Electronic Supplementary Material (ESI) for RSC Advances

Supplemental Information

"Dissociation energies of C_α-H bonds in amino acids – a re-examination"

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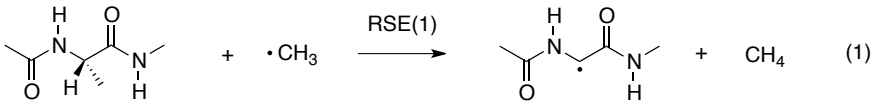
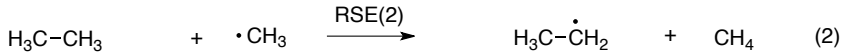
The IMOMO method mentioned in the text is based on an idea originally proposed by Morokuma et al. ((a) T. Vreven, K. Morokuma, *J. Chem. Phys.* **1999**, *111*, 8799; (b) T. Vreven, K. Morokuma, *J. Comp. Chem.* **2000**, *21*, 1419) and involves calculations at lower level on a larger molecular systems, and higher-level calculations for a smaller reference system. In the systems studied here the higher-level method equates to G3B3 and the lower-level method to G3(MP2)-RAD (see also E. I. Izgorodina, D. R. B. Brittain, J. L. Hodgson, E. H. Krenske, C. Y. Lin, M. Namazian, M. L. Coote, *J. Phys. Chem. A* **2007**, *111*, 10754, for the application of this strategy to the calculation of radical stabilization and bond dissociation energies). The RSE of alanyl radical **2H_b** can thus be obtained in the following way:



(1)



(2)

RSE(1) IMOMO(G3B3/G3(MP2)-RAD) = RSE(1) G3(MP2)-RAD
+ RSE(2) G3B3 − RSE(2) G3(MP2)-RAD

Table S1. Total energies of peptide models, amino acids, anhydrides and reference systems in Hartree.

System	H_{298} B3LYP/6-31G(d) [a.u.]	H_{298} G3(MP2)-RAD [a.u.]	H_{298} G3B3 [a.u.]	H_{298} G4-5H [a.u.]	H_{298} W1RO [a.u.]	H_{298} G2(MP2) [a.u.]	H_{298} G3X(MP2)-RAD [a.u.]	$G_{solv.}$ B3LYP/6-31G(d) [kcal/mol]
CH_4	-40.4693510	-40.4169999	-40.4544536	-40.460604		-40.405849	-40.4188481	3.29
$\bullet CH_3$	-39.8044070	-39.7518765	-39.7895467	-39.795364		-39.739661	-39.7533909	2.98
CH_3NH_2	-95.784448	-95.6808713	-95.7579170					
$\bullet CH_2NH_2$	-95.140791	-95.0328567	-95.1108822					
CH_3CHCH_2	-117.822453	-117.6662905	-117.7797155					
$\bullet CH_2CHCH_2$	-117.189239	-117.0285033	-117.1416547					
3H_a	-377.7910035	-377.3822685	-377.6646443	-377.7217460				
3_a	-377.1643090	-376.7460668	-377.0293563	-377.0863812				
3H_b	-417.0791835	-416.6203750	-416.9409716					
3_b	-416.4527109	-415.9817492	-416.3031673					
4H_a	-264.4572682	-264.1774801	-264.3771516	-264.4170515				
4_a	-263.8334805	-263.5449422	-263.7456465	-263.7856841				
4H_b	-303.7452297	-303.4147559	-303.6526214					
4_b	-303.1235712	-302.7828142	-303.0219614					
5H_a	-284.3365448	-284.0472385	-284.2493855	-284.2931825	-284.4997116	-284.0029182	-284.0511497	
5_a	-283.7168552	-283.4185933	-283.6221765	-283.6656951	-283.8734810	-283.3739639	-283.4222416	
5H_b	-323.6253926	-323.2856566	-323.5239870					
5_b	-323.0102522	-322.6595893	-322.8996172					
6H_a	-415.888512	-415.4210565	-415.7429686					-2.34
6_a	-415.260998	-414.7856127	-415.1085792					-2.68

6H_b	-494.465387	-493.8979223	-494.2963331		1.66
6_b	-493.844074	-493.2661897	-493.6657485		1.09

Table S2. Complete list of Cα-H BDE of peptide models, , amino acids and anhydrides with different reference systems.

Reference	C-H BDE of reference	System	BDE Cα-H B3LYP[a]	BDE Cα-H G3(MP2)-RAD	BDE Cα-H G3B3 or IMOMO
CH_4 / $•CH_3$	+439.3 ± 0.4 (exp.)	**2H_a**	+337.7	+365.2	+363.8
		2H_b	+340.4	+373.8	+372.3[b]
		3H_a	+338.9	+363.4	+361.7
		3H_b	+338.3	+369.7	+368.1
		4H_a	+331.2	+353.7	+351.6
		4H_b	+325.6	+352.2	+349.4
		5H_a	+320.5	+343.5	+340.3
		5H_b	+308.5	+336.8	+332.9
		6H_a	+341.0	+361.4	+359.2
		6H_b	+324.7	+351.6	+349.2
CH_3NH_2 / $•CH_2NH_2$	+392.9 ± 8.4 (exp.) +383.4 (B3LYP)[c] +394.4 (G3(MP2)-RAD)[c] +392.4 (G3B3)[c]	**2H_a**	+347.2	+363.7	+364.3
		2H_b	+350.0	+372.3	+372.8[b]
		3H_a	+348.1	+361.9	+362.0
		3H_b	+348.1	+368.2	+368.6
		4H_a	+341.3	+352.3	+352.1
		4H_b	+335.5	+350.7	+349.9
		5H_a	+330.2	+342.0	+340.8
		5H_b	+318.2	+335.3	+333.4
		6H_a	+350.5	+359.9	+359.7

		6H_b	+334.2	+350.1	+349.7
CH_3CHCH_2 / $•CH_2CHCH_2$	+368.6 ± 2.9 (exp.) +335.9 (B3LYP)[c] +367.3 (G3(MP2)-RAD)[c] +368.8 (G3B3)[c]	**2H_a**	+350.3	+366.3	+363.6
		2H_b	+353.1	+374.9	+372.1[b]
		3H_a	+351.3	+364.5	+361.3
		3H_b	+351.3	+370.8	+367.9
		4H_a	+344.4	+354.8	+351.4
		4H_b	+338.6	+353.2	+349.2
		5H_a	+333.3	+344.6	+340.1
		5H_b	+321.3	+337.9	+332.7
		6H_a	+353.6	+362.5	+359.0
		6H_b	+337.3	+352.7	+349.2
5H_a/5_a	+331.0[d]	**2H_a**	+348.3	+352.7	+354.5
		2H_b	+351.0	+361.3	+362.7[b]
		3H_a	+349.4	+350.8	+352.2
		3H_a (C_5)	+348.9	+353.4	+350.4
		3H_b	+348.8	+357.2	+358.8
		3H_b (C_5)	+344.8	+357.1	+354.5
		4H_a	+341.8	+341.2	+342.3
		4H_b	+336.2	+339.7	+340.1
		6H_a	+351.5	+348.9	+349.9
		6H_b	+335.3	+339.1	+339.9

[a] B3LYP/6-31G(d); [b] IMOMO(G3B3,G3(MP2)-RAD); [c] BDE calculated with isodesmic reaction with CH_4/$•CH_3$ as reference systems.;
[d] BDE(C_α-H) value for **5H_a** taken from ref. 5

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Structures of all systems

3H_a (C_7 trans)

1\1\GINC-BORIX\SP\RQCISD(T)-FC\6-31G(d)\C3H6N2O2\MOSCH\06-Nov-2012\0\\
#P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,-0.921023,-1.05226,-0.2
38896\C,0,0.234642,-0.864712,0.636937\C,0,1.317725,0.061158,0.044053\O
,0,2.417828,-0.362457,-0.27934\N,0,0.932085,1.361175,-0.056078\H,0,-0.
941367,-1.859984,-0.846334\H,0,-0.125774,-0.456559,1.58704\H,0,0.69834
7,-1.83515,0.815044\H,0,-0.028763,1.629434,0.135719\H,0,1.55954,2.0113
11,-0.508676\C,0,-1.920939,-0.144107,-0.339104\O,0,-1.955331,0.9251,0.
26093\H,0,-2.727959,-0.466637,-1.022013\\Version=AM64L-G09RevC.01\Stat
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491\MP4DQ=-376.8237261\MP4SDTQ=-376.8790904\MP4SDQ=-376.8390876\QCISD=
-376.8409516\QCISD(T)=-376.8744704\RMSD=9.299e-09\PG=C01 [X(C3H6N2O2)]
\\@

3H_a (C_5 trans)

1\1\GINC-TOFU\SP\RQCISD(T)-FC\6-31G(d)\C3H6N2O2\MOSCH\07-Nov-2012\0\\#
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708\C,0,0.044702,-0.5153,0.001272\C,0,1.460797,0.065563,-0.000056\O,0,
1.666513,1.272505,-0.000998\N,0,2.458762,-0.857723,-0.000152\H,0,-0.48
9127,1.50688,0.000961\H,0,-0.098847,-1.157123,0.88167\H,0,-0.100364,-1
.157718,-0.878441\H,0,3.415488,-0.533847,-0.001769\H,0,2.282238,-1.851
142,-0.000382\C,0,-2.234611,0.369436,-0.000222\O,0,-2.762409,-0.732442
,-0.001297\H,0,-2.809317,1.316032,-0.000533\\Version=AM64L-G09RevC.01\
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8404319\MP4DQ=-376.8227185\MP4SDTQ=-376.8769322\MP4SDQ=-376.8377234\QC
ISD=-376.8395487\QCISD(T)=-376.8723939\RMSD=5.913e-09\PG=C01 [X(C3H6N2
O2)]\\@

3H_a (C_7 cis)

1\1\GINC-BORIX\SP\RQCISD(T)-FC\6-31G(d)\C3H6N2O2\MOSCH\06-Nov-2012\0\\
#P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,0.897258,-0.219557,0.43
4102\C,0,-0.334012,-0.891537,0.059649\C,0,-1.58908,-0.005041,-0.022299
\O,0,-2.695857,-0.514829,-0.094848\N,0,-1.360891,1.335662,-0.021413\H,
0,1.034909,0.040513,1.404923\H,0,-0.568992,-1.711206,0.746866\H,0,-0.1
93265,-1.342964,-0.929249\H,0,-2.147255,1.958373,-0.138451\H,0,-0.4239
6,1.709805,-0.024321\C,0,2.019845,-0.149505,-0.350468\O,0,3.08639,0.30
9277,0.007355\H,0,1.839211,-0.546342,-1.369929\\Version=AM64L-G09RevC.
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76.835837\MP4DQ=-376.8180743\MP4SDTQ=-376.8728484\MP4SDQ=-376.8332661\

