L-G03RevE
.01\State=2-A\HF=-1065.111476\RMSD=9.604e-09\RMSF=2.699e-05\Thermal=0.
\Dipole=1.0224096,0.8444635,0.3691542\PG=C01 [X(C14H14N1O1S1)]\\@

ROBHandHLYP/6-311G**

1\1\GINC-GOMBERG01\FOpt\ROBHandHLYP\6-311G(d,p)\C14H14N1O1S1(2)\CARLHS
\15-Jun-2010\1\1\#robhandhlyp/6-311G** opt=(grad,readfc,nofreeze) geom=
checkpoint guess=read scfcyc=300 optcyc=300\\Louis' cyclized product N
Me (cyclic sultam) hypervalent intermediate - TS for ri\\0,2\S\C,1,r12
\N,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r2
6,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,
r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,
0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a781
4,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C
1,r117,4,a4117,2,dih14,0\C,17,r1718,1,a1718,2,dih15,0\C,18,r1819,17,
a171819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a1920
21,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1
171823,17,a171823,17,a171823,17,a171823,17,a171823,17,a171823,17,a171823,17
,dih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih
22,0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0
\C,3,r328,1,a1328,4,dih25,0\H,28,r2829,3,a32829,5,dih26,0\H,28,r2830,3
,a32830,5,dih27,0\H,28,r2831,3,a32831,5,dih28,0\\r2829=1.08494695\r283
0=1.08918999\r2831=1.08001683\ a32829=108.38787392\ a32830=111.73670229\
a32831=110.61614629\ di h26=-56.41800069\ di h27=63.67453752\ di h28=-174.82
746823\r14=1.47441312\r35=1.45934078\r26=1.36991657\r67=1.38555688\r78
=1.38353671\r89=1.39016689\r910=1.38299134\r511=1.08717832\r512=1.0918
2844\r713=1.07784276\r814=1.0763008\r915=1.07660108\r1016=1.07707254\r
328=1.45429824\ a213=88.4971935\ a214=102.58777366\ a135=116.3921192\ a126
=111.30612707\ a267=119.5235231\ a678=118.93623715\ a789=120.73158749\ a89
10=120.35872952\ a6511=112.02552613\ a6512=109.8856006\ a6713=120.7323186
5\ a7814=119.67186983\ a8915=119.72975195\ a91016=121.04343557\ a1328=116.
15393357\ di h1=116.2490083\ di h2=10.84987796\ di h3=-1.07343194\ di h4=173.7
033929\ di h5=-0.36962103\ di h6=-0.14401318\ di h7=-0.3442769\ di h8=135.7634
6795\ di h9=-104.58586344\ di h10=179.39179409\ di h11=180.06283278\ di h12=17
9.96878794\ di h13=180.36031993\ a4117=101.01325272\ di h14=194.73974647\r1
718=1.38279677\r1819=1.38627398\r1920=1.38375175\r2021=1.38673751\r212
2=1.38238594\ a11718=118.56589979\ a171819=119.14789382\ a181920=120.3242
087\ a192021=119.98095648\ a202122=120.10573455\ di h15=227.9381137\ di h16=
169.48033394\ di h17=-0.75322221\ di h18=-0.15244685\ di h19=-0.11356241\r18
23=1.07518612\r1924=1.076916\r2025=1.07642901\r2126=1.07684599\r2227=1
.07688201\ a171823=119.28834778\ a181924=119.64256582\ a192025=120.053077
21\ a202126=120.04898378\ a212227=120.52372044\ di h20=-11.46321452\ di h21=
179.03765297\ di h22=180.07624048\ di h23=180.09161652\ di h24=180.07153632\
di h25=44.56867353\r117=1.89673401\r13=1.69771452\r12=1.90045563\\Versi
on=AM64L-G03RevE.01\State=2-A\HF=-1069.674035\RMSD=3.674e-09\RMSF=3.88
7e-05\Thermal=0.\Dipole=0.9875359,0.7799881,0.3527227\PG=C01 [X(C14H14
N1O1S1)]\\@

ROBHandHLYP/6-311++G**

```
1\1\GINC-GOMBERG06\FOpt\ROBHandHLYP\6-311++G(d,p)\C14H14N1O1S1(2)\CARL
HS\16-Jun-2010\1\1\#robhandhlyp/6-311++G** opt=(grad,readfc,nofreeze) g
eom=checkpoint guess=read scfcyc=300 optcyc=300\Louis' cyclized produ
ct NME (cyclic sultam) hypervalent intermediate - TS for ri\0,2\S\C,1
,r12\N,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,
2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\
C,8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,d
ih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,
a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13
,0\C,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819
,17,a171819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a
192021,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a1718
23,1,dih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18
,dih22,0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih
24,0\C,3,r328,1,a1328,4,dih25,0\H,28,r2829,3,a32829,5,dih26,0\H,28,r28
30,3,a32830,5,dih27,0\H,28,r2831,3,a32831,5,dih28,0\H,28,r2829=1.08532958\
r2830=1.08925025\r2831=1.07995077\ a32829=108.34402391\ a32830=111.66749
41\ a32831=110.73299463\ diH26=-58.3492147\ diH27=61.65278394\ diH28=-176.
81040483\r14=1.47657075\r35=1.4584999\r26=1.36967292\r67=1.38618394\r7
8=1.38417526\r89=1.39089008\r910=1.38362571\r511=1.08744799\r512=1.091
83967\r713=1.07789648\r814=1.07634134\r915=1.0766393\r1016=1.07712399\
r328=1.45417436\ a213=88.41039688\ a214=102.56847404\ a135=116.51601626\ a
126=111.46817867\ a267=119.47961938\ a678=118.91849151\ a789=120.74701497
\ a8910=120.35346624\ a6511=111.95464108\ a6512=110.03090115\ a6713=120.76
393401\ a7814=119.66079727\ a8915=119.73330021\ a91016=121.06377488\ a1328
=117.18802307\ diH1=116.54739735\ diH2=11.22917932\ diH3=-2.03375201\ diH4
=174.65250398\ diH5=-0.14457573\ diH6=-0.26180284\ diH7=-0.19236801\ diH8=
134.6486716\ diH9=-105.70263657\ diH10=179.51231813\ diH11=180.02690743\ d
ih12=179.95158353\ diH13=180.29122769\ a4117=100.99102992\ diH14=195.0286
3937\r1718=1.38339244\r1819=1.38697167\r1920=1.38431131\r2021=1.387330
37\r2122=1.38311705\ a11718=118.41676482\ a171819=119.17116189\ a181920=1
20.34111813\ a192021=119.94391147\ a202122=120.12207075\ diH15=229.409234
41\ diH16=169.16734179\ diH17=-0.75790996\ diH18=-0.26250017\ diH19=-0.025
57011\r1823=1.07530651\r1924=1.07695884\r2025=1.07645278\r2126=1.07689
37\r2227=1.07698935\ a171823=119.41201134\ a181924=119.6249966\ a192025=1
20.07479265\ a202126=120.05670263\ a212227=120.42381749\ diH20=-11.744713
46\ diH21=179.0136172\ diH22=180.05630309\ diH23=180.20720245\ diH24=180.2
879422\ diH25=46.56864206\r117=1.89863838\r13=1.69677836\r12=1.89710644
\Version=AM64L-G03RevE.01\State=2-A\HF=-1069.6847351\RMSD=2.445e-09\R
MSF=3.755e-05\Thermal=0.\Dipole=1.0211086,0.7794426,0.3549401\PG=C01 [
X(C14H14N1O1S1)]\@
```

Transition state 11 (Y = NMe)

ROHF/6-31G*

```
1\1\GINC-GOMBERG07\FTS\ROHF\6-31G(d)\C14H14N1O1S1(2)\CARLHS\15-Jun-201
0\1\#rohlf/6-31G* opt=(grad,ts,readfc,noeigentest,nofreeze) geom=check
point guess=read optcyc=400 scfcyc=300\Louis' cyclized product NMe (c
yclic sultam) hypervalent intermediate - TS TS2\0,2\S\C,1,r12\N,1,r13
,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126
,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a7
89,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r5
12,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih1
1,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r117,
4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a171819,
1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,18,d
ih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,dih20,0
\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,0\H,2
1,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\C,3,r32
8,5,a5328,6,dih25,0\H,28,r2829,3,a32829,5,dih26,0\H,28,r2830,3,a32830,
5,dih27,0\H,28,r2831,3,a32831,5,dih28,0\H,28,r2829=1.08333914\r2830=1.0859
3571\r2831=1.07801669\ a32829=107.97422157\ a32830=111.72706109\ a32831=1
10.85519956\ di26=-53.40577741\ di27=66.48027884\ di28=-171.68598702\r
328=1.4598585\ a5328=112.25476261\ di25=204.09872617\r14=1.466366\r35=1
.46606169\r26=1.36715478\r67=1.38993856\r78=1.38401237\r89=1.39259497\r
910=1.38497823\r511=1.08501323\r512=1.08823019\r713=1.07700699\r814=1
.07536061\r915=1.07575824\r1016=1.07570439\ a213=87.56078797\ a214=101.7
7714024\ a135=117.92798408\ a126=108.09367705\ a267=119.31350463\ a678=119
.01114859\ a789=120.70691596\ a8910=120.28513286\ a6511=111.95020077\ a651
2=109.72262364\ a6713=120.78089186\ a7814=119.68254283\ a8915=119.6870314
\ a91016=120.93847996\ di1=114.02331877\ di2=9.27383469\ di3=0.1665445\
di4=173.22556597\ di5=-0.34561409\ di6=-0.16490009\ di7=-0.13244996\ d
ih8=135.80461514\ di9=-104.92196079\ di10=179.52264964\ di11=180.09285
765\ di12=180.06695334\ di13=180.4177743\ a4117=103.05712234\ di14=195.
5186202\r1718=1.38483157\r1819=1.38851547\r1920=1.38374384\r2021=1.388
80432\r2122=1.38249958\ a11718=119.27965838\ a171819=119.43046563\ a18192
0=120.27572494\ a192021=119.99193819\ a202122=120.06135817\ di15=226.604
60172\ di16=172.47765037\ di17=-0.67693916\ di18=-0.1659422\ di19=0.06
582194\r1823=1.07262349\r1924=1.07542741\r2025=1.0753687\r2126=1.07540
3\r2227=1.07482127\ a171823=119.47745191\ a181924=119.63788573\ a192025=1
20.06642512\ a202126=120.09200342\ a212227=120.29737267\ di20=-8.1144250
6\ di21=179.26592347\ di22=180.08896099\ di23=180.22144015\ di24=180.0
0872096\r117=1.83605197\r13=1.67964727\r12=2.04415083\ Version=AM64L-G
03RevE.01\ State=2-A\ HF=-1064.9451616\ RMSD=3.228e-09\ RMSF=2.768e-06\ The
rmal=0.\ Dipole=0.9555112,0.9404023,-0.0012056\ PG=C01 [X(C14H14N1O1S1)]
\@
```

ROHF/6-311G**

```
1\1\GINC-GOMBERG02\FTS\ROHF\6-311G(d,p)\C14H14N1O1S1(2)\CARLHS\15-Jun-
2010\1\#rohlf/6-311G** opt=(grad,ts,readfc,noeigentest,nofreeze) geom=
checkpoint guess=read optcyc=400 scfcyc=300\Louis' cyclized product N
Me (cyclic sultam) hypervalent intermediate - TS TS1\0,2\S\C,1,r12\N,
1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1
,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89
,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H
,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6
,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,
r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a17
1819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,
18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,d
ih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,
0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\C,
3,r328,5,a5328,6,dih25,0\H,28,r2829,3,a32829,5,dih26,0\H,28,r2830,3,a3
2830,5,dih27,0\H,28,r2831,3,a32831,5,dih28,0\H,28,r2829=1.08372506\r2830=1
.08684376\r2831=1.07867104\ a32829=108.04953113\ a32830=111.62717834\ a32
```

831=110.87494786\dih26=-52.13624933\dih27=67.82689876\dih28=-170.45103
68\r328=1.46066182\ a5328=112.29791869\dih25=204.31315523\r14=1.461158\
r35=1.46614975\r26=1.36548338\r67=1.38947693\r78=1.38282211\r89=1.3922
9573\r910=1.38367971\r511=1.08523807\r512=1.08889561\r713=1.07699567\r
814=1.07539946\r915=1.07579288\r1016=1.0757575\ a213=87.7424975\ a214=10
1.70152712\ a135=117.73642656\ a126=108.20794763\ a267=119.29096727\ a678=
118.9987705\ a789=120.72059736\ a8910=120.29846382\ a6511=111.79445033\ a6
512=109.58402167\ a6713=120.78696069\ a7814=119.68731902\ a8915=119.69264
89\ a91016=121.00202812\dih1=113.89536934\dih2=9.64264125\dih3=0.124362
2\dih4=172.85489822\dih5=-0.48040456\dih6=-0.16439832\dih7=-0.18152164
\dih8=136.30546031\dih9=-104.27169898\dih10=179.45201216\dih11=180.061
75482\dih12=180.09637089\dih13=180.38187564\ a4117=102.62841916\dih14=1
95.42886333\r1718=1.38318537\r1819=1.38800778\r1920=1.38288973\r2021=1
.38814604\r2122=1.38163447\ a11718=119.38817523\ a171819=119.32153346\ a1
81920=120.29549543\ a192021=120.00388286\ a202122=120.03855149\dih15=224
.77353368\dih16=172.64263948\dih17=-0.60872975\dih18=-0.16003498\dih19
=0.02727606\r1823=1.07290715\r1924=1.0754944\r2025=1.07542646\r2126=1.
07543746\r2227=1.07519789\ a171823=119.40417222\ a181924=119.61987263\ a1
92025=120.05484386\ a202126=120.10349954\ a212227=120.27236531\dih20=-7.
89451392\dih21=179.34274231\dih22=180.07166367\dih23=180.23152916\dih2
4=180.01953164\r117=1.84154389\r13=1.67584206\r12=2.03367161\\Version=
AM64L-G03RevE.01\State=2-A\HF=-1065.1105546\RMSD=1.700e-09\RMSF=3.727e
-06\Thermal=0.\Dipole=1.0052328,0.9681985,0.0046986\PG=C01 [X(C14H14N1
O1S1)]\@

ROBHandHLYP/6-311G**

1\1\GINC-GOMBERG01\FTS\ROBHandHLYP\6-311G(d,p)\C14H14N1O1S1(2)\CARLHS\
15-Jun-2010\1\#\robhandhlyp/6-311G** opt=(grad,ts,readfc,noeigentest,n
ofreeze) geom=checkpoint guess=read optcyc=400 scfcyc=300\\Louis' cycl
ized product NMe (cyclic sultam) hypervalent intermediate - TS TS1\\0,
2\S\C,1,r12\N,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,di
h2,0\C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,
dih5,0\C,8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6
511,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,
r814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,
8,dih13,0\C,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,1
8,r1819,17,a171819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r20
21,19,a192021,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,1
7,a171823,1,dih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a19
2025,18,dih22,0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227
20,dih24,0\C,3,r328,5,a5328,6,dih25,0\H,28,r2829,3,a32829,5,dih26,0\H
,28,r2830,3,a32830,5,dih27,0\H,28,r2831,3,a32831,5,dih28,0\\r2829=1.08
462758\r2830=1.08864583\r2831=1.08065089\ a32829=108.19132094\ a32830=11
1.78851115\ a32831=110.62782022\dih26=-52.86957521\dih27=67.15753627\di
h28=-171.19058662\r328=1.45699713\ a5328=111.95608762\dih25=201.0977950
6\r14=1.47481408\r35=1.46368069\r26=1.36642856\r67=1.38809322\r78=1.38
39916\r89=1.38908296\r910=1.3863134\r511=1.08687305\r512=1.09189114\r7
13=1.07833284\r814=1.07636116\r915=1.07706031\r1016=1.07724023\ a213=86
.78580275\ a214=102.47656171\ a135=117.36777545\ a126=105.89117894\ a267=1
18.77264612\ a678=119.18490239\ a789=120.73186451\ a8910=120.26782179\ a65
11=111.55085702\ a6512=109.41030053\ a6713=120.60230909\ a7814=119.635466
76\ a8915=119.78566322\ a91016=120.94966691\dih1=113.95116833\dih2=12.94
825792\dih3=-0.89598342\dih4=171.46781207\dih5=-0.59037405\dih6=-0.246
62237\dih7=-0.13201134\dih8=140.82698663\dih9=-100.33386733\dih10=179.
43236348\dih11=180.14483059\dih12=180.18081248\dih13=180.45114448\ a411
7=103.37340575\dih14=194.53321475\r1718=1.38255579\r1819=1.38561699\r1
920=1.38340347\r2021=1.38681896\r2122=1.38167481\ a11718=118.34797397\ a
171819=119.1435209\ a181920=120.25337414\ a192021=120.07024309\ a202122=1
20.11910312\dih15=223.93281564\dih16=172.31593719\dih17=-0.71100927\di
h18=-0.08347702\dih19=-0.04718652\r1823=1.07530306\r1924=1.07656552\r2
025=1.07637663\r2126=1.07652333\r2227=1.07629464\ a171823=119.09268821\
a181924=119.66462486\ a192025=120.01589044\ a202126=120.0702695\ a212227=
120.66286293\dih20=-8.51897311\dih21=179.18343503\dih22=180.12675131\di
h23=180.09034828\dih24=179.76406191\r117=1.8355785\r13=1.6920425\r12=
2.12283779\\Version=AM64L-G03RevE.01\State=2-A\HF=-1069.6725844\RMSD=8

.251e-09\RMSF=1.579e-05\Thermal=0.\Dipole=0.9706172,0.9245,-0.088756\PG=C01 [X(C14H14N1O1S1)]\@

ROBHandHLYP/6-311++G**

1\1\GINC-GOMBERG03\FTS\ROBHandHLYP\6-311++G(d,p)\C14H14N1O1S1(2)\CARLH
S\16-Jun-2010\1\#\robhandhlyp/6-311++G** opt=(grad,ts,readfc,noeigente
st,nofreeze) geom=checkpoint guess=read optcyc=400 scfcyc=300\Louis'
cyclized product NME (cyclic sultam) hypervalent intermediate - TS TS1
\0,2\S\C,1,r12\N,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,
2,dih2,0\C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a67
8,2,dih5,0\C,8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,
6,a6511,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,
8,r814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91
016,8,dih13,0\C,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0
\C,18,r1819,17,a171819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20
r2021,19,a192021,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r18
23,17,a171823,1,dih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19
a192025,18,dih22,0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a21
2227,20,dih24,0\C,3,r328,5,a5328,6,dih25,0\H,28,r2829,3,a32829,5,dih26
0\H,28,r2830,3,a32830,5,dih27,0\H,28,r2831,3,a32831,5,dih28,0\r2829=
1.08493542\r2830=1.08874363\r2831=1.08055302\ a32829=108.06271696\ a3283
0=111.77277342\ a32831=110.75401609\ di26=-54.17068123\ di27=65.7232281
5\ di28=-172.5122129\r328=1.45726437\ a5328=111.82475216\ di25=199.6952
2371\r14=1.47713801\r35=1.46324108\r26=1.36592354\r67=1.38891054\r78=1
.38460885\r89=1.38981922\r910=1.38706515\r511=1.0870406\r512=1.0919741
9\r713=1.07840146\r814=1.07639669\r915=1.07710601\r1016=1.07731197\ a21
3=86.60707848\ a214=102.31873542\ a135=117.48180404\ a126=105.79872996\ a2
67=118.6912677\ a678=119.17949637\ a789=120.75078331\ a8910=120.25610799\
a6511=111.47341158\ a6512=109.48218696\ a6713=120.63221742\ a7814=119.624
37234\ a8915=119.79205144\ a91016=120.95585227\ di1=114.02480289\ di2=13
.68664109\ di3=-2.14594118\ di4=172.56017375\ di5=-0.27975016\ di6=-0.
35849381\ di7=-0.03246861\ di8=139.77180083\ di9=-101.45674465\ di10=1
79.63555922\ di11=180.09599252\ di12=180.15061321\ di13=180.40474858\ a
4117=103.44739208\ di14=194.67653683\r1718=1.38297611\r1819=1.38635326
\r1920=1.38386165\r2021=1.38742064\r2122=1.38233766\ a11718=118.2865004
\ a171819=119.17102948\ a181920=120.2604448\ a192021=120.03987535\ a202122
=120.13479588\ di15=224.70703568\ di16=172.26622731\ di17=-0.70876154\
di18=-0.20973978\ di19=0.05513551\r1823=1.07544162\r1924=1.07661111\r
2025=1.0764289\r2126=1.07657604\r2227=1.07641453\ a171823=119.2104567\ a
181924=119.65185715\ a192025=120.03703731\ a202126=120.07342294\ a212227=
120.570436\ di20=-8.51352673\ di21=179.17657727\ di22=180.09199128\ di
23=180.21711659\ di24=179.94850016\r117=1.83558611\r13=1.69129502\r12=
2.13125555\ \Version=AM64L-G03RevE.01\State=2-A\HF=-1069.6830762\RMSD=6
.718e-09\RMSF=2.839e-05\Thermal=0.\Dipole=0.994367,0.9285389,-0.108395
7\PG=C01 [X(C14H14N1O1S1)]\@

Transition state 13 (Y = NMe)

ROHF/6-31G*

```
1\1\GINC-GOMBERG05\FTS\ROHF\6-31G(d)\C14H14N1O1S1(2)\CARLHS\15-Jun-201
0\1\#rohlf/6-31G* opt=(grad,ts,readfc,noeigentest,nofreeze) geom=check
point guess=read optcyc=400 scfcyc=300\Louis' cyclized product NMe (c
yclic sultam) hypervalent intermediate - TS TS2\0,2\S\C,1,r12\N,1,r13
,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126
,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a7
89,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r5
12,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih1
1,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,r117,
4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a171819,
1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,18,d
ih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,dih20,0
\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,0\H,2
1,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\C,3,r32
8,5,a5328,6,dih25,0\H,28,r2829,3,a32829,5,dih26,0\H,28,r2830,3,a32830,
5,dih27,0\H,28,r2831,3,a32831,5,dih28,0\H,28,r2829=1.08348612\r2830=1.0864
0422\r2831=1.0767623\ a32829=107.75378273\ a32830=111.77949661\ a32831=11
0.89924588\ di26=-54.32503469\ di27=65.39715659\ di28=-172.61439618\ r3
28=1.45853697\ a5328=112.70962533\ di25=202.20571523\ r14=1.46628719\ r35
=1.463061\ r26=1.37266281\ r67=1.38707623\ r78=1.38407692\ r89=1.39220669\
r910=1.3829796\ r511=1.0846631\ r512=1.08890798\ r713=1.07616211\ r814=1.0
7523094\ r915=1.07503282\ r1016=1.07531958\ a213=89.43920119\ a214=105.105
71159\ a135=115.26846863\ a126=112.77695078\ a267=119.82497208\ a678=118.8
2232427\ a789=120.84091772\ a8910=120.25841281\ a6511=112.33296615\ a6512=
110.25016509\ a6713=120.82960994\ a7814=119.63256665\ a8915=119.7687219\ a
91016=120.90990866\ di1=114.44433876\ di2=15.21267125\ di3=-6.27010692
\ di4=177.8152649\ di5=-0.00676413\ di6=-0.04484246\ di7=-0.21573425\ d
ih8=133.18017396\ di9=-106.61991583\ di10=179.78198293\ di11=180.09231
798\ di12=179.97301912\ di13=180.14880508\ a4117=99.11265595\ di14=195.
39455613\ r1718=1.38108726\ r1819=1.38961386\ r1920=1.38575622\ r2021=1.38
799026\ r2122=1.3862962\ a11718=118.62419352\ a171819=118.80261699\ a18192
0=120.30325973\ a192021=120.08103799\ a202122=120.00731035\ di15=227.855
40551\ di16=169.51954477\ di17=-0.73484091\ di18=-0.25934185\ di19=0.0
127294\ r1823=1.07356733\ r1924=1.07608105\ r2025=1.07556899\ r2126=1.0760
5425\ r2227=1.07608354\ a171823=120.06424365\ a181924=119.75260838\ a19202
5=119.99394249\ a202126=120.02630729\ a212227=120.43259158\ di20=-11.126
46531\ di21=179.21140524\ di22=180.07243143\ di23=180.292914\ di24=180
.38575305\ r13=1.6908395\ r12=1.82320477\ r117=2.07189461\ \Version=AM64L-
G03RevE.01\State=2-A\HF=-1064.9445528\ RMSD=1.552e-09\ RMSF=3.264e-07\Th
ermal=0.\Dipole=0.9506372,0.6700635,0.8355838\PG=C01 [X(C14H14N1O1S1)]
\@
```

