

Supplementary Materials

An *ab-initio* and DFT study of radical addition reactions of imidoyl and thioyl radicals to methanimine

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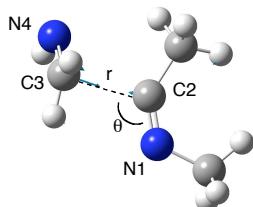
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Table S1, Figures S1 and S2, a full list of reference 19 and BHandHLYP/6-311G**, BHandHLYP/cc-pVDZ, BHandHLYP/aug-cc-pVDZ and BHandHLYP/cc-pVTZ Gaussian Archive entries for the optimized structures in this study and higher-level calculated single-point energies (22 pages).

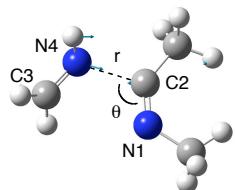
Table S1 Calculated energy barriers^a for the forward ($\Delta E_1^\ddagger, \Delta E_3^\ddagger$) and reverse ($\Delta E_2^\ddagger, \Delta E_4^\ddagger$) reactions of N-methylmethyylimidoyl radical (**1_{Me}**) with methanimine and imaginary frequencies (ν)^b of transition states **5** and **6** (Scheme 4)

Method	5					6				
	ΔE_1^\ddagger	$\Delta E_1^\ddagger + ZPE$	ΔE_2^\ddagger	$\Delta E_2^\ddagger + ZPE$	ν	ΔE_3^\ddagger	$\Delta E_3^\ddagger + ZPE$	ΔE_4^\ddagger	$\Delta E_4^\ddagger + ZPE$	ν
BHandHLYP/6-311G**	13.6	18.2	114.9	108.2	341i	31.6	35.0	187.1	180.3	410i
BHandHLYP/cc-pVDZ	12.3	16.9	119.9	113.3	331i	29.1	32.4	190.1	182.5	399i
BHandHLYP/aug-cc-pVDZ	13.4	18.0	119.3	112.3	315i	33.8	37.1	191.8	183.9	394i
BHandHLYP/cc-pVTZ	16.6	21.3	112.0	105.4	341i	35.9	39.3	189.0	182.0	411i
QCISD/cc-pVDZ //BHandHLYP/cc-pVTZ	18.5	—	115.2	—	—	34.8	—	171.6	—	—
CCSD(T)/cc-pVDZ //BHandHLYP/cc-pVTZ	13.7	—	111.2	—	—	28.8	—	167.7	—	—
ROMP2/6-311G** //BHandHLYP/cc-pVTZ	7.4	—	104.4	—	—	29.2	—	182.5	—	—
G2//MP2(full)/6-31G*	13.9	—	96.9	—	—	41.3	—	179.9	—	—
G3(MP2)-RAD //BHandHLYP/cc-pVTZ	11.9	—	94.4	—	—	27.8	—	169.4	—	—

^a Energies in kJ mol⁻¹. ^b Frequencies in cm⁻¹.



	r	θ
BHandHLYP/6-311G**	2.204 Å	113.2°
BHandHLYP/cc-pVDZ	2.219	113.4
BHandHLYP/aug-cc-pVDZ	2.221	113.1
BHandHLYP/cc-pVTZ	2.194	113.4



	r	θ
BHandHLYP/6-311G**	2.094 Å	113.1°
BHandHLYP/cc-pVDZ	2.101	112.9
BHandHLYP/aug-cc-pVDZ	2.113	113.4
BHandHLYP/cc-pVTZ	2.097	113.2

Fig. S1 Optimized structure of transition states **5** (upper) and **6** (lower) for the radical addition of N-methylmethyylimidoyl radical to the carbon and nitrogen ends of methanimine.

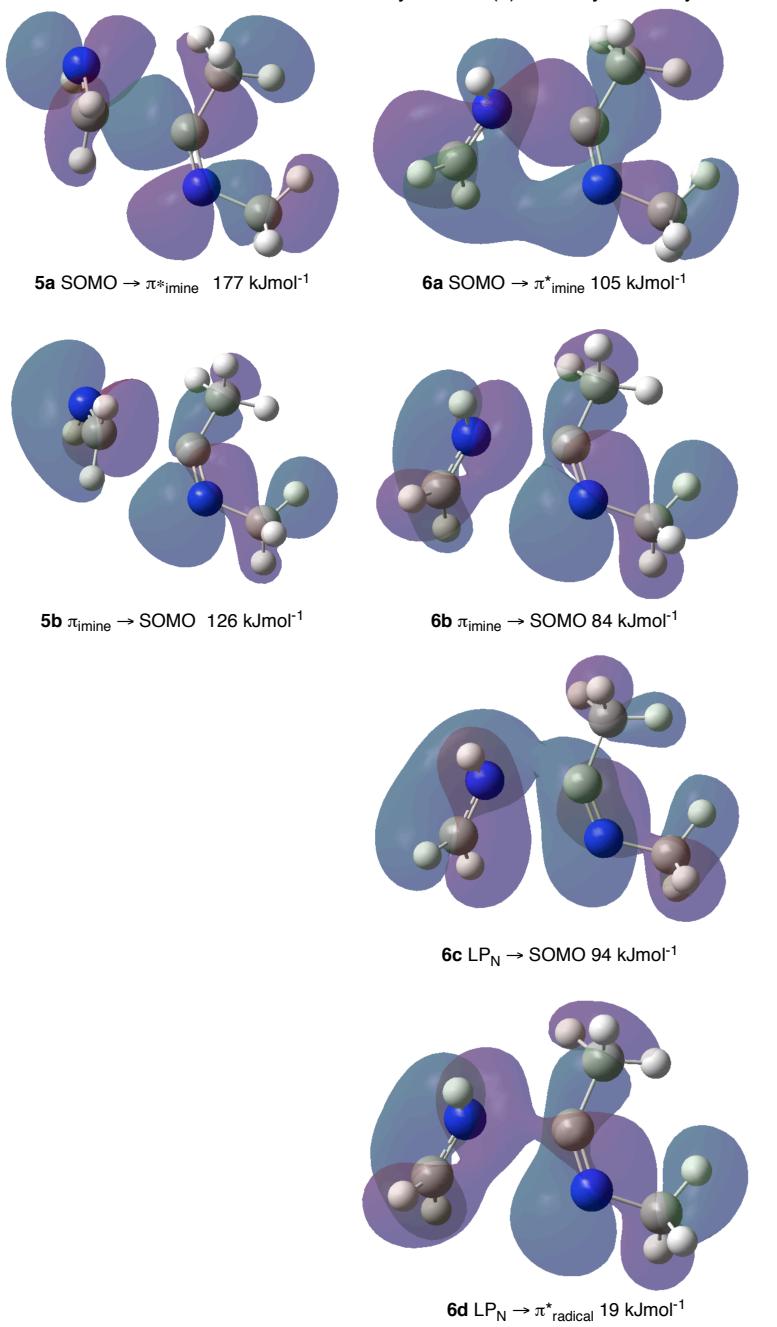


Fig. S2 BHandHLYP/6-311G** calculated Kohn-Sham orbitals involved in transition states **5** (left) and **6** (right).

Full list of Reference 19

Gaussian 03, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,

K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004; *Gaussian 09*, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

Gaussian Archive entries

Methylimidoyl radical

BHandHLYP/6-311G**

```
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BHandHLYP/cc-pVDZ

```
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BHandHLYP/aug-cc-pVDZ

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aug-cc-pVDZ freq=noraman opt=(z-matrix,readfc,maxcycle=100) geom=check guess=read Nosymm\imidoyl radical
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BHandHLYP/cc-pVTZ

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3\H,1,r4,2,a4,3,d4,0\H,3,r5,2,a5,1,d5,0\H,3,r6,2,a6,1,d6,0\H,3,r7,2,a7,1,d7,0\|r2=1.21445169\|r3=1.47881268\|a3=137
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QCISD/cc-pVDZ// BHandHLYP/cc-pVTZ
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CCSD(T)/cc-pVDZ// BHandHLYP/cc-pVTZ
 CCSD(T)= -132.9140174

ROMP2/6-311G// BHandHLYP/cc-pVTZ**
 MP2= -132.9132966

G2//MP2(full)/6-31G*
 G2= -133.0380908

G3(MP2)-RAD// BHandHLYP/cc-pVTZ
 G3(MP2)-RAD= -133.0875179

N-methylmethyylimidoyl radical

BHandHLYP/6-311G**

1\\$\\$GINC-GOMBERG03\\$\\$FOpt\\$\\$UBHandHLYP\\$\\$6-311G(d,p)\\$\\$C3H6N1(2)\\$\\$HIROSHI\\$\\$09-Sep-2010\\$\\$#BHandHLYP/
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BHandHLYP/cc-pVDZ

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BHandHLYP/aug-cc-pVDZ

1\\$\\$GINC-GOMBERG04\\$\\$FOpt\\$\\$UBHandHLYP\\$\\$Aug-CC-pVDZ\\$\\$C3H6N1(2)\\$\\$HIROSHI\\$\\$09-Sep-2010\\$\\$#BHandHLY
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BHandHLYP/cc-pVTZ

1\\$\\$GINC-GOMBERG07\\$\\$FOpt\\$\\$UBHandHLYP\\$\\$CC-pVTZ\\$\\$C3H6N1(2)\\$\\$HIROSHI\\$\\$30-Aug-2010\\$\\$#BHandHLYP/cc-
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 3\C,1,r4,2,a4,3,d4,0\H,3,r5,2,a5,1,d5,0\H,3,r6,2,a6,1,d6,0\H,3,r7,2,a7,1,d7,0\H,4,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,
 4,r10,1,a10,2,d10,0\r2=1.21066505\r3=1.48289772\r3=137.16762244\r4=1.44949461\r4=127.89924042\d4=-0.000
 04775\r5=1.08759827\r5=112.20604721\d5=0.00032868\r6=1.08259794\r6=109.71517403\d6=121.16131312\r7=1
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QCISD/cc-pVDZ// BHandHLYP/cc-pVTZ

QCISD=-172.0856121

CCSD(T)/cc-pVDZ// BHandHLYP/cc-pVTZ

CCSD(T)= -172.1039435

ROMP2/6-311G// BHandHLYP/cc-pVTZ**

MP2= -172.1001698

G2//MP2(full)/6-31G*

G2= -172.2553978

G3(MP2)-RAD// BHandHLYP/cc-pVTZ

G3(MP2)-RAD= -172.3205397

Metanethioyl radical**BHandHLYP/6-311G****

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 21\r5=113.12111637\d5=-0.00577679\r6=1.08725063\r6=109.07782568\d6=237.9522664\r7=1.08725126\r7=109.0
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 C2H3S1)]\@\n

BHandHLYP/cc-pVDZ

1\GINC-GOMBERG02\FOpt\UBHandHLYP\CC-pVDZ\C2H3S1(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/c
 c-pVDZ opt=(z-matrix,readfc) freq=noraman geom=check guess=read\thioly radical\0,2\\$C,1,r2\|C,2,r3,1,a3\H,3,r
 5,2,a5,1,d5,0\H,3,r6,2,a6,1,d6,0\H,3,r7,2,a7,1,d7,0\r2=1.57217435\r3=1.4708255\r3=138.39402525\r5=1.09600701
 \a5=113.11028321\d5=-0.00335332\r6=1.09531363\r6=109.09458435\d6=237.91091598\r7=1.09531399\r7=109.09
 432061\d7=122.08207376\Version=AM64L-G03RevE.01\State=2-A\HF=-476.0847623\S2=0.759487\S2-1=0.\\$2A
 =0.750063\RMSD=5.642e-09\RMSF=1.419e-04\Thermal=0.\Dipole=0.4720575,0.0000053,0.6827866\PG=C01 [X(
 C2H3S1)]\@\n

BHandHLYP/aug-cc-pVDZ

1\GINC-GOMBERG01\FOpt\UBHandHLYP\Aug-CC-pVDZ\C2H3S1(2)\HIROSHI\09-Sep-2010\1\#BHandH
 LYP/aug-cc-pVDZ opt=(z-matrix,readfc) freq=noraman geom=check guess=read Nosymm\thioly radical\0,2\\$C,1,r
 2\|C,2,r3,1,a3\H,3,r5,2,a5,1,d5,0\H,3,r6,2,a6,1,d6,0\H,3,r7,2,a7,1,d7,0\r2=1.57178426\r3=1.47070311\r3=138.55414
 929\r5=1.09358611\r5=112.8270289\d5=-0.0004122\r6=1.09286429\r6=109.02292412\d6=237.9319806\r7=1.0928
 6437\r7=109.02285818\d7=122.06711546\Version=AM64L-G03RevE.01\HF=-476.0913678\S2=0.760839\S2-1=0.
 \\$2A=0.750079\RMSD=3.624e-09\RMSF=8.971e-06\Thermal=0.\Dipole=0.4674733,0.0000006,0.7213886\PG=C0
 1 [X(C2H3S1)]\@\n