QCISD=-376.8348806\QCISD(T)=-376.8678975\RMSD=6.588e-09\PG=C01 [X(C3H6
N2O2)]\\@

3H_a (C_5 cis)
1\1\GINC-LIEBIG\SP\RQCISD(T)-FC\6-31G(d)\C3H6N2O2\MOSCH\07-Nov-2012\0\
\#P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,-0.912229,0.077245,0.1
8493\C,0,0.275044,-0.739755,0.233582\C,0,1.502365,0.15378,0.000412\O,0
,1.423083,1.372608,0.01644\N,0,2.674118,-0.516412,-0.173459\H,0,-0.763
688,1.078495,0.272509\H,0,0.235955,-1.53216,-0.525402\H,0,0.403227,-1.
235047,1.209903\H,0,3.514837,0.022232,-0.328176\H,0,2.722205,-1.520542
,-0.258754\C,0,-2.166383,-0.377614,-0.083792\O,0,-3.163241,0.317465,-0
.156211\H,0,-2.190651,-1.477847,-0.233417\\Version=AM64L-G09RevC.01\St
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595\MP4DQ=-376.8157986\MP4SDTQ=-376.8704408\MP4SDQ=-376.830982\QCISD=-
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\@

3_a (β_2 trans)
1\1\GINC-HP3\SP\UQCISD(T)-FC\6-31G(d)\C3H5N2O2(2)\ROOT\07-Dec-2012\0\\
#P QCISD(T,e4t)/6-31G(d) scf=tight\\whatever\\0,2\N,0,-0.848962,0.5528
72,-0.160647\C,0,0.057582,-0.463292,0.026339\C,0,1.483398,-0.219599,0.
01761\O,0,2.301617,-1.127828,-0.118872\N,0,1.870938,1.133824,0.092029\
H,0,-0.487232,1.44764,-0.475757\H,0,-0.335679,-1.463448,0.137271\H,0,1
.424229,1.676631,0.825449\H,0,2.881948,1.217597,0.131435\C,0,-2.224612
,0.388518,-0.106314\O,0,-2.773267,-0.65182,0.193921\H,0,-2.762114,1.31
814,-0.364273\\Version=AM64L-G09RevC.01\State=2-A\HF=-375.1236733\MP2=
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1344\MP4SDQ=-376.1925898\QCISD=-376.1975965\QCISD(T)=-376.2309391\S2=0
.831483\S2-1=0.799105\S2A=0.753109\RMSD=3.084e-09\PG=C01 [X(C3H5N2O2)]
\\@

3_a (α_L trans)
1\1\GINC-HP3\SP\UQCISD(T)-FC\6-31G(d)\C3H5N2O2(2)\ROOT\07-Dec-2012\0\\
#P QCISD(T,e4t)/6-31G(d) scf=tight\\whatever\\0,2\N,0,-1.049604,-1.088
791,0.069129\C,0,0.336332,-1.062545,-0.010561\C,0,1.3206,0.029496,0.00
1145\O,0,2.508411,-0.298561,-0.099961\N,0,0.914353,1.31973,0.162888\H,
0,-1.432449,-2.024159,0.151925\H,0,0.787011,-2.045136,-0.053573\H,0,1.
633268,2.021033,0.054316\H,0,-0.062095,1.573856,0.041334\C,0,-2.020769
,-0.115323,0.006457\O,0,-1.854602,1.086836,-0.13793\H,0,-3.026426,-0.5
58131,0.102757\\Version=AM64L-G09RevC.01\State=2-A\HF=-375.1200351\MP2
=-376.1529062\MP3=-376.1693357\MP4D=-376.1926122\MP4DQ=-376.1746954\MP

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729907\MP4SDQ=-376.1907016\QCISD=-376.1946188\QCISD(T)=-376.2283936\S2
=0.804952\S2-1=0.780656\S2A=0.752036\RMSD=3.271e-09\PG=C01 [X(C3H5N2O2
)]\\@

3_a (C_s trans)
1\1\GINC-HP1\SP\UQCISD(T)-FC\6-31G(d)\C3H5N2O2(2)\LOCAL\07-Dec-2012\0\
\#P QCISD(T,e4t)/6-31G(d) scf=tight\\whatever\\0,2\N,0,0.881496,0.5601
3,0.00377\C,0,-0.067976,-0.419946,-0.009033\C,0,-1.445684,0.041074,-0.
003655\O,0,-1.710953,1.250489,0.003512\N,0,-2.420899,-0.92862,-0.04661
4\H,0,0.502363,1.506257,0.008653\H,0,0.269383,-1.446905,-0.03194\H,0,-
3.36518,-0.613735,0.128989\H,0,-2.205018,-1.882956,0.204579\C,0,2.2440
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322,0.012372\\Version=AM64L-G09RevC.01\State=2-A\HF=-375.1322129\MP2=-
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DTQ=-376.2419472\PUHF=-375.1375289\PMP2-0=-376.1700486\PMP3-0=-376.184
6889\MP4SDQ=-376.2031744\QCISD=-376.2066781\QCISD(T)=-376.2398417\S2=0
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\@

3_a (α_R cis)
1\1\GINC-HP1\SP\UQCISD(T)-FC\6-31G(d)\C3H5N2O2(2)\LOCAL\07-Dec-2012\0\
\#P QCISD(T,e4t)/6-31G(d) scf=tight\\whatever\\0,2\N,0,0.953543,-0.779
824,0.227782\C,0,-0.406579,-1.000966,0.124465\C,0,-1.461326,-0.008237,
-0.004279\O,0,-2.600266,-0.358207,-0.31584\N,0,-1.137851,1.333513,0.20
1941\H,0,1.523607,-1.54799,0.572043\H,0,-0.727504,-2.033356,0.172296\H
,0,-1.964159,1.918574,0.260363\H,0,-0.44351,1.54492,0.910067\C,0,1.722
276,0.278783,-0.24356\O,0,2.930828,0.303195,-0.115117\H,0,1.130998,1.0
64645,-0.734939\\Version=AM64L-G09RevC.01\State=2-A\HF=-375.1178067\MP
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1705208\MP4SDQ=-376.1874014\QCISD=-376.1920475\QCISD(T)=-376.2254391\S
2=0.824559\S2-1=0.794315\S2A=0.753016\RMSD=2.855e-09\PG=C01 [X(C3H5N2O
2)]\\@

3_a (C_s cis)
1\1\GINC-HP1\SP\UQCISD(T)-FC\6-31G(d)\C3H5N2O2(2)\LOCAL\07-Dec-2012\0\
\#P QCISD(T,e4t)/6-31G(d) scf=tight\\whatever\\0,2\N,0,0.890446,0.0777
32,0.003709\C,0,-0.267347,-0.646946,-0.010886\C,0,-1.502255,0.117497,-
0.003875\O,0,-1.484133,1.353689,0.000174\N,0,-2.676274,-0.605267,-0.04

7242\H,0,0.761255,1.090382,0.014652\H,0,-0.200317,-1.727682,-0.042914\
H,0,-3.517047,-0.074602,0.137469\H,0,-2.68756,-1.572992,0.243629\C,0,2
.178766,-0.413407,-0.002847\O,0,3.16907,0.290495,0.009534\H,0,2.209981
,-1.518702,-0.020119\\Version=AM64L-G09RevC.01\State=2-A\HF=-375.12792
2\MP2=-376.1617843\MP3=-376.1778774\MP4D=-376.2012609\MP4DQ=-376.18346
\MP4SDTQ=-376.2381071\PUHF=-375.1339914\PMP2-0=-376.1665123\PMP3-0=-37
6.181018\MP4SDQ=-376.1992467\QCISD=-376.2027927\QCISD(T)=-376.2359909\
S2=0.796922\S2-1=0.775752\S2A=0.751635\RMSD=3.198e-09\PG=C01 [X(C3H5N2
O2)]\\@

3H_b (C_5 trans)

1\1\GINC-LIEBIG\SP\RQCISD(T)-FC\6-31G(d)\C4H8N2O2\MOSCH\08-Nov-2012\0\
\#P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,0.881613,-0.708772,0.2
34176\C,0,-0.056326,0.338476,-0.121863\C,0,-1.456872,-0.294686,-0.0985
\O,0,-1.664638,-1.389678,0.411119\C,0,0.036391,1.546268,0.831463\N,0,-
2.444108,0.456874,-0.654735\C,0,2.202004,-0.633035,-0.063906\H,0,0.175
256,0.679494,-1.139528\H,0,-0.206818,1.245024,1.855479\H,0,1.056977,1.
935597,0.806556\H,0,-0.649285,2.34691,0.532114\H,0,-3.385332,0.089862,
-0.656455\H,0,0.46698,-1.557091,0.606196\H,0,-2.264017,1.33263,-1.1214
46\O,0,2.744601,0.326743,-0.592664\H,0,2.752823,-1.547801,0.230193\\Ve
rsion=AM64L-G09RevC.01\State=1-A\HF=-414.7811677\MP2=-415.971532\MP3=-
415.9961886\MP4D=-416.0235704\MP4DQ=-416.0031718\MP4SDTQ=-416.06413\MP
4SDQ=-416.0195693\QCISD=-416.021813\QCISD(T)=-416.0596658\RMSD=6.511e-
09\PG=C01 [X(C4H8N2O2)]\\@

3H_b ($C_{7ax.}$ trans)

1\1\GINC-LIEBIG\SP\RQCISD(T)-FC\6-31G(d)\C4H8N2O2\MOSCH\07-Nov-2012\0\
\#P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,-0.788878,-0.911219,0.
513438\C,0,0.327316,-0.603707,-0.392466\C,0,1.02023,0.718564,0.032664\
O,0,2.12099,0.736259,0.565259\C,0,1.317614,-1.76139,-0.4207\N,0,0.2919
73,1.83073,-0.258332\C,0,-2.013771,-0.344811,0.405841\H,0,-0.118646,-0
.454418,-1.381781\H,0,1.796285,-1.88473,0.55574\H,0,0.814572,-2.691042
,-0.705608\H,0,2.112336,-1.556327,-1.142506\H,0,0.623636,2.714443,0.10
443\H,0,-0.612618,-1.53763,1.288472\H,0,-0.683995,1.738186,-0.528302\O
,0,-2.32456,0.503215,-0.425079\H,0,-2.733003,-0.732789,1.150325\\Versi
on=AM64L-G09RevC.01\State=1-A\HF=-414.7813812\MP2=-415.9738486\MP3=-41
5.9980492\MP4D=-416.0256151\MP4DQ=-416.0049949\MP4SDTQ=-416.0668395\MP
4SDQ=-416.0217019\QCISD=-416.0239693\QCISD(T)=-416.0623116\RMSD=8.236e
-09\PG=C01 [X(C4H8N2O2)]\\@

3H_b ($C_{7eq.}$ trans)