ROHF/6-311G**

```
1\1\GINC-GOMBERG07\FTS\ROHF\6-311G(d,p)\C14H14N1O1S1(2)\CARLHS\15-Jun-
2010\1\#rohlf/6-311G** opt=(grad,ts,readfc,noeigentest,nofreeze) geom=
checkpoint guess=read optcyc=400 scfcyc=300\Louis' cyclized product N
Me (cyclic sultam) hypervalent intermediate - TS TS2\0,2\S\C,1,r12\N,
1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1
,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89
,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H
,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6
,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,1,
r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,18,r1819,17,a17
1819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r2021,19,a192021,
18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,17,a171823,1,d
ih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a192025,18,dih22,
0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227,20,dih24,0\C,
3,r328,5,a5328,6,dih25,0\H,28,r2829,3,a32829,5,dih26,0\H,28,r2830,3,a3
2830,5,dih27,0\H,28,r2831,3,a32831,5,dih28,0\H,28,r2829=1.08387186\r2830=1
.08722745\r2831=1.0774043\ a32829=107.79822675\ a32830=111.6728961\ a3283
```

1=110.95678741\ dih26=-52.52056724\ dih27=67.27706591\ dih28=-170.8059351
3\r328=1.45976513\ a5328=112.62905912\ dih25=202.67521525\ r14=1.46131902
\ r35=1.46340972\ r26=1.37026409\ r67=1.3868878\ r78=1.38278089\ r89=1.3919
9198\ r910=1.38166397\ r511=1.084856\ r512=1.08954097\ r713=1.07618051\ r81
4=1.07533675\ r915=1.07508301\ r1016=1.07541082\ a213=89.52353626\ a214=10
4.76402809\ a135=115.15793807\ a126=112.53837679\ a267=119.74299552\ a678=
118.8176025\ a789=120.85981456\ a8910=120.25912323\ a6511=112.13234727\ a6
512=110.05654698\ a6713=120.83258745\ a7814=119.63561218\ a8915=119.76835
892\ a91016=120.96135889\ dih1=114.18591315\ dih2=15.51145505\ dih3=-6.440
64692\ dih4=177.69019875\ dih5=-0.07497569\ dih6=-0.06453167\ dih7=-0.2395
4155\ dih8=133.49959801\ dih9=-106.24033808\ dih10=179.75477823\ dih11=180
.05723322\ dih12=180.00967958\ dih13=180.12864953\ a4117=98.82740841\ dih1
4=195.21280552\ r1718=1.37998177\ r1819=1.3890521\ r1920=1.38488274\ r2021
=1.38725803\ r2122=1.38542214\ a11718=118.84796852\ a171819=118.72198731\
a181920=120.32706215\ a192021=120.08392239\ a202122=120.00321217\ dih15=2
25.31275126\ dih16=169.85973372\ dih17=-0.65264095\ dih18=-0.25914793\ dih
19=-0.03925025\ r1823=1.07379335\ r1924=1.07614125\ r2025=1.07557773\ r212
6=1.07607405\ r2227=1.07635919\ a171823=119.97318484\ a181924=119.7218373
4\ a192025=119.98844546\ a202126=120.03289357\ a212227=120.4013405\ dih20=
-10.66507479\ dih21=179.3200768\ dih22=180.04047721\ dih23=180.31171041\ d
ih24=180.38902767\ r13=1.68627071\ r12=1.82784453\ r117=2.06546964\ \Versi
on=AM64L-G03RevE.01\ State=2-A\ HF=-1065.1099125\ RMSD=8.196e-09\ RMSF=3.0
32e-06\ Thermal=0.\ Dipole=1.0023866,0.7026126,0.807983\ PG=C01 [X(C14H14
N1O1S1)]\ \e

ROBHandHLYP/6-311G**

1\1\GINC-GOMBERG02\FTS\ROBHandHLYP\6-311G(d,p)\C14H14N1O1S1(2)\CARLHS\
16-Jun-2010\1\#\robhandhlyp/6-311G** opt=(grad,ts,readfc,noeigentest,n
ofreeze) geom=checkpoint guess=read optcyc=400 scfcyc=300\Louis' cycl
ized product NMe (cyclic sultam) hypervalent intermediate - TS TS2\0,
2\S\C,1,r12\N,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,di
h2,0\C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,
dih5,0\C,8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6
511,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,
r814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,
8,dih13,0\C,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0\C,1
8,r1819,17,a171819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20,r20
21,19,a192021,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r1823,1
7,a171823,1,dih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19,a19
2025,18,dih22,0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a212227
20,dih24,0\C,3,r328,5,a5328,6,dih25,0\H,28,r2829,3,a32829,5,dih26,0\H
28,r2830,3,a32830,5,dih27,0\H,28,r2831,3,a32831,5,dih28,0\ r2829=1.08
49051\ r2830=1.08928693\ r2831=1.07958661\ a32829=108.05514565\ a32830=111
.88515492\ a32831=110.59277844\ dih26=-54.89866625\ dih27=65.09460152\ dih
28=-173.2279678\ r328=1.45443748\ a5328=112.86994462\ dih25=201.15033742\
r14=1.47579932\ r35=1.46000412\ r26=1.37390055\ r67=1.38404556\ r78=1.3839
883\ r89=1.38904297\ r910=1.38283574\ r511=1.0867277\ r512=1.09248082\ r713
=1.07730187\ r814=1.07630455\ r915=1.07615679\ r1016=1.07662878\ a213=88.8
4975745\ a214=105.47814858\ a135=114.58787438\ a126=112.64345253\ a267=119
.4796186\ a678=118.94308429\ a789=120.86397775\ a8910=120.29827668\ a6511=
112.11155912\ a6512=110.14468522\ a6713=120.72381985\ a7814=119.5984449\ a
8915=119.80039958\ a91016=121.03227619\ dih1=114.33330234\ dih2=18.465627
26\ dih3=-8.81770222\ dih4=178.74789812\ dih5=-0.08689119\ dih6=-0.0761714
\ dih7=-0.19821524\ dih8=134.47314937\ dih9=-105.49992478\ dih10=179.77313
89\ dih11=180.10914928\ dih12=180.06962579\ dih13=180.09288414\ a4117=98.4
5224959\ dih14=193.97833437\ r1718=1.37551745\ r1819=1.38872817\ r1920=1.3
85083\ r2021=1.38613432\ r2122=1.38680977\ a11718=117.04534373\ a171819=11
8.20550916\ a181920=120.24434276\ a192021=120.26093185\ a202122=120.00967
019\ dih15=224.54122954\ dih16=168.60157569\ dih17=-0.72723667\ dih18=-0.2
1682974\ dih19=-0.08447207\ r1823=1.07634577\ r1924=1.07736419\ r2025=1.07
655021\ r2126=1.07732226\ r2227=1.07780697\ a171823=120.0894222\ a181924=1
19.77516663\ a192025=119.89320689\ a202126=120.03568737\ a212227=120.7140
693\ dih20=-11.98716064\ dih21=179.23583685\ dih22=180.11609369\ dih23=180
.24747025\ dih24=180.33843053\ r13=1.70636652\ r12=1.82665743\ r117=2.2.1608
0615\ \Version=AM64L-G03RevE.01\ State=2-A\ HF=-1069.671585\ RMSD=4.582e-0

9\RMSF=1.254e-05\Thermal=0.\Dipole=0.9447776,0.6042294,0.8697799\PG=C0
1 [X(C14H14N1O1S1)]\@

ROBHandHLYP/6-311++G**

1\1\GINC-GOMBERG04\FTS\ROBHandHLYP\6-311++G(d,p)\C14H14N1O1S1(2)\CARLH
S\16-Jun-2010\1\#\robhandhlyp\6-311++G** opt=(grad,ts,readfc,noeigente
st,nofreeze) geom=checkpoint guess=read optcyc=400 scfcyc=300\Louis'
cyclized product NME (cyclic sultam) hypervalent intermediate - TS TS2
\0,2\S\C,1,r12\N,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,
2,dih2,0\C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a67
8,2,dih5,0\C,8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,
6,a6511,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,
8,r814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91
016,8,dih13,0\C,1,r117,4,a4117,2,dih14,0\C,17,r1718,1,a11718,2,dih15,0
\C,18,r1819,17,a171819,1,dih16,0\C,19,r1920,18,a181920,17,dih17,0\C,20
r2021,19,a192021,18,dih18,0\C,21,r2122,20,a202122,19,dih19,0\H,18,r18
23,17,a171823,1,dih20,0\H,19,r1924,18,a181924,17,dih21,0\H,20,r2025,19
a192025,18,dih22,0\H,21,r2126,20,a202126,19,dih23,0\H,22,r2227,21,a21
2227,20,dih24,0\C,3,r328,5,a5328,6,dih25,0\H,28,r2829,3,a32829,5,dih26
0\H,28,r2830,3,a32830,5,dih27,0\H,28,r2831,3,a32831,5,dih28,0\r2829=
1.08513183\r2830=1.08938827\r2831=1.07949837\ a32829=107.93441471\ a3283
0=111.85884915\ a32831=110.71883913\ di h26=-55.59333377\ di h27=64.2540443
2\ di h28=-173.95596882\r328=1.45438782\ a5328=112.89979349\ di h25=199.485
80341\r14=1.47796422\r35=1.4596743\r26=1.37387671\r67=1.38454609\r78=1
.38465688\r89=1.38967762\r910=1.38353577\r511=1.08683102\r512=1.092488
95\r713=1.07738442\r814=1.07636078\r915=1.07622961\r1016=1.0767036\ a21
3=88.78930225\ a214=105.34092847\ a135=114.61932174\ a126=112.59919317\ a2
67=119.45718882\ a678=118.93044472\ a789=120.86641409\ a8910=120.29879029
\ a6511=112.10799536\ a6512=110.2493331\ a6713=120.74808337\ a7814=119.593
16049\ a8915=119.80375384\ a91016=121.03186215\ di h1=114.566379\ di h2=18.8
7345859\ di h3=-9.35407114\ di h4=179.18507119\ di h5=0.01143718\ di h6=-0.099
44234\ di h7=-0.14341321\ di h8=134.16695333\ di h9=-105.73734684\ di h10=179.
81940994\ di h11=180.10429054\ di h12=180.02987558\ di h13=180.02504459\ a411
7=98.27269871\ di h14=194.14610776\r1718=1.37607654\r1819=1.38953851\r19
20=1.38556315\r2021=1.38674211\r2122=1.38751785\ a11718=117.04865001\ a1
71819=118.24816336\ a181920=120.25784839\ a192021=120.22316679\ a202122=1
20.01666035\ di h15=224.61433342\ di h16=168.87852436\ di h17=-0.74137107\ di
h18=-0.30972744\ di h19=0.00345565\r1823=1.07638948\r1924=1.07737503\r20
25=1.07657012\r2126=1.07732573\r2227=1.07789218\ a171823=120.19042211\ a
181924=119.7501871\ a192025=119.91591174\ a202126=120.05063687\ a212227=1
20.5901899\ di h20=-11.70570894\ di h21=179.2232865\ di h22=180.1045297\ di h2
3=180.36101032\ di h24=180.53724264\r13=1.70508422\r12=1.8275581\r117=2.
15665819\ \Version=AM64L-G03RevE.01\State=2-A\HF=-1069.6824669\RMSD=3.9
72e-09\RMSF=1.685e-05\Thermal=0.\Dipole=0.9744132,0.6146028,0.8363016\
PG=C01 [X(C14H14N1O1S1)]\@

Sulfinamide 4 (Y = NMe)

ROHF/6-31G*

```
1\1\GINC-GOMBERG02\FOpt\RHF\6-31G(d)\C8H9N1O1S1\CARLHS\14-Jun-2010\1\
#RHF/6-31G* opt=grad\Louis' cyclized product NMe (cyclic sultam)\0,1
\S\C,1,r12\N,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih
2,0\C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,d
ih5,0\C,8,r89,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a65
11,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r
814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8
,dih13,0\C,3,r317,1,a1317,2,dih14,0\H,17,r1718,3,a31718,1,dih15,0\H,17
,r1719,3,a31719,1,dih16,0\H,17,r1720,3,a31720,1,dih17,0\|r1718=1.08341
749\r1719=1.0828688\r1720=1.08655574\|a31718=108.63320449\|a31719=109.51
661139\|a31720=112.65767681\|dih15=167.68927993\|dih16=49.90384282\|dih17=
-71.28482239\r12=1.78231736\r13=1.68938562\r14=1.4708165\r35=1.4581898
5\r26=1.38184337\r67=1.38356167\r78=1.38683696\r89=1.38881307\r910=1.3
8552032\r511=1.08439084\r512=1.08936298\r713=1.07572012\r814=1.0752223
5\r915=1.07472736\r1016=1.07502476\r317=1.45150584\|a213=88.49045856\|a2
14=107.53736847\|a135=113.26845782\|a126=111.98468975\|a267=119.5704908\|a
678=118.94759789\|a789=120.98919336\|a8910=120.15956148\|a6511=112.267252
67\|a6512=110.84146611\|a6713=120.79527059\|a7814=119.51116098\|a8915=119.
89899056\|a91016=120.74424718\|a1317=115.10527172\|dih1=112.21660739\|dih2
=29.67326683\|dih3=-18.59076028\|dih4=183.52729065\|dih5=0.11664926\|dih6=
0.09631996\|dih7=0.10218095\|dih8=134.40119628\|dih9=-104.5360136\|dih10=1
80.29737555\|dih11=180.25431847\|dih12=180.04351496\|dih13=179.53168247\|d
ih14=167.05615117\|Version=AM64L-G03RevE.01\|State=1-A\HF=-834.9361285\
RMSD=5.848e-09\RMSF=5.056e-05\Thermal=0.\Dipole=1.0229922,0.6054162,1.
1244357\PG=C01 [X(C8H9N1O1S1)]\|@
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ROHF/6-311G**

```
1\1\GINC-GOMBERG02\FOpt\RHF\6-311G(d,p)\C8H9N1O1S1\CARLHS\14-Jun-2010\
1\#RHF/6-311G** opt=(grad,readfc) geom=checkpoint guess=read\Louis'
cyclized product NMe (cyclic sultam)\0,1\S\C,1,r12\N,1,r13,2,a213\O,1
,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,3,dih3,0\C
,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a789,6,dih6,0
\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r512,6,a6512,
2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11,0\H,9,r91
5,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,3,r317,1,a1317,2,d
ih14,0\H,17,r1718,3,a31718,1,dih15,0\H,17,r1719,3,a31719,1,dih16,0\H,1
7,r1720,3,a31720,1,dih17,0\|r1718=1.08402551\r1719=1.08351999\r1720=1.
0875006\|a31718=108.76396022\|a31719=109.49678283\|a31720=112.54331434\|d
ih15=166.64475421\|dih16=48.81449456\|dih17=-72.18404604\r12=1.78276199\r
13=1.68562038\r14=1.46681118\r35=1.45827676\r26=1.37996527\r67=1.38289
305\r78=1.3860037\r89=1.38822658\r910=1.38462091\r511=1.08455892\r512=
1.09004905\r713=1.07572034\r814=1.07534247\r915=1.07474535\r1016=1.075
08802\r317=1.45255441\|a213=88.56663471\|a214=107.01381479\|a135=113.0149
7766\|a126=111.77405877\|a267=119.48720474\|a678=118.95265475\|a789=121.01
027302\|a8910=120.14604191\|a6511=112.13158874\|a6512=110.56611282\|a6713=
120.79519247\|a7814=119.50218676\|a8915=119.91010746\|a91016=120.80187196
\|a1317=114.93134977\|dih1=111.71166606\|dih2=30.1533313\|dih3=-19.1931213
\|dih4=183.91750194\|dih5=0.27818586\|dih6=-0.00434609\|dih7=0.14890782\|d
ih8=134.4990712\|dih9=-104.35926179\|dih10=180.33950679\|dih11=180.1803778
6\|dih12=180.06544502\|dih13=179.48644274\|dih14=166.93232142\|Version=AM
64L-G03RevE.01\|State=1-A\HF=-835.0525358\RMSD=5.690e-09\RMSF=1.324e-04
\Thermal=0.\Dipole=1.067896,0.6510544,1.1271696\PG=C01 [X(C8H9N1O1S1)]
\|@
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ROBHandHLYP/6-311G**

```
1\1\GINC-GOMBERG02\FOpt\RBHandHLYP\6-311G(d,p)\C8H9N1O1S1\CARLHS\14-Ju
n-2010\1\#bhandhlyp/6-311G** opt=(grad,readfc) geom=checkpoint guess=
read\Louis' cyclized product NMe (cyclic sultam)\0,1\S\C,1,r12\N,1,r
13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a1
26,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,
```

a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,
r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,di
h11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,3,r31
7,1,a1317,2,dih14,0\H,17,r1718,3,a31718,1,dih15,0\H,17,r1719,3,a31719,
1,dih16,0\H,17,r1720,3,a31720,1,dih17,0\|r1718=1.0848992\r1719=1.08443
27\r1720=1.08944256\|a31718=108.84027094\|a31719=109.44251326\|a31720=112
.71451647\|dih15=168.19731293\|dih16=50.41692898\|dih17=-70.62391291\r12=
1.7914233\r13=1.70408787\r14=1.48012463\r35=1.45652306\r26=1.38145823\
r67=1.38153832\r78=1.38558402\r89=1.38679807\r910=1.38433314\r511=1.08
643121\r512=1.09250573\r713=1.07693867\r814=1.0763416\r915=1.07592164\
r1016=1.07631301\r317=1.44913742\|a213=87.70299751\|a214=106.68970571\|a1
35=112.74036579\|a126=111.90423902\|a267=119.37205174\|a678=119.06133344\
a789=120.9392832\|a8910=120.22166339\|a6511=112.21090943\|a6512=110.53874
889\|a6713=120.68674838\|a7814=119.52970334\|a8915=119.88874356\|a91016=12
0.85257548\|a1317=114.29920905\|dih1=111.9882702\|dih2=31.14366269\|dih3=-
20.27965227\|dih4=184.89118987\|dih5=0.23440384\|dih6=0.11792004\|dih7=0.1
1824968\|dih8=134.71969118\|dih9=-104.41907999\|dih10=180.39411145\|dih11=
180.25548492\|dih12=180.03246531\|dih13=179.47439016\|dih14=166.62647175\
\Version=AM64L-G03RevE.01\State=1-A\HF=-838.2148654\|RMSD=5.415e-09\|RMS
F=2.234e-05\|Thermal=0.\|Dipole=1.0125919,0.5707849,1.0551538\|PG=C01 [X(
C8H9N1O1S1)]\|@

ROBHandHLYP/6-311++G**

1\1\GINC-GOMBERG02\FOpt\RBHandHLYP\6-311++G(d,p)\C8H9N1O1S1\CARLHS\14-
Jun-2010\1\#bhandhlyp/6-311++G** opt=(grad,readfc) geom=checkpoint gu
ess=read\|Louis' cyclized product NMe (cyclic sultam)\|0,1\S\C,1,r12\N
,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,
1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r8
9,7,a789,6,dih6,0\C,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\
H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,
6,dih11,0\H,9,r915,8,a8915,7,dih12,0\H,10,r1016,9,a91016,8,dih13,0\C,3
,r317,1,a1317,2,dih14,0\H,17,r1718,3,a31718,1,dih15,0\H,17,r1719,3,a31
719,1,dih16,0\H,17,r1720,3,a31720,1,dih17,0\|r1718=1.08498689\r1719=1.
08430972\r1720=1.08937095\|a31718=108.73388565\|a31719=109.60527764\|a317
20=112.6182301\|dih15=166.8398795\|dih16=48.93161521\|dih17=-72.15884419\
r12=1.79097278\r13=1.70183372\r14=1.48361124\r35=1.45636432\r26=1.3813
4631\r67=1.38226231\r78=1.38595867\r89=1.38757812\r910=1.38467855\r511
=1.08657795\r512=1.09248841\r713=1.07699754\r814=1.07638917\r915=1.075
98676\r1016=1.07632099\r317=1.44897608\|a213=87.90936003\|a214=106.66573
092\|a135=113.15903371\|a126=111.93268351\|a267=119.32836904\|a678=119.060
49874\|a789=120.94068997\|a8910=120.23269383\|a6511=112.15598368\|a6512=11
0.69932753\|a6713=120.68922921\|a7814=119.52711631\|a8915=119.8948008\|a91
016=120.86534612\|a1317=114.91749504\|dih1=112.337936\|dih2=29.88614222\|d
ih3=-19.4522704\|dih4=184.78289358\|dih5=0.2077495\|dih6=0.18587037\|dih7=
0.02251155\|dih8=133.81061672\|dih9=-105.28656126\|dih10=180.3467858\|dih1
1=180.21620052\|dih12=180.01172045\|dih13=179.39809971\|dih14=166.8644099
3\|Version=AM64L-G03RevE.01\State=1-A\HF=-838.2250841\|RMSD=3.753e-09\|R
MSF=6.343e-05\|Thermal=0.\|Dipole=1.065483,0.5997312,1.0722611\|PG=C01 [X(
C8H9N1O1S1)]\|@

Radical 15 (Y = NMe)

ROHF/6-31G*

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1\1\GINC-GOMBERG02\FOpt\ROHF\6-31G(d)\C14H14N1O1S1(2)\CARLHS\14-Jun-20
10\1\#rohlf/6-31G* opt=grad scfcyc=300\Louis' biaryl intermediate tra
nsition state NMe\0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234,1,dih1,
0\N,4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,dih
4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910,7
,dih7,0\C,10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,r1
213,2,a21213,3,dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,13,a
131415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih14,
0\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,11,r1120,
10,a101120,9,dih17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,12,a1213
22,2,dih19,0\H,14,r1423,13,a131423,12,dih20,0\H,15,r1524,14,a141524,13
,dih21,0\H,6,r625,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0\O,4,r42
7,3,a3427,2,dih24,0\C,5,r528,4,a4528,27,dih25,0\H,28,r2829,5,a52829,4,
dih26,0\H,28,r2830,5,a52830,4,dih27,0\H,28,r2831,5,a52831,4,dih28,0\
r2829=1.08333087\r2830=1.08281395\r2831=1.08706262\ a52829=108.5157585\ a
52830=109.2672491\ a52831=113.53324864\ dih26=197.49648034\ dih27=-44.855
93663\ dih28=76.91285084\ r528=1.4512749\ a4528=115.6749284\ dih25=167.222
85114\ r12=1.54640767\ r23=1.51661617\ r34=1.78012354\ r45=1.67059881\ r56=
1.45892825\ r17=1.40429082\ r78=1.3865806\ r89=1.38640746\ r910=1.37812582
\ r1011=1.38813571\ r212=1.51080231\ r1213=1.33370898\ r1314=1.43629078\ r1
415=1.43319184\ r216=1.08704097\ r817=1.07624452\ r918=1.07528028\ r1019=1
.0754625\ r1120=1.07238624\ r1221=1.07605131\ r1322=1.07584444\ r1423=1.07
240084\ r1524=1.0767985\ r625=1.08101568\ r626=1.08351405\ r427=1.47566781
\ a123=112.20647869\ a234=119.04193403\ a345=103.45424203\ a456=117.161087
48\ a217=120.95741249\ a178=119.326099\ a789=121.74049696\ a8910=119.01800
013\ a91011=119.86465465\ a3212=110.33047184\ a21213=123.25312039\ a121314
=121.06980421\ a131415=118.18605997\ a3216=107.15977374\ a7817=119.012728
61\ a8918=120.2123417\ a91019=120.52633895\ a101120=118.54147735\ a21221=1
16.52849464\ a121322=120.186872\ a131423=120.90206184\ a141524=118.785209
98\ a7625=111.97138999\ a7626=109.0745965\ a3427=104.13845603\ dih1=80.876
99647\ dih2=-59.34348511\ dih3=61.66075444\ dih4=-66.58526867\ dih5=182.11
509298\ dih6=-0.39680209\ dih7=-0.71052101\ dih8=0.83070632\ dih9=206.3647
9616\ dih10=-16.69587828\ dih11=4.1204113\ dih12=9.8511832\ dih13=-36.5806
0203\ dih14=179.7221795\ dih15=179.82127579\ dih16=180.7345792\ dih17=180.
16970772\ dih18=165.76112074\ dih19=182.52340899\ dih20=182.47938825\ dih2
1=166.3807726\ dih22=-55.50466177\ dih23=-173.46820024\ dih24=50.81998055
\ Version=AM64L-G03RevE.01\ State=2-A\ HF=-1064.9951921\ RMSD=8.173e-09\ R
MSF=2.231e-05\ Thermal=0.\ Dipole=0.1783709,-1.5358603,-1.1403557\ PG=C01
[X(C14H14N1O1S1)]\ \e
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ROHF/6-311G**

```
1\1\GINC-GOMBERG02\FOpt\ROHF\6-311G(d,p)\C14H14N1O1S1(2)\CARLHS\14-Jun
-2010\1\#rohlf/6-311G** opt=(grad,readfc) geom=checkpoint guess=read s
cfcyc=300\Louis' biaryl intermediate NMe\0,2\C\C,1,r12\C,2,r23,1,a12
3\S,3,r34,2,a234,1,dih1,0\N,4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,dih
3,0\C,1,r17,2,a217,3,dih4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,d
ih6,0\C,9,r910,8,a8910,7,dih7,0\C,10,r1011,9,a91011,8,dih8,0\C,2,r212,
3,a3212,4,dih9,0\C,12,r1213,2,a21213,3,dih10,0\C,13,r1314,12,a121314,2
,dih11,0\C,14,r1415,13,a131415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H
,8,r817,7,a7817,1,dih14,0\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a910
19,8,dih16,0\H,11,r1120,10,a101120,9,dih17,0\H,12,r1221,2,a21221,3,dih
18,0\H,13,r1322,12,a121322,2,dih19,0\H,14,r1423,13,a131423,12,dih20,0\
H,15,r1524,14,a141524,13,dih21,0\H,6,r625,7,a7625,1,dih22,0\H,6,r626,7
,a7626,1,dih23,0\O,4,r427,3,a3427,2,dih24,0\C,5,r528,4,a4528,27,dih25,
0\H,28,r2829,5,a52829,4,dih26,0\H,28,r2830,5,a52830,4,dih27,0\H,28,r28
31,5,a52831,4,dih28,0\
r2829=1.08390123\r2830=1.08338767\r2831=1.08810
115\ a52829=108.59964699\ a52830=109.26943705\ a52831=113.45457675\ dih26=
197.63345049\ dih27=-44.71858711\ dih28=77.00605665\ r528=1.45212794\ a452
8=115.68336981\ dih25=167.24895404\ r12=1.54562149\ r23=1.5154204\ r34=1.7
8166814\ r45=1.66563281\ r56=1.45932101\ r17=1.40340064\ r78=1.38545139\ r8
```