BHandHLYP/cc-pVTZ

1\GINC-GOMBERG02\FOpt\UBHandHLYP\CC-pVTZ\C2H3S1(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/cc
 pVTZ opt=(z-matrix,readfc) freq=noraman geom=check guess=read\thioly radical\0,2\\$C,1,r2\|C,2,r3,1,a3\H,3,r
 5,2,a5,1,d5,0\H,3,r6,2,a6,1,d6,0\H,3,r7,2,a7,1,d7,0\r2=1.55751058\r3=1.46385176\r3=139.52523463\r5=1.08581553\r
 5=113.03426256\d5=-0.00065356\r6=1.08506775\r6=109.19336844\d6=237.98552705\r7=1.08506788\r7=109.193
 25302\d7=122.01302459\Version=AM64L-G03RevE.01\State=2-A\HF=-476.1245623\S2=0.76105\S2-1=0.\\$2A=0

.750083\RMSD=2.588e-09\RMSF=4.443e-06\Thermal=0.\Dipole=0.4588958,0.0000011,0.6882033\PG=C01 [X(C2H3S1)]\\@

QCISD/cc-pVDZ// BHandHLYP/cc-pVTZ
QCISD= -475.37340

CCSD(T)/cc-pVDZ//BHandHLYP/cc-pVTZ
CCSD(T)= -475.3872354

ROMP2/6-311G//BHandHLYP/cc-pVTZ**
MP2= -475.3683385

G2//MP2(full)/6-31G*
G2= -475.5209139

G3(MP2)-RAD//BHandHLYP/cc-pVTZ
G3(MP2)-RAD= -475.6136536

Methanimine

BHandHLYP/6-311G**

```
1\1\GINC-GOMBERG02\POpt\RBHandHLYP\6-311G(d,p)\C1H3N1\HIROSHI\09-Sep-2010\1\#BHandHLYP/6-3
11G** freq=NoRaman opt=(z-matrix,readfc) Nosymm geom=check guess=read\CH2=NH\0,1\N\C,1,r2\H,1,r3,2,a3
\H,2,r4,1,a4,3,d4,0\H,2,r5,1,a5,3,d5,0\r2=1.25413846\r3=1.01249646\r4=1.08802165\r5=1.08367443\a3=110.9137
5617\4=124.89458375\5=118.99139202\4=0.\d5=180.\\"Version=AM64L-G03RevE.01\HF=-94.5934707\RMSD
=6.449e-09\RMSF=2.502e-05\Thermal=0.\Dipole=0.5680793,0.,0.5758014\PG=CS [SG(C1H3N1)]\\@
```

BHandHLYP/cc-pVDZ

```
1\1\GINC-GOMBERG01\POpt\RBHandHLYP\CC-pVDZ\C1H3N1\HIROSHI\09-Sep-2010\1\#BHandHLYP/cc-p
VDZ freq=NoRaman opt=(z-matrix,readfc) Nosymm geom=check guess=read\CH2=NH\0,1\N\C,1,r2\H,1,r3,2,a3\
H,2,r4,1,a4,3,d4,0\H,2,r5,1,a5,3,d5,0\r2=1.25886548\r3=1.01970644\r4=1.09715447\r5=1.09333695\4=110.32601
168\4=125.1696549\5=118.89089929\4=0.\d5=180.\\"Version=AM64L-G03RevE.01\HF=-94.5716949\RMSD=3.
206e-09\RMSF=1.389e-04\Thermal=0.\Dipole=0.533966,0.,0.5256717\PG=CS [SG(C1H3N1)]\\@
```

BHandHLYP/aug-cc-pVDZ

```
1\1\GINC-GOMBERG02\POpt\RBHandHLYP\Aug-CC-pVDZ\C1H3N1\HIROSHI\09-Sep-2010\1\#BHandHLYP/
aug-cc-pVDZ freq=NoRaman opt=(z-matrix,readfc) Nosymm geom=check guess=read\CH2=NH\0,1\N\C,1,r2\H,1,
r3,2,a3\H,2,r4,1,a4,3,d4,0\H,2,r5,1,a5,3,d5,0\r2=1.26024279\r3=1.01501675\r4=1.09317658\r5=1.08913878\4=11
1.14734246\4=124.34601268\5=118.99546352\4=0.\d5=180.\\"Version=AM64L-G03RevE.01\HF=-94.5821712\
RMSD=2.319e-09\RMSF=7.139e-05\Thermal=0.\Dipole=0.5516007,0.,0.6189252\PG=CS [SG(C1H3N1)]\\@
```

BHandHLYP/cc-pVTZ

```
1\1\GINC-GOMBERG05\POpt\RBHandHLYP\CC-pVTZ\C1H3N1\HIROSHI\27-Aug-2010\1\#BHandHLYP/cc-p
VTZ freq=NoRaman opt=(z-matrix,calcfc) Nosymm geom=check guess=read\CH2=NH\0,1\N\C,1,r2\H,1,r3,2,a3\
H,2,r4,1,a4,3,d4,0\H,2,r5,1,a5,3,d5,0\r2=1.25145146\r3=1.01003455\r4=1.08509196\r5=1.08140227\4=111.35709
142\4=124.58560688\5=119.14509351\4=0.\d5=180.\\"Version=AM64L-G03RevE.01\HF=-94.6048743\RMSD
=2.690e-09\RMSF=7.802e-06\Thermal=0.\Dipole=0.5477502,0.,0.5792374\PG=CS [SG(C1H3N1)]\\@
```

QCISD/cc-pVDZ// BHandHLYP/cc-pVTZ
QCISD= -94.36266970

CCSD(T)/cc-pVDZ// BHandHLYP/cc-pVTZ
CCSD(T)= -94.37228760

ROMP2/6-311G// BHandHLYP/cc-pVTZ**
MP2= -94.37443680

G2//MP2(full)/6-31G*
G2= -94.46328760

G3(MP2)-RAD// BHandHLYP/cc-pVTZ

G3(MP2)-RAD= -94.4957814

Transition state for attacking of methylimidoyl radical at nitrogen end of methanimine

BHandHLYP/6-311G**

```
1\1\GINC-GOMBERG02\FTS\UBHandHLYP\6-311G(d,p)\C3H7N2(2)\HIROSHI\08-Sep-2010\1\#BHandHLYP/
6-311G** opt=(TS,z-matrix,readfc,maxcycle=100) Nosymm geom=check guess=read\TS nitrogen\0,2\C\N,1,r2\C,
1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,
d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\H,2,r12,1,a12,3,d12,0\r2=1.22690732\r3=1.48020387\a3=136.192
84056\r4=2.0900568\a4=112.69824726\d4=156.80612954\r5=1.28359952\a5=113.97165018\d5=5.53628596\r6=1.
08397378\a6=108.84404446\d6=121.21872838\r7=1.08992343\a7=111.48471224\d7=0.28331246\r8=1.0859186\a8
=110.35620942\d8=239.27647217\r9=1.01068875\a9=100.42347879\d9=124.67827366\r10=1.08298143\a10=123.8
3910541\d10=110.0725598\r11=1.07907123\a11=118.66572091\d11=-65.73867921\r12=1.01888443\a12=114.6555
9456\d12=2.71521668\Version=AM64L-G03RevE.01\HF=-227.8194472\S2=0.803754\S2-1=0.\$2A=0.750698\R
MSD=8.879e-09\RMSF=6.107e-06\Thermal=0.\Dipole=0.2986291,0.3177732,-0.4558025\PG=C01 [X(C3H7N2)]\@
@
```

BHandHLYP/cc-pVDZ

```
1\1\GINC-GOMBERG02\FTS\UBHandHLYP\CC-pVDZ\C3H7N2(2)\HIROSHI\08-Sep-2010\1\#BHandHLYP/cc-
pVDZ opt=(TS,z-matrix,readfc,maxcycle=100) Nosymm geom=check guess=read\TS nitrogen\0,2\C\N,1,r2\C,1,r3,
2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0
\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\H,2,r12,1,a12,3,d12,0\r2=1.2336836\r3=1.48213377\a3=136.0643886
1\r4=2.09780645\a4=112.56467368\d4=156.40267105\r5=1.28687402\a5=114.096577\d5=6.42807978\r6=1.09209
849\a6=108.89859394\d6=122.26411216\r7=1.09768033\a7=111.53376941\d7=1.22053367\r8=1.09399458\a8=110
.36280815\d8=240.2280019\r9=1.01760422\a9=100.43328964\d9=125.11724086\r10=1.09187685\a10=124.055608
18\d10=110.27492209\r11=1.08829356\a11=118.52473129\d11=-65.58000236\r12=1.02605151\a12=113.51728157
\d12=2.74789354\Version=AM64L-G03RevE.01\HF=-227.770387\S2=0.804785\S2-1=0.\$2A=0.750737\RMSD=5
.463e-09\RMSF=9.264e-06\Thermal=0.\Dipole=0.2748203,0.2946517,-0.4695022\PG=C01 [X(C3H7N2)]\@\@
```

BHandHLYP/aug-cc-pVDZ

```
1\1\GINC-GOMBERG02\FTSUB\UBHandHLYP\Aug-CC-pVDZ\C3H7N2(2)\HIROSHI\08-Sep
-2010\1\#BHandHLYP/aug-cc-pVDZ opt=(TS,z-matrix,readfc,maxcycle=100) Nosymm geom=check guess=read\TS
nitrogen\0,2\C\N,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3
,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\H,2,r12,1,a12,3,d12,0\r2=1.2333336
6\r3=1.48117645\a3=136.06416952\r4=2.10721146\a4=112.88459566\d4=158.17584642\r5=1.28759284\a5=113.80
01223\d5=6.14007823\r6=1.08961561\a6=109.00706859\d6=120.66068327\r7=1.09497285\a7=111.19140713\d7=-
0.30580158\r8=1.09132794\a8=110.27206456\d8=238.77190946\r9=1.0132334\a9=99.61770682\d9=124.55134517
\r10=1.08832712\a10=123.5902352\d10=108.78484789\r11=1.08471887\a11=118.72115442\d11=-67.64160828\r1
2=1.02093659\a12=114.65299575\d12=2.44610687\Version=AM64L-G03RevE.01\HF=-227.7903297\S2=0.80367
2\S2-1=0.\$2A=0.750735\RMSD=4.428e-09\RMSF=7.623e-06\Thermal=0.\Dipole=0.3186047,0.3190477,-0.49129
36\PG=C01 [X(C3H7N2)]\@\@
```

BHandHLYP/cc-pVTZ

```
1\1\GINC-GOMBERG05\FTS\UBHandHLYP\CC-pVTZ\C3H7N2(2)\HIROSHI\27-Aug-2010\1\#bhandhlyp/cc-pV
TZ opt=(TS,z-matrix,calcfc,maxcycle=100) Nosymm geom=check guess=read\TS nitrogen\0,2\C\N,1,r2\C,1,r3,2,a
3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H
,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\H,2,r12,1,a12,3,d12,0\r2=1.22413133\r3=1.47637237\a3=136.07735886
r4=2.09126063\a4=112.76809511\d4=157.44967723\r5=1.28058903\a5=114.06058243\d5=6.90462004\r6=1.08178
639\a6=109.12069602\d6=122.01149203\r7=1.08738884\a7=111.37452862\d7=1.03740459\r8=1.08367739\a8=110
.33697109\d8=240.15742393\r9=1.00816916\a9=99.94520813\d9=126.15924616\r10=1.08036976\a10=123.671547
77\d10=109.60469221\r11=1.07680381\a11=118.7853685\d11=-66.44727621\r12=1.01630603\a12=115.16922537
\d12=2.2796572\Version=AM64L-G03RevE.01\HF=-227.8444368\S2=0.802695\S2-1=0.\$2A=0.750676\RMSD=5
.900e-09\RMSF=4.422e-06\Thermal=0.\Dipole=0.3166936,0.3154407,-0.4678795\PG=C01 [X(C3H7N2)]\@\@
```

QCISD/cc-pVDZ// BHandHLYP/cc-pVTZ

QCISD= -227.2512476

CCSD(T)/cc-pVDZ// BHandHLYP/cc-pVTZ
CCSD(T)= -227.2763676

ROMP2/6-311G// BHandHLYP/cc-pVTZ**
MP2= -227.2778322

G2//MP2(full)/6-31G*
G2= -227.4868107

G3(MP2)-RAD// BHandHLYP/cc-pVTZ
G3(MP2)-RAD= -227.5727838

Transition state for attacking of methylimidoyl radical at carbon end of methanimine

BHandHLYP/6-311G**

```
1\GINC-GOMBERG03\FTS\SUBBHandHLYP\6-311G(d,p)\C3H7N2(2)\HIROSHI\08-Sep-2010\1\#BHandHLYP/  
6-311G** opt=(TS,ReadFC,Z-matrix,NoEigenTest,maxcycle=100) Nosymm geom=check guess=read\TS at carbon\  
\0,2\C\N,1,r2\C,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,  
,0\H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\H,2,r12,1,a12,3,d12,0\r2=1.22199899\r3=1.47910  
47\r3=137.82895412\r4=2.22013517\r4=112.98046058\r4=176.71397919\r5=1.28916563\r5=106.70934419\r5=-1  
36.71822881\r6=1.08381395\r6=109.38727432\r6=130.57441972\r7=1.08867157\r7=111.29600922\r7=8.3498928  
8\r8=1.08582542\r8=109.35861759\r8=247.55543903\r9=1.0835973\r9=88.13050592\r9=-11.20573701\r10=1.082  
68763\r10=89.27079754\r10=-255.59138462\r11=1.01257159\r11=109.87698014\r11=89.91409848\r12=1.019463  
6\r12=116.04415964\r12=0.63716448\Version=AM64L-G03RevE.01\HF=-227.8250841\S2=0.806279\S2-1=0.\$2  
A=0.750742\RMSD=3.760e-09\RMSF=4.895e-06\Thermal=0.\Dipole=0.8692574,0.0567465,0.3331451\PG=C01 [  
X(C3H7N2)]\@\n
```