1\1\GINC-LIEBIG\SP\RQCISD(T)-FC\6-31G(d)\C4H8N2O2\MOSCH\07-Nov-2012\0\
\#P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,0.93964,0.5127,-0.9589
98\C,0,-0.299291,0.875668,-0.243754\C,0,-1.318971,-0.285947,-0.128204\
O,0,-2.460576,-0.145532,-0.546933\C,0,-0.015751,1.527885,1.118185\N,0,
-0.870285,-1.40142,0.500667\C,0,1.937332,-0.283498,-0.508102\H,0,-0.80
435,1.5994,-0.886104\H,0,0.517813,0.845502,1.782407\H,0,0.590374,2.430
067,0.984624\H,0,-0.962491,1.811944,1.588715\H,0,-1.503432,-2.185039,0
.578768\H,0,1.060127,0.900848,-1.884858\H,0,0.104074,-1.495618,0.77620
5\O,0,1.949276,-0.898754,0.554338\H,0,2.782886,-0.336422,-1.21943\\Ver
sion=AM64L-G09RevC.01\State=1-A\HF=-414.7773213\MP2=-415.9699839\MP3=-
415.9941904\MP4D=-416.0217228\MP4DQ=-416.0010529\MP4SDTQ=-416.0629364\
MP4SDQ=-416.0177282\QCISD=-416.01999\QCISD(T)=-416.0584285\RMSD=6.243e
-09\PG=C01 [X(C4H8N2O2)]\\@

3H_b (α' cis)

1\1\GINC-TOFU\SP\RQCISD(T)-FC\6-31G(d)\C4H8N2O2\MOSCH\07-Nov-2012\0\\#
P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,-0.956661,0.041664,-0.29
7952\C,0,0.293377,0.549789,0.259709\C,0,1.481061,-0.427357,0.085268\O,
0,2.630372,-0.054556,0.2699\C,0,0.656828,1.936589,-0.283283\N,0,1.1486
43,-1.701207,-0.256286\C,0,-2.125139,-0.100807,0.405773\H,0,0.137869,0
.625163,1.344362\H,0,0.754685,1.912722,-1.375086\H,0,-0.117567,2.66361
4,-0.021021\H,0,1.615183,2.25404,0.132034\H,0,1.884575,-2.391212,-0.30
3892\H,0,-1.069383,0.061646,-1.307178\H,0,0.185606,-1.989537,-0.337531
\O,0,-3.205463,-0.356392,-0.089164\H,0,-1.970876,0.018667,1.497281\\Ve
rsion=AM64L-G09RevC.01\State=1-A\HF=-414.7761594\MP2=-415.9667981\MP3=
-415.9911736\MP4D=-416.0188915\MP4DQ=-415.9984669\MP4SDTQ=-416.0597664
\MP4SDQ=-416.0149785\QCISD=-416.0170133\QCISD(T)=-416.0549444\RMSD=7.6
38e-09\PG=C01 [X(C4H8N2O2)]\\@

3H_b (β_2 trans)

1\1\GINC-STEAK\SP\RQCISD(T)-FC\6-31G(d)\C4H8N2O2\MOSCH\04-Nov-2012\0\\
#P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,0.797753,-0.788588,-0.0
16827\C,0,-0.069517,0.379033,-0.233994\C,0,-1.543405,-0.044467,-0.2226
94\O,0,-2.367994,0.476958,-0.952482\C,0,0.160905,1.475422,0.822103\N,0
,-1.861571,-1.047366,0.666465\C,0,2.157956,-0.725048,-0.152689\H,0,0.1
17365,0.802994,-1.226634\H,0,-0.025491,1.09247,1.831864\H,0,1.191611,1
.828164,0.7652\H,0,-0.518758,2.31196,0.632055\H,0,-2.850377,-1.209798,
0.81101\H,0,0.37969,-1.698552,-0.171221\H,0,-1.252375,-1.233508,1.4522
87\O,0,2.811433,0.29552,-0.27233\H,0,2.621923,-1.731513,-0.119886\\Ver
sion=AM64L-G09RevC.01\State=1-A\HF=-414.7730491\MP2=-415.964275\MP3=-4
15.9888731\MP4D=-416.0166628\MP4DQ=-415.9962624\MP4SDTQ=-416.0573149\M
P4SDQ=-416.0126513\QCISD=-416.0147609\QCISD(T)=-416.0527474\RMSD=8.700
e-09\PG=C01 [X(C4H8N2O2)]\\@

3H_b (C_s cis)

1\1\GINC-STEAK\SP\RQCISD(T)-FC\6-31G(d)\C4H8N2O2\MOSCH\04-Nov-2012\0\\
#P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,-0.975626,-0.169987,-0.
16187\C,0,0.238595,0.522519,0.221714\C,0,1.410129,-0.455752,0.015008\O
,0,1.35512,-1.347254,-0.819785\C,0,0.477712,1.800862,-0.608502\N,0,2.5
17323,-0.210506,0.769286\C,0,-2.19921,0.022964,0.402173\H,0,0.166586,0
.7926,1.28361\H,0,0.560687,1.546973,-1.670006\H,0,-0.363531,2.489764,-
0.483349\H,0,1.397156,2.310794,-0.299632\H,0,3.309961,-0.829527,0.6671
53\H,0,-0.871313,-0.901632,-0.858797\H,0,2.517003,0.44557,1.535513\O,0
,-3.217308,-0.569387,0.094038\H,0,-2.17428,0.798479,1.197212\\Version=
AM64L-G09RevC.01\State=1-A\HF=-414.7743674\MP2=-415.9647795\MP3=-415.9
891274\MP4D=-416.0167807\MP4DQ=-415.9963794\MP4SDTQ=-416.0576676\MP4SD
Q=-416.0129257\QCISD=-416.0150109\QCISD(T)=-416.0528385\RMSD=7.308e-09
\PG=C01 [X(C4H8N2O2)]\\@

3H_b ($C_{7eq.}$ cis)

1\1\GINC-LIEBIG\SP\RQCISD(T)-FC\6-31G(d)\C4H8N2O2\MOSCH\07-Nov-2012\0\
\#P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,-0.938627,-0.131934,0.
540324\C,0,0.34733,0.564891,0.475455\C,0,1.526596,-0.350343,0.067869\O
,0,2.677318,0.038987,0.202855\C,0,0.346525,1.799171,-0.436673\N,0,1.19
1719,-1.565082,-0.442331\C,0,-2.066879,0.064705,-0.211438\H,0,0.594578
,0.90407,1.488631\H,0,0.16867,1.53557,-1.484341\H,0,-0.409777,2.524149
,-0.120651\H,0,1.332946,2.262932,-0.370256\H,0,1.931556,-2.170092,-0.7
68867\H,0,-1.085147,-0.753408,1.329476\H,0,0.229219,-1.832378,-0.58168
6\O,0,-3.117685,-0.521249,-0.018323\H,0,-1.932182,0.795819,-1.025788\\
Version=AM64L-G09RevC.01\State=1-A\HF=-414.7720111\MP2=-415.9624221\MP
3=-415.9869397\MP4D=-416.0146231\MP4DQ=-415.9942477\MP4SDTQ=-416.05537
61\MP4SDQ=-416.0107218\QCISD=-416.0127757\QCISD(T)=-416.0506344\RMSD=5
.213e-09\PG=C01 [X(C4H8N2O2)]\\@

3H_b (α_R trans)

1\1\GINC-LIEBIG\SP\RQCISD(T)-FC\6-31G(d)\C4H8N2O2\MOSCH\07-Nov-2012\0\
\#P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,-0.992907,0.115377,0.6
69497\C,0,0.384019,0.619589,0.579866\C,0,1.364929,-0.425254,-0.007316\
O,0,2.394341,-0.082355,-0.568388\C,0,0.50677,1.964062,-0.14592\N,0,1.0
31327,-1.72601,0.217091\C,0,-1.769083,-0.196352,-0.418861\H,0,0.710367
,0.754201,1.618851\H,0,0.179095,1.880638,-1.186943\H,0,-0.110213,2.718
412,0.352463\H,0,1.548348,2.291363,-0.148333\H,0,0.145219,-1.982174,0.
624581\H,0,-1.525756,0.334954,1.504344\H,0,1.64608,-2.445147,-0.136105
\O,0,-2.969776,-0.386968,-0.373092\H,0,-1.178415,-0.2955,-1.349751\\Ve
rsion=AM64L-G09RevC.01\State=1-A\HF=-414.7731367\MP2=-415.9641619\MP3=
-415.9886626\MP4D=-416.016467\MP4DQ=-415.9960599\MP4SDTQ=-416.0572084\

MP4SDQ=-416.0125138\QCISD=-416.0145208\QCISD(T)=-416.0524179\RMSD=8.38
2e-09\PG=C01 [X(C4H8N2O2)]\\@

3_b (C_5 trans)
1\1\GINC-HP1\SP\UQCISD(T)-FC\6-31G(d)\C4H7N2O2(2)\LOCAL\07-Dec-2012\0\
\#P QCISD(T,e4t)/6-31G(d) scf=tight\\whatever\\0,2\N,0,-0.812808,-0.74
8439,0.014848\C,0,0.133794,0.250988,-0.010957\C,0,1.493128,-0.292422,-
0.005455\O,0,1.693478,-1.516362,-0.016223\C,0,-0.201532,1.708279,-0.01
9691\N,0,2.530549,0.612417,-0.031943\C,0,-2.187868,-0.691111,0.013623\
H,0,0.377518,2.233465,-0.790411\H,0,-1.26383,1.859484,-0.205739\H,0,0.
035418,2.181618,0.946571\H,0,3.447019,0.220513,0.136576\H,0,-0.372248,
-1.670411,0.016592\H,0,2.387228,1.565017,0.270298\O,0,-2.873311,0.3182
6,-0.002564\H,0,-2.62176,-1.707116,0.030957\\Version=AM64L-G09RevC.01\
State=2-A\HF=-414.1662535\MP2=-415.3354102\MP3=-415.3601298\MP4D=-415.
3867214\MP4DQ=-415.3661682\MP4SDTQ=-415.4275766\PUHF=-414.1719132\PMP2
-0=-415.3397454\PMP3-0=-415.362999\MP4SDQ=-415.3834017\QCISD=-415.3872
46\QCISD(T)=-415.4255684\S2=0.79148\S2-1=0.7717\S2A=0.751315\RMSD=4.76
4e-09\PG=C01 [X(C4H7N2O2)]\\@

3_b (C_{7ax} trans)
1\1\GINC-HP3\SP\UQCISD(T)-FC\6-31G(d)\C4H7N2O2(2)\ROOT\07-Dec-2012\0\\
#P QCISD(T,e4t)/6-31G(d) scf=tight\\whatever\\0,2\N,0,-0.867288,1.0371
45,-0.23739\C,0,0.457158,0.644419,-0.006756\C,0,1.004326,-0.730809,-0.
025441\O,0,2.224172,-0.882641,0.111857\C,0,1.417541,1.783976,0.12434\N
,0,0.162979,-1.782222,-0.26323\C,0,-2.09109,0.438544,-0.048707\H,0,1.3
86439,2.446011,-0.755653\H,0,1.191036,2.40289,1.00455\H,0,2.426623,1.3
84484,0.221259\H,0,0.598801,-2.687529,-0.145787\H,0,-0.951438,2.012575
,-0.506209\H,0,-0.823772,-1.697094,-0.028063\O,0,-2.313891,-0.691494,0
.35977\H,0,-2.907382,1.130505,-0.319388\\Version=AM64L-G09RevC.01\Stat
e=2-A\HF=-414.1600091\MP2=-415.327369\MP3=-415.3523775\MP4D=-415.37900
32\MP4DQ=-415.3584296\MP4SDTQ=-415.4201212\PUHF=-414.166404\PMP2-0=-41
5.3323079\PMP3-0=-415.3556901\MP4SDQ=-415.3758143\QCISD=-415.3799277\Q
CISD(T)=-415.4185249\S2=0.797917\S2-1=0.77568\S2A=0.751544\RMSD=9.742e
-09\PG=C01 [X(C4H7N2O2)]\\@