9=1.38580289\r910=1.37699091\r1011=1.38747937\r212=1.50990716\r1213=1.33250452\r1314=1.4362043\r1415=1.43306936\r216=1.08688842\r817=1.0762833\r918=1.07528836\r1019=1.07546171\r1120=1.07238753\r1221=1.07632138\r1322=1.07594471\r1423=1.07241771\r1524=1.07693444\r625=1.0814805\r626=1.08346496\r427=1.47239391\|a123=112.11327562\|a234=118.8856565\|a345=103.61082211\|a456=117.15007372\|a217=120.93293155\|a178=119.31656244\|a789=121.74175576\|a8910=119.03074439\|a91011=119.84705232\|a3212=110.33751202\|a21213=123.24583532\|a121314=121.09154426\|a131415=118.19076865\|a3216=107.0996706\|a7817=119.00395902\|a8918=120.20709717\|a91019=120.54127848\|a101120=118.52272945\|a21221=116.59559322\|a121322=120.12792292\|a131423=120.91302299\|a141524=118.89121848\|a7625=111.8338649\|a7626=109.01109217\|a3427=103.81724216\|dih1=80.92086843\|dih2=-59.32282679\|dih3=61.58236513\|dih4=-66.83922913\|dih5=182.14856323\|dih6=-0.40014236\|dih7=-0.69089025\|dih8=0.83875858\|dih9=206.49876223\|dih10=-16.39353354\|dih11=3.90414799\|dih12=9.90976714\|dih13=-36.47836303\|dih14=179.7360282\|dih15=179.80566797\|dih16=180.69571935\|dih17=180.06215428\|dih18=165.92531123\|dih19=182.35870216\|dih20=182.56220327\|dih21=166.38337638\|dih22=-55.49197599\|dih23=-173.36718918\|dih24=50.67272547\|Version=AM64L-G03RevE.01\|State=2-A\|HF=-1065.1607656\|RMSD=6.541e-09\|RMSF=1.459e-05\|Thermal=0.\|Dipole=0.229843,-1.541948,-1.1981231\|PG=C01 [X(C14H14N1O1S1)]\|@

ROBHandHLYP/6-311G**

1\1\GINC-GOMBERG02\FOpt\ROBHandHLYP\6-311G(d,p)\C14H14N1O1S1(2)\CARLHS
15-Jun-2010\1\1\#robhandhlyp/6-311G** opt=(grad,readfc) geom=checkpoin
t guess=read scfcyc=300\\Louis' biaryl intermediate NMe\\0,2\C\C,1,r12
C,2,r23,1,a123\S,3,r34,2,a234,1,dih1,0\N,4,r45,3,a345,2,dih2,0\C,5,r5
6,4,a456,3,dih3,0\C,1,r17,2,a217,3,dih4,0\C,7,r78,1,a178,2,dih5,0\C,8,
r89,7,a789,1,dih6,0\C,9,r910,8,a8910,7,dih7,0\C,10,r1011,9,a91011,8,di
h8,0\C,2,r212,3,a3212,4,dih9,0\C,12,r1213,2,a21213,3,dih10,0\C,13,r131
4,12,a121314,2,dih11,0\C,14,r1415,13,a131415,12,dih12,0\H,2,r216,3,a32
16,4,dih13,0\H,8,r817,7,a7817,1,dih14,0\H,9,r918,8,a8918,7,dih15,0\H,1
0,r1019,9,a91019,8,dih16,0\H,11,r1120,10,a101120,9,dih17,0\H,12,r1221,
2,a21221,3,dih18,0\H,13,r1322,12,a121322,2,dih19,0\H,14,r1423,13,a1314
23,12,dih20,0\H,15,r1524,14,a141524,13,dih21,0\H,6,r625,7,a7625,1,dih2
2,0\H,6,r626,7,a7626,1,dih23,0\O,4,r427,3,a3427,2,dih24,0\C,5,r528,4,a
4528,27,dih25,0\H,28,r2829,5,a52829,4,dih26,0\H,28,r2830,5,a52830,4,di
h27,0\H,28,r2831,5,a52831,4,dih28,0\\r2829=1.08532279\r2830=1.08453772
r2831=1.08984722\|a52829=108.73181555\|a52830=109.15287882\|a52831=113.5
5694602\|dih26=198.65454284\|dih27=-43.74580906\|dih28=77.94153753\r528=1
.44794448\|a528=115.29256759\|dih25=170.1116073\r12=1.54215694\r23=1.50
290767\r34=1.78341555\r45=1.6848667\r56=1.45633523\r17=1.40043636\r78=
1.38620846\r89=1.3835237\r910=1.37830467\r1011=1.38495734\r212=1.49854
382\r1213=1.34556784\r1314=1.41488972\r1415=1.40852638\r216=1.09126634
r817=1.07769515\r918=1.07631413\r1019=1.07648669\r1120=1.07461847\r12
21=1.07712291\r1322=1.07713535\r1423=1.07457914\r1524=1.07852754\r625=
1.08501789\r626=1.08572826\r427=1.48494648\|a123=111.74365373\|a234=118.
64871704\|a345=103.39000853\|a456=116.1954911\|a217=121.10508439\|a178=119
.19166076\|a789=121.72681445\|a8910=119.09395949\|a91011=119.80767422\|a32
12=110.71928213\|a21213=122.69107345\|a121314=121.25017769\|a131415=119.0
0226551\|a3216=107.0958384\|a7817=118.78180015\|a8918=120.21940897\|a91019
=120.49466156\|a101120=118.96221483\|a21221=116.96181757\|a121322=119.757
53536\|a131423=120.45265847\|a141524=119.37628446\|a7625=112.03900939\|a76
26=109.08693409\|a3427=103.47000838\|dih1=81.77507034\|dih2=-60.41416515\
dih3=61.65503941\|dih4=-67.1280446\|dih5=181.73016362\|dih6=-0.32992392\
dih7=-0.72775802\|dih8=0.82463025\|dih9=207.13981617\|dih10=-15.88389577\
dih11=4.6185753\|dih12=7.95579856\|dih13=-34.96440447\|dih14=179.79120487\
dih15=179.80195748\|dih16=180.75982575\|dih17=180.10869785\|dih18=167.021
71289\|dih19=182.86858791\|dih20=181.71075975\|dih21=168.41202022\|dih22=-
54.34870943\|dih23=-172.40272344\|dih24=48.75132462\|Version=AM64L-G03Re
vE.01\|State=2-A\|HF=-1069.7129715\|RMSD=6.045e-09\|RMSF=3.902e-05\|Thermal
=0.\|Dipole=0.1680489,-1.4258734,-1.1358152\|PG=C01 [X(C14H14N1O1S1)]\|@

ROBHandHLYP/6-311++G**

1\1\GINC-GOMBERG05\FOpt\ROBHandHLYP\6-311++G(d,p)\C14H14N1O1S1(2)\CARL

```
HS\16-Jun-2010\1\#\robhandhlyp/6-311++G** opt=(grad,readfc) geom=check
point guess=read scfcyc=300\Louis' biaryl intermediate NMe\0,2\C\C,1
,r12\C,2,r23,1,a123\S,3,r34,2,a234,1,dih1,0\N,4,r45,3,a345,2,dih2,0\C,
5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,dih4,0\C,7,r78,1,a178,2,dih5,0\
C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910,7,dih7,0\C,10,r1011,9,a91011,
8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,r1213,2,a21213,3,dih10,0\C,13,
r1314,12,a121314,2,dih11,0\C,14,r1415,13,a131415,12,dih12,0\H,2,r216,3
,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih14,0\H,9,r918,8,a8918,7,dih15,0
\H,10,r1019,9,a91019,8,dih16,0\H,11,r1120,10,a101120,9,dih17,0\H,12,r1
221,2,a21221,3,dih18,0\H,13,r1322,12,a121322,2,dih19,0\H,14,r1423,13,a
131423,12,dih20,0\H,15,r1524,14,a141524,13,dih21,0\H,6,r625,7,a7625,1,
dih22,0\H,6,r626,7,a7626,1,dih23,0\O,4,r427,3,a3427,2,dih24,0\C,5,r528
,4,a4528,27,dih25,0\H,28,r2829,5,a52829,4,dih26,0\H,28,r2830,5,a52830,
4,dih27,0\H,28,r2831,5,a52831,4,dih28,0\r2829=1.08552799\r2830=1.0845
876\r2831=1.08967061\ a52829=108.66135523\ a52830=109.23497804\ a52831=11
3.47146908\ di h26=200.54430818\ di h27=-41.83695135\ di h28=79.84327912\r52
8=1.44878624\ a4528=115.54317394\ di h25=168.73444921\r12=1.54232831\r23=
1.50339038\r34=1.78550998\r45=1.68502887\r56=1.45656083\r17=1.400345\r
78=1.38670689\r89=1.38421509\r910=1.37904032\r1011=1.3855847\r212=1.49
871417\r1213=1.34616247\r1314=1.41507228\r1415=1.40903787\r216=1.09151
361\r817=1.07776094\r918=1.07635598\r1019=1.0765434\r1120=1.07475374\r
1221=1.07724409\r1322=1.07721497\r1423=1.07472741\r1524=1.07861769\r62
5=1.08514068\r626=1.08572985\r427=1.48672874\ a123=111.87980442\ a234=11
9.01688611\ a345=103.57272996\ a456=116.4754065\ a217=121.07883686\ a178=1
19.21205348\ a789=121.70718704\ a8910=119.09657828\ a91011=119.80003246\ a
3212=110.73080295\ a21213=122.72894857\ a121314=121.21615576\ a131415=119
.01901486\ a3216=107.30697504\ a7817=118.82916069\ a8918=120.21945909\ a91
019=120.49366571\ a101120=118.92683975\ a21221=116.96496674\ a121322=119.
76046009\ a131423=120.47894431\ a141524=119.3193833\ a7625=111.97253475\ a
7626=109.15106978\ a3427=103.6313534\ di h1=81.15387\ di h2=-59.2066207\ di h
3=60.82479499\ di h4=-67.28034546\ di h5=181.96512207\ di h6=-0.45784802\ di h
7=-0.70737972\ di h8=0.85919579\ di h9=206.66190784\ di h10=-15.74991287\ di h
11=4.36381514\ di h12=8.0719961\ di h13=-35.53819607\ di h14=179.66395442\ di
h15=179.80940456\ di h16=180.76436799\ di h17=180.00714349\ di h18=167.04794
074\ di h19=182.7845934\ di h20=181.81971524\ di h21=168.49132228\ di h22=-54.
2132695\ di h23=-172.19036272\ di h24=50.07710667\ \Version=AM64L-G03RevE.0
1\State=2-A\HF=-1069.7228512\RMSE=3.260e-09\RMSF=6.475e-05\Thermal=0.\
Dipole=0.1476788,-1.4094646,-1.1680156\PG=C01 [X(C14H14N1O1S1)]\@
```

Transition state 14 (Y = NMe)

ROHF/6-31G*

```
1\1\GINC-GOMBERG02\FTS\ROHF\6-31G(d)\C14H14N1O1S1(2)\CARLHS\15-Jun-201
0\1\#rohff/6-31G* opt=(grad,ts,readfc,nofreeze,noeigentest) geom=check
point guess=read optcyc=400 scfcyc=300\Biaryl TS with nitrogen (sulta
m)\0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234,1,dih1,0\N,4,r45,3,a34
5,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,dih4,0\C,7,r78,1,a
178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910,7,dih7,0\C,10,r1
011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,r1213,2,a21213,3,
dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,13,a131415,12,dih12
,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih14,0\H,9,r918,8,a8
918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,11,r1120,10,a101120,9,di
h17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,12,a121322,2,dih19,0\H,
14,r1423,13,a131423,12,dih20,0\H,15,r1524,14,a141524,13,dih21,0\H,6,r6
25,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0\O,4,r427,3,a3427,2,dih
24,0\C,5,r528,4,a4528,27,dih25,0\H,28,r2829,5,a52829,4,dih26,0\H,28,r2
830,5,a52830,4,dih27,0\H,28,r2831,5,a52831,4,dih28,0\r2829=1.08344689
\r2830=1.08306852\r2831=1.08712839\ a52829=108.56158582\ a52830=109.3607
1915\ a52831=113.40007428\ di26=199.24456173\ di27=-43.06895462\ di28=7
8.72062384\ r528=1.45022528\ a4528=115.94546066\ di25=169.319395\ r23=1.4
2414004\ r34=1.78358332\ r45=1.67325743\ r56=1.45703211\ r17=1.38729349\ r7
8=1.3916963\ r89=1.3868818\ r910=1.38190712\ r1011=1.39009574\ r212=1.4198
8817\ r1213=1.3754203\ r1314=1.39175055\ r1415=1.39135637\ r216=1.074779\ r
817=1.07683201\ r918=1.07527997\ r1019=1.07583344\ r1120=1.07324967\ r1221
=1.07481172\ r1322=1.07568863\ r1423=1.07441512\ r1524=1.07616626\ r625=1.
08052268\ r626=1.08408556\ r427=1.47485807\ a123=103.25065342\ a234=119.87
883754\ a345=103.50426378\ a456=118.05814177\ a217=119.40814697\ a178=116.
9649699\ a789=121.57286447\ a8910=119.82219669\ a91011=119.76908175\ a3212
=116.42726772\ a21213=120.59725323\ a121314=120.75453325\ a131415=119.525
76781\ a3216=117.11662229\ a7817=119.14436675\ a8918=119.85500136\ a91019=
120.36566527\ a101120=119.98396888\ a21221=119.00385175\ a121322=119.6594
4436\ a131423=120.2811706\ a141524=119.8848705\ a7625=111.35400247\ a7626=
108.68806989\ a3427=104.87309841\ di1=82.6403351\ di2=-73.27213404\ di3
=66.71744462\ di4=-61.70198834\ di5=182.15834893\ di6=-0.18229377\ di7
=-0.41605364\ di8=0.41075467\ di9=195.65512589\ di10=-12.96474099\ di1
1=4.85414819\ di12=3.71820929\ di13=-16.51406412\ di14=179.78654232\ di
h15=179.89755342\ di16=180.39753163\ di17=180.159296\ di18=169.4599477
\ di19=182.84401901\ di20=179.67978122\ di21=173.54219768\ di22=-58.17
908825\ di23=-175.53577555\ di24=37.10542064\ r12=2.04697457\ \Version=A
M64L-G03RevE.01\State=2-A\HF=-1064.9419366\RMSD=7.007e-09\RMSF=1.933e-
05\Thermal=0.\Dipole=0.1465169,-1.5522067,-1.1907461\PG=C01 [X(C14H14N
1O1S1)]\@
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ROHF/6-311G**

```
1\1\GINC-GOMBERG03\FTS\ROHF\6-311G(d,p)\C14H14N1O1S1(2)\CARLHS\15-Jun-
2010\1\#rohff/6-311G** opt=(grad,ts,readfc,nofreeze,noeigentest) geom=
checkpoint guess=read optcyc=400 scfcyc=300\Biaryl TS with nitrogen (
sultam)\0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234,1,dih1,0\N,4,r45,
3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,dih4,0\C,7,r7
8,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910,7,dih7,0\C,
10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,r1213,2,a212
13,3,dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,13,a131415,12,
dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih14,0\H,9,r918
,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,11,r1120,10,a101120
,9,dih17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,12,a121322,2,dih19
,0\H,14,r1423,13,a131423,12,dih20,0\H,15,r1524,14,a141524,13,dih21,0\H
,6,r625,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0\O,4,r427,3,a3427,
2,dih24,0\C,5,r528,4,a4528,27,dih25,0\H,28,r2829,5,a52829,4,dih26,0\H,
28,r2830,5,a52830,4,dih27,0\H,28,r2831,5,a52831,4,dih28,0\r2829=1.084
01864\r2830=1.08363148\r2831=1.08814191\ a52829=108.64385653\ a52830=109
.35898301\ a52831=113.32479029\ di26=199.50726203\ di27=-42.80467958\ di
h28=78.94237195\ r528=1.45105768\ a4528=115.99347133\ di25=169.09089067\
```

r23=1.42272408\r34=1.78447871\r45=1.66824053\r56=1.45736312\r17=1.3864
351\r78=1.39065792\r89=1.38620815\r910=1.38074444\r1011=1.38943219\r21
2=1.41892508\r1213=1.37434969\r1314=1.39110291\r1415=1.39103031\r216=1
.0745977\r817=1.07688378\r918=1.0752957\r1019=1.07584828\r1120=1.07323
886\r1221=1.07491272\r1322=1.07581527\r1423=1.07442591\r1524=1.0762128
2\r625=1.08104813\r626=1.08410944\r427=1.47147144\al23=103.02210523\al2
34=119.78489488\al345=103.67602428\al456=118.07139636\al217=119.39419378\
al78=116.9512623\al789=121.57477168\al8910=119.833294\al91011=119.7610994
5\al3212=116.3972792\al21213=120.58482245\al21314=120.77408109\al31415=1
19.51404923\al3216=117.10781157\al7817=119.12755694\al8918=119.84668682\al
91019=120.39028334\al101120=119.95594934\al21221=119.0250109\al21322=119
.65063633\al31423=120.29505175\al41524=119.92441345\al7625=111.22396743
\al7626=108.63570823\al3427=104.61170233\alh1=82.72553681\alh2=-73.34902
33\alh3=66.57925777\alh4=-61.96338119\alh5=182.17179904\alh6=-0.166047
26\alh7=-0.40519305\alh8=0.41599022\alh9=195.69765821\alh10=-12.912548
05\alh11=4.81765175\alh12=3.7760096\alh13=-16.35605816\alh14=179.80904
493\alh15=179.87918993\alh16=180.37952389\alh17=180.06180363\alh18=169
.44588903\alh19=182.75968993\alh20=179.66781833\alh21=173.50661819\alh
22=-58.18167252\alh23=-175.43530026\alh24=36.90931588\r12=2.0483323\\V
ersion=AM64L-G03RevE.01\State=2-A\HF=-1065.1074611\RMSD=8.614e-09\RMSF
=5.198e-05\Thermal=0.\Dipole=0.2025179,-1.5689908,-1.2684083\PG=C01 [X
(C14H14N1O1S1)]\@

ROBHandHLYP/6-311G**

1\1\GINC-GOMBERG02\FTS\ROBHandHLYP\6-311G(d,p)\C14H14N1O1S1(2)\CARLHS\
16-Jun-2010\1\#\robhandhlyp/6-311G** opt=(grad,ts,readfc,nofreeze,noei
gentest) geom=checkpoint guess=read optcyc=400 scfcyc=300\\Biaryl TS w
ith nitrogen (sultam)\0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234,1,d
ih1,0\N,4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3
,dih4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a89
10,7,dih7,0\C,10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,1
2,r1213,2,a21213,3,dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,
13,a131415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,di
h14,0\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,11,r1
120,10,a101120,9,dih17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,12,a
121322,2,dih19,0\H,14,r1423,13,a131423,12,dih20,0\H,15,r1524,14,a14152
4,13,dih21,0\H,6,r625,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0\O,4
,r427,3,a3427,2,dih24,0\C,5,r528,4,a4528,27,dih25,0\H,28,r2829,5,a5282
9,4,dih26,0\H,28,r2830,5,a52830,4,dih27,0\H,28,r2831,5,a52831,4,dih28,
0\r2829=1.08541168\r2830=1.08496724\r2831=1.08994547\al52829=108.79887
437\al52830=109.26062536\al52831=113.38749597\alh26=200.56635002\alh27=-
41.78177051\alh28=79.91079156\r528=1.44631085\al4528=115.64978828\alh25
=173.31401362\r23=1.41137996\r34=1.79210385\r45=1.68778595\r56=1.45377
296\r17=1.38003222\r78=1.39231028\r89=1.38453718\r910=1.38173161\r1011
=1.38907666\r212=1.40952856\r1213=1.37606954\r1314=1.38960863\r1415=1.
3885739\r216=1.07625497\r817=1.07850019\r918=1.07633336\r1019=1.077053
09\r1120=1.07595109\r1221=1.07615686\r1322=1.07676241\r1423=1.07568269
\r1524=1.07763155\r625=1.0845745\r626=1.08656776\r427=1.48298487\al23=
101.59734941\al234=119.53934741\al345=103.4145054\al456=117.47854181\al217
=120.04730178\al178=116.51205174\al789=121.46642938\al8910=120.00360261\al
91011=119.70876696\al3212=117.08884569\al21213=120.42132267\al21314=120.
70689602\al31415=119.63171292\al3216=117.53444466\al7817=118.94772449\al89
18=119.80524551\al91019=120.37947135\al101120=120.35539172\al21221=119.21
656971\al21322=119.69505123\al31423=120.21972822\al41524=120.19619569\
al7625=111.29528006\al7626=108.69844887\al3427=104.41590531\alh1=82.14052
46\alh2=-76.87494664\alh3=69.13450118\alh4=-59.74831577\alh5=181.03238
601\alh6=-0.0681596\alh7=-0.44562234\alh8=0.36646063\alh9=193.11673255
\alh10=-10.90732436\alh11=4.13072903\alh12=3.03690689\alh13=-13.831680
16\alh14=179.8383536\alh15=179.86976121\alh16=180.40050347\alh17=180.2
2569468\alh18=171.1560464\alh19=182.2295665\alh20=179.57420292\alh21=1
74.35605344\alh22=-57.95011994\alh23=-175.35118931\alh24=32.79628091\r
12=2.14194612\\Version=AM64L-G03RevE.01\State=2-A\HF=-1069.6693956\RMS
D=6.687e-09\RMSF=4.086e-05\Thermal=0.\Dipole=0.2175673,-1.5298433,-1.0
812436\PG=C01 [X(C14H14N1O1S1)]\@

ROBHandHLYP/6-311++G**

```
1\1\GINC-GOMBERG02\FTS\ROBHandHLYP\6-311++G(d,p)\C14H14N1O1S1(2)\CARLH
S\17-Jun-2010\1\1\#robhandhlyp/6-311++G** opt=(grad,ts,readfc,nofreeze,
noeigentest) geom=checkpoint guess=read optcyc=400 scfcyc=300\Biaryl
TS with nitrogen (sultam)\0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234
,1,dih1,0\N,4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a2
17,3,dih4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8
,a8910,7,dih7,0\C,10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0
\C,12,r1213,2,a21213,3,dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1
415,13,a131415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,
1,dih14,0\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,1
1,r1120,10,a101120,9,dih17,0\H,12,r1221,2,a21221,3,dih18,0\H,13,r1322,
12,a121322,2,dih19,0\H,14,r1423,13,a131423,12,dih20,0\H,15,r1524,14,a1
41524,13,dih21,0\H,6,r625,7,a7625,1,dih22,0\H,6,r626,7,a7626,1,dih23,0
\O,4,r427,3,a3427,2,dih24,0\C,5,r528,4,a4528,27,dih25,0\H,28,r2829,5,a
52829,4,dih26,0\H,28,r2830,5,a52830,4,dih27,0\H,28,r2831,5,a52831,4,di
h28,0\r2829=1.0856204\r2830=1.08498099\r2831=1.08976597\ a52829=108.71
470444\ a52830=109.3378832\ a52831=113.33444595\ di h26=201.99541372\ di h27
=-40.35325513\ di h28=81.40096887\ r528=1.44723401\ a4528=115.8420027\ di h2
5=171.58352711\ r23=1.41172626\ r34=1.79458124\ r45=1.68760328\ r56=1.4541
3719\ r17=1.37984026\ r78=1.39280517\ r89=1.38529289\ r910=1.38248108\ r101
1=1.38977675\ r212=1.40974058\ r1213=1.37654326\ r1314=1.39005411\ r1415=1
.38931259\ r216=1.07632485\ r817=1.07858375\ r918=1.07637709\ r1019=1.0771
0216\ r1120=1.07608279\ r1221=1.07627725\ r1322=1.07685955\ r1423=1.075789
81\ r1524=1.07771751\ r625=1.08464011\ r626=1.08655045\ r427=1.4845814\ a12
3=101.55158746\ a234=119.80534144\ a345=103.69765071\ a456=117.8086672\ a2
17=119.72464731\ a178=116.50385369\ a789=121.4414719\ a8910=120.01686807\
a91011=119.70166819\ a3212=117.11918183\ a21213=120.44171445\ a121314=120
.67894308\ a131415=119.63956942\ a3216=117.8215715\ a7817=118.99974601\ a8
918=119.79888185\ a91019=120.37849582\ a101120=120.34747908\ a21221=119.2
1565347\ a121322=119.71483992\ a131423=120.23842893\ a141524=120.14925\ a7
625=111.27344527\ a7626=108.74746879\ a3427=104.4934987\ di h1=82.14209203
\ di h2=-75.64448479\ di h3=67.85836571\ di h4=-60.47194117\ di h5=181.2055796
\ di h6=-0.1765374\ di h7=-0.3915557\ di h8=0.37262071\ di h9=193.08256525\ di h
10=-10.79175156\ di h11=3.96821559\ di h12=3.11135462\ di h13=-13.64607375\ d
i h14=179.72908536\ di h15=179.89191659\ di h16=180.38347271\ di h17=180.1218
903\ di h18=171.23828789\ di h19=182.16756872\ di h20=179.62309293\ di h21=174
.4022409\ di h22=-57.48523218\ di h23=-174.80194469\ di h24=34.15816137\ r12=
2.14404982\ \Version=AM64L-G03RevE.01\State=2-A\HF=-1069.6791908\RMSE=2
.088e-09\RMSEF=3.247e-05\Thermal=0.\Dipole=0.2066432,-1.5073811,-1.1275
625\PG=C01 [X(C14H14N1O1S1)]\@
```

HAT Product (Scheme 7)

ROHF/6-31G*