BHandHLYP/cc-pVDZ

```
1\GINC-GOMBERG03\FTS\SUBBHandHLYP\CC-pVDZ\C3H7N2(2)\HIROSHI\08-Sep-2010\1\#BHandHLYP/cc-  
pVDZ opt=(TS,ReadFC,Z-matrix,NoEigenTest,maxcycle=100) Nosymm geom=check guess=read\TS at carbon\  
\0,2\CC\N,1,r2\CC,1,r3,2,a3\CC,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\  
H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\H,2,r12,1,a12,3,d12,0\r2=1.22881367\r3=1.4808952  
6\r3=137.86645637\r4=2.23449892\r4=113.15903705\r4=174.73601837\r5=1.29181815\r5=105.92051434\r5=-13  
3.32429164\r6=1.09184889\r6=109.27007355\r6=132.50009089\r7=1.09637234\r7=111.37315247\r7=10.0828012  
4\r8=1.09403051\r8=109.31553274\r8=249.42912042\r9=1.09224156\r9=88.04666384\r9=-7.55832516\r10=1.091  
54331\r10=89.37190427\r10=-252.07399074\r11=1.01979743\r11=109.39370491\r11=89.65103987\r12=1.026675  
92\r12=114.84221618\r12=0.79677458\Version=AM64L-G03RevE.01\HF=-227.7756576\S2=0.807676\S2-1=0.\$2  
A=0.750792\RMSD=7.441e-09\RMSF=1.221e-05\Thermal=0.\Dipole=0.808088,0.0936083,0.2833273\PG=C01 [  
X(C3H7N2)]\@\n
```

BHandHLYP/aug-cc-pVDZ

```
1\GINC-GOMBERG04\FTS\SUBBHandHLYP\Aug-CC-pVDZ\C3H7N2(2)\HIROSHI\08-Sep-2010\1\#BHandHLY  
P/aug-cc-pVDZ opt=(TS,ReadFC,Z-matrix,NoEigenTest,maxcycle=100) Nosymm geom=check guess=read\TS at c  
arbon\  
\0,2\CC\N,1,r2\CC,1,r3,2,a3\CC,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\  
H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\H,2,r12,1,a12,3,d12,0\r2=1.22874011\r3=1.  
47980267\r3=137.52605954\r4=2.23478509\r4=112.73032421\r4=178.48694808\r5=1.29232009\r5=107.3618205  
8\r5=-141.04180789\r6=1.08961004\r6=109.38450947\r6=125.71458442\r7=1.09369663\r7=110.9911948\r7=3.7  
8128183\r8=1.09085735\r8=109.49138455\r8=242.68327169\r9=1.0885599\r9=87.80353177\r9=-15.87391717\r1  
0=1.08781242\r10=88.34941206\r10=-259.80423632\r11=1.01498282\r11=110.28340893\r11=90.45524193\r12=1  
.02147022\r12=115.9390881\r12=0.52341206\Version=AM64L-G03RevE.01\HF=-227.7967935\S2=0.804168\S2-  
1=0.\$2A=0.750739\RMSD=6.002e-09\RMSF=1.211e-05\Thermal=0.\Dipole=0.889278,0.0159645,0.3015108\PG=  
C01 [X(C3H7N2)]\@\n
```

BHandHLYP/cc-pVTZ

```
1\GINC-GOMBERG03\FTS\SUBBHandHLYP\CC-pVTZ\C3H7N2(2)\HIROSHI\08-Sep-2010\1\#BHandHLYP/cc-  
pVTZ opt=(TS,CalcFC,Z-matrix,NoEigenTest,maxcycle=100) Nosymm\TS at carbon\  
\0,2\CC\N,1,r2\CC,1,r3,2,a3\CC,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\  
H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\H,2,r12,1,a12,3,d12,0\r2=1.21948716\r3=1.47514264\r3=137.61235956\r4=2.  
20898206\r4=112.99029225\r4=177.21733312\r5=1.28691898\r5=107.17811117\r5=-137.15193129\r6=1.0816617
```

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 9\|a6=109.4643926\|d6=128.82894241\|r7=1.08613107\|a7=111.19273713\|d7=6.69479864\|r8=1.08348942\|a8=109.47
 68882\|d8=245.84312733\|r9=1.08073271\|a9=88.24562035\|d9=-11.81215437\|r10=1.08049778\|a10=89.11556869\|d1
 0=-256.17236127\|r11=1.01007428\|a11=110.34280851\|d11=90.11812863\|r12=1.0168354\|a12=116.47879086\|d12=0
 .56340758\|Version=AM64L-G03RevE.01\|HF=-227.8505567\|S2=0.804323\|S2-1=0.\|S2A=0.750696\|RMSD=3.211
 e-09\|RMSF=2.367e-06\|Thermal=0.\|Dipole=0.8732495,0.0609185,0.323832\|Polar=61.9765302,5.1193177,43.16696
 45,10.0621366,5.9045143,64.082182\|PG=C01 [X(C3H7N2)]\|@

QCISD/cc-pVDZ// BHandHLYP/cc-pVTZ

QCISD= -227.2564731

CCSD(T)/cc-pVDZ// BHandHLYP/cc-pVTZ

CCSD(T)= -227.2810421

ROMP2/6-311G// BHandHLYP/cc-pVTZ**

MP2= -227.2845258

G2//MP2(full)/6-31G*

G2= -227.4951941

G3(MP2)-RAD// BHandHLYP/cc-pVTZ

G3(MP2)-RAD= -227.5779539

Transition state for attacking of N-methylmethyliimidoyl radical at nitrogen end of methanimine**BHandHLYP/6-311G****

1\|GINC-GOMBERG01\FTS\UBHandHLYP\6-311G(d,p)\C4H9N2(2)\HIROSHI\08-Sep-2010\1\#BHandHLYP/6-311G** opt=(TS,z-matrix,readfc,NoEigenTest,maxcycle=100) Nosymm geom=check guess=read\|TS nitrogen N-Me\|0,2\|CN,1,r2\|C,1,r3,2,a3\|N,1,r4,2,a4,3,d4,0\|C,4,r5,1,a5,2,d5,0\|H,3,r6,1,a6,2,d6,0\|H,3,r7,1,a7,2,d7,0\|H,3,r8,1,a8,2,d8,0\|H,4,r9,1,a9,2,d9,0\|H,5,r10,4,a10,1,d10,0\|H,5,r11,4,a11,1,d11,0\|C,2,r12,1,a12,3,d12,0\|H,12,r13,2,a13,1,d13,0\|H,12,r14,2,a14,1,d14,0\|H,12,r15,2,a15,1,d15,0\|r2=1.22142836\|r3=1.48147519\|a3=137.5713336\|r4=2.09361791\|a4=13.04553192\|d4=159.33822775\|r5=1.28622809\|a5=113.72747748\|d5=3.7127954\|r6=1.08379907\|a6=108.51387626\|d6=126.02716659\|r7=1.08827117\|a7=112.7173866\|d7=4.7665447\|r8=1.08624216\|a8=109.96761526\|d8=243.59391894\|r9=1.01069585\|a9=98.83330644\|d9=121.47280054\|r10=1.08303755\|a10=123.90292107\|d10=107.0919918\|r11=1.07915357\|a11=118.69267105\|d11=-68.59458242\|r12=1.45212792\|a12=124.59202203\|d12=2.59588848\|r13=1.08503193\|r14=1.08889192\|r15=1.08511114\|a13=108.78651231\|a14=114.05928499\|a15=108.80907931\|d13=119.84561055\|d14=-1.66221283\|d15=236.53994645\|Version=AM64L-G03RevE.01\|HF=-267.1085456\|S2=0.805727\|S2-1=0.\|S2A=0.750741\|RMSD=4.456e-09\|RMSF=2.244e-05\|Thermal=0.\|Dipole=0.4090889,0.3864564,-0.1506491\|PG=C01 [X(C4H9N2)]\|@

BHandHLYP/cc-pVDZ

1\|GINC-GOMBERG04\FTS\UBHandHLYP\CC-pVDZ\C4H9N2(2)\HIROSHI\08-Sep-2010\1\#BHandHLYP/cc-pVDZ opt=(TS,z-matrix,readfc,NoEigenTest,maxcycle=100) Nosymm geom=check guess=read\|TS nitrogen N-Me\|0,2\|CN,1,r2\|C,1,r3,2,a3\|N,1,r4,2,a4,3,d4,0\|C,4,r5,1,a5,2,d5,0\|H,3,r6,1,a6,2,d6,0\|H,3,r7,1,a7,2,d7,0\|H,3,r8,1,a8,2,d8,0\|H,4,r9,1,a9,2,d9,0\|H,5,r10,4,a10,1,d10,0\|H,5,r11,4,a11,1,d11,0\|C,2,r12,1,a12,3,d12,0\|H,12,r13,2,a13,1,d13,0\|H,12,r14,2,a14,1,d14,0\|H,12,r15,2,a15,1,d15,0\|r2=1.22892231\|r3=1.48331603\|a3=137.43540558\|r4=2.10105314\|a4=112.87854302\|d4=158.72239495\|r5=1.28912228\|a5=113.9026411\|d5=4.71721665\|r6=1.09191647\|a6=108.52848767\|d6=127.0294526\|r7=1.09596319\|a7=112.77886092\|d7=5.68411544\|r8=1.09428624\|a8=109.9921611\|d8=244.50095986\|r9=1.01756101\|a9=98.84842694\|d9=122.10754168\|r10=1.09192902\|a10=124.12638543\|d10=107.41586127\|r11=1.08837522\|a11=118.54947955\|d11=-68.30485525\|r12=1.45079491\|a12=124.01349692\|d12=2.8020992\|r13=1.09363748\|r14=1.09703893\|r15=1.09370376\|a13=108.94925852\|a14=114.33675934\|a15=108.97391078\|d13=119.61037666\|d14=-1.98800175\|d15=236.09674766\|Version=AM64L-G03RevE.01\|HF=-267.05131\|S2=0.806735\|S2-1=0.\|S2A=0.750778\|RMSD=7.627e-09\|RMSF=1.430e-05\|Thermal=0.\|Dipole=0.3573203,0.3597695,-0.1895585\|PG=C01 [X(C4H9N2)]\|@

BHandHLYP/aug-cc-pVDZ

1\|GINC-GOMBERG04\FTS\UBHandHLYP\Aug-CC-pVDZ\C4H9N2(2)\HIROSHI\08-Sep-2010\1\#BHandHLYP/aug-cc-pVDZ opt=(TS,z-matrix,readfc,NoEigenTest,maxcycle=100) Nosymm geom=check guess=read\|TS nitrogen

This journal is (c) The Royal Society of Chemistry 2011
 n N-Me\O,2\C\N,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,
 1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\C,2,r12,1,a12,3,d12,0\H,12,r13,2,a13,1,d
 13,0\H,12,r14,2,a14,1,d14,0\H,12,r15,2,a15,1,d15,0\r2=1.22693049\r3=1.48247854\aa=137.51166483\r4=2.112946
 35\aa=113.43130158\dd=161.22674128\r5=1.29024132\aa=113.49053056\dd=3.68426445\r6=1.08946777\aa=108.
 69620649\dd=122.93550504\r7=1.09332572\aa=112.41000613\dd=1.68265772\r8=1.09142219\aa=109.97420499\dd
 8=240.53875103\r9=1.01319654\aa=97.75812532\dd=120.57595098\r10=1.08834838\aa=103.66138607\dd=105.
 37100848\r11=1.0847803\aa=118.74001044\dd=70.94098323\r12=1.45286268\aa=124.42530541\dd=2.33398
 095\r13=1.09020711\r14=1.09375312\r15=1.09054129\aa=108.7285282\aa=113.88784087\aa=108.7277081\dd
 3=121.27453181\dd=0.24279833\dd=238.024382\Version=AM64L-G03RevE.01\HF=-267.0712376\S2=0.8057
 32\S2-1=0.\\$2A=0.750788\RMSD=9.720e-09\RMSF=7.282e-06\Thermal=0.\Dipole=0.4658897,0.3839722,-0.1677
 43\PG=C01 [X(C4H9N2)]\@\@