3_b (α_L cis)
1\1\GINC-HP3\SP\UQCISD(T)-FC\6-31G(d)\C4H7N2O2(2)\ROOT\07-Dec-2012\0\\
#P QCISD(T,e4t)/6-31G(d) scf=tight\\whatever\\0,2\N,0,0.963669,0.58042
8,0.247444\C,0,-0.417071,0.636767,0.069131\C,0,-1.26301,-0.553565,-0.0
18489\O,0,-2.440983,-0.474683,-0.373609\C,0,-1.044474,1.992211,0.05354
9\N,0,-0.683502,-1.783703,0.287273\C,0,1.889972,-0.306731,-0.288396\H,
0,-0.832412,2.549015,0.979501\H,0,-0.665079,2.59884,-0.780659\H,0,-2.1
24718,1.887418,-0.052546\H,0,-1.372674,-2.52113,0.378757\H,0,1.40866,1

.400025,0.654685\H,0,0.038769,-1.804416,0.997777\O,0,3.086288,-0.17216
2,-0.120391\H,0,1.43135,-1.124167,-0.863301\\Version=AM64L-G09RevC.01\
State=2-A\HF=-414.1596603\MP2=-415.3243678\MP3=-415.350546\MP4D=-415.3
773204\MP4DQ=-415.3570514\MP4SDTQ=-415.4175309\PUHF=-414.1670756\PMP2-
0=-415.3302126\PMP3-0=-415.3544561\MP4SDQ=-415.3740938\QCISD=-415.3786
232\QCISD(T)=-415.4166819\S2=0.81027\S2-1=0.784249\S2A=0.751952\RMSD=6
.555e-09\PG=C01 [X(C4H7N2O2)]\\@

3_b (β_2 trans)

1\1\GINC-PHOBOS\SP\UQCISD(T)-FC\6-31G(d)\C4H7N2O2(2)\MOSCH\07-Dec-2012
\0\\#P QCISD(T,e4t)/6-31G(d) scf=tight\\whatever\\0,2\N,0,0.747809,-0.
754619,-0.217619\C,0,-0.130268,0.303581,-0.033012\C,0,-1.550507,-0.016
973,0.012135\O,0,-2.42996,0.833743,-0.126036\C,0,0.338291,1.716561,0.0
39791\N,0,-1.866055,-1.38745,0.144522\C,0,2.127483,-0.759594,-0.125224
\H,0,0.962713,1.895292,0.922303\H,0,0.954209,1.97721,-0.829425\H,0,-0.
539169,2.364762,0.069474\H,0,-2.871464,-1.513604,0.207498\H,0,0.317672
,-1.620789,-0.529447\H,0,-1.385562,-1.8734,0.896412\O,0,2.822615,0.172
37,0.22935\H,0,2.538095,-1.745346,-0.413789\\Version=AM64L-G09RevC.01\
State=2-A\HF=-414.161334\MP2=-415.3261792\MP3=-415.3529212\MP4D=-415.3
795904\MP4DQ=-415.3592523\MP4SDTQ=-415.4197098\PUHF=-414.1702212\PMP2-
0=-415.3333023\PMP3-0=-415.3577324\MP4SDQ=-415.3763475\QCISD=-415.3814
876\QCISD(T)=-415.419869\S2=0.828594\S2-1=0.796598\S2A=0.753375\RMSD=5
.861e-09\PG=C01 [X(C4H7N2O2)]\\@

3_b (C_5 cis)

1\1\GINC-PHOBOS\SP\UQCISD(T)-FC\6-31G(d)\C4H7N2O2(2)\MOSCH\07-Dec-2012
\0\\#P QCISD(T,e4t)/6-31G(d) scf=tight\\whatever\\0,2\N,0,-0.913574,-0
.303846,-0.005363\C,0,0.264468,0.404418,-0.021375\C,0,1.44174,-0.46244
,-0.005949\O,0,1.320544,-1.692492,-0.071161\C,0,0.258003,1.89809,-0.06
9391\N,0,2.687933,0.139463,0.029823\C,0,-2.210828,0.156728,0.036198\H,
0,-0.410786,2.268204,-0.857764\H,0,-0.079809,2.350768,0.875096\H,0,1.2
53853,2.286646,-0.293767\H,0,3.443192,-0.514346,0.19319\H,0,-0.781112,
-1.31674,-0.023481\H,0,2.795425,1.032612,0.490073\O,0,-3.179592,-0.581
653,0.038393\H,0,-2.289192,1.255923,0.070673\\Version=AM64L-G09RevC.01
\State=2-A\HF=-414.1638992\MP2=-415.3320447\MP3=-415.3571773\MP4D=-415
.383908\MP4DQ=-415.3633993\MP4SDTQ=-415.424542\PUHF=-414.1705411\PMP2-
0=-415.3372605\PMP3-0=-415.3606659\MP4SDQ=-415.3805859\QCISD=-415.3846
772\QCISD(T)=-415.4228954\S2=0.803805\S2-1=0.780156\S2A=0.752132\RMSD=
5.624e-09\PG=C01 [X(C4H7N2O2)]\\@

3_b (β_2 cis)

1\1\GINC-PHOBOS\SP\UQCISD(T)-FC\6-31G(d)\C4H7N2O2(2)\MOSCH\07-Dec-2012
\0\\#P QCISD(T,e4t)/6-31G(d) scf=tight\\whatever\\0,2\N,0,0.886108,-0.

310871,-0.076869\C,0,-0.271311,0.440582,0.014601\C,0,-1.551455,-0.2540
41,-0.016301\O,0,-2.615739,0.337006,-0.208356\C,0,-0.217791,1.928088,0
.106606\N,0,-1.497241,-1.652379,0.108921\C,0,2.19613,0.107958,0.064089
\H,0,0.226554,2.27514,1.050953\H,0,0.372511,2.364483,-0.710403\H,0,-1.
238952,2.307955,0.04548\H,0,-2.429226,-2.052428,0.134659\H,0,0.789644,
-1.278771,-0.375081\H,0,-0.907185,-2.015891,0.850635\O,0,3.145801,-0.6
3159,-0.116422\H,0,2.290651,1.163417,0.363637\\Version=AM64L-G09RevC.0
1\State=2-A\HF=-414.1622751\MP2=-415.32676\MP3=-415.353421\MP4D=-415.3
800953\MP4DQ=-415.3597801\MP4SDTQ=-415.4201212\PUHF=-414.1710591\PMP2-
0=-415.3337971\PMP3-0=-415.3581811\MP4SDQ=-415.376844\QCISD=-415.38181
4\QCISD(T)=-415.4200298\S2=0.827551\S2-1=0.795852\S2A=0.75362\RMSD=6.0
00e-09\PG=C01 [X(C4H7N2O2)]\\@

4H_a (1)
1\1\GINC-STEAK\SP\RQCISD(T)-FC\6-31G(d)\C2H6N2O1\MOSCH\04-Nov-2012\0\\
#P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,-1.821175,0.191047,-0.0
79978\C,0,-0.713912,-0.74764,0.141155\C,0,0.666598,-0.089412,0.00742\O
,0,1.682879,-0.760039,-0.108432\N,0,0.637914,1.268381,0.053322\H,0,-1.
987862,0.305603,-1.078154\H,0,-0.779859,-1.121985,1.169838\H,0,-0.7080
61,-1.630005,-0.514508\H,0,1.508038,1.779544,0.053146\H,0,-0.245967,1.
73244,0.217364\H,0,-2.682605,-0.178965,0.314916\\Version=AM64L-G09RevC
.01\State=1-A\HF=-262.996114\MP2=-263.7542962\MP3=-263.7759489\MP4D=-2
63.7929467\MP4DQ=-263.7809317\MP4SDTQ=-263.8146187\MP4SDQ=-263.7897136
\QCISD=-263.7912991\QCISD(T)=-263.8130423\RMSD=9.911e-09\PG=C01 [X(C2H
6N2O1)]\\@

4H_a (3)
1\1\GINC-BORIX\SP\RQCISD(T)-FC\6-31G(d)\C2H6N2O1\MOSCH\06-Nov-2012\0\\
#P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,1.972674,-0.047177,-0.0
51507\C,0,0.711938,-0.755892,0.095895\C,0,-0.537248,0.14094,0.013947\O
,0,-0.460971,1.361023,0.034833\N,0,-1.728463,-0.523675,-0.080915\H,0,1
.949201,0.759429,0.572821\H,0,0.648932,-1.548172,-0.661122\H,0,0.69970
3,-1.263302,1.071405\H,0,-2.58245,0.013486,-0.020499\H,0,-1.790051,-1.
526903,0.011243\H,0,2.00481,0.362948,-0.984615\\Version=AM64L-G09RevC.
01\State=1-A\HF=-262.99403\MP2=-263.7516517\MP3=-263.7736458\MP4D=-263
.790701\MP4DQ=-263.7786645\MP4SDTQ=-263.8124052\MP4SDQ=-263.7874993\QC
ISD=-263.7890629\QCISD(T)=-263.8107481\RMSD=7.747e-09\PG=C01 [X(C2H6N2
O1)]\\@

4H_a (6)
1\1\GINC-LIEBIG\SP\RQCISD(T)-FC\6-31G(d)\C2H6N2O1\MOSCH\07-Nov-2012\0\
\#P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,-1.781293,0.096784,-0.
477251\C,0,-0.832286,-0.387832,0.533067\C,0,0.608643,-0.154515,0.06767

3\O,0,1.359531,-1.05505,-0.264913\N,0,0.980018,1.169754,0.013528\H,0,-1.714082,1.10797,-0.573819\H,0,-0.959477,0.059637,1.538758\H,0,-0.951245,-1.468456,0.633964\H,0,1.950011,1.360575,-0.20074\H,0,0.481944,1.874291,0.538516\H,0,-2.73261,-0.105303,-0.175743\\Version=AM64L-G09RevC.01\State=1-A\HF=-262.985346\MP2=-263.7427913\MP3=-263.7648557\MP4D=-263.782079\MP4DQ=-263.7700832\MP4SDTQ=-263.8035992\MP4SDQ=-263.7787963\QCISD=-263.7803832\QCISD(T)=-263.8020826\RMSD=7.032e-09\PG=C01 [X(C2H6N2O1)]\\@

4_a (1)
1\1\GINC-HP3\SP\UQCISD(T)-FC\6-31G(d)\C2H5N2O1(2)\ROOT\07-Dec-2012\0\\
#P QCISD(T,e4t)/6-31G(d) scf=tight\\whatever\\0,2\N,0,-1.859835,0.091112,-0.000446\C,0,-0.728445,-0.69511,0.079605\C,0,0.596286,-0.137632,0.015084\O,0,1.612971,-0.834492,-0.063785\N,0,0.654534,1.271924,-0.035175\H,0,-1.765869,0.933432,-0.559658\H,0,-0.845015,-1.756367,0.255061\H,0,1.615228,1.594118,0.019911\H,0,0.057927,1.750613,0.633628\H,0,-2.735975,-0.390663,-0.157448\\Version=AM64L-G09RevC.01\State=2-A\HF=-262.3811831\MP2=-263.1146481\MP3=-263.1372954\MP4D=-263.1532977\MP4DQ=-263.1414443\MP4SDTQ=-263.1745783\PUHF=-262.3890008\PMP2-0=-263.120785\PMP3-0=-263.141334\MP4SDQ=-263.1508261\QCISD=-263.1549381\QCISD(T)=-263.1767983\S2=0.813148\S2-1=0.785664\S2A=0.751293\RMSD=9.677e-09\PG=C01 [X(C2H5N2O1)]\\@