```
1\1\GINC-GOMBERG01\FOpt\ROHF\6-31G(d)\C14H14N1O1S1(2)\CARLHS\22-Jun-20
10\0\0\#roh/6-31G* opt=(grad, cartesian) optcyc=200 scfcyc=300\HAT pro
duct\0,2\S,-0.365744371,-0.318795007,-0.1491019865\C,-0.5587295751,0.
0736393634,3.8813073852\N,0.6304545552,0.2321210253,1.0699870546\O,-1.
7230185446,-0.4474878923,0.4115070426\C,0.2354776953,1.3814862248,1.88
10567843\C,0.2584976756,1.0764650637,3.364610487\C,1.0651244871,1.7993
864927,4.2283875091\C,1.0626789117,1.5310068853,5.5916676645\C,0.25064
8145,0.533787673,6.0969381768\C,-0.5616015835,-0.1949331066,5.23651147
12\H,-0.7686113008,1.6526431667,1.5882458332\H,0.8823601361,2.22414798
59,1.6591482437\H,-1.1881060789,-0.4876311863,3.2137697297\H,1.6948861
986,2.0999322337,6.2500626936\H,0.2463010201,0.3222637021,7.151431606\
H,-1.197780134,-0.9697564556,5.6259604595\C,-0.4470423294,1.1186602234
,-1.2229310146\C,-1.6684657882,1.7204749482,-1.4665641233\C,-1.7314274
958,2.8013352726,-2.3353933358\C,-0.5836465275,3.2635616252,-2.9544517
767\C,0.6375084168,2.6479382851,-2.7115616664\C,0.708170449,1.57091897
6,-1.8481859876\H,-2.5471211779,1.3421935943,-0.9808117092\H,-2.676462
8433,3.276630443,-2.5270837433\H,-0.6363758501,4.0993575513,-3.6288670
32\H,1.5281508601,3.0062409309,-3.1953442347\H,1.6523252813,1.09264188
81,-1.6565148526\C,1.9556970887,-0.2196548215,1.0956559316\H,2.4883947
389,0.0000249712,2.0014026809\H,1.6998532402,2.5785383989,3.8419352715
\H,2.1314851106,-1.1747607501,0.6358850022\Version=AM64L-G03RevE.01\S
tate=2-A\HF=-1065.0124176\RMSE=5.515e-09\RMSE=6.557e-06\Thermal=0.\Dip
ole=1.0158357,0.9760532,-0.4128913\PG=C01 [X(C14H14N1O1S1)]\@
```

ROHF/6-311G**

```
1\1\GINC-GOMBERG01\FOpt\ROHF\6-311G(d,p)\C14H14N1O1S1(2)\CARLHS\22-Jun
-2010\0\0\#roh/6-311G** opt=(grad, cartesian, readfc) geom=checkpoint gu
ess=read optcyc=200 scfcyc=300\HAT product\0,2\S,-0.2893636605,-0.31
03442613,-0.1223717826\C,-0.5859842791,0.134770321,3.8144790214\N,0.73
55468987,0.271519702,1.0478836694\O,-1.6247540241,-0.4586602927,0.4752
127237\C,0.3638434377,1.4227110727,1.867747633\C,0.303199658,1.0985580
097,3.3464003505\C,1.1058963502,1.7705551008,4.2524204055\C,1.02991043
24,1.4899243439,5.6104877083\C,0.1473768839,0.5316721499,6.0678697364\
C,-0.661755612,-0.1452501715,5.1645648376\H,-0.6087910527,1.7597027379
,1.5375828028\H,1.0670622014,2.2303125776,1.6907663531\H,-1.215172259,
-0.384776017,3.1136736285\H,1.660591672,2.0195617258,6.3023369287\H,0.
085733955,0.310554217,7.118630316\H,-1.353885476,-0.8895151907,5.51653
78417\C,-0.4348350966,1.1151809431,-1.2058460441\C,-1.67140294,1.69977
07852,-1.3996993546\C,-1.7830936395,2.7721748924,-2.273408346\C,-0.669
0189548,3.2407877497,-2.9445915804\C,0.5678728034,2.6407944945,-2.7498
424391\C,0.6874864407,1.5735063183,-1.881614919\H,-2.5227471603,1.3137
675835,-0.8724283795\H,-2.7408567436,3.2353424728,-2.4280865993\H,-0.7
600966259,4.0700357382,-3.6230955984\H,1.4327028793,3.0040352527,-3.27
50105232\H,1.6438626753,1.1057962887,-1.7271192468\C,2.0311280414,-0.2
530238377,1.1235842896\H,2.5559050547,-0.0459756551,2.0372174499\H,1.7
961190462,2.5198272277,3.9036669868\H,2.1813995036,-1.2109385737,0.660
7116946\Version=AM64L-G03RevE.01\State=2-A\HF=-1065.180257\RMSE=6.097
e-09\RMSE=8.452e-06\Thermal=0.\Dipole=1.0019379,1.0091439,-0.4688672\PG
=C01 [X(C14H14N1O1S1)]\@
```

ROBHandHLYP/6-311G**

```
1\1\GINC-GOMBERG01\FOpt\ROBHandHLYP\6-311G(d,p)\C14H14N1O1S1(2)\CARLHS
\23-Jun-2010\0\0\#robhandhlyp/6-311G** opt=(grad, cartesian, readfc) geom
=checkpoint guess=read optcyc=200 scfcyc=300\HAT product\0,2\S,-0.15
49754184,-0.3444069567,-0.1016781494\C,-0.618906182,0.2789375869,3.637
1879406\N,0.9619706027,0.3145865224,0.9723021116\O,-1.4608773821,-0.54
5591189,0.5734662414\C,0.6175173273,1.4704230195,1.7955295149\C,0.3978
93421,1.1453173546,3.252210136\C,1.195366391,1.7259188155,4.225447998\
C,0.9847071866,1.4525971478,5.5676736859\C,-0.0276980754,0.5910945887,
5.9442045509\C,-0.8277815062,0.0055435703,4.9752478163\H,-0.278889885,
```

1.9138092803,1.3783802872\H,1.4136336122,2.2034333083,1.698477195\H,-1
.2378254848,-0.1739597232,2.8802656282\H,1.611688165,1.9107089965,6.31
3384274\H,-0.1940576767,0.3747718992,6.9856175025\H,-1.6187300335,-0.6
652717664,5.2642630974\C,-0.406230624,1.1001270586,-1.1455924466\C,-1.
6833433471,1.6057054845,-1.2814715898\C,-1.8928385479,2.6820041616,-2.
1289970169\C,-0.8347010181,3.2277489548,-2.8322305487\C,0.4419365938,2
.7034157767,-2.6935215044\C,0.6614982538,1.6328913246,-1.8488648095\H,
-2.4840887766,1.153884119,-0.7232750518\H,-2.8825263229,3.0899745466,-
2.2395802117\H,-1.0015934082,4.0612358618,-3.4924792121\H,1.2631341281
,3.1301662559,-3.2427520009\H,1.6501485485,1.2236079811,-1.7277308776\
C,2.1092132785,-0.4142693823,1.253885133\H,2.5429808985,-0.2818440587,
2.2270416929\H,1.9857919446,2.3990751245,3.9353483362\H,2.2414637475,-
1.3392579578,0.7268998421\\Version=AM64L-G03RevE.01\State=2-A\HF=-1069
.720847\RMSD=9.156e-09\RMSF=6.509e-05\Thermal=0.\Dipole=0.6960534,1.01
65657,-0.516299\PG=C01 [X(C14H14N1O1S1)]\\@

ROBHandHLYP/6-311++G**

1\1\GINC-GOMBERG02\FOpt\ROBHandHLYP\6-311++G(d,p)\C14H14N1O1S1(2)\CARL
HS\24-Jun-2010\0\#\robhandhlyp/6-311++G** opt=(grad, cartesian, readfc)
geom=checkpoint guess=read optcyc=200 scfcyc=300\\HAT product\\0,2\S,-
0.1741988983,-0.3478932944,-0.1134951744\C,-0.5946758792,0.2722832994,
3.6338432953\N,0.9593188162,0.289464045,0.960780689\O,-1.4808978825,-0
.5479441243,0.5644413545\C,0.6428135732,1.4550945699,1.7836929177\C,0.
4174388333,1.1417334034,3.2423398339\C,1.2062096605,1.7403243899,4.212
2328499\C,0.9924921276,1.4810555505,5.5575256881\C,-0.0143214938,0.614
9506542,5.9406288838\C,-0.8063047638,0.0118949483,4.9748771807\H,-0.24
29095455,1.9195172277,1.3660548794\H,1.45673003,2.1677059104,1.6833359
22\H,-1.2081902327,-0.1956566099,2.8816677216\H,1.6133563002,1.9527937
915,6.299906078\H,-0.1826734267,0.4089421312,6.9838307126\H,-1.5927891
721,-0.6622401544,5.2685161245\C,-0.4166057965,1.1122445444,-1.1377003
626\C,-1.7012793139,1.5850315924,-1.3192218477\C,-1.9079931732,2.66566
48645,-2.1629486298\C,-0.8398704932,3.2466253409,-2.8223078628\C,0.444
3967185,2.7531822889,-2.6418528452\C,0.6607399952,1.6792002312,-1.7997
605823\H,-2.5127371779,1.1106486559,-0.7960838094\H,-2.9037714728,3.04
82368814,-2.3056788058\H,-1.0045386129,4.0829400571,-3.4796418365\H,1.
2742772585,3.2059376973,-3.1562309065\H,1.6554781226,1.2955666329,-1.6
477313627\C,2.062179363,-0.4892607241,1.2758896221\H,2.4810607133,-0.3
804607025,2.2581826968\H,1.9940895931,2.4147135778,3.917937797\H,2.197
0566398,-1.3999189712,0.7256293434\\Version=AM64L-G03RevE.01\State=2-A
\HF=-1069.7307985\RMSD=6.307e-09\RMSF=1.197e-06\Thermal=0.\Dipole=0.67
25966,1.0366398,-0.5370166\PG=C01 [X(C14H14N1O1S1)]\\@

Transition state 18

ROHF/6-31G*

```
1\1\GINC-GOMBERG01\FTS\ROHF\6-31G(d)\C14H14N1O1S1(2)\CARLHS\21-Jun-201
0\1\#rohf/6-31G* opt=(grad,ts,readfc,noeigentest) geom=checkpoint gue
ss=read optcyc=200 scfcyc=300\Louis' starting radical\0,2\C\H,1,r12\
C,2,r13,1,a123\C,3,r34,2,a234,1,d1,0\C,4,r45,3,a345,2,d2,0\C,5,r56,4,a
456,3,d3,0\C,6,r67,5,a567,4,d4,0\C,7,r78,6,a678,5,d5,0\C,8,r89,7,a789,
6,d6,0\N,9,r910,8,a8910,3,d7,0\S,10,r1011,9,a91011,8,d8,0\H,1,r112,2,a
2112,3,d9,0\H,1,r113,2,a2113,3,d10,0\H,4,r414,3,a3414,8,d11,0\H,5,r515
,4,a4515,3,d12,0\H,6,r616,5,a5616,4,d13,0\H,7,r717,6,a6717,5,d14,0\H,9
,r918,8,a8918,7,d15,0\H,9,r919,8,a8919,7,d16,0\C,11,r1120,10,a101120,9
,d17,0\O,11,r1121,10,a101121,9,d18,0\C,20,r2022,11,a112022,21,d19,0\C,
22,r2223,20,a202223,11,d20,0\C,23,r2324,22,a222324,20,d21,0\C,24,r2425
,23,a232425,22,d22,0\C,25,r2526,24,a242526,23,d23,0\H,22,r2227,23,a232
227,24,d24,0\H,23,r2328,24,a242328,25,d25,0\H,24,r2429,25,a252429,26,d
26,0\H,25,r2530,26,a262530,20,d27,0\H,26,r2631,20,a202631,22,d28,0\
r2227=1.07464703\r2328=1.07507828\r2429=1.07530027\r2530=1.07506056\r263
1=1.07291906\ a232227=120.39241205\ a242328=120.10573761\ a252429=119.994
35007\ a262530=119.70093727\ a202631=119.31626827\ d24=180.46470009\ d25=1
79.90465526\ d26=179.80039936\ d27=180.41460012\ d28=179.20436501\ r2526=1
.38878583\ a242526=120.15024426\ d23=-0.01049669\ r2425=1.38300042\ a23242
5=120.17843531\ d22=-0.12667792\ r2324=1.38947034\ a222324=120.00697131\ d
21=-0.29583144\ r2223=1.38164224\ a202223=119.47975787\ d20=176.31030023\
r2022=1.38916344\ a112022=120.15161145\ d19=174.12668461\ r12=1.30044475\
r13=1.37349564\ r34=1.37786292\ r45=1.38782487\ r56=1.38780773\ r67=1.3857
5248\ r78=1.38992177\ r89=1.51986005\ r910=1.46529752\ r112=1.08254185\ r11
3=1.07883083\ r414=1.07537407\ r515=1.07577141\ r616=1.07549691\ r717=1.07
691872\ r918=1.08679912\ r919=1.08003014\ r1011=1.67900407\ r1120=1.793435
14\ r1121=1.47180682\ a123=143.70551603\ a234=129.79395452\ a345=118.19993
91\ a456=119.89337605\ a567=120.64629734\ a678=120.03112909\ a789=122.2031
1084\ a8910=113.19186337\ a91011=118.46431815\ a2112=105.3633744\ a2113=10
9.97600458\ a3414=121.16265824\ a4515=120.10498173\ a5616=119.75517838\ a6
717=119.7558398\ a8918=109.66686286\ a8919=110.50255815\ a101120=98.05198
749\ a101121=111.76282529\ d1=180.12765195\ d2=180.55658442\ d3=0.08101473
\ d4=0.02679204\ d5=-0.14214253\ d6=182.03630931\ d7=26.34273017\ d8=92.356
5473\ d9=95.62297235\ d10=-143.15111495\ d11=179.72872824\ d12=179.7972232
2\ d13=179.52243811\ d14=179.35685438\ d15=84.736617\ d16=-33.16402567\ d17
=70.10653609\ d18=-39.76099019\ Version=AM64L-G03RevE.01\ State=2-A\ HF=-
1064.9376542\ RMSD=2.850e-09\ RMSF=6.699e-06\ Thermal=0.\ Dipole=0.375228,
-1.0578917,-0.9477359\ PG=C01 [X(C14H14N1O1S1)]\ \e
```

ROHF/6-311G**

```
1\1\GINC-GOMBERG02\FTS\ROHF\6-311G(d,p)\C14H14N1O1S1(2)\CARLHS\21-Jun-
2010\1\#rohf/6-311G** opt=(grad,ts,readfc,noeigentest) geom=checkpoin
t guess=read optcyc=200 scfcyc=300\Louis' starting radical\0,2\C\H,1
,r12\C,2,r13,1,a123\C,3,r34,2,a234,1,d1,0\C,4,r45,3,a345,2,d2,0\C,5,r5
6,4,a456,3,d3,0\C,6,r67,5,a567,4,d4,0\C,7,r78,6,a678,5,d5,0\C,8,r89,7,
a789,6,d6,0\N,9,r910,8,a8910,3,d7,0\S,10,r1011,9,a91011,8,d8,0\H,1,r11
2,2,a2112,3,d9,0\H,1,r113,2,a2113,3,d10,0\H,4,r414,3,a3414,8,d11,0\H,5
,r515,4,a4515,3,d12,0\H,6,r616,5,a5616,4,d13,0\H,7,r717,6,a6717,5,d14,
0\H,9,r918,8,a8918,7,d15,0\H,9,r919,8,a8919,7,d16,0\C,11,r1120,10,a101
120,9,d17,0\O,11,r1121,10,a101121,9,d18,0\C,20,r2022,11,a112022,21,d19
,0\C,22,r2223,20,a202223,11,d20,0\C,23,r2324,22,a222324,20,d21,0\C,24,
r2425,23,a232425,22,d22,0\C,25,r2526,24,a242526,23,d23,0\H,22,r2227,23
,a232227,24,d24,0\H,23,r2328,24,a242328,25,d25,0\H,24,r2429,25,a252429
,26,d26,0\H,25,r2530,26,a262530,20,d27,0\H,26,r2631,20,a202631,22,d28,
0\ r2227=1.07490934\ r2328=1.07509884\ r2429=1.07537376\ r2530=1.07508899
\ r2631=1.07328157\ a232227=120.3878925\ a242328=120.11646955\ a252429=119
.98609877\ a262530=119.67607768\ a202631=119.20487222\ d24=180.42715758\ d
25=179.87680347\ d26=179.77537432\ d27=180.36035588\ d28=179.25699293\ r25
26=1.38831669\ a242526=120.16512168\ d23=-0.03042579\ r2425=1.38196221\ a2
32425=120.19171219\ d22=-0.13383929\ r2324=1.38892336\ a222324=119.986468
```

68\d21=-0.22612693\r2223=1.38056892\ a202223=119.4269899\d20=176.600726
41\r2022=1.3878271\ a112022=120.06007506\d19=175.17734941\r12=1.2966105
5\r13=1.37705944\r34=1.37773698\r45=1.38671804\r56=1.38721894\r67=1.38
461783\r78=1.38932639\r89=1.51905764\r910=1.46423844\r112=1.0834032\r1
13=1.07957887\r414=1.07539624\r515=1.07579081\r616=1.07553544\r717=1.0
7694819\r918=1.08732181\r919=1.08028144\r1011=1.67224575\r1120=1.79507
961\r1121=1.4677491\ a123=143.44462815\ a234=129.58557645\ a345=118.18251
113\ a456=119.87639426\ a567=120.65144986\ a678=120.05243337\ a789=122.083
547\ a8910=113.16275214\ a91011=118.59076492\ a2112=105.43644283\ a2113=10
9.75039082\ a3414=121.15768873\ a4515=120.10567485\ a5616=119.74856162\ a6
717=119.74875116\ a8918=109.48430104\ a8919=110.11970703\ a101120=98.3955
2123\ a101121=111.480882\d1=180.53472366\d2=180.28164071\d3=0.10516328\
d4=-0.00263985\d5=-0.14110334\d6=181.97907228\d7=25.54759234\d8=94.625
97563\d9=95.90138511\d10=-142.98832184\d11=179.70958497\d12=179.751493
14\d13=179.45368066\d14=179.25770746\d15=83.69573057\d16=-34.03308813\
d17=70.08471078\d18=-39.50026095\\Version=AM64L-G03RevE.01\State=2-A\H
F=-1065.1052853\RMSD=9.703e-09\RMSF=6.816e-06\Thermal=0.\Dipole=0.3436
369,-1.1409683,-0.9751211\PG=C01 [X(C14H14N1O1S1)]\@

ROBHandHLYP/6-311G**

1\1\GINC-GOMBERG02\FTS\ROBHandHLYP\6-311G(d,p)\C14H14N1O1S1(2)\CARLHS\
21-Jun-2010\1\#\robhandhlyp/6-311G** opt=(grad,ts,readfc,noeigentest)
geom=checkpoint guess=read optcyc=200 scfcyc=300\\Louis' starting radi
cal\\0,2\C\H,1,r12\C,2,r13,1,a123\C,3,r34,2,a234,1,d1,0\C,4,r45,3,a345
,2,d2,0\C,5,r56,4,a456,3,d3,0\C,6,r67,5,a567,4,d4,0\C,7,r78,6,a678,5,d
5,0\C,8,r89,7,a789,6,d6,0\N,9,r910,8,a8910,3,d7,0\S,10,r1011,9,a91011,
8,d8,0\H,1,r112,2,a2112,3,d9,0\H,1,r113,2,a2113,3,d10,0\H,4,r414,3,a34
14,8,d11,0\H,5,r515,4,a4515,3,d12,0\H,6,r616,5,a5616,4,d13,0\H,7,r717,
6,a6717,5,d14,0\H,9,r918,8,a8918,7,d15,0\H,9,r919,8,a8919,7,d16,0\C,11
,r1120,10,a101120,9,d17,0\O,11,r1121,10,a101121,9,d18,0\C,20,r2022,11,
a112022,21,d19,0\C,22,r2223,20,a202223,11,d20,0\C,23,r2324,22,a222324,
20,d21,0\C,24,r2425,23,a232425,22,d22,0\C,25,r2526,24,a242526,23,d23,0
\H,22,r2227,23,a232227,24,d24,0\H,23,r2328,24,a242328,25,d25,0\H,24,r2
429,25,a252429,26,d26,0\H,25,r2530,26,a262530,20,d27,0\H,26,r2631,20,a
202631,22,d28,0\\r2227=1.07622082\r2328=1.07625657\r2429=1.07638464\r2
530=1.07625874\r2631=1.07587696\ a232227=120.68105474\ a242328=120.08285
25\ a252429=119.95711022\ a262530=119.74787486\ a202631=118.80862457\d24=
180.6761722\d25=179.98444118\d26=179.68813439\d27=180.39060007\d28=179
.35380986\r2526=1.38589004\ a242526=120.12153711\d23=-0.12310086\r2425=
1.38275535\ a232425=120.22971184\d22=-0.09304115\r2324=1.38708311\ a2223
24=120.05425434\d21=-0.19000105\r2223=1.38129451\ a202223=119.1440497\d
20=176.56782386\r2022=1.38492914\ a112022=120.44679285\d19=175.49221318
\r12=1.2764165\r13=1.41061187\r34=1.37442606\r45=1.38778283\r56=1.3856
1284\r67=1.38406207\r78=1.38899266\r89=1.51359357\r910=1.46097247\r112
=1.08500644\r113=1.08108437\r414=1.07689771\r515=1.07702662\r616=1.076
52228\r717=1.07820476\r918=1.08918159\r919=1.08264261\r1011=1.69437473
\r1120=1.80143136\r1121=1.47959914\ a123=144.01269479\ a234=130.76367078
\ a345=118.07835251\ a456=119.91680542\ a567=120.6218754\ a678=120.0345077
1\ a789=121.90914567\ a8910=113.20941705\ a91011=118.04071709\ a2112=105.0
0723206\ a2113=110.11118709\ a3414=121.39862199\ a4515=120.0269519\ a5616=
119.76623027\ a6717=119.89298275\ a8918=109.54126155\ a8919=110.40731904\
a101120=96.87926191\ a101121=112.26276593\d1=177.96262428\d2=182.375464
7\d3=0.28896924\d4=-0.05208079\d5=-0.25693186\d6=182.00601035\d7=28.23
175622\d8=90.58166239\d9=97.28439621\d10=-141.5771685\d11=179.49616124
\d12=179.82075175\d13=179.31941516\d14=179.14304532\d15=86.70759296\d1
6=-31.03355623\d17=68.15260492\d18=-40.68592825\\Version=AM64L-G03RevE
.01\State=2-A\HF=-1069.6650142\RMSD=3.724e-09\RMSF=3.098e-05\Thermal=0
.\Dipole=0.4130287,-1.0259463,-0.9439965\PG=C01 [X(C14H14N1O1S1)]\@

ROBHandHLYP/6-311++G**

1\1\GINC-GOMBERG02\FTS\ROBHandHLYP\6-311++G(d,p)\C14H14N1O1S1(2)\CARLH
S\22-Jun-2010\1\#\robhandhlyp/6-311++G** opt=(grad,ts,readfc,noeigente
st) geom=checkpoint guess=read optcyc=200 scfcyc=300\\Louis' starting
radical\\0,2\C\H,1,r12\C,2,r13,1,a123\C,3,r34,2,a234,1,d1,0\C,4,r45,3,

a345,2,d2,0\C,5,r56,4,a456,3,d3,0\C,6,r67,5,a567,4,d4,0\C,7,r78,6,a678
,5,d5,0\C,8,r89,7,a789,6,d6,0\N,9,r910,8,a8910,3,d7,0\S,10,r1011,9,a91
011,8,d8,0\H,1,r112,2,a2112,3,d9,0\H,1,r113,2,a2113,3,d10,0\H,4,r414,3
,a3414,8,d11,0\H,5,r515,4,a4515,3,d12,0\H,6,r616,5,a5616,4,d13,0\H,7,r
717,6,a6717,5,d14,0\H,9,r918,8,a8918,7,d15,0\H,9,r919,8,a8919,7,d16,0\
C,11,r1120,10,a101120,9,d17,0\O,11,r1121,10,a101121,9,d18,0\C,20,r2022
,11,a112022,21,d19,0\C,22,r2223,20,a202223,11,d20,0\C,23,r2324,22,a222
324,20,d21,0\C,24,r2425,23,a232425,22,d22,0\C,25,r2526,24,a242526,23,d
23,0\H,22,r2227,23,a232227,24,d24,0\H,23,r2328,24,a242328,25,d25,0\H,2
4,r2429,25,a252429,26,d26,0\H,25,r2530,26,a262530,20,d27,0\H,26,r2631,
20,a202631,22,d28,0\\r2227=1.07626719\r2328=1.07631622\r2429=1.0764595
2\r2530=1.07631427\r2631=1.07591375\ a232227=120.56472885\ a242328=120.1
017844\ a252429=119.98122734\ a262530=119.72263669\ a202631=119.01515088\
d24=180.57612089\ d25=179.89054913\ d26=179.69533083\ d27=180.49805468\ d2
8=179.16549459\ r2526=1.38654626\ a242526=120.14152828\ d23=-0.08587681\ r
2425=1.38317334\ a232425=120.18355093\ d22=-0.14714257\ r2324=1.38755037\
a222324=120.06544334\ d21=-0.33307837\ r2223=1.38199629\ a202223=119.2084
2669\ d20=176.02154798\ r2022=1.38570476\ a112022=120.54411794\ d19=173.81
271286\ r12=1.27682989\ r13=1.41044705\ r34=1.37495351\ r45=1.38855538\ r56
=1.38625952\ r67=1.3848843\ r78=1.38938311\ r89=1.51334387\ r910=1.4611267
9\ r112=1.08509425\ r113=1.08117726\ r414=1.07695983\ r515=1.0770595\ r616=
1.07655803\ r717=1.07829755\ r918=1.08933799\ r919=1.08290946\ r1011=1.692
49394\ r1120=1.80204523\ r1121=1.48232789\ a123=143.82423337\ a234=130.649
72446\ a345=118.06608754\ a456=119.91896422\ a567=120.62287444\ a678=120.0
093354\ a789=121.91514948\ a8910=113.16173586\ a91011=118.84167799\ a2112=
104.86850595\ a2113=110.07012389\ a3414=121.42407589\ a4515=120.02335509\
a5616=119.76798143\ a6717=119.8715036\ a8918=109.61341662\ a8919=110.4919
227\ a101120=97.06044976\ a101121=112.66835834\ d1=178.34200089\ d2=182.19
667583\ d3=0.21054314\ d4=-0.00156361\ d5=-0.22854732\ d6=181.90245393\ d7=
28.02923687\ d8=91.21364174\ d9=96.65068741\ d10=-142.23640968\ d11=179.47
256422\ d12=179.80438925\ d13=179.36891521\ d14=179.10043633\ d15=86.66294
944\ d16=-31.09313528\ d17=65.93536485\ d18=-43.08596296\\Version=AM64L-G
03RevE.01\State=2-A\HF=-1069.675621\RMSD=6.545e-09\RMSF=2.222e-05\Ther
mal=0.\Dipole=0.4732905,-1.0231084,-0.9681994\PG=C01 [X(C14H14N1O1S1)]
\\@

Radical 16

ROHF/6-31G*