BHandHLYP/cc-pVTZ

1\1\GINC-GOMBERG07\FTS\UBHandHLYP\CC-pVTZ\C4H9N2(2)\HIROSHI\30-Aug-2010\1\#BHandHLYP/cc-p
 VTZ opt=(TS,z-matrix,calcfc,maxcycle=100) Nosymm\TS nitrogen N-Me\O,2\C\N,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d
 4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d1
 0,0\H,5,r11,4,a11,1,d11,0\C,2,r12,1,a12,3,d12,0\H,12,r13,2,a13,1,d13,0\H,12,r14,2,a14,1,d14,0\H,12,r15,2,a15,1,d1
 5,0\r2=1.21787884\r3=1.47773293\aa=137.50141465\r4=2.09724904\aa=113.16030159\dd=160.3428751\r5=1.283
 17313\aa=113.75969165\dd=5.07583215\r6=1.08163909\aa=108.80038979\dd=125.94277802\r7=1.08580948\aa=1
 12.55906564\dd=4.66330313\r8=1.08391464\aa=109.99060817\dd=243.61355486\r9=1.0081237\aa=98.22853559
 \dd=122.8691349\r10=1.08042337\aa=123.74429804\dd=106.39006396\r11=1.07688909\aa=118.80869594\dd=11
 =-69.52996988\r12=1.4484275\aa=124.97090825\dd=2.28990822\r13=1.08267201\r14=1.08624406\r15=1.08281
 169\aa=108.87356702\aa=113.93829417\aa=108.89890815\dd=119.88186578\r14=-1.59016509\dd=236.657
 5606\Version=AM64L-G03RevE.01\HF=-267.1370785\S2=0.804441\S2-1=0.\\$2A=0.750716\RMSD=9.446e-09\R
 MSF=8.326e-06\Thermal=0.\Dipole=0.4394733,0.3856607,-0.1623572\PG=C01 [X(C4H9N2)]\@\@

QCISD/cc-pVDZ// BHandHLYP/cc-pVTZ

QCISD= -266.4350179

CCSD(T)/cc-pVDZ// BHandHLYP/cc-pVTZ

CCSD(T)= -266.4652808

ROMP2/6-311G// BHandHLYP/cc-pVTZ**

MP2= -266.4634749

G2//MP2(full)/6-31G*

G2= -266.465373

G3(MP2)-RAD// BHandHLYP/cc-pVTZ

G3(MP2)-RAD= -266.8057314

Transition state for attacking of N-methylmethyliimidoyl radical at carbon end of methanimine**BHandHLYP/6-311G****

1\1\GINC-GOMBERG05\FTS\UBHandHLYP\6-311G(d,p)\C4H9N2(2)\HIROSHI\08-Sep-2010\1\#BHandHLYP/6-
 311G** opt=(TS,z-matrix,readfc,NoEigenTest,maxcycle=100) Nosymm geom=check guess=read\TS carbon N-Me\O,2\C\N,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\C,2,r12,1,a12,3,d12,0\H,12,r13,2,a13,1,d13,0\H,12,r14,2,a14,1,d14,0\H,12,r15,2,a15,1,d15,0\r2=1.21735334\r3=1.48187703\aa=138.07350275\r4=2.20413863\aa=1
 13.24299259\dd=177.45483926\r5=1.29079651\aa=107.29993157\dd=-137.80924395\r6=1.08362402\aa=109.1504
 7023\dd=137.94691711\r7=1.08752969\aa=112.07994827\dd=15.62924868\r8=1.08637467\aa=109.22241316\dd=2
 54.89722739\r9=1.08350921\aa=88.33623998\dd=-12.15579164\r10=1.08281666\aa=10=89.32953473\dd=10=-256.683
 02499\r11=1.01252835\aa=109.82500619\dd=89.99788548\r12=1.45395191\aa=125.54436682\dd=0.8969399
 6\r13=1.08805821\aa=1.08418193\r15=1.08450072\aa=113.55721091\aa=108.71657828\aa=108.61101566\dd
 3=-2.7445825\dd=124.52615504\dd=118.68378355\Version=AM64L-G03RevE.01\HF=-267.1154181\S2=0.80
 4111\S2-1=0.\\$2A=0.750687\RMSD=8.351e-09\RMSF=3.283e-06\Thermal=0.\Dipole=0.9334248,0.0701695,0.681
 3521\PG=C01 [X(C4H9N2)]\@\@

BHandHLYP/cc-pVDZ

```
1\GINC-GOMBERG05\FTSUBHandHLYP\CC-pVDZ\C4H9N2(2)\HIROSHI\08-Sep-2010\1\#BHandHLYP/cc-p
VDZ opt=(TS,z-matrix,readfc,NoEigenTest,maxcycle=100) Nosymm geom=check guess=read\TS carbon N-Me\0,
2\C\N,1,r2\C,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\
H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\C,2,r12,1,a12,3,d12,0\H,12,r13,2,a13,1,d13,0\H,12,r
14,2,a14,1,d14,0\H,12,r15,2,a15,1,d15,0\r2=1.22461752\r3=1.48348777\r3=138.11358846\r4=2.21894366\r4=113.
38253795\d4=175.99084049\r5=1.29329031\r5=106.67169769\d5=-136.04938648\r6=1.0917079\r6=109.04139626
\d6=139.41617942\r7=1.09524655\r7=112.13867075\d7=16.94890444\r8=1.09450577\r8=109.22209744\d8=256.3
1887328\r9=1.09213771\r9=88.25579529\d9=-10.10124142\r10=1.09159953\r10=89.25479973\d10=-254.7704679
4\r11=1.01977941\r11=109.35347596\d11=89.85722356\r12=1.45289247\r12=124.90711079\d12=1.11725565\r13
=1.09621606\r14=1.09273333\r15=1.0930611\r13=113.81542903\r14=108.86137675\r15=108.75380313\d13=-3.0
9828332\d14=-124.993366\d15=118.41547355\Version=AM64L-G03RevE.01\HF=-267.057713\S2=0.805751\S2-
1=0.\$2A=0.750733\RMSD=3.604e-09\RMSF=5.825e-06\Thermal=0.\Dipole=0.8566912,0.088304,0.6103856\PG=
C01 [X(C4H9N2)]\@\@
```

BHandHLYP/aug-cc-pVDZ

```
1\GINC-GOMBERG05\FTSUBHandHLYP\Aug-CC-pVDZ\C4H9N2(2)\HIROSHI\08-Sep-2010\1\#BHandHLYP
/aug-cc-pVDZ opt=(TS,z-matrix,readfc,NoEigenTest,maxcycle=100) Nosymm geom=check guess=read\TS carbon
N-Me\0,2\C\N,1,r2\C,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,
a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\C,2,r12,1,a12,3,d12,0\H,12,r13,2,a13,1,d1
3,0\H,12,r14,2,a14,1,d14,0\H,12,r15,2,a15,1,d15,0\r2=1.22329169\r3=1.4823981\r3=137.97605706\r4=2.22076957
\r4=113.10688785\d4=179.06748257\r5=1.29381908\r5=107.98343357\d5=-141.76349505\r6=1.08928103\r6=109.
20965289\d6=130.60306319\r7=1.09250588\r7=111.90102278\d7=8.45845781\r8=1.09116818\r8=109.30360901\d
8=247.35606877\r9=1.08836937\r9=87.96851018\d9=-16.49193582\r10=1.08779474\r10=88.4380429\d10=-260.5
4114974\r11=1.01490304\r11=110.22323606\d11=90.50726652\r12=1.45427643\r12=125.4211772\d12=0.593386
56\r13=1.09303111\r14=1.08971554\r15=1.0897689\r13=113.42556908\r14=108.64875812\r15=108.58953878\d1
3=-0.93012492\d14=-122.62512681\d15=120.53147922\Version=AM64L-G03RevE.01\HF=-267.0789976\S2=0.8
01731\S2-1=0.\$2A=0.750679\RMSD=4.144e-09\RMSF=8.117e-06\Thermal=0.\Dipole=0.9706431,0.0286208,0.66
29229\PG=C01 [X(C4H9N2)]\@\@
```

BHandHLYP/cc-pVTZ

```
1\GINC-GOMBERG01\FTSUBHandHLYP\CC-pVTZ\C4H9N2(2)\HIROSHI\31-Aug-2010\1\#BHandHLYP/cc-p
VTZ opt=(TS,z-matrix,calcfc,maxcycle=100) Nosymm\TS carbon N-Me\0,2\C\N,1,r2\C,1,r3,2,a3\C,1,r4,2,a4,3,d4,
0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,
0\H,5,r11,4,a11,1,d11,0\C,2,r12,1,a12,3,d12,0\H,12,r13,2,a13,1,d13,0\H,12,r14,2,a14,1,d14,0\H,12,r15,2,a15,1,d15,
0\r2=1.21431265\r3=1.47797707\r3=137.91155709\r4=2.19406763\r4=113.35831737\d4=177.66595546\r5=1.288
51567\r5=107.73893417\d5=-137.33840378\r6=1.08143818\r6=109.24791642\d6=134.49582848\r7=1.08500267\r7=112.01083976\d7=12.21473131\r8=1.08392546\r8=109.32152442\d8=251.40925493\r9=1.08065002\r9=88.4102
7217\d9=-11.8819486\r10=1.08061999\r10=89.27696483\d10=-256.38525231\r11=1.01000632\r11=110.287457\d
11=90.11683213\r12=1.45015185\r12=125.90826898\d12=0.79150385\r13=1.08547593\r14=1.08191849\r15=1.08
217746\r13=113.48888462\r14=108.79467662\r15=108.70913225\d13=-2.40596759\r14=-124.1231697\d15=119.
01641184\Version=AM64L-G03RevE.01\HF=-267.1444295\S2=0.802016\S2-1=0.\$2A=0.750644\RMSD=8.114e-
09\RMSF=4.417e-06\Thermal=0.\Dipole=0.937225,0.0853104,0.6709149\PG=C01 [X(C4H9N2)]\@\@
```

QCISD/cc-pVDZ// BHandHLYP/cc-pVTZ

QCISD= -266.4412339

CCSD(T)/cc-pVDZ// BHandHLYP/cc-pVTZ

CCSD(T)= -266.4710137

ROMP2/6-311G// BHandHLYP/cc-pVTZ**

MP2= -266.4717801

G2//MP2(full)/6-31G*

G2= -266.7133842

G3(MP2)-RAD// BHandHLYP/cc-pVTZ

G3(MP2)-RAD= -266.811796

Transition state for attacking of methanethioyl radical at nitrogen end of methanimine

BHandHLYP/6-311G**

```
1\GINC-GOMBERG01\FTS\UBHandHLYP\6-311G(d,p)\C3H6N1S1(2)\HIROSHI\08-Sep-2010\1\#BHandHLYP/6-311G** opt=(TS,NoEigenTest,z-matrix,ReadFC,maxcycle=100) Nosymm geom=check guess=read\TS N\0,2\CS,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\r2=1.60821568\r3=1.48037455\aa=132.49329659\r4=2.05071757\aa=110.01772655\d4=124.05140202\r5=1.25172286\aa=119.3233182\d5=11.65499958\r6=1.08875225\aa=112.24520318\d6=54.15263862\r7=1.08632121\aa=107.35125019\d7=-64.08827737\r8=1.08523064\aa=112.06667071\d8=177.46655727\r9=1.01023457\aa=123.1093826\d9=175.79335549\r10=1.0827228\aa=10=123.69189733\d10=166.47284373\r11=1.08406738\aa=117.4624703\d11=-12.74952236\Version=AM64L-G03RevE.01\HF=-570.6935469\S2=0.759253\S2-1=0.\$2A=0.750051\RMSD=5.779e-09\RMSF=2.092e-05\Thermal=0.\Dipole=-0.6549526,-1.2913895,-1.4010116\PG=C01 [X(C3H6N1S1)]\@\@
```

BHandHLYP/cc-pVDZ

```
1\GINC-GOMBERG02\FTS\UBHandHLYP\CC-pVDZ\C3H6N1S1(2)\HIROSHI\08-Sep-2010\1\#BHandHLYP/cc-pVDZ opt=(TS,NoEigenTest,z-matrix,ReadFC,maxcycle=100) Nosymm geom=check guess=read\TS N\0,2\CS,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\r2=1.6106448\r3=1.48363111\aa=131.97473026\r4=2.04995223\aa=109.75495645\d4=123.00609238\r5=1.25629177\aa=118.90815932\d5=12.34751302\r6=1.0968379\aa=112.42609232\d6=53.1882647\r7=1.09429778\aa=107.20908696\d7=-64.90610369\r8=1.09337431\aa=112.16268989\d8=176.70397871\r9=1.01632785\aa=124.20201835\d9=177.16046865\r10=1.09107812\aa=10=123.68610284\d10=167.30658574\r11=1.093193\aa=117.17809895\d11=-11.93046621\Version=AM64L-G03RevE.01\HF=-570.6522061\S2=0.759404\S2-1=0.\$2A=0.750052\RMSD=4.190e-09\RMSF=3.263e-05\Thermal=0.\Dipole=-0.6021939,-1.2410618,-1.3030996\PG=C01 [X(C3H6N1S1)]\@\@
```