4_a (3)
1\1\GINC-HP3\SP\UQCISD(T)-FC\6-31G(d)\C2H5N2O1(2)\ROOT\07-Dec-2012\0\\
#P QCISD(T,e4t)/6-31G(d) scf=tight\\whatever\\0,2\N,0,1.894221,-0.050116,0.093055\C,0,0.699634,-0.706012,-0.031291\C,0,-0.494752,0.103205,-0.01218\O,0,-0.434733,1.342096,-0.009224\N,0,-1.712394,-0.568807,-0.059964\H,0,1.805951,0.956282,-0.021155\H,0,0.703256,-1.788537,-0.077753\H,0,-2.505613,0.017187,0.168158\H,0,-1.756523,-1.50271,0.327153\H,0,2.728709,-0.469681,-0.293418\\Version=AM64L-G09RevC.01\State=2-A\HF=-262.3840641\MP2=-263.1222886\MP3=-263.1429142\MP4D=-263.1589919\MP4DQ=-263.1469632\MP4SDTQ=-263.1810349\PUHF=-262.3889625\PMP2-0=-263.1258898\PMP3-0=-263.145168\MP4SDQ=-263.1564728\QCISD=-263.1593818\QCISD(T)=-263.1811773\S2=0.780054\S2-1=0.763975\S2A=0.75051\RMSD=6.544e-09\PG=C01 [X(C2H5N2O1)]\\@

4H_b (1)
1\1\GINC-STEAK\SP\RQCISD(T)-FC\6-31G(d)\C3H8N2O1\MOSCH\04-Nov-2012\0\\
#P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,-1.290308,1.17113,-0.265184\C,0,-0.661083,-0.152306,-0.406846\C,0,0.850444,-0.087481,-0.115523\O,0,1.595917,-1.005211,-0.432371\C,0,-1.30704,-1.146547,0.565738\N,0

,1.251672,1.041027,0.527226\H,0,-1.103277,1.738337,-1.090777\H,0,-0.74
1401,-0.566148,-1.423578\H,0,-1.252769,-0.76822,1.592766\H,0,-2.361811
,-1.308558,0.311701\H,0,-0.786922,-2.106374,0.51509\H,0,2.208074,1.111
025,0.842474\H,0,-2.302115,1.069146,-0.209332\H,0,0.549414,1.705383,0.
82611\\Version=AM64L-G09RevC.01\State=1-A\HF=-302.0333262\MP2=-302.925
2238\MP3=-302.9554135\MP4D=-302.9757679\MP4DQ=-302.9612111\MP4SDTQ=-30
3.0011281\MP4SDQ=-302.9712474\QCISD=-302.9732643\QCISD(T)=-302.9997686
\RMSD=8.201e-09\PG=C01 [X(C3H8N2O1)]\\@

4H_b (2)

1\1\GINC-TOFU\SP\RQCISD(T)-FC\6-31G(d)\C3H8N2O1\MOSCH\07-Nov-2012\0\\#
P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,1.056511,1.416112,-0.022
171\C,0,0.6679,0.049101,0.371919\C,0,-0.82358,-0.207325,0.063282\O,0,-
1.290484,-1.338775,0.028179\C,0,1.536886,-1.072074,-0.209018\N,0,-1.55
3334,0.922216,-0.131233\H,0,1.939979,1.662125,0.42081\H,0,0.738672,0.0
14025,1.468303\H,0,1.521271,-1.044252,-1.305869\H,0,2.57613,-0.965407,
0.122559\H,0,1.159781,-2.048617,0.103763\H,0,-2.551798,0.844264,-0.256
119\H,0,1.230561,1.440471,-1.027537\H,0,-1.100202,1.821088,-0.034609\\
Version=AM64L-G09RevC.01\State=1-A\HF=-302.0331826\MP2=-302.925422\MP3
=-302.9557793\MP4D=-302.9761373\MP4DQ=-302.9614929\MP4SDTQ=-303.001541
1\MP4SDQ=-302.9715703\QCISD=-302.9735841\QCISD(T)=-303.0001774\RMSD=7.
573e-09\PG=C01 [X(C3H8N2O1)]\\@

4H_b (4)

1\1\GINC-TOFU\SP\RQCISD(T)-FC\6-31G(d)\C3H8N2O1\MOSCH\07-Nov-2012\0\\#
P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,1.349267,-1.036777,-0.65
1103\C,0,0.636832,0.220045,-0.422975\C,0,-0.778628,-0.149023,0.045035\
O,0,-0.962661,-1.018337,0.886358\C,0,1.277251,1.147203,0.630935\N,0,-1
.793784,0.603023,-0.473645\H,0,2.354233,-0.870999,-0.647701\H,0,0.5783
09,0.763909,-1.376955\H,0,1.303787,0.644546,1.603726\H,0,2.304075,1.39
7858,0.338631\H,0,0.718878,2.084845,0.74172\H,0,-2.73965,0.34309,-0.22
7601\H,0,1.140315,-1.65382,0.134052\H,0,-1.659769,1.164204,-1.30147\\V
ersion=AM64L-G09RevC.01\State=1-A\HF=-302.0287989\MP2=-302.9204137\MP3
=-302.9507912\MP4D=-302.971188\MP4DQ=-302.9565942\MP4SDTQ=-302.9967004
\MP4SDQ=-302.9667401\QCISD=-302.968769\QCISD(T)=-302.9952654\RMSD=4.46
4e-09\PG=C01 [X(C3H8N2O1)]\\@

4H_b (5)

1\1\GINC-STEAK\SP\RQCISD(T)-FC\6-31G(d)\C3H8N2O1\MOSCH\04-Nov-2012\0\\
#P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,1.537069,-0.963187,-0.4
68604\C,0,0.653286,0.199467,-0.410615\C,0,-0.778188,-0.178602,0.025717
\O,0,-0.992482,-1.132629,0.762237\C,0,1.225406,1.229553,0.577474\N,0,-
1.778967,0.622436,-0.44773\H,0,1.376875,-1.498173,0.38736\H,0,0.620259

,0.649837,-1.411815\H,0,1.256783,0.80415,1.587125\H,0,2.245043,1.49171
6,0.28205\H,0,0.616495,2.140122,0.613235\H,0,-2.715966,0.480906,-0.095
63\H,0,1.221651,-1.58074,-1.21716\H,0,-1.591021,1.45596,-0.984186\\Ver
sion=AM64L-G09RevC.01\State=1-A\HF=-302.0305427\MP2=-302.9218719\MP3=-
302.9522955\MP4D=-302.9727087\MP4DQ=-302.9581235\MP4SDTQ=-302.9981928\
MP4SDQ=-302.9682564\QCISD=-302.970271\QCISD(T)=-302.9967419\RMSD=9.722
e-09\PG=C01 [X(C3H8N2O1)]\\@

4H_b (6)

1\1\GINC-LIEBIG\SP\RQCISD(T)-FC\6-31G(d)\C3H8N2O1\MOSCH\07-Nov-2012\0\
\#P QCISD(T,FC,E4T)/6-31G(d)\\whatever\\0,1\N,0,-1.338464,-1.184268,-0
.244455\C,0,-0.690262,-0.023227,0.363349\C,0,0.815847,-0.133994,0.0533
89\O,0,1.359226,-1.226701,-0.046959\C,0,-1.363921,1.265256,-0.126173\N
,0,1.520899,1.033636,-0.011797\H,0,-0.698275,-1.973792,-0.167891\H,0,-
0.737772,-0.029763,1.470638\H,0,-1.233292,1.385687,-1.20657\H,0,-2.440
059,1.213889,0.070997\H,0,-0.98806,2.155738,0.393635\H,0,1.065205,1.92
3926,-0.135784\H,0,-2.184832,-1.418919,0.269002\H,0,2.496242,0.963057,
-0.267981\\Version=AM64L-G09RevC.01\State=1-A\HF=-302.027194\MP2=-302.
9189241\MP3=-302.9495384\MP4D=-302.9699223\MP4DQ=-302.955324\MP4SDTQ=-
302.9952811\MP4SDQ=-302.9653963\QCISD=-302.9673909\QCISD(T)=-302.99388
16\RMSD=8.491e-09\PG=C01 [X(C3H8N2O1)]\\@

4_b (1)

1\1\GINC-EVGENIX\SP\UQCISD(T)-FC\6-31G(d)\C3H7N2O1(2)\MOSCH\07-Dec-201
2\0\\#P QCISD(T,e4t)/6-31G(d) scf=tight\\whatever\\0,2\N,0,-0.985722,1
.451063,-0.044434\C,0,-0.643721,0.107452,-0.012205\C,0,0.752007,-0.265
993,-0.013253\O,0,1.142068,-1.434332,-0.1315\C,0,-1.719409,-0.918498,0
.108716\N,0,1.664992,0.808932,0.051796\H,0,-0.336434,2.048792,-0.54674
5\H,0,-2.310597,-0.784428,1.027093\H,0,-2.422124,-0.872799,-0.736944\H
,0,-1.264379,-1.910188,0.127754\H,0,2.614717,0.465051,0.147912\H,0,-1.
953071,1.65517,-0.266785\H,0,1.447193,1.515333,0.748634\\Version=AM64L
-G09RevC.01\State=2-A\HF=-301.4223746\MP2=-302.2897137\MP3=-302.321158
\MP4D=-302.340433\MP4DQ=-302.3259852\MP4SDTQ=-302.365336\PUHF=-301.429
7806\PMP2-0=-302.2954767\PMP3-0=-302.3249142\MP4SDQ=-302.336634\QCISD=
-302.3409245\QCISD(T)=-302.3674844\S2=0.807902\S2-1=0.781901\S2A=0.751
175\RMSD=5.072e-09\PG=C01 [X(C3H7N2O1)]\\@

4_b (6)

1\1\GINC-EVGENIX\SP\UMP2-Full\GTlarge\C3H7N2O1(2)\MOSCH\07-Dec-2012\0\
\#P UMP2(Full)/gtlarge scf=tight geom=check guess=read\\whatever\\0,2\
N,0,1.291715,-1.244253,0.136943\C,0,0.657728,-0.033366,-0.009709\C,0,-
0.78875,-0.104365,-0.013714\O,0,-1.380433,-1.195418,-0.064187\C,0,1.47
8238,1.21674,-0.050488\N,0,-1.498146,1.098651,-0.024312\H,0,0.662572,-