```
1\1\GINC-X80\FOpt\ROHF\6-31G(d)\C12H10N1O2S1(2)\SHK563\15-May-2010\1\
# ROHF/6-31G* opt=grad optcyc=300 scfcyc=300 freq=noraman\Louis' sulf
inate pyridyl\0,2\SC,1,r12\O,1,r13,2,a213\O,1,r14,3,a214,2,dih1,0\C,
3,r35,1,a135,4,dih2,0\C,5,r26,3,a126,1,dih3,0\C,6,r67,5,a267,3,dih4,0\
C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a789,6,dih6,0\N,9,r910,8,a8910,7,dih
7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a67
13,2,dih10,0\H,8,r814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\C,1
,r117,3,a4117,5,dih14,0\C,16,r1718,1,a11718,3,dih15,0\C,17,r1819,16,a1
71819,1,dih16,0\C,18,r1920,17,a181920,16,dih17,0\C,19,r2021,18,a192021
,17,dih18,0\C,20,r2122,19,a202122,18,dih19,0\H,17,r1823,16,a171823,1,d
ih20,0\H,18,r1924,17,a181924,16,dih21,0\H,19,r2025,18,a192025,17,dih22
,0\H,20,r2126,19,a202126,18,dih23,0\H,21,r2227,20,a212227,19,dih24,0\
r13=1.62705358\r14=1.46227578\r35=1.4253892\r26=1.50480663\r67=1.38759
577\r78=1.38951439\r89=1.38122536\r910=1.33033881\r511=1.08047083\r512
=1.08481934\r713=1.07504792\r814=1.07389598\r915=1.07505409\r1718=1.38
244752\r1819=1.38730481\r1920=1.38399576\r2021=1.38880187\r2122=1.3817
7459\r1823=1.07295451\r1924=1.07482843\r2025=1.07517792\r2126=1.074764
9\r2227=1.07514122\ a213=27.0819486\ a214=108.66954751\ a135=116.63830934
\ a126=110.7049768\ a267=123.56406807\ a678=119.26428718\ a789=118.9802431
2\ a8910=122.36196183\ a6511=110.16636319\ a6512=110.60407472\ a6713=119.9
4433699\ a7814=120.77069689\ a8915=121.1021773\ a4117=94.64030102\ a11718=
119.19721557\ a171819=119.06075971\ a181920=120.10094601\ a192021=120.367
24737\ a202122=119.89822489\ a171823=119.56065366\ a181924=119.75812441\ a
192025=119.8837903\ a202126=120.16365246\ a212227=120.35374288\ dih1=-44.
63298596\ dih2=-76.45880171\ dih3=118.10554324\ dih4=-49.14229035\ dih5=0.
13078765\ dih6=0.11583398\ dih7=-0.16465588\ dih8=13.53702883\ dih9=-105.8
2011186\ dih10=180.5267757\ dih11=180.14603719\ dih12=179.98630481\ dih14=
173.92998982\ dih15=116.26859853\ dih16=177.56013746\ dih17=-0.31129646\ d
ih18=-0.07666052\ dih19=0.03958091\ dih20=-2.54326667\ dih21=179.72487764
\ dih22=180.12015292\ dih23=180.02273311\ dih24=179.71875127\r117=1.78085
282\r12=4.94113585\Version=EM64L-G03RevE.01\State=2-A\HF=-1061.788218
4\RMSD=5.520e-09\RMSF=2.867e-05\Thermal=0.\Dipole=0.7842532,-0.0385078
,-1.0849969\PG=C01 [X(C12H10N1O2S1)]\@
```

ROHF/6-311G**

```
1\1\GINC-X82\FOpt\ROHF\6-311G(d,p)\C12H10N1O2S1(2)\SHK563\16-May-2010\
1\# ROHF/6-311G** opt=grad optcyc=300 geom=checkpoint gues
s=check freq=noraman\Louis' sulfinate pyridyl\0,2\SC,1,r12\O,1,r13,
2,a213\O,1,r14,3,a214,2,dih1,0\C,3,r35,1,a135,4,dih2,0\C,5,r26,3,a126,
1,dih3,0\C,6,r67,5,a267,3,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a78
9,6,dih6,0\N,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r51
2,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11
,0\H,9,r915,8,a8915,7,dih12,0\C,1,r117,3,a4117,5,dih14,0\C,16,r1718,1,
a11718,3,dih15,0\C,17,r1819,16,a171819,1,dih16,0\C,18,r1920,17,a181920
,16,dih17,0\C,19,r2021,18,a192021,17,dih18,0\C,20,r2122,19,a202122,18,
dih19,0\H,17,r1823,16,a171823,1,dih20,0\H,18,r1924,17,a181924,16,dih21
,0\H,19,r2025,18,a192025,17,dih22,0\H,20,r2126,19,a202126,18,dih23,0\H
,21,r2227,20,a212227,19,dih24,0\ r13=1.62063365\r14=1.45712671\r35=1.4
2385792\r26=1.50408866\r67=1.38577957\r78=1.38919311\r89=1.37986786\r9
10=1.33013055\r511=1.08067432\r512=1.08598767\r713=1.07537815\r814=1.0
7389994\r915=1.07553337\r1718=1.38086056\r1819=1.38608263\r1920=1.3835
6273\r2021=1.38773415\r2122=1.38118611\r1823=1.07317245\r1924=1.074840
59\r2025=1.07528057\r2126=1.07475745\r2227=1.07552076\ a213=27.02636432
\ a214=108.17470885\ a135=117.32483017\ a126=110.51936122\ a267=123.474139
42\ a678=119.27681117\ a789=118.98861401\ a8910=122.2884328\ a6511=110.150
93407\ a6512=110.49877642\ a6713=119.81496869\ a7814=120.753182\ a8915=121
.13249858\ a4117=94.71499194\ a11718=119.28215167\ a171819=118.94317004\ a
181920=120.10459872\ a192021=120.40806657\ a202122=119.85261515\ a171823=
119.45078769\ a181924=119.75131841\ a192025=119.85261098\ a202126=120.190
30321\ a212227=120.36428932\ dih1=-44.42966534\ dih2=-76.64563831\ dih3=11
```

8.09021524\ dih4=-47.41222954\ dih5=0.26895426\ dih6=0.00753698\ dih7=-0.1677582\ dih8=14.98540185\ dih9=-104.52510184\ dih10=180.60726863\ dih11=180.05570979\ dih12=180.04024333\ dih14=174.02404505\ dih15=108.91821024\ dih16=178.60347094\ dih17=-0.19483884\ dih18=-0.09853807\ dih19=0.10767325\ dih20=-1.13110843\ dih21=179.88411865\ dih22=180.15348415\ dih23=180.11709316\ dih24=179.90946002\ r117=1.78098428\ r12=4.94274156\ \Version=EM64L-G03RevE.01\State=2-A\HF=-1061.9523172\ RMSD=5.987e-09\ RMSF=1.792e-05\ Thermal=0.\Dipole=0.874624,-0.0494284,-1.0868788\ PG=C01 [X(C12H10N1O2S1)]\@

ROBHandHLYP/6-311G**

1\1\GINC-X82\FOpt\ROBHandHLYP\6-311G(d,p)\C12H10N1O2S1(2)\SHK563\21-May-2010\1\#\ ROBHandHLYP/6-311G** opt=(grad) optcyc=300 scfcyc=300 geom=checkpoint guess=check freq=noraman\ \Louis' sulfinate pyridyl\ \0,2\SC,1,r12\O,1,r13,2,a213\O,1,r14,3,a214,2,dih1,0\ C,3,r35,1,a135,4,dih2,0\ C,5,r26,3,a126,1,dih3,0\ C,6,r67,5,a267,3,dih4,0\ C,7,r78,6,a678,2,dih5,0\ C,8,r89,7,a789,6,dih6,0\ N,9,r910,8,a8910,7,dih7,0\ H,5,r511,6,a6511,2,dih8,0\ H,5,r512,6,a6512,2,dih9,0\ H,7,r713,6,a6713,2,dih10,0\ H,8,r814,7,a7814,6,dih11,0\ H,9,r915,8,a8915,7,dih12,0\ C,1,r117,3,a4117,5,dih14,0\ C,16,r1718,1,a11718,3,dih15,0\ C,17,r1819,16,a171819,1,dih16,0\ C,18,r1920,17,a181920,16,dih17,0\ C,19,r2021,18,a192021,17,dih18,0\ C,20,r2122,19,a202122,18,dih19,0\ H,17,r1823,16,a171823,1,dih20,0\ H,18,r1924,17,a181924,16,dih21,0\ H,19,r2025,18,a192025,17,dih22,0\ H,20,r2126,19,a202126,18,dih23,0\ H,21,r2227,20,a212227,19,dih24,0\ \r13=1.65144357\ r14=1.47019684\ r35=1.42708478\ r26=1.49790722\ r67=1.38608773\ r78=1.3888829\ r89=1.37838211\ r910=1.33618022\ r511=1.08262832\ r512=1.08912419\ r713=1.07759961\ r814=1.07530571\ r915=1.0767078\ r1718=1.37972758\ r1819=1.38442522\ r1920=1.38351051\ r2021=1.38641005\ r2122=1.38119576\ r1823=1.07554519\ r1924=1.07602716\ r2025=1.07630913\ r2126=1.07596218\ r2227=1.07641613\ a213=30.90565599\ a214=109.03215841\ a135=116.05637878\ a126=111.08761348\ a267=123.45800544\ a678=119.49413177\ a789=119.27496614\ a8910=121.11042051\ a6511=109.91161955\ a6512=110.57704573\ a6713=119.58983125\ a7814=120.57675\ a8915=121.82988871\ a4117=93.40694186\ a11718=118.47978833\ a171819=118.82994437\ a181920=120.08924428\ a192021=120.40095705\ a202122=119.96503868\ a171823=119.15457827\ a181924=119.78459351\ a192025=119.85724237\ a202126=120.13646239\ a212227=120.57607293\ dih1=-46.75702746\ dih2=-79.03682223\ dih3=111.77050722\ dih4=-42.23997522\ dih5=0.32702112\ dih6=-0.02102784\ dih7=-0.14260327\ dih8=20.03637948\ dih9=-99.04263952\ dih10=180.54858984\ dih11=180.05691395\ dih12=180.103473\ dih14=172.4578847\ dih15=114.08867887\ dih16=178.21458181\ dih17=-0.30883167\ dih18=-0.00624006\ dih19=0.08460196\ dih20=-1.85569103\ dih21=179.74907265\ dih22=180.18107117\ dih23=179.95794768\ dih24=179.57691019\ r117=1.78748492\ r12=4.92489927\ \Version=EM64L-G03RevE.01\State=2-A\HF=-1066.3091232\ RMSD=2.142e-09\ RMSF=3.158e-05\ Thermal=0.\Dipole=1.3878268,-0.03593,-0.257593\ PG=C01 [X(C12H10N1O2S1)]\@

ROBHandHLYP/6-311++G**

1\1\GINC-X87\FOpt\ROBHandHLYP\6-311++G(d,p)\C12H10N1O2S1(2)\SHK563\25-May-2010\1\#\ ROBHandHLYP/6-311++G** opt=grad optcyc=300 scfcyc=300 geom=checkpoint guess=check freq=noraman\ \Louis' sulfinate pyridyl\ \0,2\SC,1,r12\O,1,r13,2,a213\O,1,r14,3,a214,2,dih1,0\ C,3,r35,1,a135,4,dih2,0\ C,5,r26,3,a126,1,dih3,0\ C,6,r67,5,a267,3,dih4,0\ C,7,r78,6,a678,2,dih5,0\ C,8,r89,7,a789,6,dih6,0\ N,9,r910,8,a8910,7,dih7,0\ H,5,r511,6,a6511,2,dih8,0\ H,5,r512,6,a6512,2,dih9,0\ H,7,r713,6,a6713,2,dih10,0\ H,8,r814,7,a7814,6,dih11,0\ H,9,r915,8,a8915,7,dih12,0\ C,1,r117,3,a4117,5,dih14,0\ C,16,r1718,1,a11718,3,dih15,0\ C,17,r1819,16,a171819,1,dih16,0\ C,18,r1920,17,a181920,16,dih17,0\ C,19,r2021,18,a192021,17,dih18,0\ C,20,r2122,19,a202122,18,dih19,0\ H,17,r1823,16,a171823,1,dih20,0\ H,18,r1924,17,a181924,16,dih21,0\ H,19,r2025,18,a192025,17,dih22,0\ H,20,r2126,19,a202126,18,dih23,0\ H,21,r2227,20,a212227,19,dih24,0\ \r13=1.65230142\ r14=1.47212388\ r35=1.42940191\ r26=1.4978395\ r67=1.38721495\ r78=1.38884971\ r89=1.37945329\ r910=1.33587354\ r511=1.08247803\ r512=1.08877225\ r713=1.0781802\ r814=1.07537298\ r915=1.07664726\ r1718=1.38039762\ r1819=1.38522072\ r1920=1.3838402\ r2021=1.38694298\ r2122=1.38170318\ r1823=1.07565809

\r1924=1.07608603\r2025=1.0763877\r2126=1.07602714\r2227=1.07643987\aa213=29.84181197\aa214=108.98670406\aa135=116.01801509\aa126=111.29562765\aa267=123.63404212\aa678=119.51185967\aa789=119.2768921\aa8910=121.11641558\aa6511=109.81913751\aa6512=110.6329513\aa6713=119.73893966\aa7814=120.61613538\aa8915=121.79143596\aa4117=93.72646655\aa11718=118.4826237\aa171819=118.85432743\aa181920=120.11053574\aa192021=120.36758549\aa202122=119.97445816\aa171823=119.33029287\aa181924=119.75722412\aa192025=119.87048742\aa202126=120.15515033\aa212227=120.46926063\ dih1=-46.87915494\ dih2=-80.11964001\ dih3=111.6474266\ dih4=-48.26582422\ dih5=0.04792244\ dih6=0.16711716\ dih7=-0.15330018\ dih8=14.66765132\ dih9=-104.51472273\ dih10=180.51547301\ dih11=180.1825945\ dih12=180.04734283\ dih14=171.28755519\ dih15=117.01193545\ dih16=177.49727674\ dih17=-0.59676237\ dih18=-0.00076131\ dih19=0.09301184\ dih20=-2.81106031\ dih21=179.56503443\ dih22=180.18900919\ dih23=180.00834372\ dih24=179.60315769\r117=1.78804096\r12=4.92118829\version=EM64L-G03RevE.01\State=2-A\HF=-1066.3212809\RMSD=5.484e-09\RMSF=1.592e-05\Thermal=0.\Dipole=0.7134605,-0.055984,-1.1643715\PG=C01 [X(C12H10N1O2S1)]\@

Intermediate A (Scheme S1)

ROHF/6-31G*

```
1\1\GINC-X97\FOpt\ROHF\6-31G(d)\C12H10N1O2S1(2)\SHK563\30-Apr-2010\1\
# ROHF/6-31G* opt=(nofreeze,grad) optcyc=300 scfcyc=300 geom=checkpoin
t guess=check freq=noraman\Louis' hypervalent intermediate pyridyl\0
,2\S\C,1,r12\O,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,d
ih2,0\C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2
,dih5,0\C,8,r89,7,a789,6,dih6,0\N,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a
6511,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8
,r814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\C,1,r117,4,a4117,2
,dih14,0\C,16,r1718,1,a11718,2,dih15,0\C,17,r1819,16,a171819,1,dih16,0\
C,18,r1920,17,a181920,16,dih17,0\C,19,r2021,18,a192021,17,dih18,0\C,20
,r2122,19,a202122,18,dih19,0\H,17,r1823,16,a171823,1,dih20,0\H,18,r192
4,17,a181924,16,dih21,0\H,19,r2025,18,a192025,17,dih22,0\H,20,r2126,19
,a202126,18,dih23,0\H,21,r2227,20,a212227,19,dih24,0\|r13=1.63265806\r
14=1.45269095\r35=1.42057242\r26=1.37100072\r67=1.38287011\r78=1.38531
466\r89=1.38954989\r910=1.32262494\r511=1.08121658\r512=1.08290745\r71
3=1.07641613\r814=1.07389337\r915=1.07513861\r1718=1.38339844\r1819=1.
38837458\r1920=1.38401232\r2021=1.388107\r2122=1.38308354\r1823=1.0723
0841\r1924=1.07545137\r2025=1.07539503\r2126=1.0754436\r2227=1.0748474
9\|a213=87.16653706\|a214=100.70189078\|a135=119.03487893\|a126=111.170822
13\|a267=117.7642646\|a678=117.32875021\|a789=119.20563175\|a8910=123.4609
3419\|a6511=113.1466153\|a6512=112.29708524\|a6713=121.83380372\|a7814=120
.96245807\|a8915=120.24162537\|a4117=102.27517369\|a11718=118.96651408\|a1
71819=119.17964771\|a181920=120.31013063\|a192021=120.03296677\|a202122=1
20.01318599\|a171823=119.81562532\|a181924=119.60732254\|a192025=120.0357
2075\|a202126=120.11917003\|a212227=120.11736283\|dih1=113.86618863\|dih2=
19.02574529\|dih3=-9.26035792\|dih4=179.41927981\|dih5=-0.74574108\|dih6=-
0.17763071\|dih7=0.3055828\|dih8=130.61165395\|dih9=-105.46060391\|dih10=1
79.36241592\|dih11=180.3295863\|dih12=180.616155\|dih14=187.25680867\|dih1
5=213.48803495\|dih16=173.58803108\|dih17=-0.67465597\|dih18=-0.16347719\
|dih19=0.06614924\|dih20=-7.25463173\|dih21=179.17647703\|dih22=180.047416
84\|dih23=180.11373452\|dih24=179.93318664\r12=1.89378282\r117=1.8692234
4\|Version=EM64L-G03RevE.01\|State=2-A\HF=-1061.7404162\|RMSD=5.152e-09\
|RMSF=8.619e-06\|Thermal=0.\|Dipole=1.3038616,0.8491485,1.1569781\|PG=C01
[X(C12H10N1O2S1)]\|e
```

ROHF/6-311G**