BHandHLYP/aug-cc-pVDZ

```
1\GINC-GOMBERG03\FTS\UBHandHLYP\Aug-CC-pVDZ\C3H6N1S1(2)\HIROSHI\08-Sep-2010\1\#BHandHLYP/aug-cc-pVDZ opt=(TS,NoEigenTest,z-matrix,ReadFC,maxcycle=100) Nosymm geom=check guess=read\TS N\0,2\CS,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\r2=1.61412925\r3=1.48211931\aa=132.42371404\r4=2.06808873\aa=109.51747194\d4=123.08930622\r5=1.25697709\aa=118.71134419\d5=12.48761385\r6=1.09412045\aa=112.18495542\d6=52.45062352\r7=1.09197898\aa=107.08938866\d7=-65.72971503\r8=1.09045325\aa=8=111.96327364\d8=175.89320769\r9=1.01279002\aa=9=124.37702692\d9=177.08613254\r10=1.08813315\aa=10=123.41111346\d10=167.08333917\r11=1.08984089\aa=11=117.54555567\d11=-12.28552456\Version=AM64L-G03RevE.01\HF=-570.6664216\S2=0.760763\S2-1=0.\$2A=0.750064\RMSD=7.481e-09\RMSF=2.696e-05\Thermal=0.\Dipole=-0.6072036,-1.212455,-1.3144656\PG=C01 [X(C3H6N1S1)]\@\@
```

BHandHLYP/cc-pVTZ

```
1\GINC-GOMBERG06\FTS\UBHandHLYP\CC-pVTZ\C3H6N1S1(2)\HIROSHI\08-Sep-2010\1\#BHandHLYP/cc-pVTZ opt=(TS,NoEigenTest,z-matrix,calcFC,maxcycle=100) Nosymm\TS N\0,2\CS,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\r2=1.6025027\r3=1.47683172\aa=132.9160687\r4=2.04748896\aa=109.79362047\d4=124.29987177\r5=1.24870174\aa=118.81734244\d5=11.51655759\r6=1.0865745\aa=112.37206165\d6=54.00624993\r7=1.08410395\aa=107.31440934\d7=-64.18102426\r8=1.08293736\aa=112.13950152\d8=177.38399843\r9=1.0803071\aa=123.65777452\d9=176.40582452\r10=1.08022821\aa=10=123.51418413\d10=167.1286625\r11=1.08213796\aa=117.50627139\d11=-12.12552879\Version=AM64L-G03RevE.01\HF=-570.7212982\S2=0.761282\S2-1=0.\$2A=0.750072\RMSD=8.589e-09\RMSF=2.640e-05\Thermal=0.\Dipole=-0.6424818,-1.2124473,-1.3081629\Par=60.8606322,18.8841305,60.1426765,-0.810439,5.1538088,78.0157318\PG=C01 [X(C3H6N1S1)]\@\@
```

QCISD/cc-pVDZ// BHandHLYP/cc-pVTZ

QCISD= -569.72860

CCSD(T)/cc-pVDZ// BHandHLYP/cc-pVTZ

CCSD(T)= -569.75440

ROMP2/6-311G***// BHandHLYP/cc-pVTZ

MP2= -569.737044

G2//MP2(full)/6-31G*

G2= -569.9782063

G3(MP2)-RAD// BHandHLYP/cc-pVTZ

G3(MP2)-RAD= -570.1013727

Transition state for attacking of methanethioyl radical at carbon end of methanimine

BHandHLYP/6-311G**

```
1\1\GINC-GOMBERG04\FTSUBBHandHLYP\6-311G(d,p)\C3H6N1S1(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP
P/6-311G** opt=(TS,z-matrix,NoEigenTest,CalcFC,Maxcycle=100) Nosymm\TS C\0,2\C\S,1,r2\C,1,r3,2,a3\C,1,r4
,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,4,r10,1,
a10,2,d10,0\H,5,r11,4,a11,1,d11,0\r2=1.57281456\r3=1.4692492\r3=135.31656873\r4=2.12269308\r4=117.479329
41\r4=181.64236971\r5=1.29977495\r5=107.33536535\r5=-148.04355659\r6=1.08567441\r6=109.19374483\r6=1
29.01401086\r7=1.08458466\r7=112.15179389\r7=5.44522459\r8=1.0881879\r8=108.67281593\r8=243.83770895
\r9=1.08327755\r9=92.81951963\r9=-21.35190054\r10=1.08318588\r10=88.87271123\r10=-266.35268126\r11=1.
01263406\r11=109.8307032\r11=93.58810075\Version=AM64L-G03RevE.01\HF=-570.6892743\S2=0.8101\S2-1
=0.\$2A=0.750999\RMSD=8.798e-09\RMSF=5.146e-06\Thermal=0.\Dipole=0.2547336,-0.1012788,0.071181\PG=
C01 [X(C3H6N1S1)]\@\n
```

BHandHLYP/cc-pVDZ

```
1\1\GINC-GOMBERG05\FTSUBBHandHLYP\CC-pVDZ\C3H6N1S1(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/
cc-pVDZ opt=(TS,z-matrix,NoEigenTest,CalcFC,Maxcycle=100) Nosymm\TS C\0,2\C\S,1,r2\C,1,r3,2,a3\C,1,r4,2
,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H
,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\r2=1.58138256\r3=1.47253302\r3=135.00549425\r4=2.13378915\r4=117.9808894
\r4=179.15092044\r5=1.302591\r5=106.44944427\r5=-139.61369753\r6=1.09316068\r6=109.20301259\r6=134.9
6517148\r7=1.09246833\r7=112.29039854\r7=10.5822477\r8=1.09691346\r8=108.19918308\r8=249.86625935\r9
=1.09172\r9=92.52242344\r9=-12.81571383\r10=1.09200124\r10=89.37059441\r10=-257.91616347\r11=1.01978
356\r11=109.354542\r11=92.82784809\Version=AM64L-G03RevE.01\HF=-570.646855\S2=0.812056\S2-1=0.\$2
A=0.751084\RMSD=9.628e-09\RMSF=1.604e-05\Thermal=0.\Dipole=0.2524188,0.0134987,0.0746712\PG=C01 [
X(C3H6N1S1)]\@\n
```

BHandHLYP/aug-cc-pVDZ

```
1\1\GINC-GOMBERG05\FTSUBBHandHLYP\Aug-CC-pVDZ\C3H6N1S1(2)\HIROSHI\09-Sep-2010\1\#BHandH
LYP/aug-cc-pVDZ opt=(TS,z-matrix,NoEigenTest,CalcFC,Maxcycle=100) Nosymm\TS C\0,2\C\S,1,r2\C,1,r3,2,a
3\C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H
,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\r2=1.58106288\r3=1.47095464\r3=135.22036521\r4=2.13363752\r4=11
7.19058132\r4=181.94119868\r5=1.30273175\r5=107.69008004\r5=-151.15106035\r6=1.09199365\r6=108.77548
301\r6=122.76468383\r7=1.08996911\r7=111.94740962\r7=0.01402326\r8=1.09275028\r8=109.04612329\r8=237
.4709193\r9=1.08814821\r9=92.29683568\r9=-24.81536726\r10=1.08831061\r10=88.39413971\r10=-269.429207
71\r11=1.01504314\r11=110.23329762\r11=93.63048929\Version=AM64L-G03RevE.01\HF=-570.6634279\S2=0.
808344\S2-1=0.\$2A=0.751055\RMSD=9.488e-09\RMSF=2.109e-05\Thermal=0.\Dipole=0.3156649,-0.1249751,0.
1236846\PG=C01 [X(C3H6N1S1)]\@\n
```

BHandHLYP/cc-pVTZ

```
1\1\GINC-GOMBERG04\FTSUBBHandHLYP\CC-pVTZ\C3H6N1S1(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/
cc-pVTZ opt=(TS,z-matrix,NoEigenTest,CalcFC,Maxcycle=100) Nosymm\TS C\0,2\C\S,1,r2\C,1,r3,2,a3\C,1,r4,2
,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H
,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\r2=1.56857776\r3=1.46570194\r3=135.41164519\r4=2.10910746\r4=117.2584563
9\r4=181.44462237\r5=1.29799898\r5=107.81223948\r5=-147.905871\r6=1.08384004\r6=109.06478841\r6=125.
82267218\r7=1.08222003\r7=112.12001384\r7=2.66961718\r8=1.0856694\r8=109.00007215\r8=240.66381795\r9
=1.08032115\r9=92.79743786\r9=-21.35794782\r10=1.08104295\r10=89.01996686\r10=-266.39075558\r11=1.01
015883\r11=110.29118371\r11=93.54893824\Version=AM64L-G03RevE.01\HF=-570.7175928\S2=0.808746\S2-1=0.
\$2A=0.751069\RMSD=5.085e-09\RMSF=7.631e-06\Thermal=0.\Dipole=0.2983785,-0.0872843,0.1287783\Polar=66.4212618,3.8818793,46.2317729,13.9478706,6.6406972,95.2747175\PG=C01 [X(C3H6N1S1)]\@\n
```

QCISD/cc-pVDZ// BHandHLYP/cc-pVTZ

QCISD=-569.7243705

CCSD(T)/cc-pVDZ// BHandHLYP/cc-pVTZ
CCSD(T)= -569.7499537

ROMP2/6-311G// BHandHLYP/cc-pVTZ**
ROMP2= -569.7393939

G2//MP2(full)/6-31G*
G2= -569.9742307

G3(MP2)-RAD// BHandHLYP/cc-pVTZ
G3(MP2)-RAD= -570.1008958

Product for attacking of methylimidoyl radical at nitrogen end of methanimine

BHandHLYP/6-311G**

```
1\1\GINC-GOMBERG01\FOpt\UBHandHLYP\6-311G(d,p)\C3H7N2(2)\HIROSHI\09-Sep-2010\1\#bhandhlyp/6-3
11G** opt=(z-matrix,readfc,maxcycle=100) Nosymm freq=Noramfreq=check geom=guess=read\product trans out NH
\0,2\CVN,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d
8,0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\H,2,r12,1,a12,3,d12,0\r2=1.2662321\r3=1.50534
924\a3=126.59278333\r4=1.37366905\a4=119.80097781\d4=179.2511971\r5=1.37379896\a5=124.45953277\d5=-2.
49412027\r6=1.08697988\a6=110.5190155\d6=112.0141487\r7=1.08219169\a7=110.50730244\d7=-8.05480988\r8
=1.08667589\a8=110.96389928\d8=231.66168672\r9=0.99758485\a9=117.32173338\d9=180.93886815\r10=1.0706
9938\a10=117.74037295\d10=173.36155341\r11=1.06863409\a11=117.31908872\d11=5.97873849\r12=1.0062766
3\12=110.62628056\d12=0.88897523\Version=AM64L-G03RevE.01\HF=-227.893661\S2=0.76018\S2-1=0.\$2A
=0.750063\RMSD=5.050e-09\RMSF=2.562e-06\Thermal=0.\Dipole=0.5516007,0.0490288,-1.1894017\PG=C01 [X
(C3H7N2)]\@\@
```

BHandHLYP/cc-pVDZ

```
1\1\GINC-GOMBERG02\FOpt\UBHandHLYP\CC-pVDZ\C3H7N2(2)\HIROSHI\09-Sep-2010\1\#bhandhlyp/cc-p
VDZ opt=(z-matrix,readfc,maxcycle=100) Nosymm freq=Noramfreq=check geom=guess=read\product trans out NH
\0,2\CVN,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,
0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\H,2,r12,1,a12,3,d12,0\r2=1.27125112\r3=1.50526
104\12=126.73019439\r4=1.37552285\13=119.61989066\d4=179.76978012\r5=1.3755373\14=124.5136226\d5=-2.8
048016\r6=1.09500099\15=110.66288586\d6=115.89432197\r7=1.09005356\16=110.60197037\d7=-4.31143228\r8
=1.09476479\17=110.86933915\d8=235.35460646\r9=1.00205517\18=117.23968902\d9=181.58906171\r10=1.0796
7249\19=117.45550874\d10=171.9241641\r11=1.07797321\11=116.95828692\d11=7.85896578\r12=1.01307412\
12=109.9996873\d12=0.56452926\Version=AM64L-G03RevE.01\HF=-227.8452891\S2=0.760746\S2-1=0.\$2A
=0.750068\RMSD=5.645e-09\RMSF=2.537e-06\Thermal=0.\Dipole=0.5450318,0.0584972,-1.1537099\PG=C01 [X(
C3H7N2)]\@\@
```

BHandHLYP/aug-cc-pVDZ

```
1\1\GINC-GOMBERG02\FOpt\UBHandHLYP\Aug-CC-pVDZ\C3H7N2(2)\HIROSHI\09-Sep-2010\1\#bhandhlyp/
aug-cc-pVDZ opt=(z-matrix,readfc,maxcycle=100) Nosymm freq=Noramfreq=check geom=guess=read\product trans
out NH\0,2\CVN,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,
0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\H,2,r12,1,a12,3,d12,0\r2=1.27366881\r3=1.5045188\13=126.51373208\r4=1.37437037\14=119.52268263\d4=180.00363657\r5=1.37317643\15=124.7921959
1\d5=-0.00089992\r6=1.09241805\16=110.77519009\d6=120.15862803\r7=1.08729631\17=110.29861817\d7=0.03
120217\r8=1.09241859\18=110.77435248\d8=239.90330125\r9=1.00001421\19=117.17984977\d9=180.00402075\r
10=1.07580022\11=117.92054408\d10=179.9977472\r11=1.07410686\12=118.02953707\d11=0.00914767\r12=1.
00865309\13=110.63991467\d14=-0.00209099\Version=AM64L-G03RevE.01\HF=-227.8665084\S2=0.760635\S
2-1=0.\$2A=0.75007\RMSD=7.709e-09\RMSF=1.176e-06\Thermal=0.\Dipole=0.5306803,0.000037,-1.2433278\PG
=C01 [X(C3H7N2)]\@\@
```