2.032621,0.008486\H,0,1.787259,1.55579,0.951221\H,0,2.40091,1.061606,-
0.626657\H,0,0.931341,2.033322,-0.531076\H,0,-1.105747,1.882117,0.4819
19\H,0,2.215237,-1.351159,-0.264012\H,0,-2.486377,0.95945,0.14867\\Ver
sion=AM64L-G09RevC.01\State=2-A\HF=-301.5397881\MP2=-302.9243025\PUHF=
-301.5449263\PMP2-0=-302.928049\S2=0.781119\S2-1=0.764068\S2A=0.750603
\RMSD=2.753e-09\PG=C01 [X(C3H7N2O1)]\\@

5H_a (1)
1\1\GINC-GOLEM\SP\RQCISD(T)-FC\6-31G(d)\C2H5N1O2\MOSCH\10-Dec-2012\0\\
#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,1\C,0,0.766138,-0.6
72994,0.267605\H,0,0.838157,-0.82137,1.363059\H,0,0.792764,-1.666082,-
0.188315\N,0,1.811947,0.164749,-0.315904\H,0,1.77729,1.09336,0.099113\
H,0,2.72367,-0.227933,-0.090532\C,0,-0.622683,-0.115742,0.015786\O,0,-
1.616143,-0.775576,-0.184865\O,0,-0.646775,1.237834,0.106819\H,0,-1.57
2899,1.503138,-0.04798\\Version=AM64L-G09RevC.01\State=1-A\HF=-282.822
732\MP2=-283.5953367\MP3=-283.6109018\MP4D=-283.6281344\MP4DQ=-283.616
5943\MP4SDTQ=-283.6509787\MP4SDQ=-283.6259578\QCISD=-283.6273751\QCISD
(T)=-283.6487413\RMSD=5.123e-09\PG=C01 [X(C2H5N1O2)]\\@

5H_a (2)
1\1\GINC-YIN\SP\RQCISD(T)-FC\6-31G(d)\C2H5N1O2\MOSCH\24-Feb-2008\0\\#p
qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,1\C,0,0.64313,-0.7951
,-0.11152\H,0,0.61268,-1.637946,0.58866\H,0,0.686717,-1.219501,-1.1205
04\N,0,1.775554,0.12396,0.077946\H,0,2.091705,0.122369,1.04486\H,0,2.5
71358,-0.13232,-0.499233\C,0,-0.6933,-0.038451,-0.004875\O,0,-1.757279
,-0.601149,0.089586\O,0,-0.556565,1.295259,-0.057647\H,0,0.420438,1.44
81,-0.11655\\Version=AM64L-G09RevC.01\State=1-A\HF=-282.8222626\MP2=-2
83.5984895\MP3=-283.6132474\MP4D=-283.6304254\MP4DQ=-283.6184943\MP4SD
TQ=-283.6537686\MP4SDQ=-283.628113\QCISD=-283.6295019\QCISD(T)=-283.65
13936\RMSD=5.917e-09\PG=C01 [X(C2H5N1O2)]\\@

5H_a (3)
1\1\GINC-AZAZEL\SP\RQCISD(T)-FC\6-31G(d)\C2H5N1O2\MOSCH\10-Dec-2012\0\
\#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,1\C,0,-0.665556,-0
.787648,0.000247\H,0,-0.659149,-1.449852,-0.872337\H,0,-0.659177,-1.44
8867,0.873631\N,0,-1.893234,-0.012567,-0.000223\H,0,-2.063268,0.531081
,0.838364\H,0,-2.062738,0.530824,-0.839088\C,0,0.687274,-0.048153,-0.0
00006\O,0,1.742861,-0.630073,-0.000187\O,0,0.618807,1.304273,0.000111\
H,0,-0.326687,1.545987,0.000152\\Version=AM64L-G09RevC.01\State=1-A\HF
=-282.8126247\MP2=-283.5872144\MP3=-283.6023901\MP4D=-283.6195403\MP4D
Q=-283.6077023\MP4SDTQ=-283.6428181\MP4SDQ=-283.6173543\QCISD=-283.618
7083\QCISD(T)=-283.640398\RMSD=4.117e-09\PG=C01 [X(C2H5N1O2)]\\@

5H_a (4)
1\1\GINC-GOLEM\SP\RQCISD(T)-FC\6-31G(d)\C2H5N1O2\MOSCH\10-Dec-2012\0\\
#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,1\C,0,-0.687991,-0.
743921,0.000131\H,0,-0.638592,-1.403691,-0.878035\H,0,-0.638575,-1.403
719,0.878268\N,0,-1.957235,-0.04272,0.000046\H,0,-1.986715,0.580138,0.
806246\H,0,-1.987446,0.578845,-0.807125\C,0,0.556383,0.155967,0.00001\
O,0,0.514322,1.360003,0.000014\O,0,1.752214,-0.493654,-0.000087\H,0,1.
609334,-1.455592,0.000063\\Version=AM64L-G09RevC.01\State=1-A\HF=-282.
8165498\MP2=-283.5900962\MP3=-283.6059206\MP4D=-283.6231315\MP4DQ=-283
.6113444\MP4SDTQ=-283.6460906\MP4SDQ=-283.6208271\QCISD=-283.6222095\Q
CISD(T)=-283.6437508\RMSD=2.633e-09\PG=C01 [X(C2H5N1O2)]\\@

5H_a (5)
1\1\GINC-NAUTILUS\SP\RQCISD(T)-FC\6-31G(d)\C2H5N1O2\MOSCH\10-Dec-2012\
0\\#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,1\C,0,-0.727982,
-0.738164,0.000034\H,0,-0.692781,-1.400427,-0.873949\H,0,-0.692672,-1.
400443,0.873976\N,0,-1.9703,0.013222,0.000132\H,0,-1.981405,0.635478,0
.807101\H,0,-1.982295,0.634286,-0.80774\C,0,0.541095,0.108102,-0.00003
9\O,0,0.573711,1.318748,-0.000041\O,0,1.657273,-0.66074,-0.000018\H,0,
2.414703,-0.045139,0.000186\\Version=AM64L-G09RevC.01\State=1-A\HF=-28
2.8277298\MP2=-283.6004368\MP3=-283.6160715\MP4D=-283.6332307\MP4DQ=-2
83.6216111\MP4SDTQ=-283.6561312\MP4SDQ=-283.6310257\QCISD=-283.6324336
\QCISD(T)=-283.6538413\RMSD=2.755e-09\PG=C01 [X(C2H5N1O2)]\\@

5_a (1)
1\1\GINC-HP3\SP\UQCISD(T)-FC\6-31G(d)\C2H4N1O2(2)\ROOT\13-Dec-2012\0\\
#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,2\C,0,-0.72554,-0.6
96499,-0.007094\H,0,-0.833718,-1.77221,0.002805\N,0,-1.851917,0.076878
,0.059716\H,0,-1.738659,1.068531,-0.106836\H,0,-2.736133,-0.319707,-0.
225775\C,0,0.586312,-0.131126,0.000656\O,0,1.63999,-0.759098,-0.003071
\O,0,0.561365,1.250433,-0.002339\H,0,1.496461,1.520314,-0.006296\\Vers
ion=AM64L-G09RevC.01\State=2-A\HF=-282.2172843\MP2=-282.9690028\MP3=-2
82.9839691\MP4D=-282.9999487\MP4DQ=-282.9883898\MP4SDTQ=-283.0227967\P
UHF=-282.223897\PMP2-0=-282.9740455\PMP3-0=-282.9871745\MP4SDQ=-282.99
84458\QCISD=-283.0016795\QCISD(T)=-283.0231737\S2=0.797347\S2-1=0.7746
17\S2A=0.750872\RMSD=3.169e-09\PG=C01 [X(C2H4N1O2)]\\@
5_a (2)
1\1\GINC-ANGIE\SP\UQCISD(T)-FC\6-31G(d)\C2H4N1O2(2)\MOSCH\13-Dec-2012\
0\\#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,2\C,0,-0.672244,
-0.710998,0.08484\H,0,-0.745189,-1.770376,0.292545\N,0,-1.835242,0.032
167,-0.014388\H,0,-1.822727,0.794643,-0.685668\H,0,-2.69797,-0.495875,
-0.057142\C,0,0.629162,-0.098151,0.016258\O,0,1.671442,-0.7227,-0.0827

57\O,0,0.644249,1.284308,0.017261\H,0,-0.154452,1.608476,0.468369\\Ver
sion=AM64L-G09RevC.01\State=2-A\HF=-282.2042565\MP2=-282.9513358\MP3=-
282.9682688\MP4D=-282.9841408\MP4DQ=-282.9726743\MP4SDTQ=-283.0067354\
PUHF=-282.2130475\PMP2-0=-282.9583167\PMP3-0=-282.9728935\MP4SDQ=-282.
9829209\QCISD=-282.987528\QCISD(T)=-283.0090856\S2=0.823607\S2-1=0.792
902\S2A=0.751601\RMSD=5.817e-09\PG=C01 [X(C2H4N1O2)]\\@

5_a (4)
1\1\GINC-EVGENIX\SP\UQCISD(T)-FC\6-31G(d)\C2H4N1O2(2)\MOSCH\13-Dec-201
2\0\\#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,2\C,0,0.674433
,-0.691251,0.018739\H,0,0.681516,-1.775468,0.027111\N,0,1.871612,-0.04
0678,-0.072691\H,0,1.807497,0.965777,0.046617\H,0,2.712052,-0.48546,0.
268404\C,0,-0.517092,0.118447,0.004384\O,0,-0.482929,1.34264,0.011315\
O,0,-1.72463,-0.529306,-0.003567\H,0,-1.585925,-1.489943,-0.034015\\Ve
rsion=AM64L-G09RevC.01\State=2-A\HF=-282.2075455\MP2=-282.9604149\MP3=
-282.9753481\MP4D=-282.9913349\MP4DQ=-282.9796094\MP4SDTQ=-283.0144783
\PUHF=-282.2136346\PMP2-0=-282.9650542\PMP3-0=-282.9782962\MP4SDQ=-282
.9898139\QCISD=-282.9930574\QCISD(T)=-283.0146954\S2=0.792737\S2-1=0.7
72159\S2A=0.750798\RMSD=7.046e-09\PG=C01 [X(C2H4N1O2)]\\@

5_a (5)
1\1\GINC-EVGENIX\SP\UQCISD(T)-FC\6-31G(d)\C2H4N1O2(2)\MOSCH\13-Dec-201
2\0\\#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,2\C,0,0.714483
,-0.680177,0.01172\H,0,0.734969,-1.761376,0.011713\N,0,1.888284,0.0119
47,-0.065317\H,0,1.80452,1.014241,0.067439\H,0,2.745792,-0.417708,0.25
0453\C,0,-0.501376,0.074096,0.002383\O,0,-0.551911,1.304925,0.008587\O
,0,-1.624712,-0.705534,-0.003472\H,0,-2.368928,-0.077427,0.002077\\Ver
sion=AM64L-G09RevC.01\State=2-A\HF=-282.218742\MP2=-282.9725578\MP3=-2
82.9867067\MP4D=-283.0027422\MP4DQ=-282.9910928\MP4SDTQ=-283.025916\PU
HF=-282.2237477\PMP2-0=-282.9762392\PMP3-0=-282.9889778\MP4SDQ=-283.00
11734\QCISD=-283.0038825\QCISD(T)=-283.0253528\S2=0.780854\S2-1=0.7643
7\S2A=0.750506\RMSD=4.156e-09\PG=C01 [X(C2H4N1O2)]\\@