```
1\1\GINC-X97\FOpt\ROHF\6-311G(d,p)\C12H10N1O2S1(2)\SHK563\03-May-2010\
1\|ROHF/6-311G** opt=grad optcyc=300 scfcyc=300 geom=checkpoint gues
s=check freq=noraman\Louis' hypervalent intermediate pyridyl\0,2\S\C
,1,r12\O,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\
C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,
0\C,8,r89,7,a789,6,dih6,0\N,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2
,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,
7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\C,1,r117,4,a4117,2,dih14,
0\C,16,r1718,1,a11718,2,dih15,0\C,17,r1819,16,a171819,1,dih16,0\C,18,r
1920,17,a181920,16,dih17,0\C,19,r2021,18,a192021,17,dih18,0\C,20,r2122
,19,a202122,18,dih19,0\H,17,r1823,16,a171823,1,dih20,0\H,18,r1924,17,a
181924,16,dih21,0\H,19,r2025,18,a192025,17,dih22,0\H,20,r2126,19,a2021
26,18,dih23,0\H,21,r2227,20,a212227,19,dih24,0\|r13=1.6252231\r14=1.44
687882\r35=1.41935179\r26=1.37017403\r67=1.38136018\r78=1.38517008\r89
=1.38831572\r910=1.32232721\r511=1.0810893\r512=1.08368049\r713=1.0765
9184\r814=1.07395164\r915=1.07569635\r1718=1.38138712\r1819=1.38801512
\r1920=1.38312488\r2021=1.38748168\r2122=1.38212067\r1823=1.07254951\r
1924=1.07550333\r2025=1.07545353\r2126=1.07543573\r2227=1.07555729\|a21
3=86.84482206\|a214=100.44627093\|a135=118.93969377\|a126=110.67613149\|a2
67=117.60682475\|a678=117.34514656\|a789=119.24312592\|a8910=123.37599314
\|a6511=113.11342338\|a6512=111.99363778\|a6713=121.83117634\|a7814=120.94
62569\|a8915=120.27053385\|a4117=102.06315409\|a11718=119.39917306\|a17181
9=119.00924545\|a181920=120.3351326\|a192021=120.0781089\|a202122=119.950
47522\|a171823=119.75785458\|a181924=119.58813666\|a192025=120.00685195\|a
```

202126=120.14608281\ a212227=120.10127179\ di h1=112.95190897\ di h2=21.597
48352\ di h3=-11.00905573\ di h4=179.86188708\ di h5=-0.72244699\ di h6=-0.217
21547\ di h7=0.36340283\ di h8=131.56891873\ di h9=-104.32256543\ di h10=179.4
2850077\ di h11=180.31907221\ di h12=180.63845869\ di h14=186.47918727\ di h15
=206.16781158\ di h16=174.28327715\ di h17=-0.53723132\ di h18=-0.14096063\ d
i h19=0.0174854\ di h20=-6.34773894\ di h21=179.34134603\ di h22=180.05054307
\ di h23=180.10977954\ di h24=179.9582747\ r12=1.90699223\ r117=1.87468237\ \\
Version=EM64L-G03RevE.01\ State=2-A\ HF=-1061.9022628\ RMSD=4.935e-09\ RMS
F=1.157e-05\ Thermal=0.\ Dipole=1.3072345,0.8387098,1.1351734\ PG=C01 [X(
C12H10N1O2S1)]\ \e

ROBHandHLYP/6-311G**

1\1\GINC-X80\Fopt\ROBHandHLYP\6-311G(d,p)\C12H10N1O2S1(2)\SHK563\04-May-2010\1\#\ ROBHandHLYP/6-311G** opt=grad optcyc=300 scfcyc=300 geom=c
heckpoint guess=check freq=noraman\ \Louis' hypervalent intermediate py
ridyl\ \0,2\ S\ C,1,r12\ O,1,r13,2,a213\ O,1,r14,2,a214,3,dih1,0\ C,3,r35,1,
a135,2,dih2,0\ C,2,r26,1,a126,3,dih3,0\ C,6,r67,2,a267,1,dih4,0\ C,7,r78,
6,a678,2,dih5,0\ C,8,r89,7,a789,6,dih6,0\ N,9,r910,8,a8910,7,dih7,0\ H,5,
r511,6,a6511,2,dih8,0\ H,5,r512,6,a6512,2,dih9,0\ H,7,r713,6,a6713,2,dih
10,0\ H,8,r814,7,a7814,6,dih11,0\ H,9,r915,8,a8915,7,dih12,0\ C,1,r117,4,
a4117,2,dih14,0\ C,16,r1718,1,a11718,2,dih15,0\ C,17,r1819,16,a171819,1,
dih16,0\ C,18,r1920,17,a181920,16,dih17,0\ C,19,r2021,18,a192021,17,dih1
8,0\ C,20,r2122,19,a202122,18,dih19,0\ H,17,r1823,16,a171823,1,dih20,0\ H
,18,r1924,17,a181924,16,dih21,0\ H,19,r2025,18,a192025,17,dih22,0\ H,20,
r2126,19,a202126,18,dih23,0\ H,21,r2227,20,a212227,19,dih24,0\ \r13=1.66
151437\ r14=1.46177364\ r35=1.42186804\ r26=1.37160965\ r67=1.38063728\ r78
=1.38565617\ r89=1.3864356\ r910=1.32852785\ r511=1.08366755\ r512=1.08663
615\ r713=1.07787166\ r814=1.07521887\ r915=1.07735681\ r1718=1.38056774\ r
1819=1.38602243\ r1920=1.38347887\ r2021=1.3860448\ r2122=1.38249648\ r182
3=1.07484019\ r1924=1.07664533\ r2025=1.07640229\ r2126=1.07660207\ r2227=
1.07606538\ a213=86.325268\ a214=100.14213405\ a135=118.14997431\ a126=110
.28867161\ a267=117.29160588\ a678=117.52401674\ a789=119.41967053\ a8910=
123.08248256\ a6511=112.87553083\ a6512=111.58777376\ a6713=121.66268728\
a7814=120.81972273\ a8915=120.53407767\ a4117=102.08391727\ a11718=117.98
324503\ a171819=118.85237937\ a181920=120.30434877\ a192021=120.09423393\
a202122=120.07524888\ a171823=119.59750077\ a181924=119.59967669\ a192025
=119.98840796\ a202126=120.11328132\ a212227=120.43964367\ di h1=113.73335
374\ di h2=21.01638442\ di h3=-10.21213339\ di h4=179.28071067\ di h5=-0.81308
435\ di h6=-0.14795478\ di h7=0.30996622\ di h8=133.08585588\ di h9=-103.74114
328\ di h10=179.29894876\ di h11=180.39952217\ di h12=180.61774779\ di h14=184
.8167852\ di h15=209.54069776\ di h16=172.95512869\ di h17=-0.75410825\ di h18
=-0.05665069\ di h19=-0.07869729\ di h20=-8.28204903\ di h21=179.00929442\ di
h22=180.07686002\ di h23=179.90368564\ di h24=179.62990663\ r12=1.9409452\ r
117=1.88147328\ \Version=EM64L-G03RevE.01\ State=2-A\ HF=-1066.282718\ RMS
D=6.719e-09\ RMSF=2.292e-05\ Thermal=0.\ Dipole=1.2324346,0.7780119,1.078
7187\ PG=C01 [X(C12H10N1O2S1)]\ \e

ROBHandHLYP/6-311++G**

1\1\GINC-X97\Fopt\ROBHandHLYP\6-311++G(d,p)\C12H10N1O2S1(2)\SHK563\08-May-2010\1\#\ ROBHandHLYP/6-311++G** opt=grad optcyc=300 scfcyc=300 ge
om=checkpoint guess=check freq=noraman\ \Louis' hypervalent intermediat
e pyridyl\ \0,2\ S\ C,1,r12\ O,1,r13,2,a213\ O,1,r14,2,a214,3,dih1,0\ C,3,r3
5,1,a135,2,dih2,0\ C,2,r26,1,a126,3,dih3,0\ C,6,r67,2,a267,1,dih4,0\ C,7,
r78,6,a678,2,dih5,0\ C,8,r89,7,a789,6,dih6,0\ N,9,r910,8,a8910,7,dih7,0\
H,5,r511,6,a6511,2,dih8,0\ H,5,r512,6,a6512,2,dih9,0\ H,7,r713,6,a6713,2,
dih10,0\ H,8,r814,7,a7814,6,dih11,0\ H,9,r915,8,a8915,7,dih12,0\ C,1,r11
7,4,a4117,2,dih14,0\ C,16,r1718,1,a11718,2,dih15,0\ C,17,r1819,16,a17181
9,1,dih16,0\ C,18,r1920,17,a181920,16,dih17,0\ C,19,r2021,18,a192021,17,
dih18,0\ C,20,r2122,19,a202122,18,dih19,0\ H,17,r1823,16,a171823,1,dih20
,0\ H,18,r1924,17,a181924,16,dih21,0\ H,19,r2025,18,a192025,17,dih22,0\ H
,20,r2126,19,a202126,18,dih23,0\ H,21,r2227,20,a212227,19,dih24,0\ \r13=
1.66365811\ r14=1.46366351\ r35=1.42168061\ r26=1.37146014\ r67=1.38132288
\ r78=1.3857448\ r89=1.38737806\ r910=1.32830788\ r511=1.08416861\ r512=1.0
8681397\ r713=1.077943\ r814=1.0752927\ r915=1.07733185\ r1718=1.38073524\

r1819=1.38690997\r1920=1.38389512\r2021=1.38673348\r2122=1.3830821\r1823=1.07489352\r1924=1.07669745\r2025=1.07646002\r2126=1.07663577\r2227=1.07619127\ra213=86.58785044\ra214=100.172032\ra135=118.58503907\ra126=110.45582242\ra267=117.23206579\ra678=117.56594203\ra789=119.40587481\ra8910=123.04971803\ra6511=112.72235742\ra6512=111.72940995\ra6713=121.64070652\ra7814=120.83271387\ra8915=120.5217029\ra4117=101.96205623\ra11718=118.1017733\ra171819=118.81003399\ra181920=120.32289323\ra192021=120.08732539\ra202122=120.06737503\ra171823=119.74439154\ra181924=119.58217607\ra192025=119.99314189\ra202126=120.11874725\ra212227=120.38552446\rdih1=114.10117135\rdih2=18.46195863\rdih3=-8.75037051\rdih4=179.09513795\rdih5=-0.82277389\rdih6=-0.21382405\rdih7=0.35978643\rdih8=131.51340415\rdih9=-105.45444109\rdih10=179.25559056\rdih11=180.35855166\rdih12=180.65980226\rdih14=185.06202125\rdih15=209.02332463\rdih16=173.12004727\rdih17=-0.73008915\rdih18=-0.15132595\rdih19=-0.04404745\rdih20=-7.96989044\rdih21=179.04514931\rdih22=180.0542803\rdih23=180.02282823\rdih24=179.9265635\r12=1.93368726\r117=1.88142768\\Version=EM64L-G03RevE.01\\State=2-A\\HF=-1066.2960867\\RMSD=5.543e-09\\RMSF=7.267e-06\\Thermal=0.\\Dipole=1.2933021,0.7862703,1.0987883\\PG=C01 [X(C12H10N1O2S1)]\\@

Transition state **B** (Scheme S1)

ROHF/6-31G*

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1\1\GINC-X82\FTS\ROHF\6-31G(d)\C12H10N1O2S1(2)\SHK563\04-May-2010\1\#\n
ROHF/6-31G* opt=(grad,nofreeze,ts,noeigentest,readfc) optcyc=300 scfcyc=300 geom=checkpoint guess=check freq=noraman\\Louis' hypervalent intermediate pyridyl ts1\\0,2\\S\\C,1,r12\\O,1,r13,2,a213\\O,1,r14,2,a214,3,dih1,0\\C,3,r35,1,a135,2,dih2,0\\C,2,r26,1,a126,3,dih3,0\\C,6,r67,2,a267,1,dih4,0\\C,7,r78,6,a678,2,dih5,0\\C,8,r89,7,a789,6,dih6,0\\N,9,r910,8,a8910,7,dih7,0\\H,5,r511,6,a6511,2,dih8,0\\H,5,r512,6,a6512,2,dih9,0\\H,7,r713,6,a6713,2,dih10,0\\H,8,r814,7,a7814,6,dih11,0\\H,9,r915,8,a8915,7,dih12,0\\C,1,r117,4,a4117,2,dih14,0\\C,16,r1718,1,a11718,2,dih15,0\\C,17,r1819,16,a171819,1,dih16,0\\C,18,r1920,17,a181920,16,dih17,0\\C,19,r2021,18,a192021,17,dih18,0\\C,20,r2122,19,a202122,18,dih19,0\\H,17,r1823,16,a171823,1,dih20,0\\H,18,r1924,17,a181924,16,dih21,0\\H,19,r2025,18,a192025,17,dih22,0\\H,20,r2126,19,a202126,18,dih23,0\\H,21,r2227,20,a212227,19,dih24,0\\r13=1.63050052\\r14=1.45360212\\r35=1.42207317\\r26=1.37247554\\r67=1.38171316\\r78=1.38825366\\r89=1.38634301\\r910=1.3273414\\r511=1.08083726\\r512=1.08290831\\r713=1.07676214\\r814=1.07390955\\r915=1.07510814\\r1718=1.38332689\\r1819=1.38811389\\r1920=1.38384167\\r2021=1.38841591\\r2122=1.38243081\\r1823=1.07247222\\r1924=1.07525768\\r2025=1.07534541\\r2126=1.07522697\\r2227=1.07494436\\a213=85.40040264\\a214=99.19618035\\a135=119.36955074\\a126=107.37658576\\a267=117.11326553\\a678=117.60845193\\a789=119.18023769\\a8910=123.26363405\\a6511=112.98508918\\a6512=111.96877128\\a6713=121.71765102\\a7814=120.90710326\\a8915=120.42942118\\a4117=103.936236\\a11718=119.16344616\\a171819=119.18466586\\a181920=120.24895817\\a192021=120.12662098\\a202122=119.97522844\\a171823=119.69807625\\a181924=119.64386437\\a192025=119.99439219\\a202126=120.135449\\a212227=120.18858268\\dih1=111.66160927\\dih2=23.71579507\\dih3=-11.31935141\\dih4=178.8593552\\dih5=-0.66468126\\dih6=-0.20187165\\dih7=0.27903771\\dih8=134.40080252\\dih9=-102.11557021\\dih10=179.51024564\\dih11=180.31193532\\dih12=180.58111796\\dih14=186.15994064\\dih15=207.96346125\\dih16=174.8466719\\dih17=-0.5413254\\dih18=-0.14898668\\dih19=0.04265149\\dih20=-5.79591957\\dih21=179.35430532\\dih22=180.07449321\\dih23=180.11178011\\dih24=179.92464323\\r17=1.82918033\\r12=2.04899838\\Version=EM64L-G03RevE.01\\State=2-A\\HF=-1061.7390218\\RMSD=1.416e-09\\RMSF=2.965e-06\\Thermal=0.\\Dipole=1.3030504,0.8459807,0.804209\\PG=C01 [X(C12H10N1O2S1)]\\@
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ROHF/6-311G**

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1\1\GINC-X120\FTS\ROHF\6-311G(d,p)\C12H10N1O2S1(2)\SHK563\06-May-2010\1\#\n
ROHF/6-311G** opt=(grad,nofreeze,ts,noeigentest,readfc) optcyc=300 scfcyc=300 geom=checkpoint guess=check freq=noraman\\Louis' hypervalent intermediate pyridyl ts1\\0,2\\S\\C,1,r12\\O,1,r13,2,a213\\O,1,r14,2,a214,3,dih1,0\\C,3,r35,1,a135,2,dih2,0\\C,2,r26,1,a126,3,dih3,0\\C,6,r67,2,a267,1,dih4,0\\C,7,r78,6,a678,2,dih5,0\\C,8,r89,7,a789,6,dih6,0\\N,9,r910,8,a8910,7,dih7,0\\H,5,r511,6,a6511,2,dih8,0\\H,5,r512,6,a6512,2,dih9,0\\H,7,r713,6,a6713,2,dih10,0\\H,8,r814,7,a7814,6,dih11,0\\H,9,r915,8,a8915,7,dih12,0\\C,1,r117,4,a4117,2,dih14,0\\C,16,r1718,1,a11718,2,dih15,0\\C,17,r1819,16,a171819,1,dih16,0\\C,18,r1920,17,a181920,16,dih17,0\\C,19,r2021,18,a192021,17,dih18,0\\C,20,r2122,19,a202122,18,dih19,0\\H,17,r1823,16,a171823,1,dih20,0\\H,18,r1924,17,a181924,16,dih21,0\\H,19,r2025,18,a192025,17,dih22,0\\H,20,r2126,19,a202126,18,dih23,0\\H,21,r2227,20,a212227,19,dih24,0\\r13=1.62385874\\r14=1.44772973\\r35=1.42047564\\r26=1.37160035\\r67=1.38027445\\r78=1.38776068\\r89=1.38549878\\r910=1.32650641\\r511=1.08080932\\r512=1.08370355\\r713=1.07689083\\r814=1.07395098\\r915=1.07565398\\r1718=1.38147328\\r1819=1.38755612\\r1920=1.38309526\\r2021=1.38762117\\r2122=1.38164676\\r1823=1.07271156\\r1924=1.0753262\\r2025=1.07542527\\r2126=1.07524514\\r2227=1.07555367\\a213=85.3222376\\a214=99.16587785\\a135=119.28892678\\a126=107.58478251\\a267=117.05225638\\a678=117.57992215\\a789=119.22389292\\a8910=123.21687718\\a6511=112.9761685\\a6512=111.73843001\\a6713=121.73086197\\a7814=120.90141982\\a8915=120.42727823\\a4117=103.48842343\\a11718=119.46391904\\a171819=119.03138644\\a181920=120.27742289\\a192021=120.15609707\\a202122=119.922841\\a171823=119.63226371\\a181924
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=119.6228162\ a192025=119.97186558\ a202126=120.16202335\ a212227=120.15973111\ dih1=111.20355219\ dih2=25.08903021\ dih3=-12.51811934\ dih4=179.45328719\ dih5=-0.63958293\ dih6=-0.24335337\ dih7=0.32840844\ dih8=134.36154728\ dih9=-101.90405564\ dih10=179.54999897\ dih11=180.2924601\ dih12=180.60572112\ dih14=185.63484357\ dih15=201.56016059\ dih16=175.39490267\ dih17=-0.45108019\ dih18=-0.13285364\ dih19=0.02475645\ dih20=-5.05738037\ dih21=179.47908078\ dih22=180.08780514\ dih23=180.13188189\ dih24=180.00098479\ r117=1.83743121\ r12=2.0355372\ \Version=EM64L-G03RevE.01\ State=2-A\ HF=-1061.9015099\ RMSD=5.466e-09\ RMSF=4.603e-06\ Thermal=0.\ Dipole=1.3072431,0.8453234,0.8307913\ PG=C01 [X(C12H10N1O2S1)]\ \e

ROBHandHLYP/6-311G**

1\1\GINC-X89\FTS\ROBHandHLYP\6-311G(d,p)\C12H10N1O2S1(2)\SHK563\12-May-2010\1\#\ ROBHandHLYP/6-311G** opt=(grad,nofreeze,ts,noeigentest,readfc) optcyc=300 scfcyc=300 geom=checkpoint guess=check freq=noraman\ \Louis' hypervalent intermediate pyridyl ts1\ \0,2\ S\ C,1, r12\ O,1, r13,2, a213\ O,1, r14,2, a214,3, dih1,0\ C,3, r35,1, a135,2, dih2,0\ C,2, r26,1, a126,3, dih3,0\ C,6, r67,2, a267,1, dih4,0\ C,7, r78,6, a678,2, dih5,0\ C,8, r89,7, a789,6, dih6,0\ N,9, r910,8, a8910,7, dih7,0\ H,5, r511,6, a6511,2, dih8,0\ H,5, r512,6, a6512,2, dih9,0\ H,7, r713,6, a6713,2, dih10,0\ H,8, r814,7, a7814,6, dih11,0\ H,9, r915,8, a8915,7, dih12,0\ C,1, r117,4, a4117,2, dih14,0\ C,16, r1718,1, a1718,2, dih15,0\ C,17, r1819,16, a171819,1, dih16,0\ C,18, r1920,17, a181920,16, dih17,0\ C,19, r2021,18, a192021,17, dih18,0\ C,20, r2122,19, a202122,18, dih19,0\ H,17, r1823,16, a171823,1, dih20,0\ H,18, r1924,17, a181924,16, dih21,0\ H,19, r2025,18, a192025,17, dih22,0\ H,20, r2126,19, a202126,18, dih23,0\ H,21, r2227,20, a212227,19, dih24,0\ \r13=1.65968566\ r14=1.46207681\ r35=1.42269274\ r26=1.37228444\ r67=1.38060994\ r78=1.38750327\ r89=1.38408676\ r910=1.33245818\ r511=1.08326036\ r512=1.08672424\ r713=1.07819002\ r814=1.07524468\ r915=1.07721552\ r1718=1.38066715\ r1819=1.385636\ r1920=1.3833778\ r2021=1.38619922\ r2122=1.38195229\ r1823=1.07505582\ r1924=1.07649337\ r2025=1.07639409\ r2126=1.07643351\ r2227=1.07612398\ a213=84.70968406\ a214=98.8739911\ a135=118.25408228\ a126=106.67545264\ a267=116.69808143\ a678=117.81826009\ a789=119.41497004\ a8910=122.72343819\ a6511=112.75473685\ a6512=111.25665724\ a6713=121.51287666\ a7814=120.77675885\ a8915=120.7829572\ a4117=103.41671254\ a1718=118.19762047\ a171819=118.89412835\ a181920=120.25417264\ a192021=120.15887503\ a202122=120.04976242\ a171823=119.43862739\ a181924=119.64190885\ a192025=119.95953842\ a202126=120.11772109\ a212227=120.47783408\ dih1=111.83365165\ dih2=25.46506022\ dih3=-12.42881136\ dih4=179.10533272\ dih5=-0.6572966\ dih6=-0.15865294\ dih7=0.2605619\ dih8=136.46043214\ dih9=-100.7881232\ dih10=179.51728464\ dih11=180.37000979\ dih12=180.54611828\ dih14=183.70156529\ dih15=204.44190829\ dih16=174.17593496\ dih17=-0.64115176\ dih18=-0.03185342\ dih19=-0.08773079\ dih20=-6.90617525\ dih21=179.18159951\ dih22=180.11108692\ dih23=179.90725001\ dih24=179.64061688\ r117=1.84576476\ r12=2.08505809\ \Version=EM64L-G03RevE.01\ State=2-A\ HF=-1066.2822372\ RMSD=5.530e-09\ RMSF=1.010e-05\ Thermal=0.\ Dipole=1.2300895,0.7583544,0.8063724\ PG=C01 [X(C12H10N1O2S1)]\ \e

ROBHandHLYP/6-311++G**

1\1\GINC-X102\FTS\ROBHandHLYP\6-311++G(d,p)\C12H10N1O2S1(2)\SHK563\14-Jun-2010\1\#\ ROBHandHLYP/6-311++G** opt=(maxstep=15,grad,nofreeze,ts,noeigentest,readfc) optcyc=300 scfcyc=300 geom=checkpoint guess=check freq=noraman\ \Louis' hypervalent intermediate pyridyl ts1\ \0,2\ S\ C,1, r12\ O,1, r13,2, a213\ O,1, r14,2, a214,3, dih1,0\ C,3, r35,1, a135,2, dih2,0\ C,2, r26,1, a126,3, dih3,0\ C,6, r67,2, a267,1, dih4,0\ C,7, r78,6, a678,2, dih5,0\ C,8, r89,7, a789,6, dih6,0\ N,9, r910,8, a8910,7, dih7,0\ H,5, r511,6, a6511,2, dih8,0\ H,5, r512,6, a6512,2, dih9,0\ H,7, r713,6, a6713,2, dih10,0\ H,8, r814,7, a7814,6, dih11,0\ H,9, r915,8, a8915,7, dih12,0\ C,1, r117,4, a4117,2, dih14,0\ C,16, r1718,1, a1718,2, dih15,0\ C,17, r1819,16, a171819,1, dih16,0\ C,18, r1920,17, a181920,16, dih17,0\ C,19, r2021,18, a192021,17, dih18,0\ C,20, r2122,19, a202122,18, dih19,0\ H,17, r1823,16, a171823,1, dih20,0\ H,18, r1924,17, a181924,16, dih21,0\ H,19, r2025,18, a192025,17, dih22,0\ H,20, r2126,19, a202126,18, dih23,0\ H,21, r2227,20, a212227,19, dih24,0\ \r13=1.66123986\ r14=1.46402874\ r35=1.42273961\ r26=1.3720946\ r67=1.38132012\ r78=1.38785459\ r89=1.38472145\ r910=1.33272754\ r511=1.08365288\ r512=1.08696215\ r713=1.0783007

2\r814=1.07531172\r915=1.07714373\r1718=1.38083859\r1819=1.38645643\r1
920=1.38385321\r2021=1.38680511\r2122=1.38253565\r1823=1.07515051\r192
4=1.07654545\r2025=1.07646507\r2126=1.07645636\r2227=1.076393\ra213=84.
7879301\ra214=98.79684424\ra135=118.85527465\ra126=106.46913058\ra267=116.
54859326\ra678=117.89236842\ra789=119.4097782\ra8910=122.64120342\ra6511=1
12.59794267\ra6512=111.31660646\ra6713=121.48079457\ra7814=120.77846076\ra
8915=120.80389771\ra4117=103.47985135\ra11718=118.46601884\ra171819=118.8
6091107\ra181920=120.26983622\ra192021=120.15696616\ra202122=120.02669432
\ra171823=119.57041382\ra181924=119.63058011\ra192025=119.96076985\ra20212
6=120.13089107\ra212227=120.40286613\rdih1=111.83872407\rdih2=23.47559575
\rdih3=-11.11384504\rdih4=178.81553056\rdih5=-0.70902255\rdih6=-0.21683926
\rdih7=0.33961687\rdih8=135.49818861\rdih9=-101.94959814\rdih10=179.470704
27\rdih11=180.35499282\rdih12=180.58254823\rdih14=183.75701013\rdih15=201.
81815417\rdih16=174.46416397\rdih17=-0.61196772\rdih18=-0.14892526\rdih19=
-0.06584841\rdih20=-6.3505768\rdih21=179.25774533\rdih22=180.08568223\rdih
23=180.08384306\rdih24=179.98751567\r117=1.84350802\r12=2.09559724\\Ver
sion=EM64L-G03RevE.01\State=2-A\HF=-1066.295387\RMSE=4.255e-09\RMSEF=6.
008e-06\Thermal=0.\Dipole=1.2896739,0.7709096,0.8088592\PG=C01 [X(C12H
10N1O2S1)]\@

Transition state C (Scheme S1)

ROHF/6-31G*