BHandHLYP/cc-pVTZ

```
1\1\GINC-GOMBERG03\FOpt\UBHandHLYP\CC-pVTZ\C3H7N2(2)\HIROSHI\30-Aug-2010\1\#bhandhlyp/cc-p
VTZ opt=(z-matrix,calcfc,maxcycle=100) Nosymm freq=Noramfreq=check geom=guess=read\product trans out NH\0,2\CVN,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\H,2,r12,1,a12,3,d12,0\r2=1.26468219\r3=1.50138182\13=126.42949385\r4
```

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 $=1.36963274\text{a}4=119.90660294\text{d}4=179.98181303\text{v}5=1.36866301\text{a}5=124.83230967\text{d}5=-0.04060536\text{r}6=1.084610$
 $34\text{a}6=110.73367117\text{d}6=120.05547903\text{r}7=1.0795902\text{a}7=110.5265587\text{d}7=-0.18646712\text{r}8=1.08460423\text{a}8=110.74$
 $51952\text{d}8=239.56461967\text{r}9=0.9953964\text{a}9=117.12108208\text{d}9=180.00876407\text{r}10=1.06762072\text{a}10=118.02522337\text{d}$
 $10=179.89222122\text{r}11=1.06585713\text{a}11=117.94664688\text{d}11=0.09693318\text{r}12=1.00408261\text{a}12=110.90939894\text{d}12=$
 $0.01973208\text{\Version=AM64L-G03RevE.01\HF=-227.9196794\$\$2=0.760436\$\$2-1=0.\$\$2A=0.750069\$\$RMSD=7.169}$
 $e-09\$\$RMSF=4.480e-06\$\$Thermal=0.\$\$Dipole=0.5311834,0.0008612,-1.194313\$\$Polar=64.3588431,0.0135201,33.9580$
 $725.2.5896917,0.0029668,53.2088513\$\$PG=C01 [X(C3H7N2)]\$\$@$

QCISD/cc-pVDZ// BHandHLYP/cc-pVTZ

QCISD=-227.3188224

CCSD(T)/cc-pVDZ// BHandHLYP/cc-pVTZ

CCSD(T)= -227.3423598

ROMP2/6-311G// BHandHLYP/cc-pVTZ**

MP2=-227.3500796

G2//MP2(full)/6-31G*

G2=-227.5564995

G3(MP2)-RAD// BHandHLYP/cc-pVTZ

G3(MP2)-RAD= -227.639364

Product for attacking of methylimidoyl radical at carbon end of methanimine**BHandHLYP/6-311G****

1\1\GINC-GOMBERG01\FOpt\UBHandHLYP\6-311G(d,p)\C3H7N2(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/
 6-311G** opt=(z-matrix,readfc,maxcycle=100) Nosymm freq=noramam geom=check guess=read\product at carbon\
 \0,2\C\N,1,r2\|C,1,r3,2,a3\|C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,
 ,0\H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\H,2,r12,1,a12,3,d12,0\|r2=1.25806047\|r3=1.50151
 258\|a3=126.31280372\|r4=1.51874633\|a4=118.07156705\|d4=178.28851354\|r5=1.44359022\|a5=110.31016205\|d5=-
 105.74935674\|r6=1.08618107\|a6=110.13639683\|d6=126.70620973\|r7=1.08431836\|a7=111.52175208\|d7=5.194106
 5\|r8=1.08733762\|a8=110.04745003\|d8=244.39694906\|r9=1.08807723\|a9=107.01357744\|d9=15.26138926\|r10=1.0
 8662205\|a10=110.09249432\|d10=-226.0090022\|r11=1.01748817\|a11=105.81502607\|d11=64.69699896\|r12=1.0126
 0072\|a12=111.0718345\|d12=0.07397879\Version=AM64L-G03RevE.01\HF=-227.8715972\\$\\$2=0.755026\\$\\$2-1=0.\\$
 \\$\\$2A=0.750018\\$\\$RMSD=2.769e-09\\$\\$RMSF=1.350e-05\\$\\$Thermal=0.\\$\\$Dipole=0.6758711,0.2272423,-0.0340036\\$\\$PG=C01
 1 [X(C3H7N2)]\\$\\$@

BHandHLYP/cc-pVDZ

1\1\GINC-GOMBERG02\FOpt\UBHandHLYP\CC-pVDZ\C3H7N2(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/c
 c-pVDZ opt=(z-matrix,readfc,maxcycle=100) Nosymm freq=noramam geom=check guess=read\product at carbon\
 \0,2\|CN,1,r2\|C,1,r3,2,a3\|C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0
 \H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\H,2,r12,1,a12,3,d12,0\|r2=1.26327848\|r3=1.502191
 19\|a3=126.26588319\|r4=1.51754587\|a4=118.21394742\|d4=178.69170557\|r5=1.44376095\|a5=111.41417245\|d5=-1
 11.29061752\|r6=1.09424101\|a6=110.14755558\|d6=126.41095383\|r7=1.09206945\|a7=111.65409824\|d7=4.7203045
 2\|r8=1.09525653\|a8=110.05204819\|d8=243.77951947\|r9=1.09666742\|a9=106.97752778\|d9=9.85568683\|r10=1.09
 542566\|a10=109.90924264\|d10=-232.08583103\|r11=1.02551138\|a11=105.53394019\|d11=60.45948079\|r12=1.0196
 11\|a12=110.38909252\|d12=0.15049658\Version=AM64L-G03RevE.01\HF=-227.823898\\$\\$2=0.754872\\$\\$2-1=0.\\$
 \\$\\$2A=0.750017\\$\\$RMSD=8.725e-09\\$\\$RMSF=4.203e-06\\$\\$Thermal=0.\\$\\$Dipole=0.6717666,0.1395465,-0.0271607\\$\\$PG=C01
 1 [X(C3H7N2)]\\$\\$@

BHandHLYP/aug-cc-pVDZ

1\1\GINC-GOMBERG02\FOpt\UBHandHLYP\Aug-CC-pVDZ\C3H7N2(2)\HIROSHI\09-Sep-2010\1\#BHandH
 LYP/aug-cc-pVDZ opt=(z-matrix,readfc,maxcycle=100) Nosymm freq=noramam geom=check guess=read\product at
 carbon\
 \0,2\|CN,1,r2\|C,1,r3,2,a3\|C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0
 \H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\H,2,r12,1,a12,3,d12,0\|r2=1.26448299\|r3=1.
 50134238\|a3=126.00533119\|r4=1.51812214\|a4=118.02986603\|d4=178.41423271\|r5=1.44358959\|a5=111.221738
 69\|d5=-103.27860268\|r6=1.09204117\|a6=110.12776804\|d6=125.00459174\|r7=1.08923281\|a7=111.50699271\|d7=3
 .45964926\|r8=1.09275255\|a8=109.9467337\|d8=242.52190652\|r9=1.09437529\|a9=107.28887872\|d9=16.86728618\|r

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 10=1.09167184\ a10=110.39620135\d10=-224.1976891\r11=1.02065555\ a11=106.44437561\d11=58.31259777\r12=1.01460965\ a12=111.27483938\d12=-0.11805798\ Version=AM64L-G03RevE.01\ HF=-227.8449432\ S2=0.755697\ S2-1=0\ S2A=0.750024\ RMSD=6.006e-09\ RMSF=7.672e-06\ Thermal=0\ Dipole=0.7425936,0.2479866,-0.1151827\ PG=C01 [X(C3H7N2)]\\@

BHandHLYP/cc-pVTZ

1\GINC-GOMBERG01\FOpt\UBHandHLYP\CC-pVTZ\C3H7N2(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/c
 c-pVTZ opt=(z-matrix,calcfc,maxcycle=100) Nosymm freq=noramanc\product at carbon\0,2\C\N,1,r2\C,1,r3,2,a3\C
 ,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,4,r1
 0,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\H,2,r12,1,a12,3,d12,0\r2=1.25595428\r3=1.49768288\ a3=126.01995418\r4=1.51496167\r4=118.27471135\d4=178.45397059\r5=1.43986354\ a5=110.87100741\d5=-104.48889719\r6=1.08423
 964\ a6=110.19809554\d6=125.54615039\r7=1.08175808\ a7=111.5412754\d7=4.02530364\r8=1.08502401\ a8=110.
 0711724\d8=243.12031053\r9=1.08639406\ a9=107.25281488\d9=16.07512536\r10=1.08440321\ a10=110.2005412
 1\d10=-225.24774505\r11=1.0153598\ a11=106.29004756\d11=60.96638743\r12=1.01020005\ a12=111.37382183\d
 12=-0.06850145\ Version=AM64L-G03RevE.01\ HF=-227.8961298\ S2=0.755473\ S2-1=0\ S2A=0.750022\ RMSD=5.139e-09\ RMSF=5.700e-06\ Thermal=0\ Dipole=0.6967741,0.2252065,-0.0726856\ Polar=48.9366298,2.5324293,4
 1.4351056,2.2097616,1.1954133,5
 4.0911737\ PG=C01 [X(C3H7N2)]\\@

QCISD/cc-pVDZ// BHandHLYP/cc-pVTZ

QCISD=-227.3028977

CCSD(T)/cc-pVDZ// BHandHLYP/cc-pVTZ

CCSD(T)= -227.3259627

ROMP2/6-311G// BHandHLYP/cc-pVTZ**

MP2=-227.3274907

G2//MP2(full)/6-31G*

G2=-227.5333547

G3(MP2)-RAD// BHandHLYP/cc-pVTZ

G3(MP2)-RAD= -227.6153914

Product for attacking of N-methylmethyliimidoyl radical at nitrogen end of methanimine**BHandHLYP/6-311G****

1\GINC-GOMBERG04\FOpt\UBHandHLYP\6-311G(d,p)\C4H9N2(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/
 6-311G** opt=(z-matrix,readfc,maxcycle=100) Nosymm freq=Noramanc\geom=check guess=read\product nitrogen
 N-Me\0,2\C\N,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,
 a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\C,2,r12,1,a12,3,d12,0\H,12,r13,2,a13,1,d1
 3,0\H,12,r14,2,a14,1,d14,0\H,12,r15,2,a15,1,d15,0\r2=1.26520578\r3=1.50488066\ a3=125.9187419\r4=1.37522642
 \ a4=119.33620695\d4=179.99998673\r5=1.37027664\ a5=124.70265422\d5=0.00537959\r6=1.08576758\ a6=110.33
 325114\d6=59.19843024\r7=1.08576929\ a7=110.33334671\d7=-59.21635924\r8=1.08404967\ a8=112.39970593\d8
 =179.99106542\r9=0.99688014\ a9=117.1888628\d9=179.99627077\r10=1.07001928\ a10=117.99358755\d10=180.0
 1734673\r11=1.06783645\ a11=117.78061122\d11=-0.01747517\r12=1.44069798\ a12=118.91518148\d12=-0.00137
 338\r13=1.08340636\r14=1.09181013\r15=1.09181028\ a13=108.96187597\ a14=112.78543209\ a15=112.78266577\d
 13=179.98205155\d14=60.89093684\d15=299.07065831\ Version=AM64L-G03RevE.01\ HF=-267.1797972\ S2=0.
 762807\ S2-1=0\ S2A=0.750089\ RMSD=7.098e-09\ RMSF=2.143e-05\ Thermal=0\ Dipole=0.4888514,-0.0001565,-1
 .048034\ PG=C01 [X(C4H9N2)]\\@

BHandHLYP/cc-pVDZ

1\GINC-GOMBERG05\FOpt\UBHandHLYP\CC-pVDZ\C4H9N2(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/cc-
 pVDZ opt=(z-matrix,readfc,maxcycle=100) Nosymm freq=Noramanc\geom=check guess=read\product nitrogen N-
 Me\0,2\C\N,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,
 2,d8,0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\C,2,r12,1,a12,3,d12,0\H,12,r13,2,a13,1,d13,0
 \ H,12,r14,2,a14,1,d14,0\H,12,r15,2,a15,1,d15,0\r2=1.27152899\r3=1.50415171\ a3=125.98470385\r4=1.37577959\ a
 4=119.16182709\d4=179.99944388\r5=1.37152938\ a5=124.81559828\d5=0.00553098\r6=1.09396355\ a6=110.3694
 9387\d6=59.05800974\r7=1.09396482\ a7=110.36970056\d7=-59.07115905\r8=1.09203308\ a8=112.47373659\d8=1

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 79.99344382\r9=1.00139272\aa9=117.03584546\dd9=179.9962837\r10=1.07872117\aa10=117.90447275\d10=180.018
 18044\r11=1.07710591\aa11=117.63351779\d11=-0.01852345\r12=1.43966018\aa12=118.46590254\d12=-0.0010210
 7\r13=1.09235219\r14=1.10023894\r15=1.10023996\aa13=109.22982968\aa14=112.97495351\aa15=112.97133316\d1
 3=179.9771641\d14=60.78777914\d15=299.16320418\\Version=AM64L-G03RevE.01\\HF=-267.1236797\\S2=0.764
 002\\S2-1=0.\\S2A=0.7501\\RMSD=4.446e-09\\RMSF=1.308e-04\\Thermal=0.\\Dipole=0.453597,-0.0001604,-1.04715
 31\\PG=C01 [X(C4H9N2)]\\@