5H_b (1)
1\1\GINC-ANGIE\SP\RQCISD(T)-FC\6-31G(d)\C3H7N1O2\MOSCH\11-Dec-2012\0\\
#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,1\C,0,0.671415,-0.1
26671,-0.399621\H,0,0.666284,-0.456378,-1.445956\N,0,1.537474,1.040862
,-0.290972\H,0,1.188552,1.777058,-0.903942\H,0,1.44637,1.422739,0.6510
48\C,0,-0.781273,0.166211,-0.013067\O,0,-1.162275,1.156264,0.572894\O,
0,-1.622385,-0.829247,-0.389362\H,0,-2.511319,-0.56609,-0.083578\C,0,1
.2175,-1.275867,0.464347\H,0,1.219089,-0.993667,1.524292\H,0,0.612351,
-2.179434,0.349797\H,0,2.247779,-1.48844,0.166933\\Version=AM64L-G09Re

vC.01\State=1-A\HF=-321.8643929\MP2=-322.7704397\MP3=-322.7946635\MP4D
=-322.8151989\MP4DQ=-322.8010609\MP4SDTQ=-322.8417756\MP4SDQ=-322.8117
286\QCISD=-322.8135704\QCISD(T)=-322.839702\RMSD=5.594e-09\PG=C01 [X(C
3H7N1O2)]\\@

5H_b (2)

1\1\GINC-ANGIE\SP\RQCISD(T)-FC\6-31G(d)\C3H7N1O2\MOSCH\11-Dec-2012\0\\
#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,1\C,0,-0.666234,-0.
141571,-0.366779\H,0,-0.680791,-0.278093,-1.466868\N,0,-1.03173,-1.359
069,0.369317\H,0,-0.40034,-2.116537,0.117136\H,0,-1.967815,-1.646809,0
.08905\C,0,0.778627,0.223396,-0.038812\O,0,1.195069,1.327222,0.227044\
O,0,1.594444,-0.85978,-0.126667\H,0,2.491009,-0.541355,0.089467\C,0,-1
.61063,1.002181,-0.006319\H,0,-1.596547,1.176076,1.073204\H,0,-1.31514
1,1.924226,-0.512922\H,0,-2.63494,0.752401,-0.305839\\Version=AM64L-G0
9RevC.01\State=1-A\HF=-321.8610711\MP2=-322.7669647\MP3=-322.7913469\M
P4D=-322.8119207\MP4DQ=-322.7978584\MP4SDTQ=-322.8383285\MP4SDQ=-322.8
084444\QCISD=-322.8102904\QCISD(T)=-322.8363434\RMSD=3.321e-09\PG=C01
[X(C3H7N1O2)]\\@

5H_b (5)

1\1\GINC-STEAK\SP\RQCISD(T)-FC\6-31G(d)\C3H7N1O2\MOSCH\08-Dec-2012\0\\
#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,1\C,0,0.662911,-0.1
82969,-0.42529\H,0,0.726834,-0.669141,-1.403616\N,0,1.255061,1.152709,
-0.545863\H,0,1.172212,1.642049,0.343993\H,0,2.251217,1.059861,-0.7394
38\C,0,-0.826935,-0.059346,-0.134377\O,0,-1.702122,-0.717455,-0.64772\
O,0,-1.075416,0.855395,0.838899\H,0,-2.042155,0.854784,0.97066\C,0,1.3
11492,-1.10246,0.632387\H,0,1.237176,-0.656794,1.630761\H,0,0.832379,-
2.088198,0.655891\H,0,2.372411,-1.246397,0.397045\\Version=AM64L-G09Re
vC.01\State=1-A\HF=-321.8602289\MP2=-322.7662972\MP3=-322.790441\MP4D=
-322.8110444\MP4DQ=-322.7969536\MP4SDTQ=-322.8376243\MP4SDQ=-322.80761
59\QCISD=-322.8094502\QCISD(T)=-322.8355735\RMSD=3.098e-09\PG=C01 [X(C
3H7N1O2)]\\@

5H_b (6)

1\1\GINC-STEAK\SP\RQCISD(T)-FC\6-31G(d)\C3H7N1O2\MOSCH\08-Dec-2012\0\\
#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,1\C,0,0.647061,-0.0
0207,0.376587\H,0,0.707155,0.026233,1.472938\N,0,1.068488,-1.356957,-0
.034943\H,0,1.403365,-1.344516,-0.998029\H,0,1.836767,-1.694822,0.5393
23\C,0,-0.856953,0.167174,0.053658\O,0,-1.408709,1.242052,0.022762\O,0
,-1.49595,-0.994941,-0.150444\H,0,-0.786857,-1.684513,-0.097024\C,0,1.
472113,1.150707,-0.198477\H,0,1.463658,1.123609,-1.295138\H,0,1.048487
,2.108642,0.112375\H,0,2.511956,1.092315,0.141009\\Version=AM64L-G09Re
vC.01\State=1-A\HF=-321.8597544\MP2=-322.7695823\MP3=-322.7931257\MP4D

=-322.8136539\MP4DQ=-322.7991145\MP4SDTQ=-322.8406415\MP4SDQ=-322.8099
88\QCISD=-322.8117921\QCISD(T)=-322.8384745\RMSD=4.167e-09\PG=C01 [X(C
3H7N1O2)]\\@

5H_b (7)
1\1\GINC-STEAK\SP\RQCISD(T)-FC\6-31G(d)\C3H7N1O2\MOSCH\08-Dec-2012\0\\
#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,1\C,0,-0.622565,0.1
77166,-0.43054\H,0,-0.674659,0.536818,-1.466159\N,0,-1.278079,-1.13244
7,-0.247841\H,0,-1.283316,-1.665049,-1.115184\H,0,-2.246255,-1.025084,
0.045024\C,0,0.878176,0.040416,-0.089698\O,0,1.689916,0.889181,-0.3747
78\O,0,1.180783,-1.081517,0.580925\H,0,0.321902,-1.572885,0.645144\C,0
,-1.245952,1.232697,0.490155\H,0,-1.219203,0.898244,1.533728\H,0,-0.68
6687,2.168136,0.412604\H,0,-2.288767,1.423969,0.21106\\Version=AM64L-G
09RevC.01\State=1-A\HF=-321.8594539\MP2=-322.7691878\MP3=-322.7925177\
MP4D=-322.8130477\MP4DQ=-322.7985672\MP4SDTQ=-322.8400612\MP4SDQ=-322.
8094384\QCISD=-322.8112481\QCISD(T)=-322.837884\RMSD=6.529e-09\PG=C01
[X(C3H7N1O2)]\\@

5H_b (9)
1\1\GINC-LIEBIG\SP\RQCISD(T)-FC\6-31G(d)\C3H7N1O2\MOSCH\11-Dec-2012\0\
\#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,1\C,0,-0.649698,0.
135858,-0.397604\H,0,-0.643974,0.483047,-1.441523\N,0,-1.535036,-1.017
605,-0.32073\H,0,-1.197645,-1.739019,-0.957487\H,0,-1.434863,-1.430169
,0.607689\C,0,0.803975,-0.19155,-0.000634\O,0,1.130433,-1.202552,0.569
703\O,0,1.736421,0.751816,-0.307918\H,0,1.317199,1.492432,-0.777231\C,
0,-1.191931,1.2695,0.491902\H,0,-1.203676,0.955561,1.54201\H,0,-0.5845
44,2.179106,0.423214\H,0,-2.216151,1.505317,0.192163\\Version=AM64L-G0
9RevC.01\State=1-A\HF=-321.8529586\MP2=-322.7599697\MP3=-322.7843897\M
P4D=-322.8049701\MP4DQ=-322.7906379\MP4SDTQ=-322.8316274\MP4SDQ=-322.8
013855\QCISD=-322.8031918\QCISD(T)=-322.829488\RMSD=6.837e-09\PG=C01 [
X(C3H7N1O2)]\\@

5H_b (10)
1\1\GINC-LIEBIG\SP\RQCISD(T)-FC\6-31G(d)\C3H7N1O2\MOSCH\11-Dec-2012\0\
\#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,1\C,0,-0.628544,0.
217521,0.363686\H,0,-0.600294,0.558112,1.419428\N,0,-0.995897,1.287542
,-0.580299\H,0,-1.921855,1.641305,-0.346296\H,0,-0.356202,2.077656,-0.
519688\C,0,0.791695,-0.249944,0.006398\O,0,1.068285,-1.302115,-0.50504
9\O,0,1.780872,0.647352,0.296956\H,0,1.41879,1.396074,0.798926\C,0,-1.
622017,-0.933027,0.249048\H,0,-1.620864,-1.322888,-0.7713\H,0,-1.35643
5,-1.744652,0.932218\H,0,-2.631921,-0.587601,0.498758\\Version=AM64L-G
09RevC.01\State=1-A\HF=-321.845838\MP2=-322.7526855\MP3=-322.777245\MP
4D=-322.7979296\MP4DQ=-322.7836723\MP4SDTQ=-322.82444\MP4SDQ=-322.7943

623\QCISD=-322.7961927\QCISD(T)=-322.8224195\RMSD=4.053e-09\PG=C01 [X(
C3H7N1O2)]\\@

5_b (1)
1\1\GINC-EVGENIX\SP\UQCISD(T)-FC\6-31G(d)\C3H6N1O2(2)\MOSCH\13-Dec-201
2\0\\#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,2\C,0,-0.65113
3,-0.049883,0.006731\N,0,-1.247048,-1.282434,-0.074336\H,0,-0.618697,-
2.066623,0.064723\H,0,-2.187788,-1.393287,0.279649\C,0,0.785238,-0.068
029,0.002849\O,0,1.461304,-1.09991,0.015545\O,0,1.366364,1.172911,-0.0
08139\H,0,2.323963,0.997464,0.003387\C,0,-1.502843,1.17746,0.006348\H,
0,-2.257419,1.140523,0.806155\H,0,-0.89266,2.069044,0.154605\H,0,-2.04
6986,1.288624,-0.942982\\Version=AM64L-G09RevC.01\State=2-A\HF=-321.25
85316\MP2=-322.1451897\MP3=-322.1684238\MP4D=-322.1877429\MP4DQ=-322.1
735565\MP4SDTQ=-322.2144739\PUHF=-321.2635794\PMP2-0=-322.1489099\PMP3
-0=-322.1707223\MP4SDQ=-322.1849246\QCISD=-322.1880881\QCISD(T)=-322.2
142208\S2=0.781622\S2-1=0.764824\S2A=0.750523\RMSD=4.537e-09\PG=C01 [X
(C3H6N1O2)]\\@