```
1\1\GINC-X88\FTS\ROHF\6-31G(d)\C12H10N1O2S1(2)\SHK563\04-May-2010\1\#\n
ROHF/6-31G* opt=(nofreeze,grad,ts,noeigentest,readfc) optcyc=300 scfcyc=300 geom=checkpoint guess=check freq=noraman\\Louis' hypervalent in
termediate pyridyl ts2\\0,2\\S\\C,1,r12\\O,1,r13,2,a213\\O,1,r14,2,a214,3,
dih1,0\\C,3,r35,1,a135,2,dih2,0\\C,2,r26,1,a126,3,dih3,0\\C,6,r67,2,a267,
1,dih4,0\\C,7,r78,6,a678,2,dih5,0\\C,8,r89,7,a789,6,dih6,0\\N,9,r910,8,a8
910,7,dih7,0\\H,5,r511,6,a6511,2,dih8,0\\H,5,r512,6,a6512,2,dih9,0\\H,7,r
713,6,a6713,2,dih10,0\\H,8,r814,7,a7814,6,dih11,0\\H,9,r915,8,a8915,7,di
h12,0\\C,1,r117,4,a4117,2,dih14,0\\C,16,r1718,1,a11718,2,dih15,0\\C,17,r1
819,16,a171819,1,dih16,0\\C,18,r1920,17,a181920,16,dih17,0\\C,19,r2021,1
8,a192021,17,dih18,0\\C,20,r2122,19,a202122,18,dih19,0\\H,17,r1823,16,a1
71823,1,dih20,0\\H,18,r1924,17,a181924,16,dih21,0\\H,19,r2025,18,a192025
,17,dih22,0\\H,20,r2126,19,a202126,18,dih23,0\\H,21,r2227,20,a212227,19,
dih24,0\\r13=1.63133537\\r14=1.45386653\\r35=1.42138891\\r26=1.37341048\\r
67=1.38284534\\r78=1.38486436\\r89=1.38963226\\r910=1.32184083\\r511=1.080
88875\\r512=1.08296324\\r713=1.07606719\\r814=1.07386964\\r915=1.07490872\\
r1718=1.37774122\\r1819=1.38969461\\r1920=1.38565869\\r2021=1.38768589\\r2
122=1.38643748\\r1823=1.0728153\\r1924=1.07581483\\r2025=1.07547166\\r2126
=1.07579907\\r2227=1.07539183\\a213=88.13433194\\a214=102.43918186\\a135=1
17.54667421\\a126=111.54841342\\a267=117.73262005\\a678=117.35499127\\a789
=119.29525958\\a8910=123.4086538\\a6511=113.27848531\\a6512=112.32367392\\
a6713=121.79852421\\a7814=120.91729365\\a8915=120.29220424\\a4117=98.9204
3933\\a11718=118.37939842\\a171819=118.19244391\\a181920=120.32653011\\a19
2021=120.24297855\\a202122=119.98379964\\a171823=120.41869207\\a181924=11
9.68033164\\a192025=119.91061113\\a202126=120.08082465\\a212227=120.55244
016\\dih1=112.67657613\\dih2=22.14680684\\dih3=-12.41636579\\dih4=181.6210
9597\\dih5=-0.77689089\\dih6=0.04134933\\dih7=0.32383248\\dih8=130.0464959
3\\dih9=-105.75397407\\dih10=179.3920145\\dih11=180.40829587\\dih12=180.47
838665\\dih14=185.35872535\\dih15=205.59497652\\dih16=175.25645125\\dih17=
-0.6045242\\dih18=-0.17407018\\dih19=0.03164139\\dih20=-5.44738695\\dih21=
179.32672099\\dih22=180.06917052\\dih23=180.1787291\\dih24=180.09765063\\r
12=1.83620309\\r117=2.07636159\\Version=EM64L-G03RevE.01\\State=2-A\\HF=-
1061.7372173\\RMSD=9.848e-09\\RMSF=2.425e-06\\Thermal=0.\\Dipole=1.2906177
,0.6563684,1.5059506\\PG=C01 [X(C12H10N1O2S1)]\\@
```

ROHF/6-311G**

```
1\1\GINC-X85\FTS\ROHF\6-311G(d,p)\C12H10N1O2S1(2)\SHK563\06-May-2010\1\
\\# ROHF/6-311G** opt=(nofreeze,grad,ts,noeigentest,readfc) optcyc=300
scfcyc=300 geom=checkpoint guess=check freq=noraman\\Louis' hypervale
nt intermediate pyridyl ts2\\0,2\\S\\C,1,r12\\O,1,r13,2,a213\\O,1,r14,2,a2
14,3,dih1,0\\C,3,r35,1,a135,2,dih2,0\\C,2,r26,1,a126,3,dih3,0\\C,6,r67,2,
a267,1,dih4,0\\C,7,r78,6,a678,2,dih5,0\\C,8,r89,7,a789,6,dih6,0\\N,9,r910
,8,a8910,7,dih7,0\\H,5,r511,6,a6511,2,dih8,0\\H,5,r512,6,a6512,2,dih9,0\\
H,7,r713,6,a6713,2,dih10,0\\H,8,r814,7,a7814,6,dih11,0\\H,9,r915,8,a8915
,7,dih12,0\\C,1,r117,4,a4117,2,dih14,0\\C,16,r1718,1,a11718,2,dih15,0\\C,
17,r1819,16,a171819,1,dih16,0\\C,18,r1920,17,a181920,16,dih17,0\\C,19,r2
021,18,a192021,17,dih18,0\\C,20,r2122,19,a202122,18,dih19,0\\H,17,r1823,
16,a171823,1,dih20,0\\H,18,r1924,17,a181924,16,dih21,0\\H,19,r2025,18,a1
92025,17,dih22,0\\H,20,r2126,19,a202126,18,dih23,0\\H,21,r2227,20,a21222
7,19,dih24,0\\r13=1.62321592\\r14=1.44793928\\r35=1.4196019\\r26=1.372132
25\\r67=1.38158205\\r78=1.38441028\\r89=1.38873051\\r910=1.32109488\\r511=1
.08085003\\r512=1.08375367\\r713=1.07624432\\r814=1.07394265\\r915=1.07549
125\\r1718=1.37681486\\r1819=1.38885297\\r1920=1.38503442\\r2021=1.3867057
\\r2122=1.38565811\\r1823=1.07298432\\r1924=1.07587031\\r2025=1.07550466\\r
2126=1.07578324\\r2227=1.0759581\\a213=87.92376615\\a214=102.10576082\\a13
5=117.67243812\\a126=111.19497271\\a267=117.59374537\\a678=117.36908277\\a
789=119.32249924\\a8910=123.33590876\\a6511=113.19357551\\a6512=112.04007
776\\a6713=121.79374975\\a7814=120.91001334\\a8915=120.30561324\\a4117=98.
78659943\\a11718=118.95224648\\a171819=118.09138708\\a181920=120.35808061
\\a192021=120.26432072\\a202122=119.93805142\\a171823=120.30960239\\a18192
```

4=119.64882817\ a192025=119.89081221\ a202126=120.10693258\ a212227=120.5
0289392\ dihl=111.99455751\ dihl2=23.416141\ dihl3=-13.37786642\ dihl4=181.90
589957\ dihl5=-0.73907548\ dihl6=-0.01873458\ dihl7=0.37619942\ dihl8=130.3417
9531\ dihl9=-105.32580641\ dihl10=179.44863134\ dihl11=180.38021922\ dihl12=18
0.5030022\ dihl14=184.90267875\ dihl15=194.71885673\ dihl16=176.31360328\ dihl
17=-0.4615499\ dihl18=-0.16929147\ dihl19=0.02977192\ dihl20=-3.96423961\ dihl
21=179.54812789\ dihl22=180.09028621\ dihl23=180.23953663\ dihl24=180.234807
34\ r12=1.84476791\ r117=2.06570079\ \Version=EM64L-G03RevE.01\ State=2-A\
HF=-1061.8998753\ RMSD=3.651e-09\ RMSF=2.271e-05\ Thermal=0.\ Dipole=1.303
1215,0.6677252,1.4805426\ PG=C01 [X(C12H10N1O2S1)]\ \@

ROBHandHLYP/6-311G**

1\1\GINC-X95\FTS\ROBHandHLYP\6-311G(d,p)\C12H10N1O2S1(2)\SHK563\13-May
-2010\1\1\# ROBHandHLYP/6-311G** opt=(nofreeze,grad,ts,noeigentest,read
fc) optcyc=300 scfcyc=300 geom=checkpoint guess=check freq=noraman\ \Lo
uis' hypervalent intermediate pyridyl ts2\ \0,2\ S\ C,1, r12\ O,1, r13,2, a21
3\ O,1, r14,2, a214,3, dihl,0\ C,3, r35,1, a135,2, dihl2,0\ C,2, r26,1, a126,3, dihl
3,0\ C,6, r67,2, a267,1, dihl4,0\ C,7, r78,6, a678,2, dihl5,0\ C,8, r89,7, a789,6, dihl
6,0\ N,9, r910,8, a8910,7, dihl7,0\ H,5, r511,6, a6511,2, dihl8,0\ H,5, r512,6, a
6512,2, dihl9,0\ H,7, r713,6, a6713,2, dihl10,0\ H,8, r814,7, a7814,6, dihl11,0\ H,
9, r915,8, a8915,7, dihl12,0\ C,1, r117,4, a4117,2, dihl14,0\ C,16, r1718,1, a171
8,2, dihl15,0\ C,17, r1819,16, a171819,1, dihl16,0\ C,18, r1920,17, a181920,16, dihl
17,0\ C,19, r2021,18, a192021,17, dihl18,0\ C,20, r2122,19, a202122,18, dihl19,
0\ H,17, r1823,16, a171823,1, dihl20,0\ H,18, r1924,17, a181924,16, dihl21,0\ H,
19, r2025,18, a192025,17, dihl22,0\ H,20, r2126,19, a202126,18, dihl23,0\ H,21, r
2227,20, a212227,19, dihl24,0\ \r13=1.65728573\ r14=1.46260579\ r35=1.423494
99\ r26=1.3751507\ r67=1.38054604\ r78=1.38466656\ r89=1.38696745\ r910=1.3
2659173\ r511=1.08331158\ r512=1.08665561\ r713=1.07737008\ r814=1.0752347
8\ r915=1.07720377\ r1718=1.37158349\ r1819=1.38912988\ r1920=1.38486817\ r
2021=1.38570719\ r2122=1.38725117\ r1823=1.07544985\ r1924=1.07713594\ r20
25=1.07647358\ r2126=1.0770762\ r2227=1.07691744\ a213=87.60261816\ a214=1
02.37899294\ a135=116.55022488\ a126=111.27040073\ a267=117.40230494\ a678
=117.52175172\ a789=119.49701083\ a8910=123.16207466\ a6511=113.05800188\
a6512=111.7323609\ a6713=121.64838496\ a7814=120.78589567\ a8915=120.4986
5659\ a4117=97.50496771\ a11718=117.05083123\ a171819=117.50280268\ a18192
0=120.29565083\ a192021=120.40441836\ a202122=120.01176378\ a171823=120.5
0843399\ a181924=119.65478944\ a192025=119.81812935\ a202126=120.112463\ a
212227=120.84163053\ dihl1=112.32310797\ dihl2=23.85119856\ dihl3=-14.132016
99\ dihl4=182.76282841\ dihl5=-0.7794007\ dihl6=0.12770155\ dihl7=0.35156489\
dihl8=130.68493681\ dihl9=-105.71830062\ dihl10=179.41026486\ dihl11=180.46925
769\ dihl12=180.41835356\ dihl14=182.24105118\ dihl15=192.37584772\ dihl16=175
.97641576\ dihl17=-0.46080978\ dihl18=-0.09752775\ dihl19=-0.02326747\ dihl20=
-4.49267523\ dihl21=179.49048321\ dihl22=180.11287371\ dihl23=180.10418884\
dihl24=180.00649379\ r12=1.8507184\ r117=2.17152088\ \Version=EM64L-G03RevE
.01\ State=2-A\ HF=-1066.2792724\ RMSD=8.769e-09\ RMSF=8.666e-06\ Thermal=0
. \Dipole=1.2209778,0.5434374,1.4903609\ PG=C01 [X(C12H10N1O2S1)]\ \@

ROBHandHLYP/6-311++G**

1\1\GINC-X102\FTS\ROBHandHLYP\6-311++G(d,p)\C12H10N1O2S1(2)\SHK563\14-
Jun-2010\1\1\# ROBHandHLYP/6-311++G** opt=(maxstep=15,nofreeze,grad,ts,
noeigentest,readfc) optcyc=300 scfcyc=300 geom=checkpoint guess=check
freq=noraman\ \Louis' hypervalent intermediate pyridyl ts2\ \0,2\ S\ C,1, r
12\ O,1, r13,2, a213\ O,1, r14,2, a214,3, dihl,0\ C,3, r35,1, a135,2, dihl2,0\ C,2,
r26,1, a126,3, dihl3,0\ C,6, r67,2, a267,1, dihl4,0\ C,7, r78,6, a678,2, dihl5,0\ C,
8, r89,7, a789,6, dihl6,0\ N,9, r910,8, a8910,7, dihl7,0\ H,5, r511,6, a6511,2, dihl
8,0\ H,5, r512,6, a6512,2, dihl9,0\ H,7, r713,6, a6713,2, dihl10,0\ H,8, r814,7, a7
814,6, dihl11,0\ H,9, r915,8, a8915,7, dihl12,0\ C,1, r117,4, a4117,2, dihl14,0\ C,
16, r1718,1, a1718,2, dihl15,0\ C,17, r1819,16, a171819,1, dihl16,0\ C,18, r1920
17, a181920,16, dihl17,0\ C,19, r2021,18, a192021,17, dihl18,0\ C,20, r2122,19,
a202122,18, dihl19,0\ H,17, r1823,16, a171823,1, dihl20,0\ H,18, r1924,17, a1819
24,16, dihl21,0\ H,19, r2025,18, a192025,17, dihl22,0\ H,20, r2126,19, a202126,1
8, dihl23,0\ H,21, r2227,20, a212227,19, dihl24,0\ \r13=1.65885646\ r14=1.46464
834\ r35=1.4236796\ r26=1.375138\ r67=1.3811482\ r78=1.38480897\ r89=1.3878
0316\ r910=1.32654815\ r511=1.08369279\ r512=1.08683261\ r713=1.07745118\ r

814=1.07532527\r915=1.07719227\r1718=1.37179941\r1819=1.38996759\r1920=1.38541276\r2021=1.38627395\r2122=1.38805261\r1823=1.07550645\r1924=1.07717307\r2025=1.07651204\r2126=1.07709098\r2227=1.07699209\ra213=87.777214\ra214=102.52097586\ra135=116.81191035\ra126=111.30731024\ra267=117.35478631\ra678=117.55404811\ra789=119.48797835\ra8910=123.13159341\ra6511=112.97242885\ra6512=111.83590094\ra6713=121.63117301\ra7814=120.79396496\ra8915=120.48836494\ra4117=97.35855432\ra11718=117.17051708\ra171819=117.45784834\ra181920=120.3175336\ra192021=120.38842199\ra202122=120.01228023\ra171823=120.68374293\ra181924=119.6277806\ra192025=119.82580411\ra202126=120.13098079\ra212227=120.80166233\rdih1=112.39921721\rdih2=22.41551237\rdih3=-13.14199537\rdih4=182.66920373\rdih5=-0.9117418\rdih6=0.1548406\rdih7=0.37719935\rdih8=130.03276335\rdih9=-106.44614436\rdih10=179.31261903\rdih11=180.45838721\rdih12=180.45068722\rdih14=182.37569977\rdih15=190.57199378\rdih16=175.87641185\rdih17=-0.49177557\rdih18=-0.18335739\rdih19=-0.02759353\rdih20=-4.46631848\rdih21=179.50831871\rdih22=180.1012363\rdih23=180.23929848\rdih24=180.30856872\r12=1.84918763\r117=2.17535902\\Version=EM64L-G03RevE.01\State=2-A\HF=-1066.2924608\RMSD=6.805e-09\RMSF=1.366e-05\Thermal=0.\Dipole=1.2717786,0.5483546,1.4967238\PG=C01 [X(C12H10N1O2S1)]\@

Sultine 17

ROHF/6-31G*

```
1\1\GINC-X126\FOpt\ROHF\6-31G(d)\C6H5N1O2S1\SHK563\14-Apr-2010\1\#\ ro
hf/6-31G* opt=grad optcyc=300 scfcyc=300 geom=checkpoint guess=check f
req=noraman\Louis' cyclic sultine pyridyl\0,1\SC,1,r12\O,1,r13,2,a2
13\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,3,di
h3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a789,6,
dih6,0\N,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r512,6,
a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11,0\H
,9,r915,8,a8915,7,dih12,0\|r12=1.79523142\r13=1.63483218\r14=1.4534280
5\r35=1.42171634\r26=1.37598628\r67=1.38327585\r78=1.38434611\r89=1.38
978155\r910=1.3211771\r511=1.08059086\r512=1.08296096\r713=1.07565148\
r814=1.0738424\r915=1.07458072\|a213=88.98733368\|a214=105.87212557\|a135
=115.99863696\|a126=111.11943842\|a267=117.44133793\|a678=117.47129326\|a
789=119.44060329\|a8910=123.26437296\|a6511=113.17467044\|a6512=112.226374
13\|a6713=121.70749964\|a7814=120.84123935\|a8915=120.4002413\|dih1=110.73
125788\|dih2=25.78011178\|dih3=-16.15849545\|dih4=184.15449155\|dih5=-0.75
583512\|dih6=0.33906925\|dih7=0.3519718\|dih8=129.39375755\|dih9=-106.3874
5971\|dih10=179.55316991\|dih11=180.50663667\|dih12=180.24443849\|Version
=EM64L-G03RevE.01\State=1-A\HF=-831.7239901\RMSD=9.497e-09\RMSF=4.081e
-05\Thermal=0.\Dipole=1.292177,0.4364759,2.1468426\PG=C01 [X(C6H5N1O2S
1)]\@
```

ROHF/6-311G**

```
1\1\GINC-X126\FOpt\ROHF\6-311G(d,p)\C6H5N1O2S1\SHK563\14-Apr-2010\1\#\
rohf/6-311G** opt=grad optcyc=300 scfcyc=300 geom=checkpoint guess=ch
eck freq=noraman\Louis' cyclic sultine pyridyl\0,1\SC,1,r12\O,1,r13
,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126
,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a7
89,6,dih6,0\N,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r5
12,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih1
1,0\H,9,r915,8,a8915,7,dih12,0\|r12=1.79776246\r13=1.62653943\r14=1.44
813856\r35=1.41985107\r26=1.37458408\r67=1.38214787\r78=1.38359763\r89
=1.38914685\r910=1.32010822\r511=1.08060148\r512=1.08370844\r713=1.075
80781\r814=1.07393114\r915=1.07516245\|a213=88.91370776\|a214=105.356110
88\|a135=116.0768479\|a126=110.80933616\|a267=117.30940208\|a678=117.48309
104\|a789=119.46792979\|a8910=123.20108915\|a6511=113.09683099\|a6512=111.
91420187\|a6713=121.70228774\|a7814=120.83277443\|a8915=120.40192056\|dih1
=110.20247362\|dih2=26.69684162\|dih3=-16.99945201\|dih4=184.77943132\|dih
5=-0.73758656\|dih6=0.3521402\|dih7=0.35422582\|dih8=129.38080775\|dih9=-1
06.2528952\|dih10=179.55408787\|dih11=180.48960911\|dih12=180.22129359\|V
ersion=EM64L-G03RevE.01\State=1-A\HF=-831.838158\RMSD=4.637e-09\RMSF=2
.651e-05\Thermal=0.\Dipole=1.2875013,0.458135,2.1702696\PG=C01 [X(C6H5
N1O2S1)]\@
```

ROBHandHLYP/6-311G**

```
1\1\GINC-X117\FOpt\ROBHandHLYP\6-311G(d,p)\C6H5N1O2S1\SHK563\15-Apr-20
10\1\#\ ROBHandHLYP/6-311G** opt=grad optcyc=300 scfcyc=300 geom=check
point guess=check freq=noraman\Louis' cyclic sultine pyridyl\0,1\SC
,1,r12\O,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\
C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,
0\C,8,r89,7,a789,6,dih6,0\N,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2
,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,
7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\|r12=1.81003117\r13=1.658
22539\r14=1.46179459\r35=1.42499722\r26=1.37791986\r67=1.38052175\r78=
1.38421588\r89=1.38705361\r910=1.32591716\r511=1.08300444\r512=1.08648
854\r713=1.07699603\r814=1.07524923\r915=1.0769981\|a213=88.3112354\|a21
4=105.00082692\|a135=115.11886557\|a126=110.93000822\|a267=117.24278402\|a
678=117.60135408\|a789=119.59924254\|a8910=123.12297461\|a6511=113.051449
9\|a6512=111.67295628\|a6713=121.59871449\|a7814=120.72749536\|a8915=120.5
3639006\|dih1=110.61352233\|dih2=27.29114424\|dih3=-17.98761546\|dih4=185.
77650182\|dih5=-0.75834535\|dih6=0.43985136\|dih7=0.39412324\|dih8=129.547
```

79805\ dih9=-106.68626123\ dih10=179.55932285\ dih11=180.54129547\ dih12=180.19132696\\ Version=EM64L-G03RevE.01\ State=1-A\ HF=-834.8198436\ RMSD=7.196e-09\ RMSF=3.407e-05\ Thermal=0.\ Dipole=1.1911658,0.3565962,2.0538604\ PG=C01 [X(C6H5N1O2S1)]\\ @

ROBHandHLYP/6-311++G**

1\1\GINC-X143\FOpt\ROBHandHLYP\6-311++G(d,p)\C6H5N1O2S1\SHK563\16-Apr-2010\1\\# ROBHandHLYP/6-311++G** opt=grad optcyc=300 scfcyc=300 geom=c heckpoint guess=check freq=noraman\\Louis' cyclic sultine pyridyl\\0,1\ S\C,1,r12\O,1,r13,2,a213\O,1,r14,2,a214,3,dih1,0\C,3,r35,1,a135,2,dih2,0\C,2,r26,1,a126,3,dih3,0\C,6,r67,2,a267,1,dih4,0\C,7,r78,6,a678,2,dih5,0\C,8,r89,7,a789,6,dih6,0\N,9,r910,8,a8910,7,dih7,0\H,5,r511,6,a6511,2,dih8,0\H,5,r512,6,a6512,2,dih9,0\H,7,r713,6,a6713,2,dih10,0\H,8,r814,7,a7814,6,dih11,0\H,9,r915,8,a8915,7,dih12,0\\r12=1.811101\r13=1.65890623\r14=1.46422341\r35=1.4253351\r26=1.37798778\r67=1.38119161\r78=1.38424546\r89=1.38784932\r910=1.32575724\r511=1.08330016\r512=1.08659635\r713=1.07705976\r814=1.07532423\r915=1.07694909\ a213=88.40565234\ a214=105.08003993\ a135=115.45844326\ a126=110.93282144\ a267=117.17493537\ a678=117.63760493\ a789=119.59265012\ a8910=123.0864784\ a6511=113.02556773\ a6512=111.82609563\ a6713=121.57563405\ a7814=120.73363321\ a8915=120.53980206\ dih1=110.69646784\ dih2=26.14961437\ dih3=-17.19439215\ dih4=185.91109571\ dih5=-0.98769189\ dih6=0.59246966\ dih7=0.33765376\ dih8=128.90779434\ dih9=-107.28972864\ dih10=179.46223848\ dih11=180.54784156\ dih12=180.18719994\\ Version=EM64L-G03RevE.01\ State=1-A\ HF=-834.8314666\ RMSD=8.324e-09\ RMSF=4.778e-05\ Thermal=0.\ Dipole=1.2420343,0.3763382,2.108562\ PG=C01 [X(C6H5N1O2S1)]\\ @

Radical E (Scheme S1)

ROHF/6-31G*

```
1\1\GINC-X81\FOpt\ROHF\6-31G(d)\C12H10N1O2S1(2)\SHK563\14-Aug-2010\1\
# rohf/6-31G* opt=grad optcyc=300 scfcyc=300 freq=noraman\Louis' biar
yl product pyridyl\0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234,1,dih1
,0\O,4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,di
h4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910,
7,dih7,0\N,10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,r
1213,2,a21213,3,dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,13,
a131415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih14
,0\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,12,r1221
,2,a21221,3,dih17,0\H,13,r1322,12,a121322,2,dih18,0\H,14,r1423,13,a131
423,12,dih19,0\H,15,r1524,14,a141524,13,dih20,0\H,6,r625,7,a7625,1,dih
21,0\H,6,r626,7,a7626,1,dih22,0\O,4,r427,3,a3427,2,dih23,0\|r12=1.5421
6934\r23=1.5169876\r34=1.7697163\r45=1.62159441\r56=1.42452631\r17=1.4
0319933\r78=1.38162653\r89=1.38584685\r910=1.37589265\r1011=1.32381907
\r212=1.51047197\r1213=1.33303229\r1314=1.43362686\r1415=1.42962652\r2
16=1.0891271\r817=1.07595821\r918=1.07384908\r1019=1.07572772\r1221=1.
07341309\r1322=1.07529934\r1423=1.07227118\r1524=1.07684759\r625=1.080
53167\r626=1.07940798\r427=1.46528069\|a123=112.47885145\|a234=120.06127
661\|a345=100.50594239\|a456=118.35765588\|a217=121.95638333\|a178=117.524
3617\|a789=120.29361283\|a8910=117.36750671\|a91011=123.13400224\|a3212=11
0.72423741\|a21213=123.46738621\|a121314=121.3133855\|a131415=118.3865172
8\|a3216=107.36770561\|a7817=119.69049262\|a8918=121.55811233\|a91019=120.
90455351\|a21221=116.25889441\|a121322=119.93770197\|a131423=121.06636158
\|a141524=118.79709411\|a7625=112.39348239\|a7626=109.94982226\|a3427=105.
25564665\|dih1=78.33985814\|dih2=-61.76753672\|dih3=68.76684851\|dih4=-60.
64706382\|dih5=180.36642962\|dih6=0.55912183\|dih7=-0.2520623\|dih8=-0.075
14479\|dih9=202.28497768\|dih10=-11.8919732\|dih11=2.36035618\|dih12=7.791
43738\|dih13=-39.40067509\|dih14=180.51823871\|dih15=179.95665214\|dih16=1
79.92781539\|dih17=170.74155505\|dih18=182.12139203\|dih19=182.41928827\|d
ih20=169.4587541\|dih21=-56.69568332\|dih22=-177.09228546\|dih23=49.20965
024\|Version=EM64L-G03RevE.01\|State=2-A\HF=-1061.7954866\|RMSD=6.175e-0
9\|RMSF=5.803e-05\|Thermal=0.\|Dipole=-0.2391359,-0.9240475,-1.0874317\|PG
=C01 [X(C12H10N1O2S1)]\|@
```

ROHF/6-311G**