BHandHLYP/aug-cc-pVDZ

1\\GINC-GOMBERG05\\FOpt\\UBHandHLYP\\Aug-CC-pVDZ\\C4H9N2(2)\\HIROSHI\\09-Sep-2010\\#BHandhIY
 P/aug-cc-pVDZ opt=(z-matrix,readfc,maxcycle=100) Nosymm freq=Noraman geom=check guess=read\\product nitr
 ogen N-Me\\0,2\\C\\N,1,r2\\C,1,r3,2,a3\\N,1,r4,2,a4,3,d4,0\\C,4,r5,1,a5,2,d5,0\\H,3,r6,1,a6,2,d6,0\\H,3,r7,1,a7,2,d7,0\\H,3,
 r8,1,a8,2,d8,0\\H,4,r9,1,a9,2,d9,0\\H,5,r10,4,a10,1,d10,0\\H,5,r11,4,a11,1,d11,0\\C,2,r12,1,a12,3,d12,0\\H,12,r13,2,a13,
 1,d13,0\\H,12,r14,2,a14,1,d14,0\\H,12,r15,2,a15,1,d15,0\\r2=1.27115624\\r3=1.50392048\\a3=125.75370829\\r4=1.377
 52717\\a4=119.23926983\\d4=180.00058201\\r5=1.3703925\\a5=125.03365911\\d5=0.00036556\\r6=1.09113834\\a6=11
 0.30057217\\d6=59.18989416\\r7=1.09114032\\a7=110.30071062\\d7=-59.21212118\\r8=1.08942034\\a8=112.1829802
 9\\d8=179.98907375\\r9=0.99927424\\a9=116.97068081\\d9=180.00009197\\r10=1.07606831\\a10=117.84810416\\d10=179.99734967\\r11=1.07397844\\a11=118.18177797\\d11=0.00124549\\r12=1.44185638\\a12=118.56694511\\d12=-0.0
 0143427\\r13=1.08870137\\r14=1.09688909\\r15=1.09688975\\a13=108.9750985\\a14=112.64701734\\a15=112.644029
 04\\d13=179.981456\\d14=60.82223906\\d15=299.13800723\\Version=AM64L-G03RevE.01\\HF=-267.1443043\\S2=0.
 763363\\S2-1=0.\\S2A=0.750097\\RMSD=4.173e-09\\RMSF=7.330e-05\\Thermal=0.\\Dipole=0.5053646,0.0000115,-1.
 0623255\\PG=C01 [X(C4H9N2)]\\@

BHandHLYP/cc-pVTZ

1\\GINC-GOMBERG07\\FOpt\\UBHandHLYP\\CC-pVTZ\\C4H9N2(2)\\HIROSHI\\30-Aug-2010\\#BHandhIY\\cc-
 pVTZ opt=(z-matrix,calcfc,maxcycle=100) Nosymm freq=Noraman\\product nitrogen N-Me\\0,2\\C\\N,1,r2\\C,1,r3,2,
 a3\\N,1,r4,2,a4,3,d4,0\\C,4,r5,1,a5,2,d5,0\\H,3,r6,1,a6,2,d6,0\\H,3,r7,1,a7,2,d7,0\\H,3,r8,1,a8,2,d8,0\\H,4,r9,1,a9,2,d9,0\\
 H,5,r10,4,a10,1,d10,0\\H,5,r11,4,a11,1,d11,0\\C,2,r12,1,a12,3,d12,0\\H,12,r13,2,a13,1,d13,0\\H,12,r14,2,a14,1,d14,0\\H
 ,12,r15,2,a15,1,d15,0\\r2=1.26229774\\r3=1.50128997\\a3=125.72396403\\r4=1.37241719\\a4=119.49485633\\d4=179.
 9996092\\r5=1.36563766\\a5=125.0759102\\d5=0.00358274\\r6=1.08322251\\a6=110.31703904\\d6=59.15376881\\r7=1
 0.08322316\\a7=110.31731335\\d7=-59.16602908\\r8=1.08154249\\a8=112.38805644\\d8=179.99397443\\r9=0.9946038
 7\\a9=116.92529502\\d9=179.99781607\\r10=1.06757363\\a10=117.95145416\\d10=180.01035767\\r11=1.06549418\\a1
 1=118.07880528\\d11=-0.01069449\\r12=1.43777286\\a12=119.12037868\\d12=-0.00134796\\r13=1.08105724\\r14=1.0
 8902563\\r15=1.089026\\a13=109.07270986\\a14=112.72958917\\a15=112.72463457\\d13=179.96717013\\d14=60.797
 55849\\d15=299.13242069\\Version=AM64L-G03RevE.01\\HF=-267.209058\\S2=0.762937\\S2-1=0.\\S2A=0.750093\\
 RMSD=5.902e-09\\RMSF=8.241e-05\\Thermal=0.\\Dipole=0.4763846,-0.0001103,-1.0440635\\PG=C01 [X(C4H9N2)]\\@

QCISD/cc-pVDZ// BHandHLYP/cc-pVTZ

QCISD=-266.5003680

CCSD(T)/cc-pVDZ// BHandHLYP/cc-pVTZ

CCSD(T)= -266.5291381

ROMP2/6-311G// BHandHLYP/cc-pVTZ**

MP2=-266.5329843

G2//MP2(full)/6-31G*

G2=-266.7714697

G3(MP2)-RAD// BHandHLYP/cc-pVTZ

G3(MP2)-RAD= -266.8702363

Product for attacking of N-methylmethyliimidoyl radical at carbon end of methanimine**BHandHLYP/6-311G****

1\\GINC-GOMBERG02\\FOpt\\UBHandHLYP\\6-311G(d,p)\\C4H9N2(2)\\HIROSHI\\09-Sep-2010\\#BHandhIY\\
 6-311G** opt=(z-matrix,readfc,maxcycle=100) Nosymm freq=Noraman geom=check guess=read\\product carbon
 N-Me\\0,2\\C\\N,1,r2\\C,1,r3,2,a3\\C,1,r4,2,a4,3,d4,0\\N,4,r5,1,a5,2,d5,0\\H,3,r6,1,a6,2,d6,0\\H,3,r7,1,a7,2,d7,0\\H,3,r8,1,
 a8,2,d8,0\\H,4,r9,1,a9,2,d9,0\\H,4,r10,1,a10,2,d10,0\\H,5,r11,4,a11,1,d11,0\\C,2,r12,1,a12,3,d12,0\\H,12,r13,2,a13,1,d1

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 3,0\H,12,r14,2,a14,1,d14,0\H,12,r15,2,a15,1,d15,0\r2=1.25645568\r3=1.50644355\|a3=128.82452158\r4=1.5216691
 4\|a4=116.9342078\r4=178.77989022\r5=1.44308453\|a5=109.83460263\|d5=-104.22435724\r6=1.08472662\|a6=109.
 18678473\|d6=140.87890258\r7=1.08120188\|a7=113.51708313\|d7=19.45542706\r8=1.08805945\|a8=109.74958596\|
 d8=258.14962502\|r9=1.08725166\|a9=107.13083674\|d9=17.27686053\|r10=1.08726871\|a10=109.7672817\|d10=-223.
 .89655921\|r11=1.01719264\|a11=105.77317859\|d11=68.69153349\|r12=1.44075412\|a12=122.63775721\|d12=1.0041
 319\|r13=1.08738557\|r14=1.08661884\|r15=1.08597383\|a13=115.85131061\|a14=108.66983146\|a15=108.29853787\|
 d13=3.75294243\|d14=-18.85651214\|d15=125.65364653\|Version=AM64L-G03RevE.01\|HF=-267.1591838\|S2=0.
 755147\|S2-1=0.\|S2A=0.750019\|RMSD=5.055e-09\|RMSF=3.562e-05\|Thermal=0.\|Dipole=0.651117,0.2730431,0.23
 514\|PG=C01 [X(C4H9N2)]\|@

BHandHLYP/cc-pVDZ

1\|GINC-GOMBERG04\FOpt\UBHandHLYP\CC-pVDZ\C4H9N2(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/cc-pVDZ opt=(z-matrix,readfc,maxcycle=100) Nosymm freq=Noraman geom=check guess=read\product carbon N-Me\|0,2\CN,1,r2\|C,1,r3,2,a3\|C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\|C,2,r12,1,a12,3,d12,0\H,12,r13,2,a13,1,d13,0\H,12,r14,2,a14,1,d14,0\H,12,r15,2,a15,1,d15,0\r2=1.26247373\r3=1.50648111\|a3=128.96598936\r4=1.52019502\|a4=116.96580672\|d4=178.81346653\r5=1.44377075\|a5=110.99285912\|d5=-107.56625743\|r6=1.09310167\|a6=109.103
 15669\|d6=137.56050481\|r7=1.08871133\|a7=113.85754076\|d7=15.74025411\|r8=1.09582779\|a8=109.61040152\|d8=254.30122962\|r9=1.09599725\|a9=107.06868979\|d9=13.75146457\|r10=1.09573163\|a10=109.82330153\|d10=-227.9
 333876\|r11=1.02536013\|a11=105.37013777\|d11=63.06226852\|r12=1.43977665\|a12=122.4552022\|d12=0.8303643
 3\|r13=1.09547731\|r14=1.09482567\|r15=1.09460076\|a13=116.20223116\|a14=108.71010564\|a15=108.44150508\|d13=0.97953544\|d14=-121.70144265\|d15=123.08104858\|Version=AM64L-G03RevE.01\|HF=-267.1033635\|S2=0.75
 4927\|S2-1=0.\|S2A=0.750018\|RMSD=5.366e-09\|RMSF=2.833e-05\|Thermal=0.\|Dipole=0.64787,0.1993485,0.22283
 29\|PG=C01 [X(C4H9N2)]\|@

BHandHLYP/aug-cc-pVDZ

1\|GINC-GOMBERG04\FOpt\UBHandHLYP\Aug-CC-pVDZ\C4H9N2(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/aug-cc-pVDZ opt=(z-matrix,readfc,maxcycle=100) Nosymm freq=Noraman geom=check guess=read\product carbon N-Me\|0,2\CN,1,r2\|C,1,r3,2,a3\|C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\|C,2,r12,1,a12,3,d12,0\H,12,r13,2,a13,1,d13,0\H,12,r14,2,a14,1,d14,0\H,12,r15,2,a15,1,d15,0\r2=1.26208691\r3=1.50557593\|a3=128.659712\r4=1.521760
 56\|a4=116.89480199\|d4=178.4521338\r5=1.44318421\|a5=110.65014631\|d5=-98.84022571\|r6=1.09092831\|a6=109.
 12112024\|d6=134.83040606\|r7=1.08571561\|a7=113.67111906\|d7=13.2752961\|r8=1.09312804\|a8=109.58098088\|d8=251.65053387\|r9=1.09363326\|a9=107.44441073\|d9=21.67336946\|r10=1.09193234\|a10=110.17797\|d10=-219.20
 083397\|r11=1.02037876\|a11=106.18535188\|d11=62.10165333\|r12=1.44119625\|a12=122.76744535\|d12=0.610771
 25\|r13=1.09221409\|r14=1.09213433\|r15=1.09097325\|a13=115.72826232\|a14=108.71425303\|a15=108.29653809\|d13=7.32202698\|d14=-115.25166875\|d15=129.12949994\|Version=AM64L-G03RevE.01\|HF=-267.1244421\|S2=0.75579\|S2-1=0.\|S2A=0.750025\|RMSD=7.804e-09\|RMSF=1.702e-05\|Thermal=0.\|Dipole=0.7335731,0.320126,0.1585
 463\|PG=C01 [X(C4H9N2)]\|@

BHandHLYP/cc-pVTZ

1\|GINC-GOMBERG01\FOpt\UBHandHLYP\CC-pVTZ\C4H9N2(2)\HIROSHI\31-Aug-2010\1\#BHandHLYP/cc-pVTZ opt=(z-matrix,calcfc,maxcycle=100) Nosymm freq=Noraman\product carbon N-Me\|0,2\CN,1,r2\|C,1,r3,2,a3\|C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\|C,2,r12,1,a12,3,d12,0\H,12,r13,2,a13,1,d13,0\H,12,r14,2,a14,1,d14,0\H,12,r15,2,a15,1,d15,0\r2=1.25372229\r3=1.50211177\|a3=128.78183944\r4=1.51896217\|a4=117.04779753\|d4=178.511
 75613\|r5=1.43925515\|a5=110.31674998\|d5=-100.49257926\|r6=1.08326359\|a6=109.20684124\|d6=135.31954835\|r7=1.0782121\|a7=113.74534446\|d7=13.6313033\|r8=1.08557103\|a8=109.59189831\|d8=252.15936248\|r9=1.08569185\|a9=107.35357228\|d9=20.36984623\|r10=1.0847037\|a10=110.06226166\|d10=-220.75497552\|r11=1.01512421\|a11=106.10456846\|d11=64.4283073\|r12=1.43698525\|a12=123.14646616\|d12=0.65644362\|r13=1.08473497\|r14=1.08432885\|r15=1.08375332\|a13=115.86044184\|a14=108.73097305\|a15=108.4232812\|d13=3.46305461\|d14=-119.0426
 9289\|d15=125.39772876\|Version=AM64L-G03RevE.01\|HF=-267.1870706\|S2=0.755588\|S2-1=0.\|S2A=0.750023\|RMSD=3.666e-09\|RMSF=2.325e-05\|Thermal=0.\|Dipole=0.6774788,0.2920059,0.1908449\|PG=C01 [X(C4H9N2)]\|@