5_b (2)
1\1\GINC-EVGENIX\SP\UQCISD(T)-FC\6-31G(d)\C3H6N1O2(2)\MOSCH\13-Dec-201
2\0\\#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,2\C,0,0.6435,0
.093857,-0.005178\N,0,1.036361,1.408659,0.062737\H,0,0.325946,2.107917
,-0.109489\H,0,1.966882,1.646057,-0.254789\C,0,-0.754034,-0.228888,0.0
00216\O,0,-1.237687,-1.358913,-0.005181\O,0,-1.557524,0.895983,-0.0011
79\H,0,-2.468171,0.553374,-0.006928\C,0,1.681484,-0.978973,0.000807\H,
0,2.289707,-0.945583,0.916069\H,0,1.195683,-1.954126,-0.057546\H,0,2.3
71415,-0.880778,-0.850668\\Version=AM64L-G09RevC.01\State=2-A\HF=-321.
2583378\MP2=-322.1432961\MP3=-322.1672408\MP4D=-322.186474\MP4DQ=-322.
1723442\MP4SDTQ=-322.2128658\PUHF=-321.2646365\PMP2-0=-322.1480615\PMP
3-0=-322.1702439\MP4SDQ=-322.1836516\QCISD=-322.1871782\QCISD(T)=-322.
2133199\S2=0.794008\S2-1=0.772352\S2A=0.750795\RMSD=7.022e-09\PG=C01 [
X(C3H6N1O2)]\\@

5_b (8)
1\1\GINC-STEAK\SP\UQCISD(T)-FC\6-31G(d)\C3H6N1O2(2)\MOSCH\10-Dec-2012\
0\\#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,2\C,0,-0.629073,
-0.072129,0.018858\N,0,-1.18852,-1.319015,-0.111309\H,0,-0.521953,-2.0
7662,0.003578\H,0,-2.112099,-1.479461,0.26987\C,0,0.818803,-0.055318,0
.009386\O,0,1.487542,-1.082393,0.049755\O,0,1.456162,1.15826,-0.026789
\H,0,0.813538,1.872178,-0.160217\C,0,-1.531719,1.123863,0.030717\H,0,-
1.092031,1.964741,0.579827\H,0,-1.784639,1.476503,-0.981249\H,0,-2.480
871,0.890332,0.529853\\Version=AM64L-G09RevC.01\State=2-A\HF=-321.2456
511\MP2=-322.1312178\MP3=-322.155375\MP4D=-322.1746377\MP4DQ=-322.1603

447\MP4SDTQ=-322.2013363\PUHF=-321.2518929\PMP2-0=-322.1359862\PMP3-0=
-322.1584158\MP4SDQ=-322.1718521\QCISD=-322.1756063\QCISD(T)=-322.2019
682\S2=0.794504\S2-1=0.773252\S2A=0.750856\RMSD=9.905e-09\PG=C01 [X(C3
H6N1O2)]\\@

5_b (10)

1\1\GINC-STEAK\SP\UQCISD(T)-FC\6-31G(d)\C3H6N1O2(2)\MOSCH\10-Dec-2012\
0\\#p qcisd(t,e4t)/6-31g(d) scf=tight\\enter title\\0,2\C,0,0.621909,0
.07616,0.022176\N,0,1.006343,1.414506,0.065435\H,0,2.002713,1.574488,0
.16065\H,0,0.474788,2.004918,0.699247\C,0,-0.789122,-0.244035,0.012237
\O,0,-1.241371,-1.369202,0.156123\O,0,-1.646036,0.830126,-0.128086\H,0
,-1.172403,1.547655,-0.583724\C,0,1.660174,-0.985635,-0.117279\H,0,2.3
53417,-0.989602,0.736735\H,0,1.17312,-1.960454,-0.172497\H,0,2.265458,
-0.844889,-1.02555\\Version=AM64L-G09RevC.01\State=2-A\HF=-321.2459778
\MP2=-322.1265738\MP3=-322.1523763\MP4D=-322.171517\MP4DQ=-322.1574691
\MP4SDTQ=-322.1976718\PUHF=-321.2542988\PMP2-0=-322.1331316\PMP3-0=-32
2.156685\MP4SDQ=-322.1689509\QCISD=-322.1736538\QCISD(T)=-322.1998602\
S2=0.817571\S2-1=0.788563\S2A=0.751468\RMSD=5.022e-09\PG=C01 [X(C3H6N1
O2)]\\@

6H_a

1\1\GINC-LIEBIG\FOpt\RB3LYP\6-31G(d)\C4H6N2O2\MOSCH\08-Jan-2013\0\\#p
b3lyp/6-31g(d) opt freq scf=tight\\enter title\\0,1\C,-1.47475195,0.02
698389,-0.02372995\C,-0.69664574,-1.26847396,0.19696919\C,1.47475195,-
0.02698389,-0.02372995\C,0.69664574,1.26847396,0.19696919\H,-0.8778976
7,-1.58884486,1.23464423\H,-1.15087063,-2.02042111,-0.45411371\H,0.877
89767,1.58884486,1.23464423\H,1.15087063,2.02042111,-0.45411371\N,0.72
561724,-1.16261776,-0.09370684\H,1.26332938,-2.01585868,-0.19179875\N,
-0.72561724,1.16261776,-0.09370684\H,-1.26332938,2.01585868,-0.1917987
5\O,2.69220905,-0.01519244,-0.12186501\O,-2.69220905,0.01519244,-0.121
86501\\Version=AM64L-G09RevC.01\State=1-A\HF=-416.0068369\RMSD=5.535e-
09\RMSF=1.293e-04\Dipole=0.,0.,0.3345826\Quadrupole=-13.8439426,10.734
8634,3.1090793,-0.9763031,0.,0.\PG=C02 [X(C4H6N2O2)]\\@

6_a

1\1\GINC-LIEBIG\FOpt\UB3LYP\6-31G(d)\C4H5N2O2(2)\MOSCH\08-Jan-2013\0\\
#p b3lyp/6-31g(d) opt freq scf=tight\\enter title\\0,2\C,-0.8286740781
,-0.9479815237,-0.7239328975\C,0.6094828767,-0.8638071566,-0.862947054
1\C,0.7940252424,1.0835114522,0.6172048015\C,-0.657923673,0.8463668385
,1.0150313568\H,1.1414400752,-1.5685623813,-1.4848668572\H,-0.63850905
31,0.3761925807,2.0139679598\H,-1.1200596148,1.8304708204,1.1347054332
\N,1.3169711426,0.161674092,-0.2734134773\H,2.301814109,0.2872470313,-
0.4830503817\N,-1.3981357306,0.0578063592,0.0417390843\H,-2.3913139683

,-0.0643174483,0.1976165426\O,1.4716208399,1.9801522388,1.0876979651\O
,-1.500917168,-1.8127369031,-1.2882914755\\Version=AM64L-G09RevC.01\St
ate=2-A\HF=-415.3658753\S2=0.75674\S2-1=0.\S2A=0.750033\RMSD=7.067e-09
\RMSF=2.020e-05\Dipole=0.3769239,0.1487557,0.3618796\Quadrupole=4.6462
133,-5.3036713,0.657458,-7.5940113,-7.1421811,-4.0437071\PG=C01 [X(C4H
5N2O2)]\\@

6H_b

1\1\GINC-EVGENIX\FOpt\RB3LYP\6-31G(d)\C6H10N2O2\MOSCH\14-Jan-2013\0\\#
p b3lyp/6-31g(d) opt freq scf=tight\\enter title\\0,1\C,-1.3317619584,
0.6223327429,0.1467252392\C,-1.1649791087,-0.8768044283,-0.135901672\C
,1.3317619584,-0.6223327429,0.1467252392\C,1.1649791087,0.8768044283,-
0.135901672\H,-1.3367520175,-0.999629925,-1.2190143777\N,0.1773847307,
-1.341781211,0.2103929363\H,0.3142443751,-2.3393533809,0.3294575133\N,
-0.1773847307,1.341781211,0.2103929363\H,-0.3142443751,2.3393533809,0.
3294575133\O,2.4380315764,-1.1247198508,0.2907047195\O,-2.4380315764,1
.1247198508,0.2907047195\H,1.3367520175,0.999629925,-1.2190143777\C,2.
2226309891,1.6874685196,0.6136442574\H,3.2140596936,1.3014619626,0.370
4779\H,2.1721671197,2.7445228569,0.3286449012\H,2.0734751231,1.6065180
804,1.6949385023\C,-2.2226309891,-1.6874685196,0.6136442574\H,-3.21405
96936,-1.3014619626,0.3704779\H,-2.1721671197,-2.7445228569,0.32864490
12\H,-2.0734751231,-1.6065180804,1.6949385023\\Version=AM64L-G09RevC.0
1\State=1-A\HF=-494.6428094\RMSD=7.522e-09\RMSF=3.048e-06\Dipole=0.,0.
,-0.3832404\Quadrupole=-9.2652372,6.3967308,2.8685064,8.8497841,0.,0.\
PG=C02 [X(C6H10N2O2)]\\@

6_b

1\1\GINC-BORIX\FOpt\UB3LYP\6-31G(d)\C6H9N2O2(2)\MOSCH\14-Jan-2013\0\\#
p b3lyp/6-31g(d) opt freq scf=tight\\enter title\\0,2\C,1.12554,0.9365
07,-0.014052\C,1.33157,-0.501294,-0.00126\C,-1.09998,-0.94555,0.055435
\C,-1.32282,0.531112,0.390753\N,0.222999,-1.33041,-0.056621\H,0.354831
,-2.32646,-0.203017\N,-0.198974,1.3424,-0.071151\H,-0.305213,2.34696,0
.013068\O,-2.00853,-1.75405,-0.045022\O,2.05868,1.7453,-0.035834\C,2.6
922,-1.10451,-0.007308\H,3.42814,-0.298849,0.009241\H,2.86505,-1.7154,
-0.905889\H,2.85691,-1.75336,0.864932\C,-2.6386,1.03301,-0.203866\H,-2
.83757,2.05893,0.125401\H,-3.46071,0.392702,0.122492\H,-2.59414,1.0189
2,-1.29712\H,-1.40413,0.567079,1.49393\\Version=AM64L-G09RevC.01\State
=2-A\HF=-494.0083042\S2=0.756386\S2-1=0.\S2A=0.75003\RMSD=9.167e-09\RM
SF=2.163e-05\Dipole=-0.1529058,-0.3985937,0.2649342\Quadrupole=-3.1460
156,1.1969218,1.9490938,-11.6152473,-0.6466644,0.8579275\PG=C01 [X(C6H
9N2O2)]\\@

Table S3. Rate constants for hydrogen abstraction by thiyl radicals[12] and BDE(C_a-H) values for selected peptide models.

System	Rate constant [M^{-1} s^{-1}]	C-H BDE (G3B3) [kJ/mol]	C-H BDE (B3LYP/6-31G(d)) [kJ/mol]
6H_a	8.0 x 10^4	+359.2[a]	+341.0
N-Ac-Gly-NH_2	3.2 x 10^4	+363.8[c] (**2H_a**)	+337.7 (**2H_a**)
N-Ac-Ala-NH_2	1.0 x 10^4	+372.3[b] (**2H_b**)	+340.4 (**2H_b**)
N-Ac-Pro-NH_2	0.18 x 10^4	+391.5[b] (Proline)[c]	+364.6 (Proline)[c]

[a] G3B3; [b] IMOMO(G3B3/G3(MP2)-RAD); [c] Taken from ref. 3.