```
1\1\GINC-X85\FOpt\ROHF\6-311G(d,p)\C12H10N1O2S1(2)\SHK563\14-Aug-2010\
1\| # rohf/6-311G** opt=grad optcyc=300 scfcyc=300 freq=noraman geom=ch
eckpoint guess=check\Louis' biaryl product pyridyl\0,2\C\C,1,r12\C,2
,r23,1,a123\S,3,r34,2,a234,1,dih1,0\O,4,r45,3,a345,2,dih2,0\C,5,r56,4,
a456,3,dih3,0\C,1,r17,2,a217,3,dih4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,
7,a789,1,dih6,0\C,9,r910,8,a8910,7,dih7,0\N,10,r1011,9,a91011,8,dih8,0
\C,2,r212,3,a3212,4,dih9,0\C,12,r1213,2,a21213,3,dih10,0\C,13,r1314,12
,a121314,2,dih11,0\C,14,r1415,13,a131415,12,dih12,0\H,2,r216,3,a3216,4
,dih13,0\H,8,r817,7,a7817,1,dih14,0\H,9,r918,8,a8918,7,dih15,0\H,10,r1
019,9,a91019,8,dih16,0\H,12,r1221,2,a21221,3,dih17,0\H,13,r1322,12,a12
1322,2,dih18,0\H,14,r1423,13,a131423,12,dih19,0\H,15,r1524,14,a141524,
13,dih20,0\H,6,r625,7,a7625,1,dih21,0\H,6,r626,7,a7626,1,dih22,0\O,4,r
427,3,a3427,2,dih23,0\|r12=1.54184636\r23=1.51584238\r34=1.77061378\r4
5=1.61412031\r56=1.42404825\r17=1.40284211\r78=1.37990593\r89=1.385525
65\r910=1.3746779\r1011=1.3231672\r212=1.50948333\r1213=1.33174688\r13
14=1.43364724\r1415=1.42962911\r216=1.08892273\r817=1.07614139\r918=1.
07382034\r1019=1.07619041\r1221=1.0737557\r1322=1.0753725\r1423=1.0722
935\r1524=1.07700807\r625=1.0816459\r626=1.07914568\r427=1.46085099\|a1
23=112.35377195\|a234=119.88651523\|a345=100.52282176\|a456=119.05435708\
|a217=121.84467347\|a178=117.50291718\|a789=120.25936364\|a8910=117.400489
46\|a91011=123.1023132\|a3212=110.71457483\|a21213=123.41932911\|a121314=1
21.31676432\|a131415=118.39119714\|a3216=107.3086195\|a7817=119.68398924\
|a8918=121.56075841\|a91019=120.90780614\|a21221=116.34482582\|a121322=119
.89125984\|a131423=121.07824044\|a141524=118.91992393\|a7625=112.29703912
\|a7626=109.94195377\|a3427=104.96073425\|dih1=78.68111952\|dih2=-61.43768
```

851\ dih3=68.43057988\ dih4=-61.21528021\ dih5=180.14658617\ dih6=0.742988
15\ dih7=-0.34935287\ dih8=-0.11529584\ dih9=202.68575821\ dih10=-12.04234
947\ dih11=2.29766535\ dih12=8.03914651\ dih13=-39.04922491\ dih14=180.681
89218\ dih15=179.87780104\ dih16=179.92836772\ dih17=170.66229822\ dih18=1
82.17755926\ dih19=182.63738223\ dih20=169.25561675\ dih21=-56.82646971\ d
ih22=-177.34016976\ dih23=49.32665199\ \Version=EM64L-G03RevE.01\State=2
-A\HF=-1061.9585295\RMSD=7.096e-09\RMSF=2.196e-05\Thermal=0.\Dipole=-0
.219518,-0.9676126,-1.1259149\PG=C01 [X(C12H10N1O2S1)]\ \@

ROBHandHLYP/6-311G**

1\1\GINC-X75\FOpt\ROBHandHLYP\6-311G(d,p)\C12H10N1O2S1(2)\SHK563\16-Au
g-2010\1\ \# ROBHandHLYP/6-311G** opt=grad optcyc=300 scfcyc=300 freq=n
oraman geom=checkpoint guess=check\ \Louis' biaryl product pyridyl\ \0,2
\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234,1,dih1,0\O,4,r45,3,a345,2,dih
2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,dih4,0\C,7,r78,1,a178,2,d
ih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910,7,dih7,0\N,10,r1011,9,a
91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,r1213,2,a21213,3,dih10,0
\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,13,a131415,12,dih12,0\H,2,
r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih14,0\H,9,r918,8,a8918,7,d
ih15,0\H,10,r1019,9,a91019,8,dih16,0\H,12,r1221,2,a21221,3,dih17,0\H,1
3,r1322,12,a121322,2,dih18,0\H,14,r1423,13,a131423,12,dih19,0\H,15,r15
24,14,a141524,13,dih20,0\H,6,r625,7,a7625,1,dih21,0\H,6,r626,7,a7626,1
,dih22,0\O,4,r427,3,a3427,2,dih23,0\ \r12=1.53938704\r23=1.50303618\r34
=1.76969002\r45=1.6485315\r56=1.4282305\r17=1.39983936\r78=1.38175496\
r89=1.38249558\r910=1.37678123\r1011=1.32507859\r212=1.49866107\r1213=
1.34490072\r1314=1.41251394\r1415=1.40679051\r216=1.09314847\r817=1.07
742337\r918=1.07520432\r1019=1.07807543\r1221=1.07460317\r1322=1.07660
35\r1423=1.07444161\r1524=1.07850256\r625=1.08569242\r626=1.08165822\r
427=1.47510015\ a123=112.34531961\ a234=119.5975252\ a345=100.17382556\ a4
56=116.89419696\ a217=122.07493025\ a178=117.52282764\ a789=120.22735194\
a8910=117.61806506\ a91011=123.03130081\ a3212=111.01629744\ a21213=122.9
2212568\ a121314=121.44482517\ a131415=119.12157086\ a3216=107.23100891\ a
7817=119.4900839\ a8918=121.49831363\ a91019=120.92072475\ a21221=116.659
21491\ a121322=119.50951308\ a131423=120.59557227\ a141524=119.42736128\ a
7625=112.22461322\ a7626=110.04333606\ a3427=104.66764859\ dih1=79.566541
17\ dih2=-63.50679386\ dih3=69.16786329\ dih4=-61.10369991\ dih5=180.06942
081\ dih6=0.60527532\ dih7=-0.26369262\ dih8=-0.14323892\ dih9=203.3071687
\ dih10=-11.29478124\ dih11=2.67043292\ dih12=6.51330949\ dih13=-37.685061
09\ dih14=180.61249152\ dih15=179.9790917\ dih16=179.91196576\ dih17=172.1
9652028\ dih18=182.44944763\ dih19=181.94430221\ dih20=170.89560068\ dih21
=-55.96007987\ dih22=-176.38013069\ dih23=46.86631714\ \Version=EM64L-G03
RevE.01\State=2-A\HF=-1066.3281852\RMSD=5.622e-09\RMSF=3.902e-05\Therm
al=0.\Dipole=-0.2909318,-0.9040077,-1.0423787\PG=C01 [X(C12H10N1O2S1)]
\ \@

ROBHandHLYP/6-311++G**

1\1\GINC-X76\FOpt\ROBHandHLYP\6-311++G(d,p)\C12H10N1O2S1(2)\SHK563\17-
Aug-2010\1\ \# ROBHandHLYP/6-311++G** opt=grad optcyc=300 scfcyc=300 fr
eq= noraman geom=checkpoint guess=check\ \Louis' biaryl product pyridyl\
\0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234,1,dih1,0\O,4,r45,3,a345,2
,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,dih4,0\C,7,r78,1,a178
,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910,7,dih7,0\N,10,r1011
,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,r1213,2,a21213,3,dih
10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,13,a131415,12,dih12,0\
H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih14,0\H,9,r918,8,a8918
,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,12,r1221,2,a21221,3,dih17,0
\H,13,r1322,12,a121322,2,dih18,0\H,14,r1423,13,a131423,12,dih19,0\H,15
,r1524,14,a141524,13,dih20,0\H,6,r625,7,a7625,1,dih21,0\H,6,r626,7,a76
26,1,dih22,0\O,4,r427,3,a3427,2,dih23,0\ \r12=1.53941025\r23=1.50367174
\r34=1.77159112\r45=1.6491649\r56=1.42767363\r17=1.39982529\r78=1.3819
9433\r89=1.38299569\r910=1.37744068\r1011=1.32550223\r212=1.49869157\r
1213=1.34566719\r1314=1.41259261\r1415=1.40742263\r216=1.09324971\r817
=1.07751412\r918=1.07527005\r1019=1.07805675\r1221=1.07492972\r1322=1.
07667612\r1423=1.0745759\r1524=1.07861487\r625=1.08593879\r626=1.08181

542\r427=1.4770445\al23=112.33611393\al234=120.07024905\al345=100.392539
9\al456=117.2451895\al217=121.83929095\al178=117.58537128\al789=120.164266
28\al8910=117.6399054\al91011=123.03423048\al3212=111.04232929\al21213=122
.93417956\al21314=121.38471283\al131415=119.14825469\al3216=107.50931875
\al7817=119.54672658\al8918=121.50705059\al91019=120.87152145\al21221=116.
69693052\al21322=119.53037803\al131423=120.61273936\al141524=119.3473978
4\al7625=112.27562639\al7626=110.0784049\al3427=104.83247256\dih1=79.2174
8479\dih2=-62.05315937\dih3=67.93377229\dih4=-61.6072192\dih5=180.2241
1247\dih6=0.47669841\dih7=-0.32162523\dih8=0.00634934\dih9=203.2212369
5\dih10=-11.52958589\dih11=2.63996095\dih12=6.66464982\dih13=-37.92196
071\dih14=180.46170789\dih15=179.9719103\dih16=180.00844644\dih17=171.
79164761\dih18=182.40209439\dih19=182.05219915\dih20=170.89706222\dih2
1=-55.36920888\dih22=-175.75179886\dih23=48.20094222\\Version=EM64L-G0
3RevE.01\State=2-A\HF=-1066.3402387\RMSE=5.257e-09\RMSF=2.158e-05\Ther
mal=0.\Dipole=-0.3065178,-0.8956313,-1.0869827\PG=C01 [X(C12H10N1O2S1)
]\@

Transition state **D** (Scheme S1)

ROHF/6-31G*

```

1\GINC-X93\FTS\ROHF\6-31G(d)\C12H10N1O2S1(2)\SHK563\16-Aug-2010\1\#\
  ROHF/6-31G* opt=(maxstep=15,grad,ts,nofreeze,noeigentest,readfc) optc
yc=300 scfcyc=300 geom=checkpoint guess=check freq=noraman\\Louis' bia
ryl ts pyridyl\\0,2\\C\\1,r12\\C,2,r23,1,a123\\S,3,r34,2,a234,1,dih1,0\\O
,4,r45,3,a345,2,dih2,0\\C,5,r56,4,a456,3,dih3,0\\C,1,r17,2,a217,3,dih4,0\\
C,7,r78,1,a178,2,dih5,0\\C,8,r89,7,a789,1,dih6,0\\C,9,r910,8,a8910,7,d
ih7,0\\N,10,r1011,9,a91011,8,dih8,0\\C,2,r212,3,a3212,4,dih9,0\\C,12,r1213
,2,a21213,3,dih10,0\\C,13,r1314,12,a121314,2,dih11,0\\C,14,r1415,13,a131
415,12,dih12,0\\H,2,r216,3,a3216,4,dih13,0\\H,8,r817,7,a7817,1,dih14,0\\H
,9,r918,8,a8918,7,dih15,0\\H,10,r1019,9,a91019,8,dih16,0\\H,12,r1221,2,a
21221,3,dih17,0\\H,13,r1322,12,a121322,2,dih18,0\\H,14,r1423,13,a131423
,12,dih19,0\\H,15,r1524,14,a141524,13,dih20,0\\H,6,r625,7,a7625,1,dih21,0\\
H,6,r626,7,a7626,1,dih22,0\\O,4,r427,3,a3427,2,dih23,0\\r23=1.42366692\\
r34=1.77270531\\r45=1.62753516\\r56=1.42420412\\r17=1.39520729\\r78=1.382
1943\\r89=1.39104896\\r910=1.37492154\\r1011=1.3323664\\r212=1.41989086\\r1
213=1.37341351\\r1314=1.3924459\\r1415=1.38984283\\r216=1.07578582\\r817=1
.0765703\\r918=1.07385252\\r1019=1.07515972\\r1221=1.07315991\\r1322=1.075
20277\\r1423=1.07432675\\r1524=1.07601511\\r625=1.07993911\\r626=1.079956\\
r427=1.46467417\\a123=103.6059306\\a234=120.32876695\\a345=100.119626\\a45
6=119.17006166\\a217=119.72670744\\a178=115.28630205\\a789=120.24140213\\a
8910=118.07853824\\a91011=122.53805218\\a3212=116.41726097\\a21213=120.55
845581\\a121314=120.93322692\\a131415=119.61037654\\a3216=117.25206682\\a7
817=119.86732942\\a8918=121.16299876\\a91019=121.2152901\\a21221=119.0089
282\\a121322=119.51818736\\a131423=120.29294807\\a141524=120.06549823\\a76
25=111.79885692\\a7626=109.65262144\\a3427=105.76283864\\dih1=81.66325524\\
dih2=-76.20417071\\dih3=74.11981015\\dih4=-55.53541265\\dih5=178.3052145
7\\dih6=0.48478158\\dih7=-0.1184047\\dih8=-0.30604059\\dih9=192.67268074\\d
ih10=-11.61329338\\dih11=-4.44564487\\dih12=2.95267059\\dih13=-18.62159622\\
dih14=180.38212505\\dih15=179.99169524\\dih16=179.78077156\\dih17=172.12
225353\\dih18=183.11930192\\dih19=179.90546703\\dih20=175.17667531\\dih21=
-57.85582666\\dih22=-177.64504657\\dih23=35.01337954\\r12=2.03948044\\Ver
sion=EM64L-G03RevE.01\\State=2-A\\HF=-1061.741733\\RMSD=7.885e-09\\RMSF=2.
069e-05\\Thermal=0.\\Dipole=-0.210277,-0.9496722,-1.2833825\\PG=C01 [X(C1
2H10N1O2S1)]\\@

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ROHF / 6-311G**

```
1\1\GINC-X88\FTS\ROHF\6-311G(d,p)\C12H10N1O2S1(2)\SHK563\19-Aug-2010\1
  \# ROHF/6-311G** opt=(maxstep=15,grad,ts,nofreeze,noeigentest,readfc)
  optcyc=300 scfcyc=300 geom=checkpoint guess=check freq=noraman\Louis
  ' biaryl ts pyridyl\0,2\C,C,1,r12\C,2,r23,1,a123\S,3,r34,2,a234,1,dih
  1,0\O,4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,r17,2,a217,3,d
  ih4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,9,r910,8,a8910
  ,7,dih7,0\N,10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a3212,4,dih9,0\C,12,
  r1213,2,a21213,3,dih10,0\C,13,r1314,12,a121314,2,dih11,0\C,14,r1415,13
  ,a131415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,7,a7817,1,dih1
  4,0\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,dih16,0\H,12,r122
  1,2,a21221,3,dih17,0\H,13,r1322,12,a21322,2,dih18,0\H,14,r1423,13,a1
  423,12,dih19,0\H,15,r1524,14,a141524,13,dih20,0\H,6,r625,7,a7625,1,d
  ih21,0\H,6,r626,7,a7626,1,dih22,0\O,4,r427,3,a3427,2,dih23,0\`r23=1.422
  21698\r34=1.77291972\r45=1.62012784\r56=1.42330253\r17=1.39537289\r78=
  1.38025484\r89=1.39102556\r910=1.37325307\r1011=1.3322413\r212=1.41897
  044\r1213=1.37215517\r1314=1.39187731\r1415=1.38914715\r216=1.07563887
  \r817=1.07678485\r918=1.07383572\r1019=1.07556857\r1221=1.0733005\r132
  2=1.07532896\r1423=1.07434578\r1524=1.07603494\r625=1.08111138\r626=1.
  07976284\r427=1.46023651\`a123=103.3187348\`a234=120.18966051\`a345=100.1
  2624799\`a456=119.82568462\`a217=119.74721076\`a178=115.21255478\`a789=120
  .24238611\`a8910=118.10973345\`a91011=122.46469447\`a3212=116.36451973\`a2
  1213=120.52286259\`a121314=120.96574624\`a131415=119.59712851\`a3216=117.
  21601605\`a7817=119.84043183\`a8918=121.16081213\`a91019=121.26021097\`a21
  221=119.05245382\`a121322=119.49428935\`a131423=120.31060217\`a141524=120
```

.13643627\ a7625=111.65933579\ a7626=109.64609576\ a3427=105.57299436\ dih
1=82.02076909\ dih2=-76.30714834\ dih3=73.91799167\ dih4=-55.71604925\ dih
5=177.92625182\ dih6=0.6091071\ dih7=-0.19650998\ dih8=-0.30048136\ dih9=1
92.82647837\ dih10=-11.77734207\ dih11=4.41612917\ dih12=3.11100979\ dih13
=-18.39754997\ dih14=180.47466915\ dih15=179.96163884\ dih16=179.80758652
\ dih17=172.05254566\ dih18=183.17543716\ dih19=179.99850248\ dih20=175.11
751189\ dih21=-57.98203282\ dih22=-177.86665672\ dih23=34.70169634\ r12=2.
04013038\ \Version=EM64L-G03RevE.01\ State=2-A\ HF=-1061.9050325\ RMSD=9.3
18e-09\ RMSF=8.384e-06\ Thermal=0.\ Dipole=-0.1898634,-0.9978266,-1.34988
33\ PG=C01 [X(C12H10N1O2S1)]\ \@

ROBHandHLYP/6-311G**

1\1\GINC-X83\FTS\ROBHandHLYP\6-311G(d,p)\C12H10N1O2S1(2)\SHK563\21-Aug
-2010\1\#\ ROBHandHLYP/6-311G** opt=(maxstep=15,grad,ts,nofreeze,noeig
entest,readfc) optcyc=300 scfcyc=300 geom=checkpoint guess=check freq=
noraman\ \Louis' biaryl ts pyridyl\ \0,2\C\C,1,r12\C,2,r23,1,a123\S,3,r3
4,2,a234,1,dih1,0\O,4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0\C,1,
r17,2,a217,3,dih4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6,0\C,
9,r910,8,a8910,7,dih7,0\N,10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a3212,
4,dih9,0\C,12,r1213,2,a21213,3,dih10,0\C,13,r1314,12,a121314,2,dih11,0
\C,14,r1415,13,a131415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,r817,
7,a7817,1,dih14,0\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,dih
16,0\H,12,r1221,2,a21221,3,dih17,0\H,13,r1322,12,a121322,2,dih18,0\H,1
4,r1423,13,a131423,12,dih19,0\H,15,r1524,14,a141524,13,dih20,0\H,6,r62
5,7,a7625,1,dih21,0\H,6,r626,7,a7626,1,dih22,0\O,4,r427,3,a3427,2,dih2
3,0\ \r23=1.41173316\ r34=1.77726787\ r45=1.65639353\ r56=1.42740069\ r17=1
.3904681\ r78=1.38356409\ r89=1.38804216\ r910=1.37555939\ r1011=1.3352264
6\ r212=1.41165934\ r1213=1.37269123\ r1314=1.39165639\ r1415=1.3864163\ r2
16=1.07689111\ r817=1.0782565\ r918=1.07522353\ r1019=1.07713277\ r1221=1.
07466431\ r1322=1.07641775\ r1423=1.07556489\ r1524=1.07740885\ r625=1.085
15775\ r626=1.082399\ r427=1.47346281\ a123=102.63889788\ a234=119.8009507
9\ a345=99.57537049\ a456=117.84794072\ a217=120.30174491\ a178=114.877674
26\ a789=120.30667763\ a8910=118.42231882\ a91011=121.84358823\ a3212=116.
84025145\ a21213=120.40595825\ a121314=120.94025339\ a131415=119.65345222
\ a3216=117.53470376\ a7817=119.60306659\ a8918=121.05181543\ a91019=121.5
4663528\ a21221=119.16917834\ a121322=119.53253219\ a131423=120.25266917\
a141524=120.40928342\ a7625=111.4439747\ a7626=109.78804971\ a3427=105.31
266104\ dih1=81.2280978\ dih2=-80.44033602\ dih3=77.11244793\ dih4=-52.271
65732\ dih5=176.06280095\ dih6=0.59277274\ dih7=-0.12539299\ dih8=-0.43444
498\ dih9=190.63468124\ dih10=-10.06805962\ dih11=3.85021025\ dih12=2.4705
242\ dih13=-16.49860941\ dih14=180.44481351\ dih15=180.02138099\ dih16=179
.69827035\ dih17=173.70014748\ dih18=182.74250115\ dih19=179.89673923\ dih
20=175.94117721\ dih21=-57.33839455\ dih22=-177.1145544\ dih23=30.3873310
2\ r12=2.12191636\ \Version=EM64L-G03RevE.01\ State=2-A\ HF=-1066.286256\ R
MSD=3.324e-09\ RMSF=2.615e-05\ Thermal=0.\ Dipole=-0.1533324,-0.9799141,-
1.2197166\ PG=C01 [X(C12H10N1O2S1)]\ \@

ROBHandHLYP/6-311++G**

1\1\GINC-X138\FTS\ROBHandHLYP\6-311++G(d,p)\C12H10N1O2S1(2)\SHK563\25-
Aug-2010\1\#\ ROBHandHLYP/6-311++G** opt=(maxstep=15,grad,ts,nofreeze,
noeigentest,readfc) optcyc=300 scfcyc=300 geom=checkpoint guess=check
freq=noraman\ \Louis' biaryl ts pyridyl\ \0,2\C\C,1,r12\C,2,r23,1,a123\S
,3,r34,2,a234,1,dih1,0\O,4,r45,3,a345,2,dih2,0\C,5,r56,4,a456,3,dih3,0
\C,1,r17,2,a217,3,dih4,0\C,7,r78,1,a178,2,dih5,0\C,8,r89,7,a789,1,dih6
,0\C,9,r910,8,a8910,7,dih7,0\N,10,r1011,9,a91011,8,dih8,0\C,2,r212,3,a
3212,4,dih9,0\C,12,r1213,2,a21213,3,dih10,0\C,13,r1314,12,a121314,2,di
h11,0\C,14,r1415,13,a131415,12,dih12,0\H,2,r216,3,a3216,4,dih13,0\H,8,
r817,7,a7817,1,dih14,0\H,9,r918,8,a8918,7,dih15,0\H,10,r1019,9,a91019,8,
dih16,0\H,12,r1221,2,a21221,3,dih17,0\H,13,r1322,12,a121322,2,dih18,
0\H,14,r1423,13,a131423,12,dih19,0\H,15,r1524,14,a141524,13,dih20,0\H,
6,r625,7,a7625,1,dih21,0\H,6,r626,7,a7626,1,dih22,0\O,4,r427,3,a3427,2
,dih23,0\ \r23=1.41246557\ r34=1.77907274\ r45=1.65705183\ r56=1.42677717\
r17=1.39029612\ r78=1.38382654\ r89=1.38861156\ r910=1.37618956\ r1011=1.3
357238\ r212=1.41149509\ r1213=1.37351964\ r1314=1.3917407\ r1415=1.387371

07\r216=1.07692779\r817=1.07833748\r918=1.07529424\r1019=1.07710662\r1
221=1.07491751\r1322=1.0765033\r1423=1.07564406\r1524=1.07753879\r625=
1.08540634\r626=1.08251197\r427=1.47526635\al23=102.5635097\al234=120.1
6471249\al345=99.9333842\al456=118.21514971\al217=119.53413006\al178=114.8
9634085\al789=120.25659668\al8910=118.44488226\al91011=121.83547295\al3212
=116.89429997\al21213=120.44156835\al121314=120.89423661\al131415=119.653
16076\al3216=117.85088514\al7817=119.65191956\al8918=121.0599568\al91019=1
21.50421568\al21221=119.18345936\al121322=119.55134547\al131423=120.28813
903\al141524=120.31864986\al7625=111.61809423\al7626=109.81530668\al3427=1
05.37318352\alh1=81.56444605\alh2=-78.5600231\alh3=75.36412478\alh4=-5
4.12670905\alh5=176.628059\alh6=0.57423422\alh7=-0.1903273\alh8=-0.326
47204\alh9=191.13243489\alh10=-9.98619477\alh11=3.7238763\alh12=2.5711
8903\alh13=-15.88453141\alh14=180.4061481\alh15=179.99401064\alh16=179
.75924854\alh17=173.53464805\alh18=182.62707113\alh19=179.91291939\alh
20=175.86517492\alh21=-56.49960987\alh22=-176.25621316\alh23=32.168219
52\r12=2.1252448\Version=EM64L-G03RevE.01\State=2-A\HF=-1066.2983124\
RMSD=6.915e-09\RMSF=1.535e-05\Thermal=0.\Dipole=-0.1747625,-0.9584951,
-1.2690548\PG=C01 [X(C12H10N1O2S1)]\@