QCISD/cc-pVDZ// BHandHLYP/cc-pVTZ

QCISD=-266.4850993

CCSD(T)/cc-pVDZ// BHandHLYP/cc-pVTZ

CCSD(T)= -266.5133616

ROMP2/6-311G// BHandHLYP/cc-pVTZ**

MP2=-266.5115454

G2//MP2(full)/6-31G*

G2=-266.7503038

G3(MP2)-RAD// BHandHLYP/cc-pVTZ

G3(MP2)-RAD= -266.8477448

Product for attacking of methanethioyl radical at nitrogen end of methanimine

BHandHLYP/6-311G**

```
1\GINC-GOMBERG02\FOpt\UBHandHLYP\6-311G(d,p)\C3H6N1S1(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/6-311G** Nosymm opt=(z-matrix,readfc,maxcycle=100) freq=noraman geom=check guess=read\product N\0,2\C\S,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\r2=1.65014931\r3=1.50189476\aa=122.41421942\r4=1.35121716\aa=123.47552516\dd=181.63610334\r5=1.35931961\aa=127.55257351\dd=0.43118204\r6=1.08756658\aa=112.52636832\dd=164.80542821\r7=1.08169126\aa=109.81170287\dd=43.35058713\r8=1.08610703\aa=109.53974489\dd=285.47083238\r9=1.00187198\aa=116.0329988\dd=180.25091351\r10=1.07018441\aa=117.60712005\dd=180.81273773\r11=1.06870792\aa=118.34026145\dd=0.23340111\Version=AM64L-G03RevE.01\HF=-570.7626251\$2=0.77074\$2-1=0.\$2A=0.750146\RMSD=7.915e-09\RMSF=2.356e-05\Thermal=0.\Dipole=-0.4074617,0.0336905,-1.9307666\PG=C01 [X(C3H6N1S1)]\@\n
```

BHandHLYP/cc-pVDZ

```
1\GINC-GOMBERG03\FOpt\UBHandHLYP\CC-pVDZ\C3H6N1S1(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/cc-pVDZ Nosymm opt=(z-matrix,readfc,maxcycle=100) freq=noraman geom=check guess=read\product N\0,2\C\S,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\r2=1.65497084\r3=1.50258143\aa=122.32196629\r4=1.35354707\aa=123.28589609\dd=180.95390543\r5=1.36106182\aa=127.40839839\dd=0.30287412\r6=1.09522442\aa=112.75913875\dd=170.90655587\r7=1.09073283\aa=109.68868709\dd=49.40083873\r8=1.09342774\aa=109.63839093\dd=291.93357241\r9=1.00627564\aa=116.02051237\dd=180.19807986\r10=1.07867016\aa=117.54249599\dd=180.59910331\r11=1.07806041\aa=117.9822451\dd=0.09654467\Version=AM64L-G03RevE.01\HF=-570.7215537\$2=0.772956\$2-1=0.\$2A=0.750167\RMSD=9.062e-09\RMSF=1.811e-05\Thermal=0.\Dipole=-0.3486142,0.0210904,-1.8223687\PG=C01 [X(C3H6N1S1)]\@\n
```

BHandHLYP/aug-cc-pVDZ

```
1\GINC-GOMBERG02\FOpt\UBHandHLYP\Aug-CC-pVDZ\C3H6N1S1(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/aug-cc-pVDZ Nosymm opt=(z-matrix,readfc,maxcycle=100) freq=noraman geom=check guess=read\product N\0,2\C\S,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\r2=1.65656821\r3=1.50197416\aa=122.32533314\r4=1.35377033\aa=123.16135247\dd=180.72779686\r5=1.36088568\aa=127.42136997\dd=0.32892929\r6=1.09276955\aa=112.55698987\dd=173.01704385\r7=1.08845076\aa=109.62900608\dd=51.58687104\r8=1.09052712\aa=109.50150689\dd=293.96531091\r9=1.00402329\aa=116.04296701\dd=180.27160427\r10=1.07610982\aa=117.52767411\dd=180.39217977\r11=1.07495517\aa=118.34243415\dd=0.13939145\Version=AM64L-G03RevE.01\HF=-570.736718\$2=0.771142\$2-1=0.\$2A=0.750158\RMSD=6.890e-09\RMSF=1.940e-05\Thermal=0.\Dipole=-0.3444435,0.0118436,-1.8635183\PG=C01 [X(C3H6N1S1)]\@\n
```

BHandHLYP/cc-pVTZ

```
1\GINC-GOMBERG03\FOpt\UBHandHLYP\CC-pVTZ\C3H6N1S1(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/cc-pVTZ Nosymm opt=(z-matrix,calcfc,maxcycle=100) freq=noraman\product N\0,2\C\S,1,r2\C,1,r3,2,a3\N,1,r4,2,a4,3,d4,0\C,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,5,r10,4,a10,1,d10,0\H,5,r11,4,a11,1,d11,0\r2=1.64500593\r3=1.49873744\aa=122.68387932\r4=1.34916552\aa=123.35553908\dd=181.86251568\r5=1.35539459\aa=127.57701396\dd=0.80951471\r6=1.08562915\aa=112.18187939\dd=154.5984987\r7=1.07833289\aa=109.91679441\dd=33.07838692\r8=1.0849972\aa=109.6815192\dd=274.82894611\r9=0.99978997\aa=115.96531643\dd=180.58620855\r10=1.0679721\aa=117.62939465\dd=181.05013968\r11=1.06677661\aa=118.34810918\dd=0.35240039\Version=AM64L-G03RevE.01\HF=-570.7908161\$2=0.772504\$2-1=0.
```

\\$2A=0.750176\RMSD=3.638e-09\RMSF=3.023e-05\Thermal=0.\Dipole=-0.3445985,0.0334623,-1.8250535\Polar=80.5562499,-1.0803085,38.9807785,10.3479566,-0.4954014,77.9309844\PG=C01 [X(C3H6N1S1)]\\@

QCISD/cc-pVDZ// BHandHLYP/cc-pVTZ
QCISD=-569.7895195

CCSD(T)/cc-pVDZ// BHandHLYP/cc-pVTZ
CCSD(T)= -569.814044

ROMP2/6-311G// BHandHLYP/cc-pVTZ**
MP2=-569.80060

G2//MP2(full)/6-31G*
G2=-570.03915

G3(MP2)-RAD// BHandHLYP/cc-pVTZ
G3(MP20-RAD)= -570.1619247

Product for attacking of methanethioyl radical at carbon end of methanimine

BHandHLYP/6-311G**

1\1\GINC-GOMBERG03\FOpt\UBHandHLYP\6-311G(d,p)\C3H6N1S1(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/6-311G** opt=(z-matrix,readfc,maxcycle=100) Nosymm freq=Noraman geom=check guess=read\product C\0,2\CS,1,r2\C,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\r2=1.61702302\r3=1.49336356\aa3=123.71622789\r4=1.51676066\aa4=122.00799136\aa4=177.65614336\r5=1.44520865\aa5=110.26808695\aa5=-102.13527932\r6=1.08805657\aa6=109.74397911\aa6=127.69930673\r7=1.08038531\aa7=111.8368445\aa7=5.21583229\r8=1.08917386\aa8=109.2208529\r8=244.15306432\r9=1.08790771\aa9=109.00280564\aa9=18.60511609\r10=1.08673657\aa10=109.7495805\aa10=-222.01059641\r11=1.01779573\aa11=106.13307648\r11=58.82612098\Version=AM64L-G03RevE.01\HF=-570.7269383\\$2=0.755415\\$2-1=0.\\$2A=0.750022\RMSD=7.198e-09\RMSF=3.223e-06\Thermal=0.\Dipole=0.1456841,0.2136182,-0.4506078\PG=C01 [X(C3H6N1S1)]\\@

BHandHLYP/cc-pVDZ

1\1\GINC-GOMBERG02\FOpt\UBHandHLYP\CC-pVDZ\C3H6N1S1(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/cc-pVDZ opt=(z-matrix,readfc,maxcycle=100) Nosymm freq=Noraman geom=check guess=read\product C\0,2\CS,1,r2\C,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\r2=1.62378297\r3=1.49490955\aa3=123.57252697\r4=1.51565562\aa4=121.97896964\aa4=177.22173594\r5=1.44515511\aa5=111.18473129\aa5=-102.91393999\r6=1.09619065\aa6=109.6040317\r6=126.74492153\r7=1.08837663\aa7=111.89714921\r7=4.2127354\r8=1.09695882\aa8=109.30772929\r8=242.88403641\r9=1.09660177\aa9=108.9641931\r9=17.50263778\r10=1.09546162\aa10=109.96624686\d10=-223.53666278\r11=1.02577603\aa11=105.74304084\r11=52.90521347\Version=AM64L-G03RevE.01\HF=-570.685777\\$2=0.755169\\$2-1=0.\\$2A=0.75002\RMSD=9.506e-09\RMSF=6.642e-06\Thermal=0.\Dipole=0.1912875,0.1796507,-0.416924\PG=C01 [X(C3H6N1S1)]\\@

BHandHLYP/aug-cc-pVDZ

1\1\GINC-GOMBERG01\FOpt\UBHandHLYP\Aug-CC-pVDZ\C3H6N1S1(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/aug-cc-pVDZ opt=(z-matrix,readfc,maxcycle=100) Nosymm freq=Noraman geom=check guess=read\product C\0,2\CS,1,r2\C,1,r3,2,a3\C,1,r4,2,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,4,r10,1,a10,2,d10,0\H,5,r11,4,a11,1,d11,0\r2=1.62543347\r3=1.49323067\aa3=123.60652487\r4=1.51815217\aa4=121.49790021\aa4=177.4074873\r5=1.44438071\aa5=110.76623375\aa5=-91.87385264\r6=1.09400177\aa6=109.57360331\r6=126.09793557\r7=1.08586566\aa7=111.79395988\r7=3.65925885\r8=1.09465784\aa8=109.19533954\r8=242.30256228\r9=1.09447293\aa9=108.86961166\r9=27.75347681\r10=1.09153233\aa10=110.43429612\d10=-212.45986767\r11=1.02078849\aa11=106.54661819\r11=53.63108959\Version=AM64L-G03RevE.01\HF=-570.702271\\$2=0.756112\\$2-1=0.\\$2A=0.750028\RMSD=5.014e-09\RMSF=9.236e-06\Thermal=0.\Dipole=0.2476721,0.3183444,-0.4841485\PG=C01 [X(C3H6N1S1)]\\@

BHandHLYP/cc-pVTZ

1\1\GINC-GOMBERG02\FOpt\UBHandHLYP\CC-pVTZ\C3H6N1S1(2)\HIROSHI\09-Sep-2010\1\#BHandHLYP/cc-pVTZ opt=(z-matrix,calcfc,maxcycle=100) Nosymm freq=Noraman\product C\0,2\CS,1,r2\C,1,r3,2,a3\C,1,r4,2

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,a4,3,d4,0\N,4,r5,1,a5,2,d5,0\H,3,r6,1,a6,2,d6,0\H,3,r7,1,a7,2,d7,0\H,3,r8,1,a8,2,d8,0\H,4,r9,1,a9,2,d9,0\H,4,r10,1,a1
0,2,d10,0\H,5,r11,4,a11,1,d11,0\r2=1.61351952\r3=1.48946985\ a3=123.71566804\r4=1.51402374\ a4=121.7004982
2\d4=177.40308711\r5=1.44071697\ a5=110.65136873\d5=-94.7144587\r6=1.08631973\ a6=109.65307924\d6=125.
99583937\r7=1.07814915\ a7=111.88823861\d7=3.65259039\r8=1.08689361\ a8=109.36247034\d8=242.30878614\r
9=1.0865325\ a9=108.8749652\d9=25.2829708\r10=1.08425933\ a10=110.22976752\d10=-215.26609784\r11=1.015
57757\ a11=106.45900406\d11=55.10514936\ Version=AM64L-G03RevE.01\HF=-570.7541245\ S2=0.755932\ S2-1
=0.\\$2A=0.750026\ RMSD=5.918e-09\ RMSF=3.945e-06\ Thermal=0.\ Dipole=0.2112091,0.2801901,-0.4387269\ Pol
ar=54.9325713,3.4494634,47.0700888,1.1564261,2.2592256,76.1831219\ PG=C01 [X(C3H6N1S1)]\@\n@

QCISD/cc-pVDZ// BHandHLYP/cc-pVTZ
QCISD=-569.7604754

CCSD(T)/cc-pVDZ// BHandHLYP/cc-pVTZ
CCSD(T)= -569.7840773

ROMP2/6-311G// BHandHLYP/cc-pVTZ**
MP2=-569.7674437

G2//MP2(full)/6-31G*
G2=-570.0045483

G3(MP2)-RAD// BHandHLYP/cc-pVTZ
G3(MP2)-RAD= -570.1277388